



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:24 PM GMT

PDB ID : 3WHE  
Title : A new conserved neutralizing epitope at the globular head of hemagglutinin in H3N2 influenza viruses  
Authors : Fujii, Y.; Sumida, T.; Shirouzu, M.; Yokoyama, S.  
Deposited on : 2013-08-25  
Resolution : 4.00 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

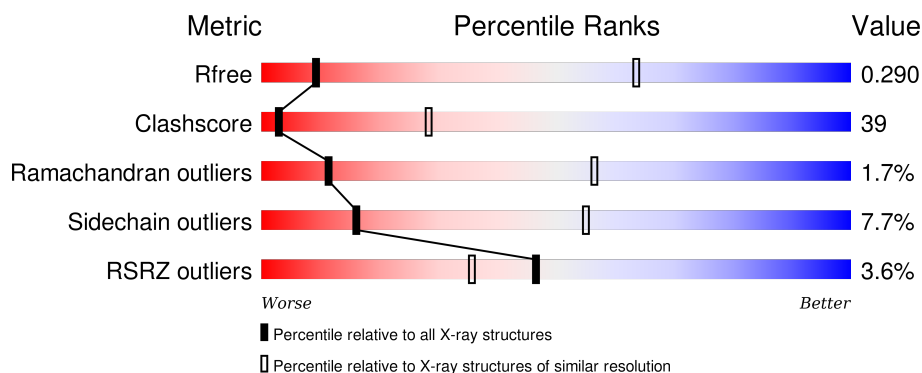
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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.






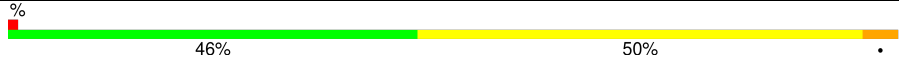
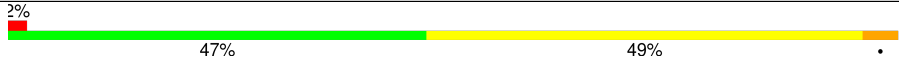
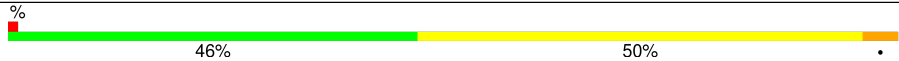
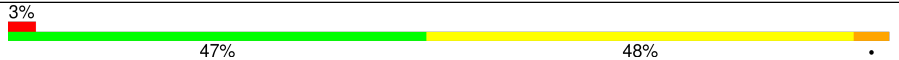
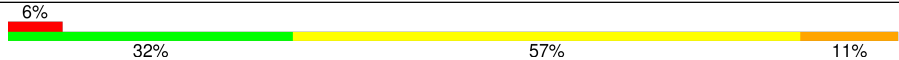
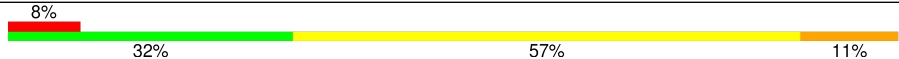
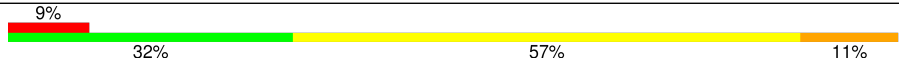
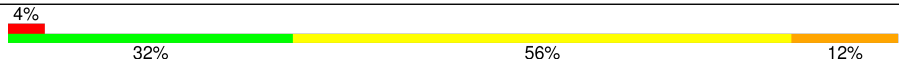
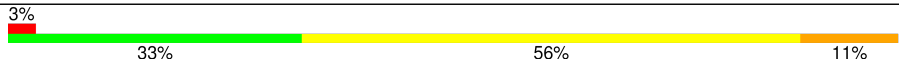
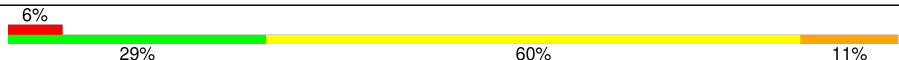
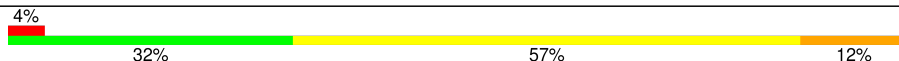
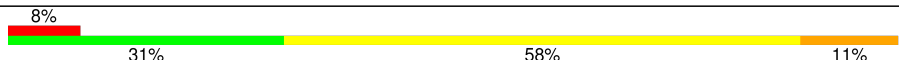
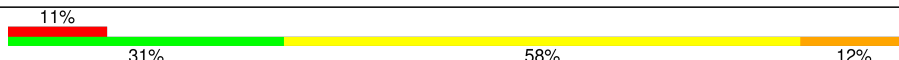
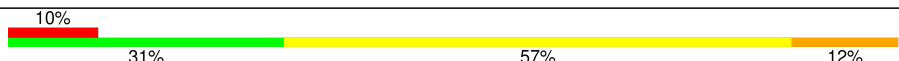
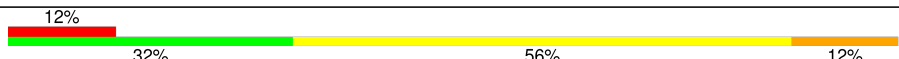
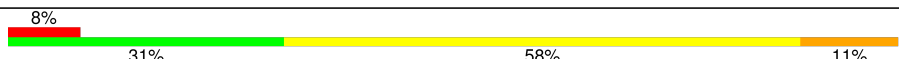
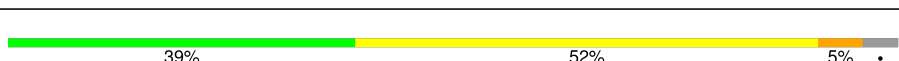
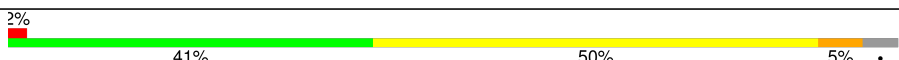
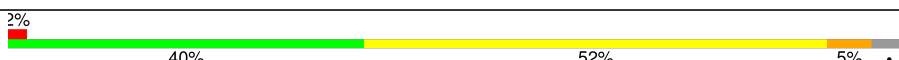
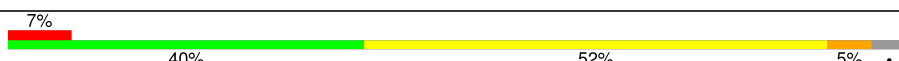
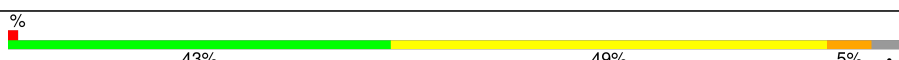
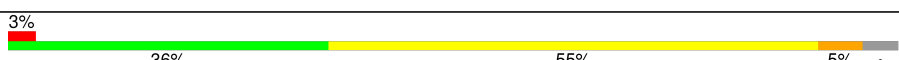
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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	493	<div> <div>2%</div> <div>49%</div> <div>46%</div> <div>•</div> </div>
1	B	493	<div> <div>2%</div> <div>46%</div> <div>49%</div> <div>•</div> </div>
1	C	493	<div> <div>2%</div> <div>46%</div> <div>49%</div> <div>•</div> </div>
1	D	493	<div> <div>2%</div> <div>47%</div> <div>48%</div> <div>•</div> </div>
1	E	493	<div> <div>2%</div> <div>46%</div> <div>49%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	493	
1	G	493	
1	H	493	
1	I	493	
1	J	493	
1	K	493	
1	L	493	
2	1	226	
2	3	226	
2	5	226	
2	7	226	
2	9	226	
2	M	226	
2	O	226	
2	Q	226	
2	S	226	
2	U	226	
2	W	226	
2	Y	226	
3	0	220	
3	2	220	
3	4	220	
3	6	220	
3	8	220	
3	N	220	

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Mol	Chain	Length	Quality of chain
3	P	220	
3	R	220	
3	T	220	
3	V	220	
3	X	220	
3	Z	220	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	K	602	-	-	X	-
5	NAG	H	608	-	-	-	X
5	NAG	H	618	-	-	-	X
6	NAG	C	610	-	-	X	-
6	NAG	F	610	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 88152 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	B	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	C	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	D	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	E	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	F	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	G	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	H	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	I	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	J	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	K	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	L	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			

- Molecule 2 is a protein called immunoglobulin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	O	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	S	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	U	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	W	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	Y	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	1	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	3	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	5	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	7	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	9	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			

- Molecule 3 is a protein called immunoglobulin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	P	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	R	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	T	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	V	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	X	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	Z	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	2	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	4	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			

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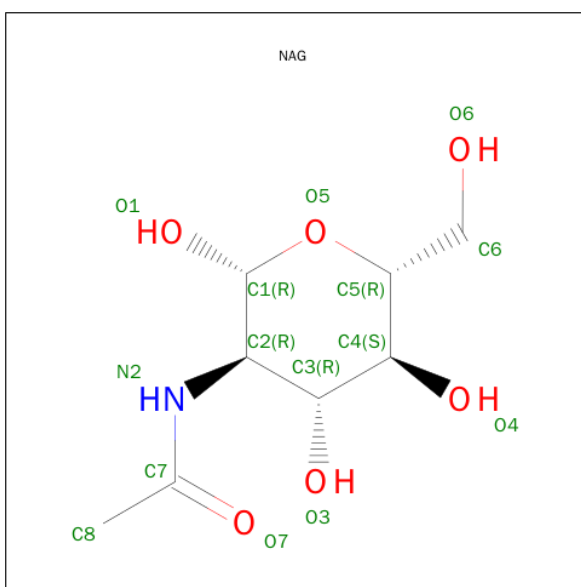
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	6	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	8	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	0	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			

- Molecule 4 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	7	Total	C	N	O	0	0
			83	46	2	35		
4	B	7	Total	C	N	O	0	0
			83	46	2	35		
4	C	7	Total	C	N	O	0	0
			83	46	2	35		
4	D	7	Total	C	N	O	0	0
			83	46	2	35		
4	E	7	Total	C	N	O	0	0
			83	46	2	35		
4	F	7	Total	C	N	O	0	0
			83	46	2	35		
4	G	7	Total	C	N	O	0	0
			83	46	2	35		
4	H	7	Total	C	N	O	0	0
			83	46	2	35		
4	I	7	Total	C	N	O	0	0
			83	46	2	35		
4	J	7	Total	C	N	O	0	0
			83	46	2	35		
4	K	7	Total	C	N	O	0	0
			83	46	2	35		
4	L	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	6	Total	C	N	O	0	0
			72	40	2	30		
6	B	6	Total	C	N	O	0	0
			72	40	2	30		
6	C	6	Total	C	N	O	0	0
			72	40	2	30		
6	D	6	Total	C	N	O	0	0
			72	40	2	30		
6	E	6	Total	C	N	O	0	0
			72	40	2	30		
6	F	6	Total	C	N	O	0	0
			72	40	2	30		
6	G	6	Total	C	N	O	0	0
			72	40	2	30		
6	H	6	Total	C	N	O	0	0
			72	40	2	30		
6	I	6	Total	C	N	O	0	0
			72	40	2	30		

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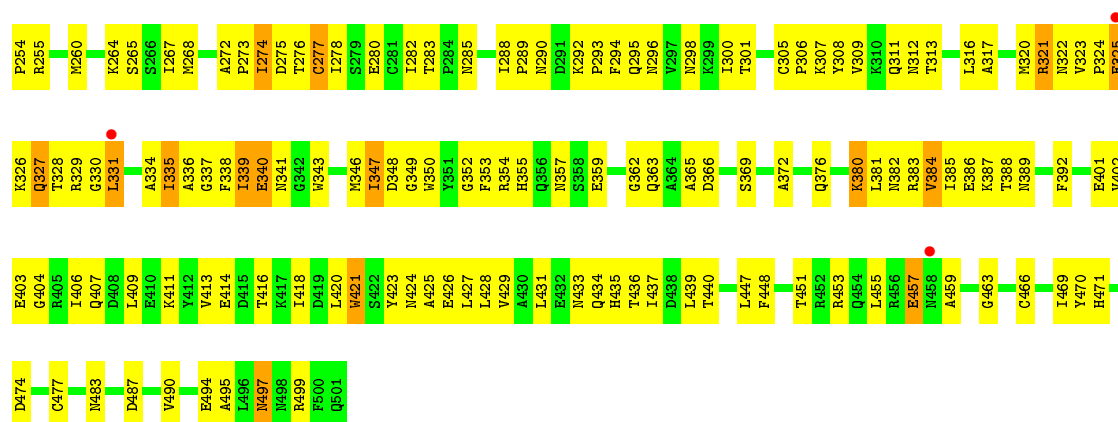
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	J	6	Total	C	N	O	0	0
			72	40	2	30		
6	K	6	Total	C	N	O	0	0
			72	40	2	30		
6	L	6	Total	C	N	O	0	0
			72	40	2	30		

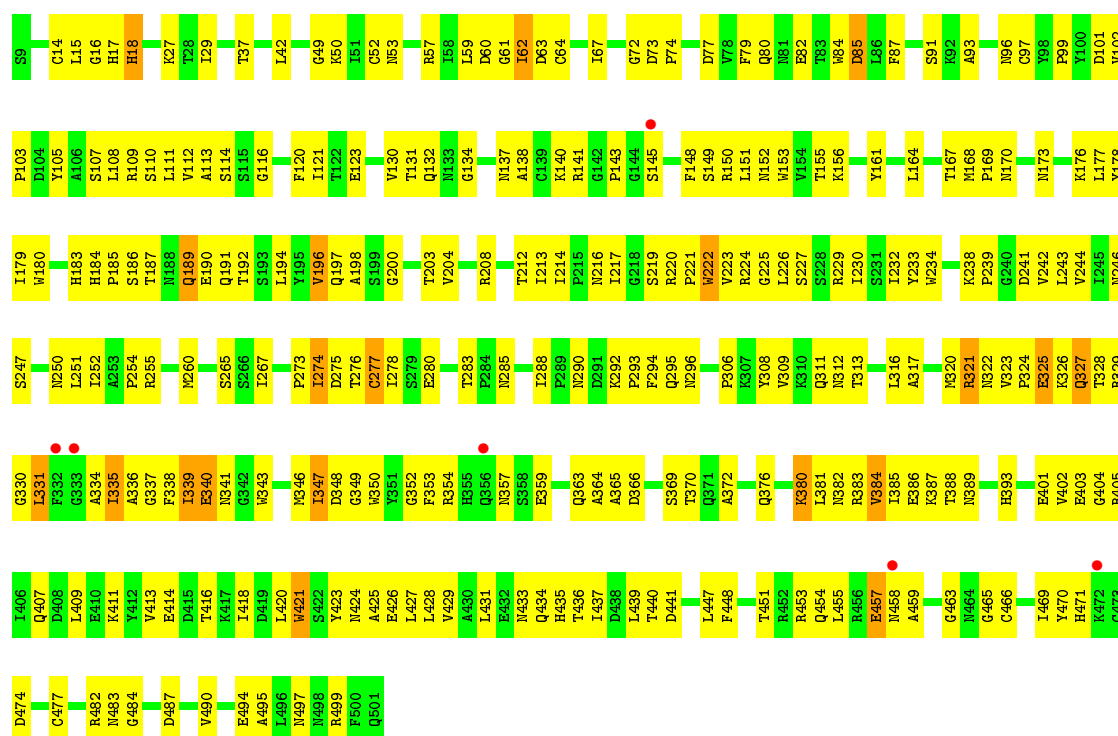
- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	3	Total	C	N	O	0	0
			39	22	2	15		
7	B	3	Total	C	N	O	0	0
			39	22	2	15		
7	C	3	Total	C	N	O	0	0
			39	22	2	15		
7	D	3	Total	C	N	O	0	0
			39	22	2	15		
7	E	3	Total	C	N	O	0	0
			39	22	2	15		
7	F	3	Total	C	N	O	0	0
			39	22	2	15		
7	G	3	Total	C	N	O	0	0
			39	22	2	15		
7	H	3	Total	C	N	O	0	0
			39	22	2	15		
7	I	3	Total	C	N	O	0	0
			39	22	2	15		
7	J	3	Total	C	N	O	0	0
			39	22	2	15		
7	K	3	Total	C	N	O	0	0
			39	22	2	15		
7	L	3	Total	C	N	O	0	0
			39	22	2	15		

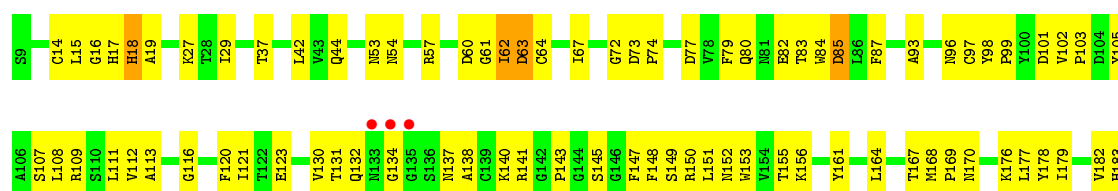


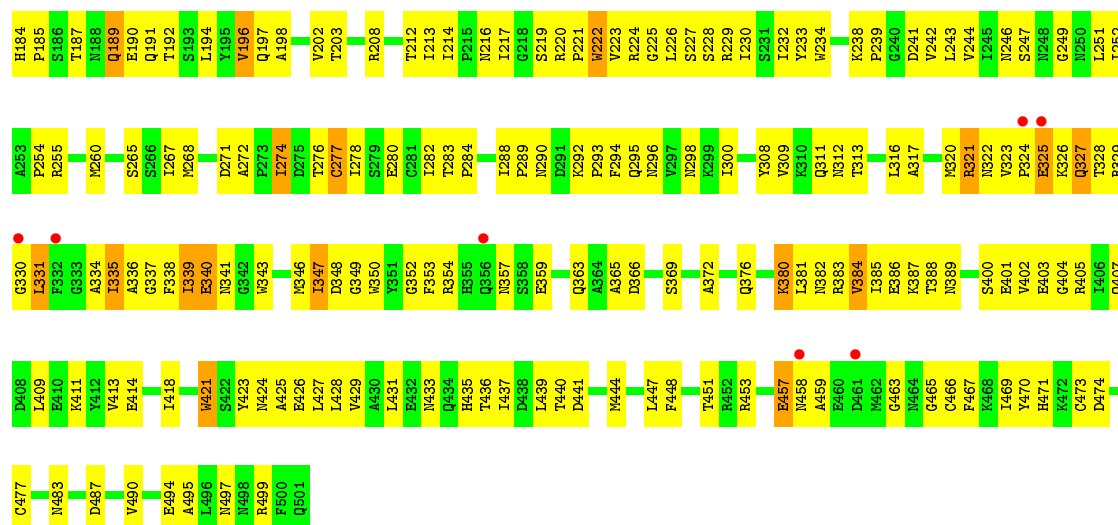


• Molecule 1: Hemagglutinin

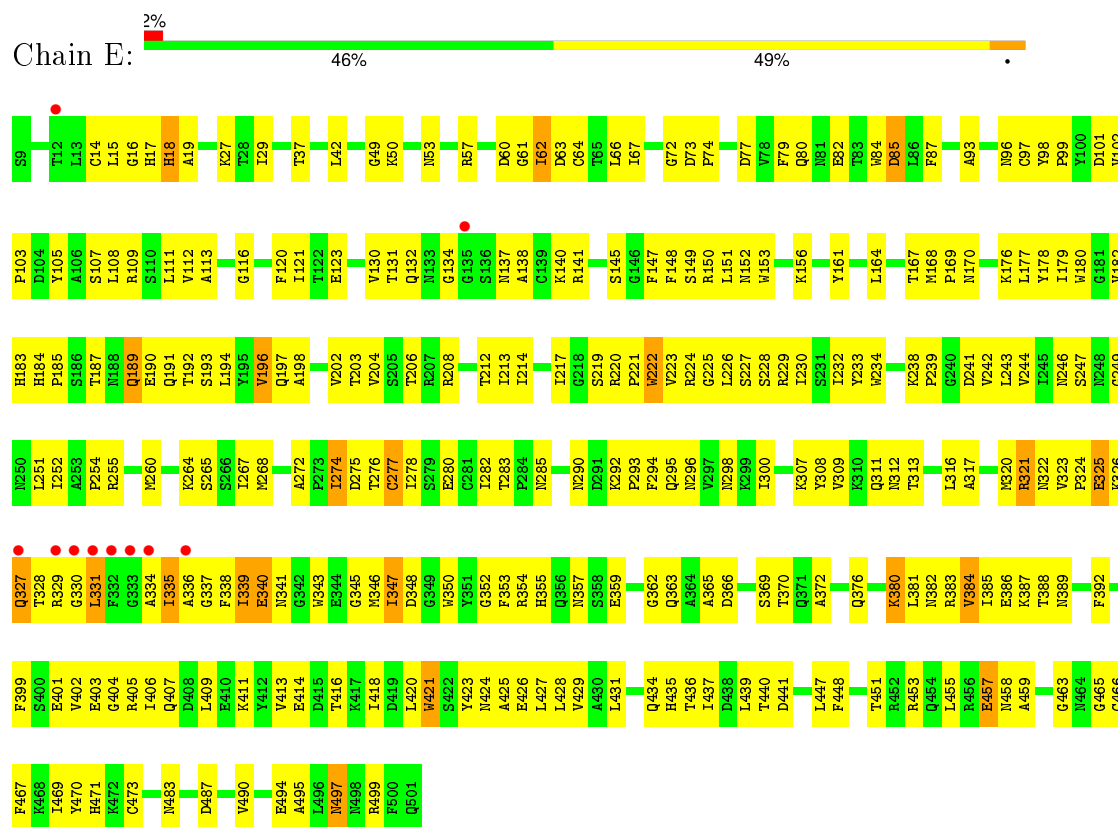


• Molecule 1: Hemagglutinin

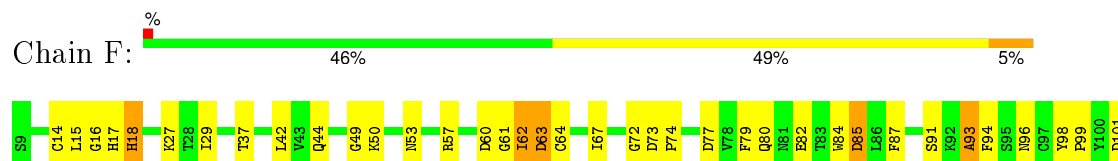


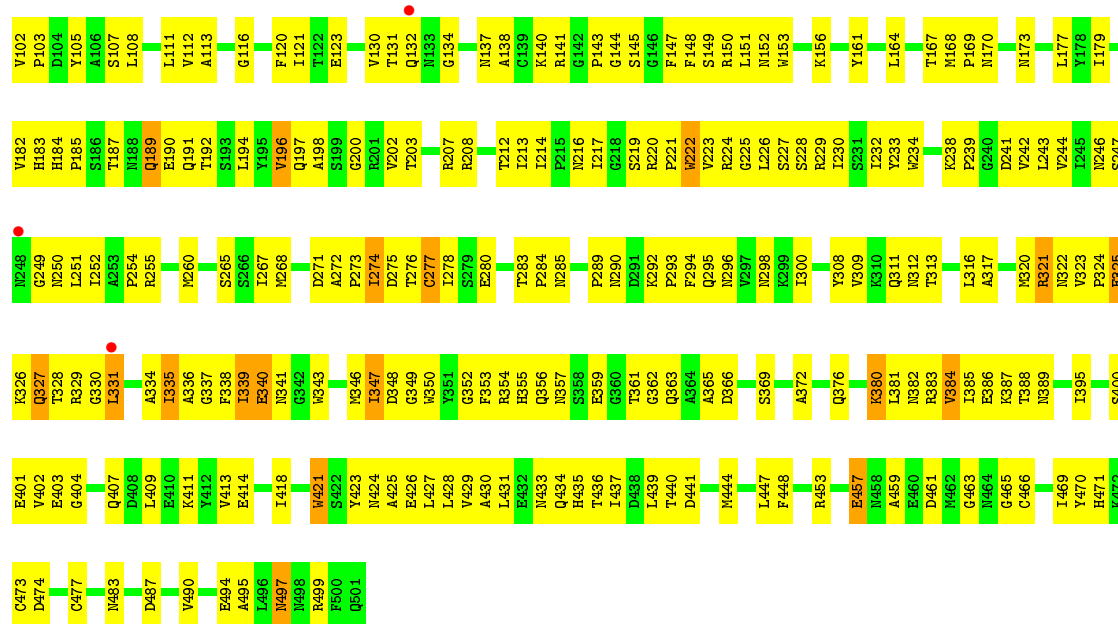


• Molecule 1: Hemagglutinin

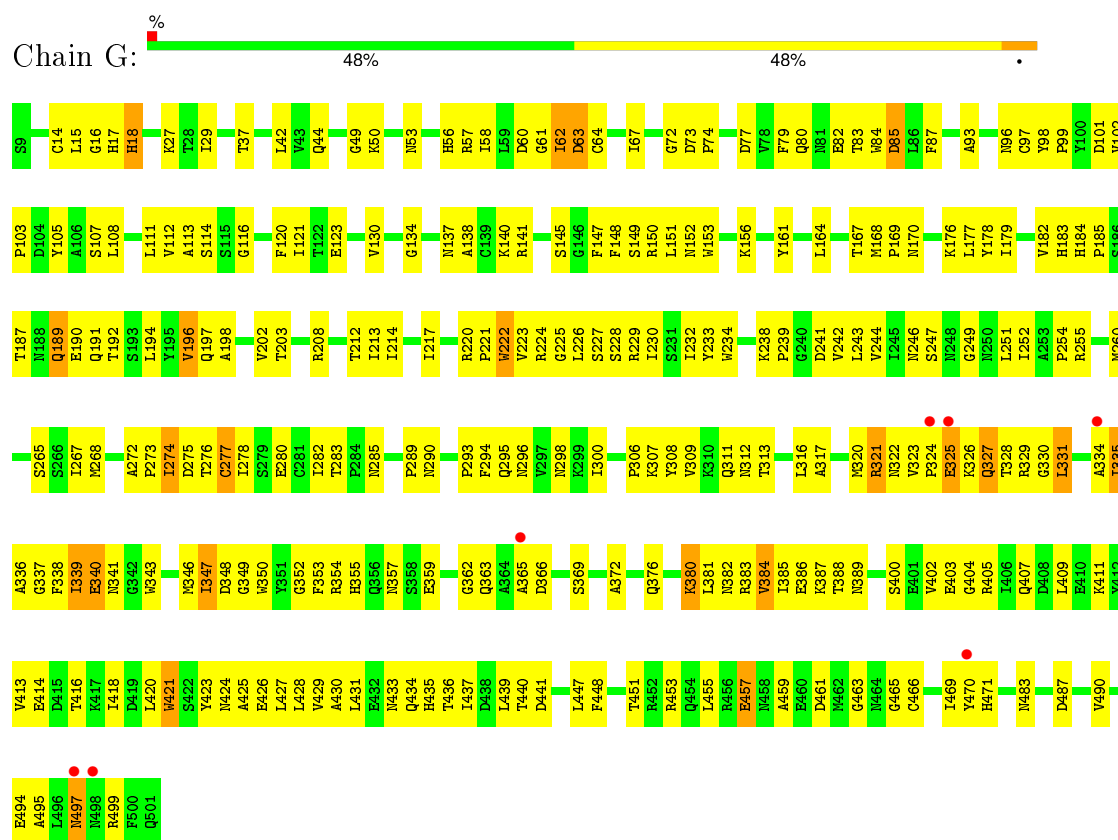


• Molecule 1: Hemagglutinin



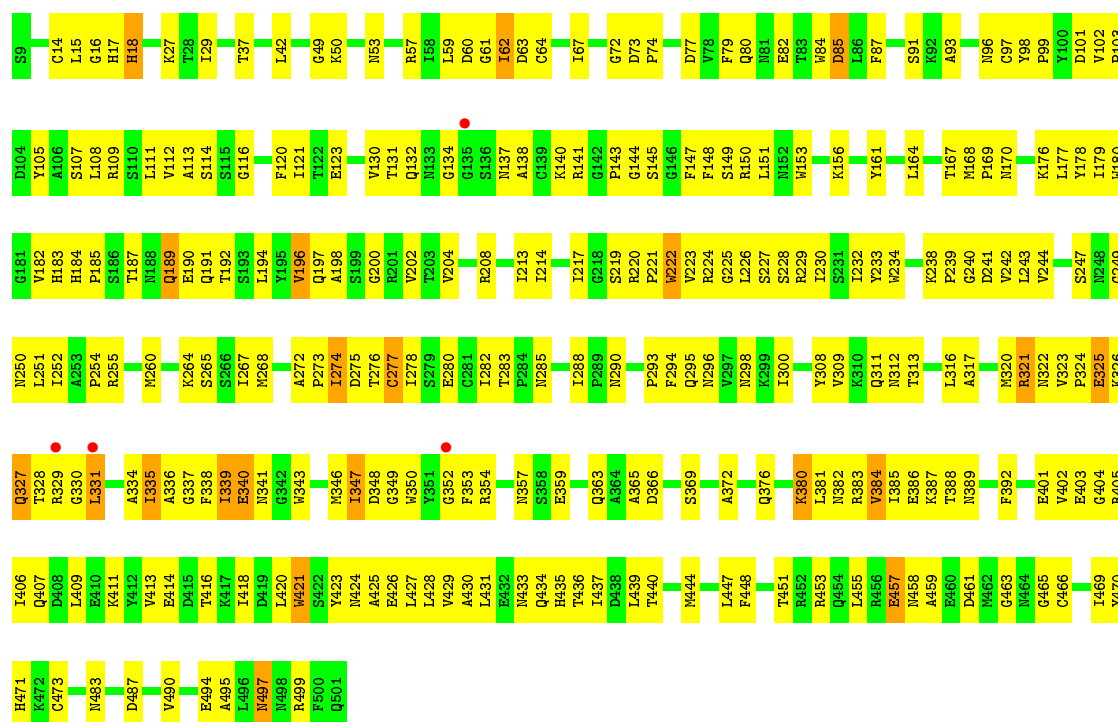


• Molecule 1: Hemagglutinin

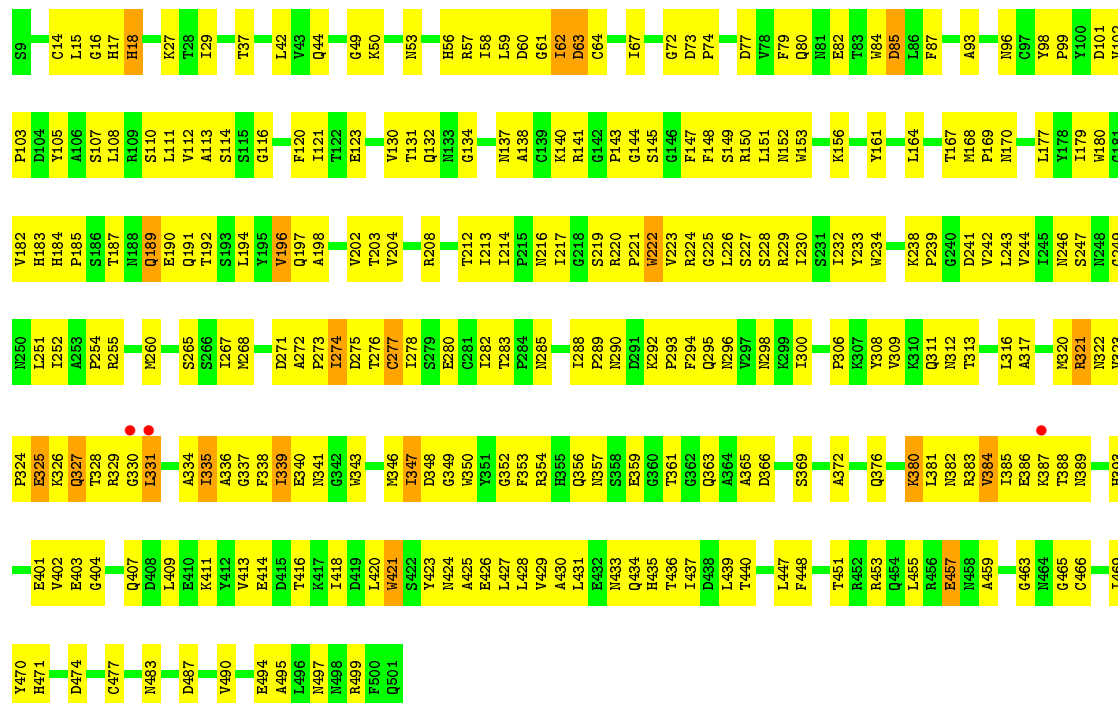


• Molecule 1: Hemagglutinin



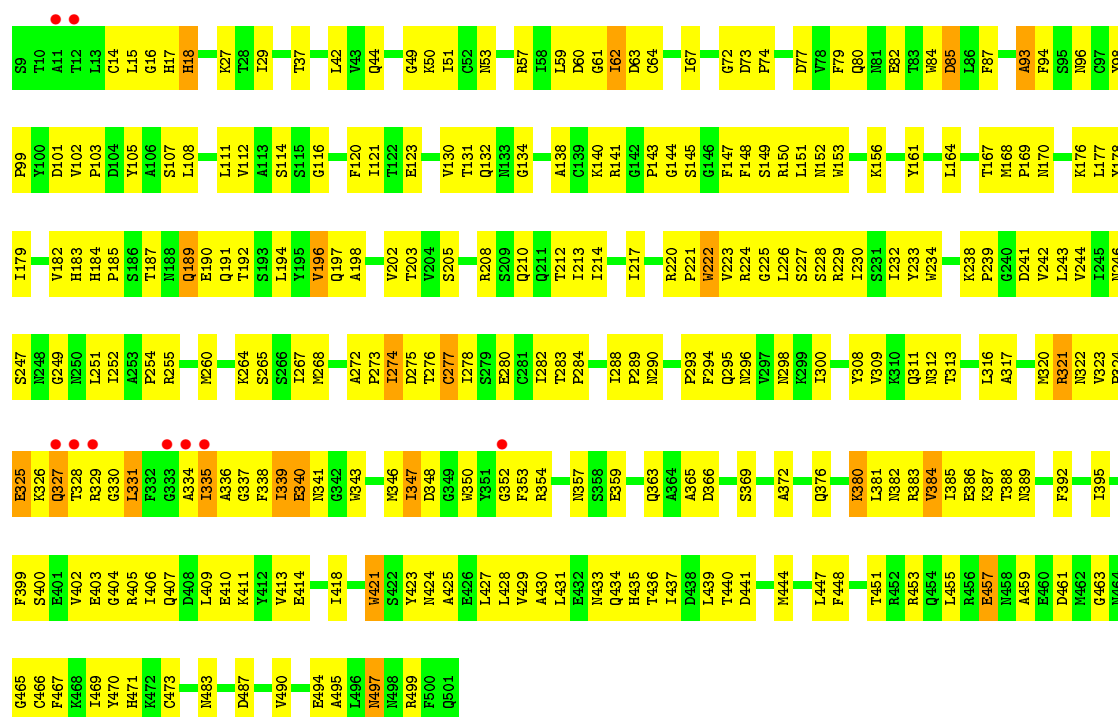


### • Molecule 1: Hemagglutinin

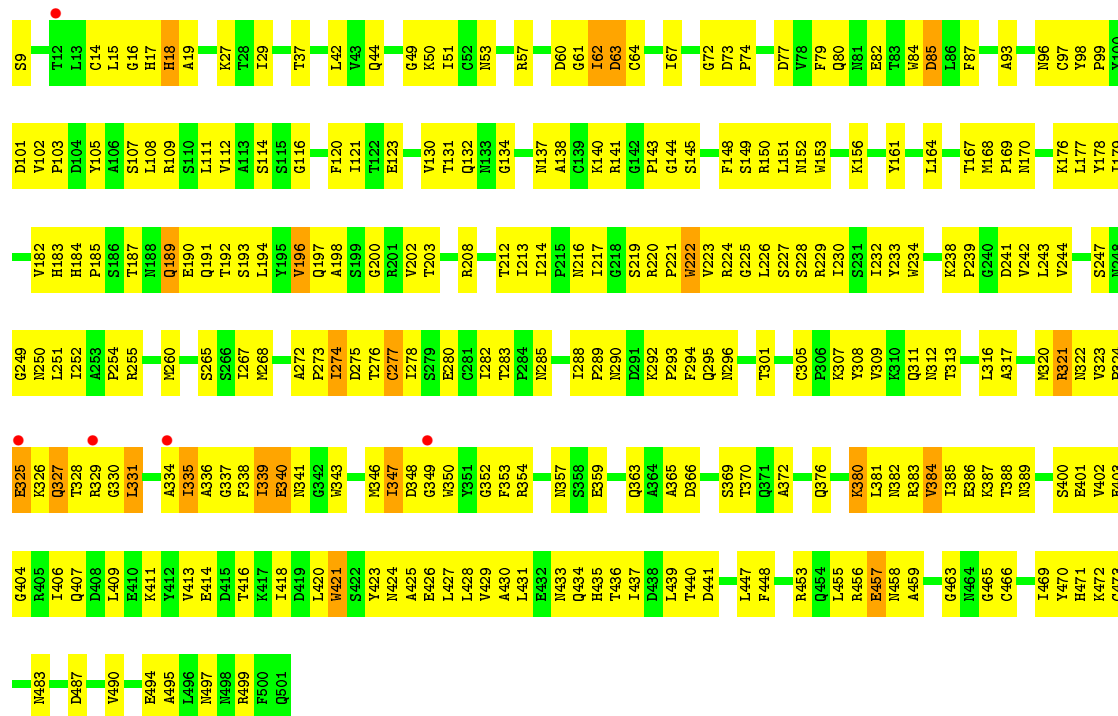


### • Molecule 1: Hemagglutinin





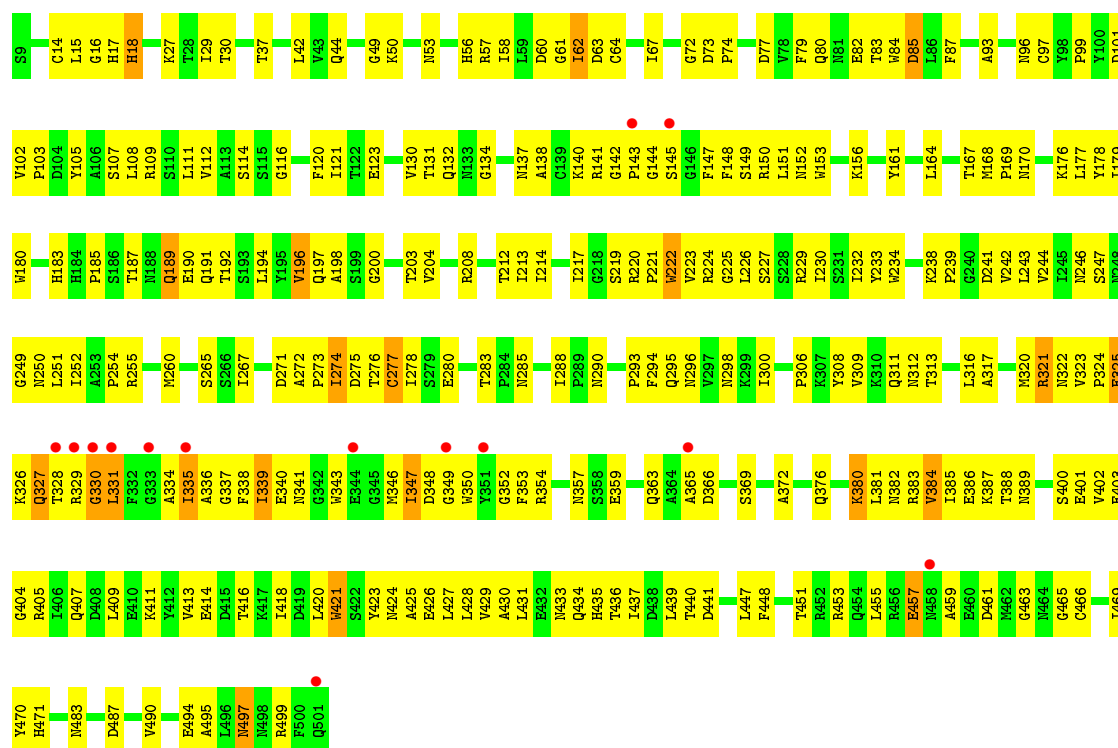
### • Molecule 1: Hemagglutinin

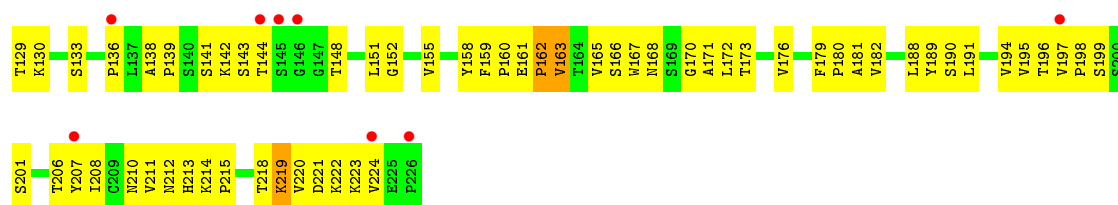


### • Molecule 1: Hemagglutinin

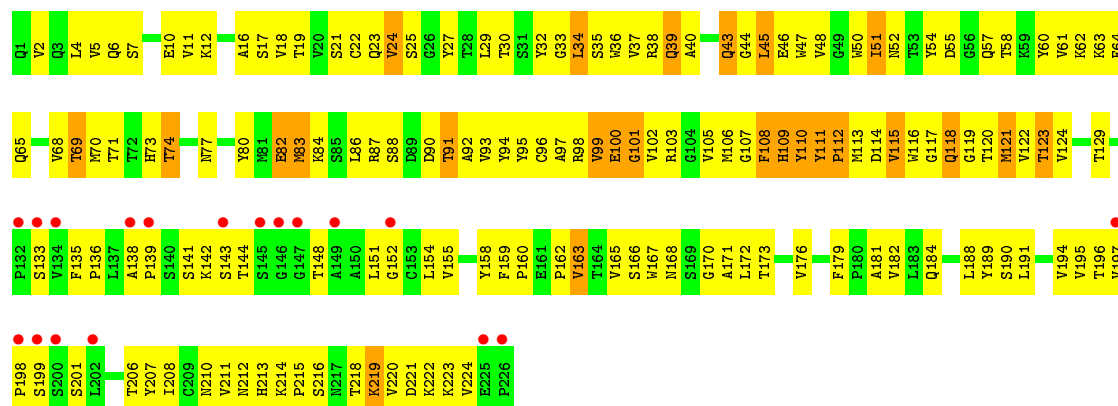




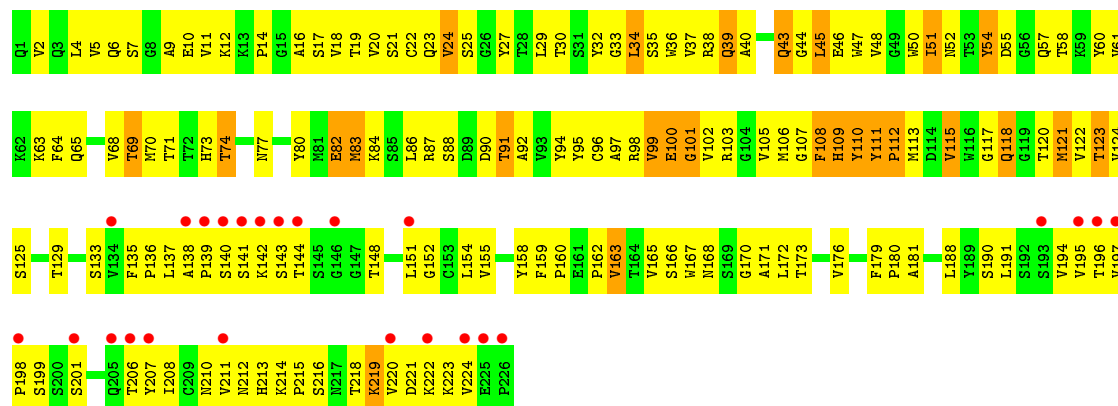




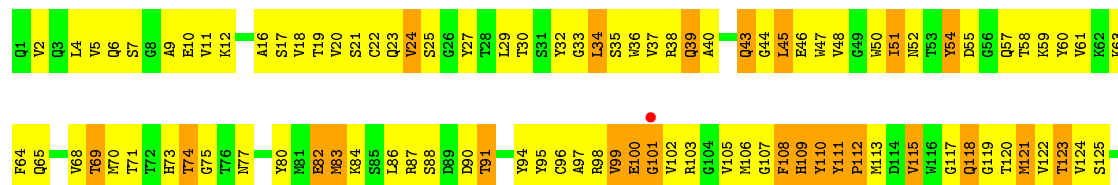
• Molecule 2: immunoglobulin heavy chain

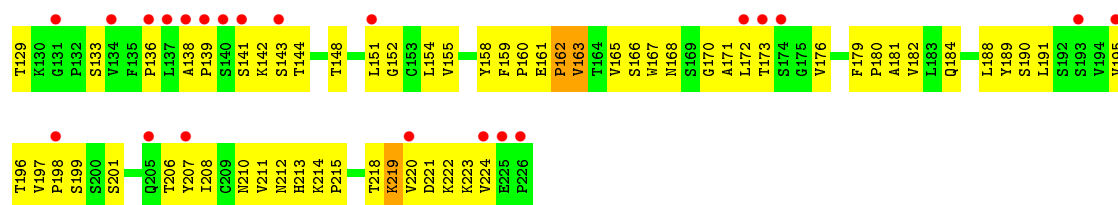


• Molecule 2: immunoglobulin heavy chain

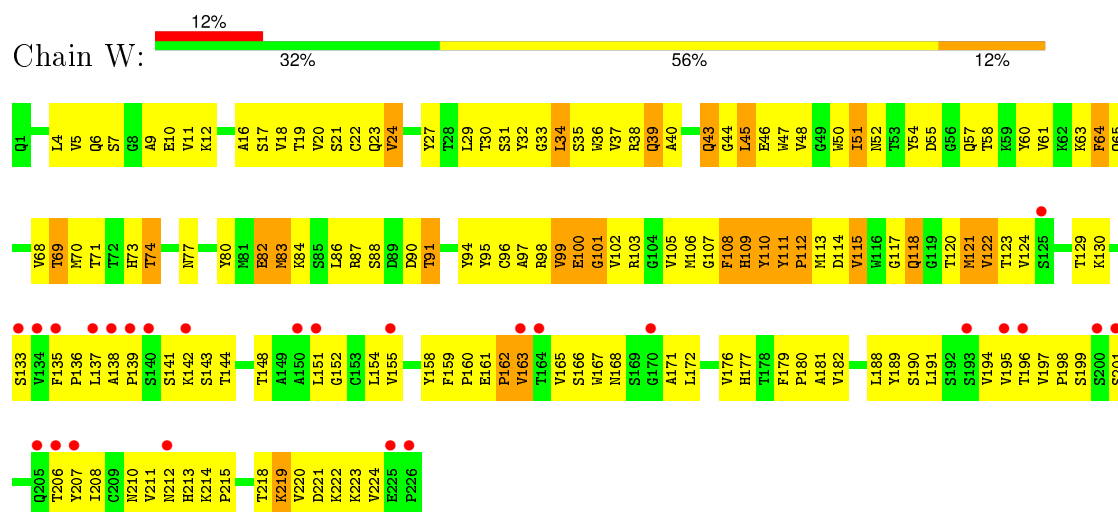


• Molecule 2: immunoglobulin heavy chain

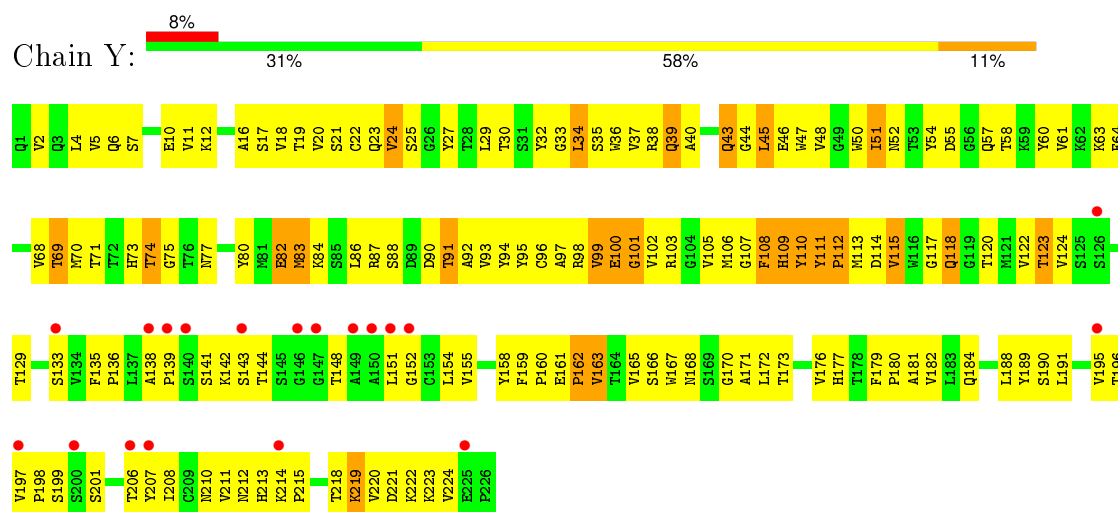




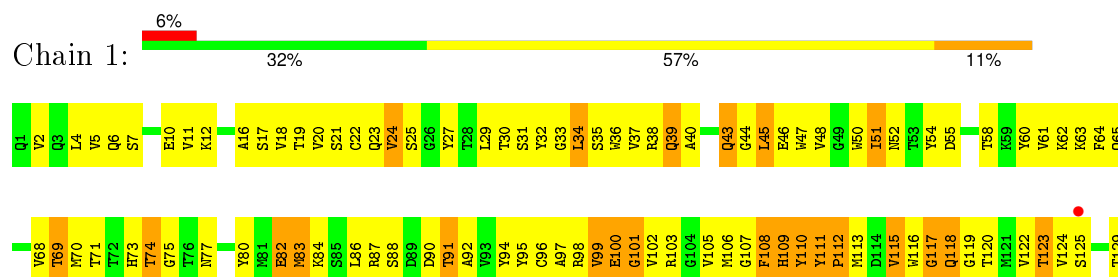
• Molecule 2: immunoglobulin heavy chain



• Molecule 2: immunoglobulin heavy chain

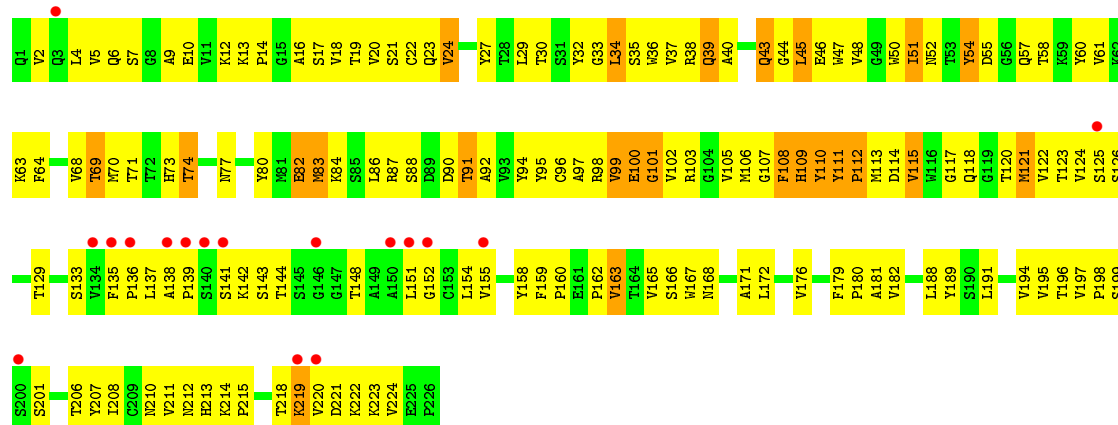


• Molecule 2: immunoglobulin heavy chain

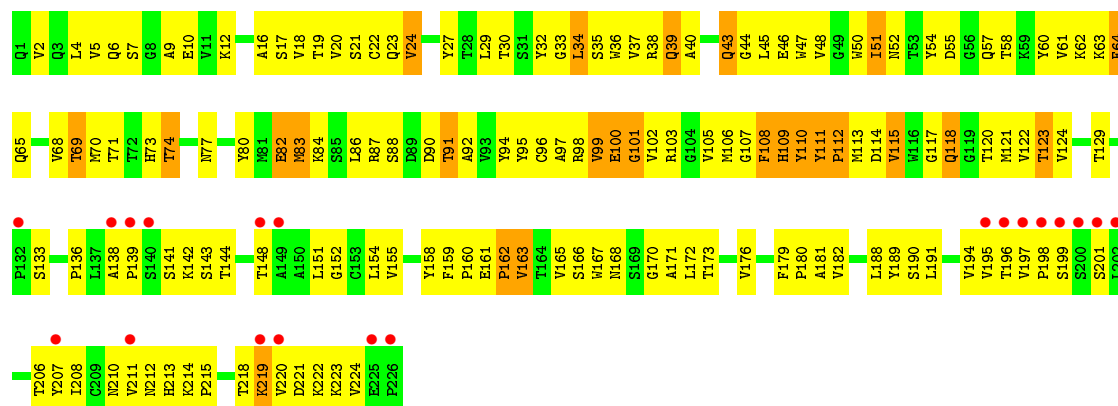




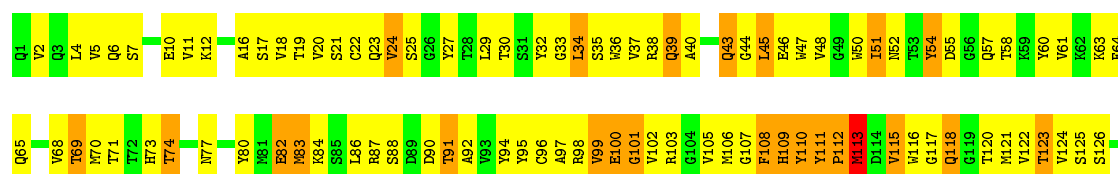
• Molecule 2: immunoglobulin heavy chain

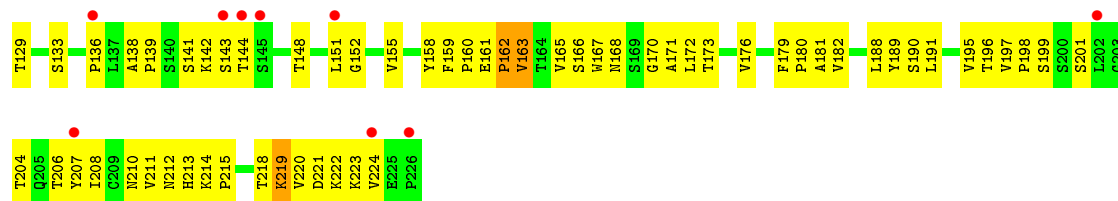


• Molecule 2: immunoglobulin heavy chain

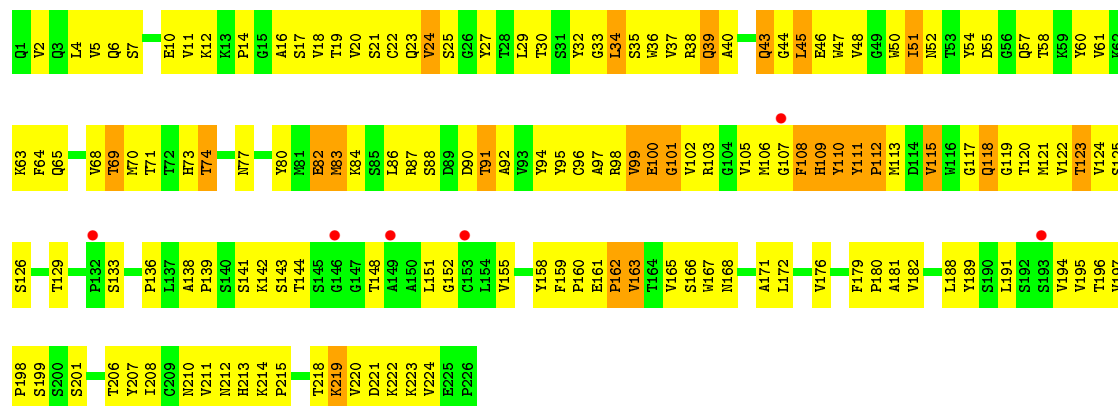


• Molecule 2: immunoglobulin heavy chain

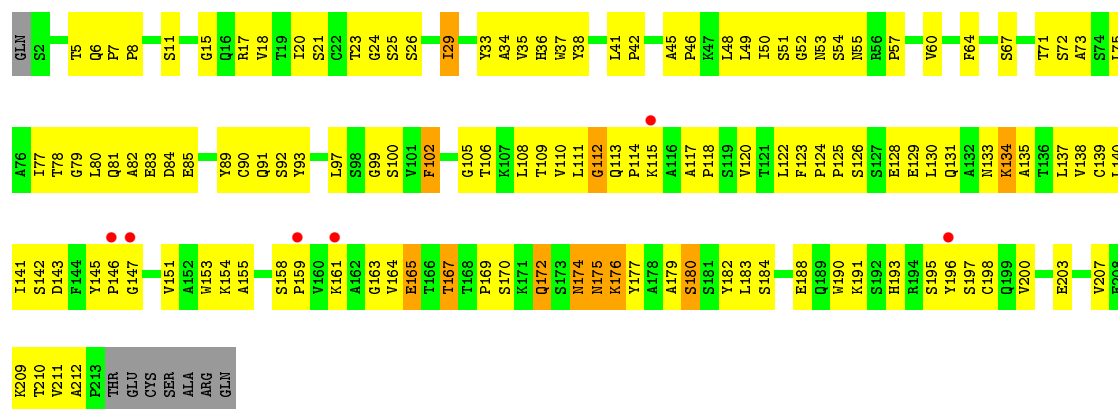




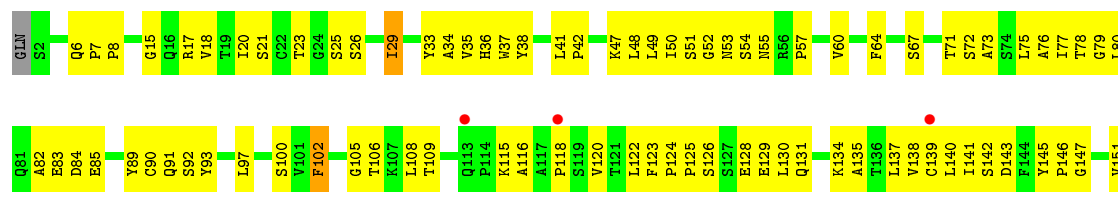
• Molecule 2: immunoglobulin heavy chain

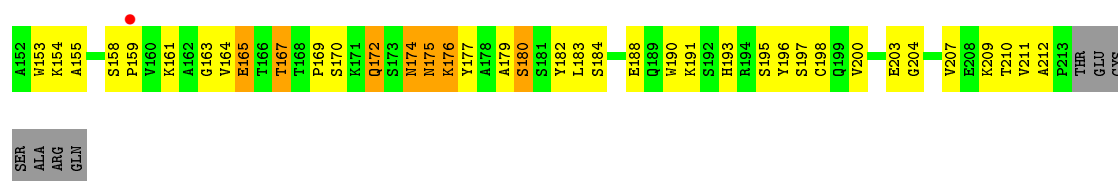


• Molecule 3: immunoglobulin light chain

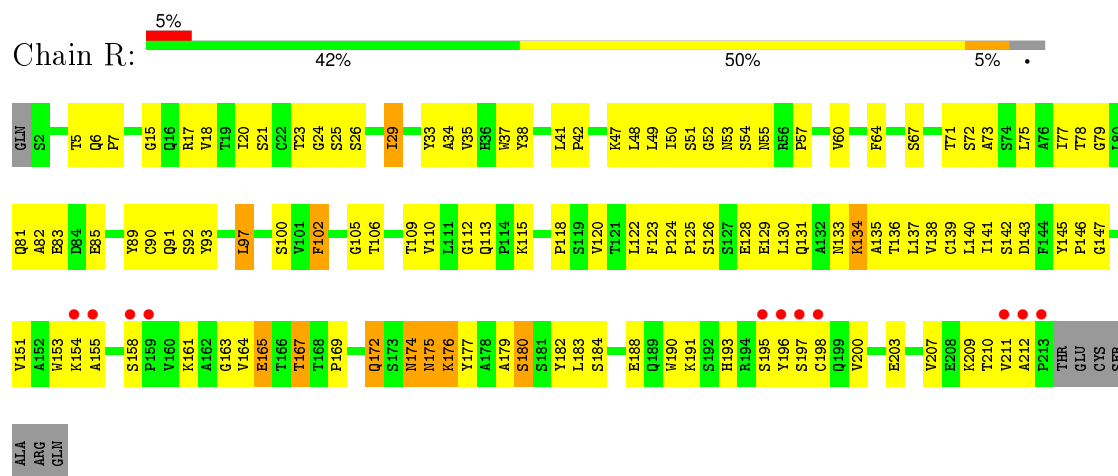


• Molecule 3: immunoglobulin light chain

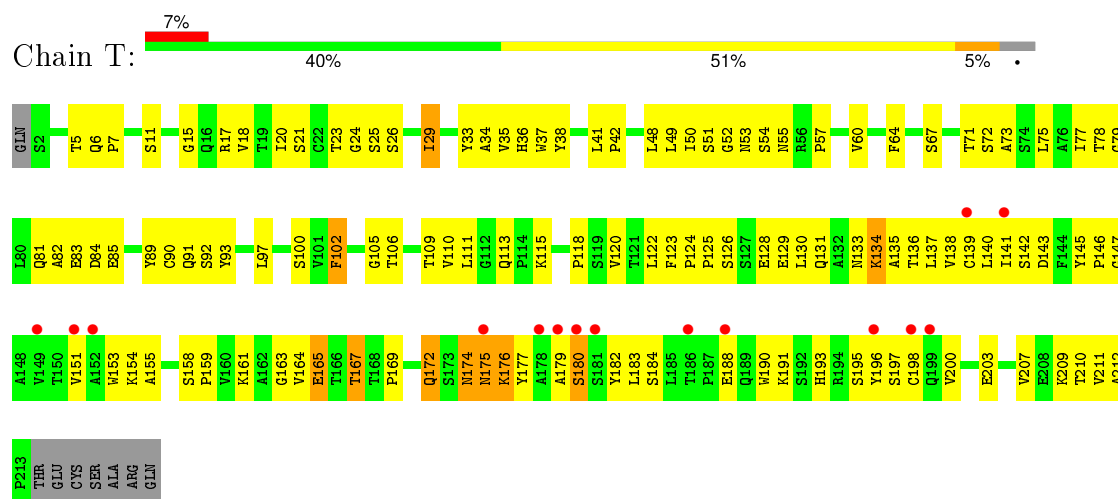




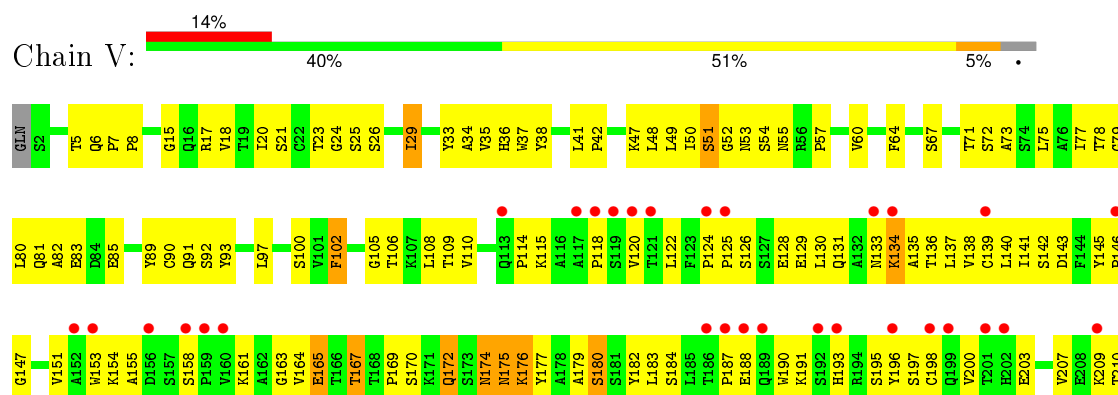
• Molecule 3: immunoglobulin light chain

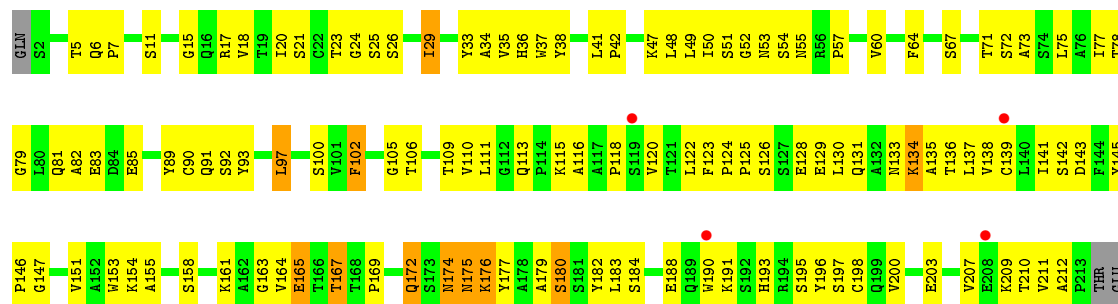


• Molecule 3: immunoglobulin light chain



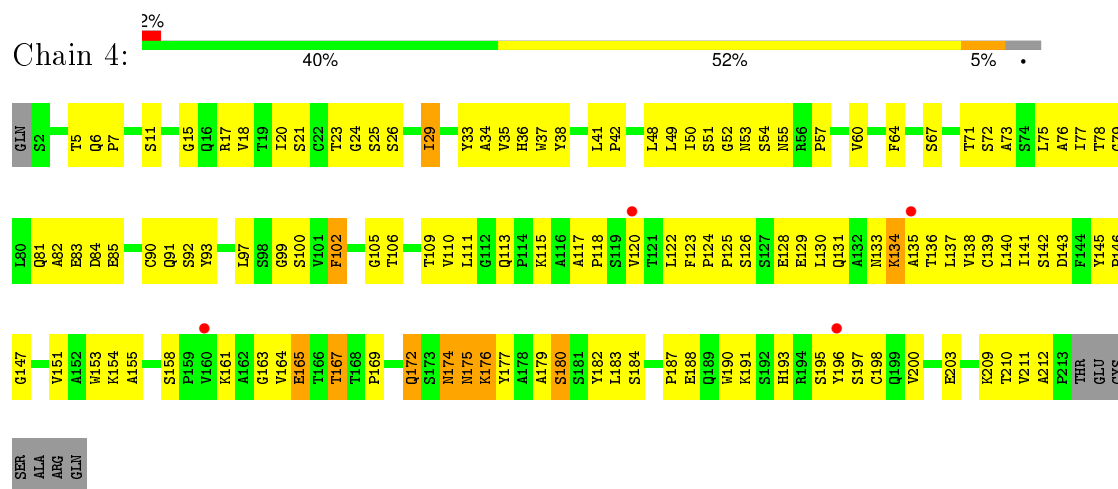
• Molecule 3: immunoglobulin light chain





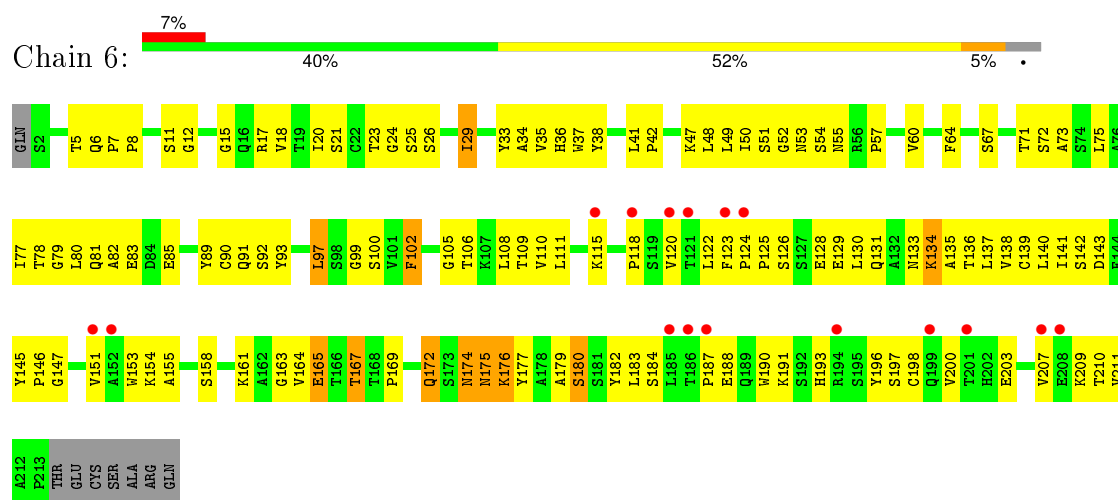
CYS  
SER  
ALA  
ARG  
GLN

• Molecule 3: immunoglobulin light chain



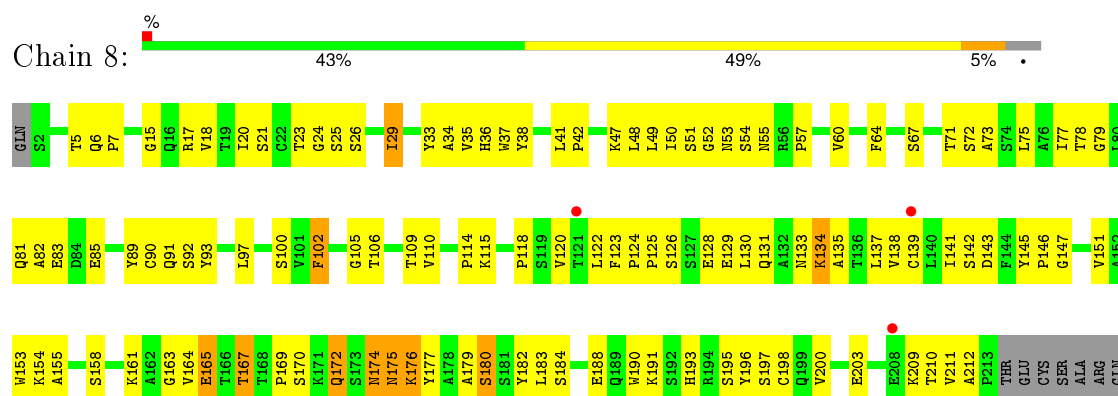
SER  
ALA  
ARG  
GLN

• Molecule 3: immunoglobulin light chain



A212  
F213  
THR  
GLU  
CYS  
SER  
ALA  
ARG  
GLN

• Molecule 3: immunoglobulin light chain



• Molecule 3: immunoglobulin light chain



Chain 0: 

39%

52%

5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	391.04Å 241.17Å 223.21Å 90.00° 123.62° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00 29.98 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-4.00) 98.2 (29.98-4.00)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 3.98Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.235 , 0.308 0.283 , 0.290	Depositor DCC
$R_{free}$ test set	7101 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	180.3	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 149.3	EDS
Estimated twinning fraction	0.063 for -h-2*k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	1 of 142111 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	88152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.25	0/3959	0.50	0/5369
1	B	0.25	0/3959	0.50	0/5369
1	C	0.25	0/3959	0.50	0/5369
1	D	0.25	0/3959	0.50	0/5369
1	E	0.25	0/3959	0.50	0/5369
1	F	0.25	0/3959	0.49	0/5369
1	G	0.25	0/3959	0.50	0/5369
1	H	0.25	0/3959	0.50	0/5369
1	I	0.25	0/3959	0.50	0/5369
1	J	0.25	0/3959	0.50	0/5369
1	K	0.25	0/3959	0.50	0/5369
1	L	0.25	0/3959	0.50	0/5369
2	1	0.25	0/1739	0.52	0/2371
2	3	0.26	0/1739	0.52	0/2371
2	5	0.25	0/1739	0.52	0/2371
2	7	0.25	0/1739	0.52	0/2371
2	9	0.26	0/1739	0.52	0/2371
2	M	0.25	0/1739	0.52	0/2371
2	O	0.25	0/1739	0.52	0/2371
2	Q	0.25	0/1739	0.53	0/2371
2	S	0.25	0/1739	0.52	0/2371
2	U	0.25	0/1739	0.52	0/2371
2	W	0.26	0/1739	0.52	0/2371
2	Y	0.25	0/1739	0.52	0/2371
3	0	0.26	0/1586	0.53	0/2166
3	2	0.26	0/1586	0.53	0/2166
3	4	0.26	0/1586	0.53	0/2166
3	6	0.26	0/1586	0.53	0/2166
3	8	0.26	0/1586	0.53	0/2166
3	N	0.26	0/1586	0.55	1/2166 (0.0%)
3	P	0.26	0/1586	0.53	0/2166
3	R	0.26	0/1586	0.55	1/2166 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	T	0.26	0/1586	0.53	0/2166
3	V	0.28	0/1586	0.55	0/2166
3	X	0.26	0/1586	0.53	0/2166
3	Z	0.26	0/1586	0.53	0/2166
All	All	0.25	0/87408	0.51	2/118872 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	112	GLY	N-CA-C	-5.23	100.03	113.10
3	N	112	GLY	N-CA-C	-5.11	100.33	113.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3878	0	3743	259	0
1	B	3878	0	3743	278	0
1	C	3878	0	3743	277	0
1	D	3878	0	3743	277	0
1	E	3878	0	3743	281	0
1	F	3878	0	3743	283	0
1	G	3878	0	3743	249	0
1	H	3878	0	3743	259	0
1	I	3878	0	3743	256	0
1	J	3878	0	3743	263	0
1	K	3878	0	3743	262	0
1	L	3878	0	3743	268	0
2	1	1697	0	1668	192	0
2	3	1697	0	1668	191	2
2	5	1697	0	1668	193	0
2	7	1697	0	1668	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	1697	0	1668	192	0
2	M	1697	0	1668	217	0
2	O	1697	0	1668	197	0
2	Q	1697	0	1668	191	0
2	S	1697	0	1668	200	0
2	U	1697	0	1668	210	0
2	W	1697	0	1668	211	0
2	Y	1697	0	1668	189	0
3	0	1549	0	1503	133	0
3	2	1549	0	1503	133	0
3	4	1549	0	1503	136	0
3	6	1549	0	1503	137	0
3	8	1549	0	1503	127	0
3	N	1549	0	1503	154	0
3	P	1549	0	1503	132	0
3	R	1549	0	1503	137	0
3	T	1549	0	1503	135	0
3	V	1549	0	1503	144	0
3	X	1549	0	1503	143	0
3	Z	1549	0	1503	133	0
4	A	83	0	70	4	0
4	B	83	0	70	5	0
4	C	83	0	70	1	0
4	D	83	0	70	4	0
4	E	83	0	70	2	0
4	F	83	0	70	2	0
4	G	83	0	70	2	0
4	H	83	0	70	2	0
4	I	83	0	70	1	0
4	J	83	0	70	4	0
4	K	83	0	70	7	0
4	L	83	0	70	5	0
5	A	28	0	26	0	0
5	B	28	0	26	0	0
5	C	28	0	26	0	0
5	D	28	0	26	0	0
5	E	28	0	26	0	0
5	F	28	0	26	0	0
5	G	28	0	26	0	0
5	H	28	0	26	0	0
5	I	28	0	26	0	0
5	J	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	28	0	26	0	0
5	L	28	0	26	0	0
6	A	72	0	61	3	0
6	B	72	0	61	3	0
6	C	72	0	61	9	0
6	D	72	0	61	7	0
6	E	72	0	61	3	0
6	F	72	0	61	11	0
6	G	72	0	61	3	0
6	H	72	0	61	3	0
6	I	72	0	61	4	0
6	J	72	0	61	3	0
6	K	72	0	61	3	0
6	L	72	0	61	4	0
7	A	39	0	34	1	0
7	B	39	0	34	1	0
7	C	39	0	34	1	0
7	D	39	0	34	1	0
7	E	39	0	34	1	0
7	F	39	0	34	1	0
7	G	39	0	34	2	0
7	H	39	0	34	1	0
7	I	39	0	34	1	0
7	J	39	0	34	1	0
7	K	39	0	34	1	0
7	L	39	0	34	1	0
All	All	88152	0	85260	6774	2

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 39.

All (6774) 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)
2:5:136:PRO:O	3:6:126:SER:HB3	1.52	1.09
3:2:143:ASP:HA	3:2:176:LYS:HG3	1.35	1.08
3:T:143:ASP:HA	3:T:176:LYS:HG3	1.35	1.08
3:0:143:ASP:HA	3:0:176:LYS:HG3	1.34	1.08
1:G:331:LEU:H	1:G:331:LEU:HD22	1.19	1.08
4:L:602:NAG:H5	2:9:57:GLN:HE22	1.17	1.07
3:N:143:ASP:HA	3:N:176:LYS:HG3	1.35	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:143:ASP:HA	3:Z:176:LYS:HG3	1.35	1.07
3:P:143:ASP:HA	3:P:176:LYS:HG3	1.34	1.06
3:8:143:ASP:HA	3:8:176:LYS:HG3	1.36	1.05
3:V:143:ASP:HA	3:V:176:LYS:HG3	1.35	1.05
3:4:143:ASP:HA	3:4:176:LYS:HG3	1.36	1.05
3:6:143:ASP:HA	3:6:176:LYS:HG3	1.36	1.03
2:O:33:GLY:HA3	2:O:99:VAL:HG22	1.41	1.02
1:D:331:LEU:H	1:D:331:LEU:HD22	1.24	1.02
3:X:143:ASP:HA	3:X:176:LYS:HG3	1.35	1.02
2:U:33:GLY:HA3	2:U:99:VAL:HG22	1.41	1.02
2:S:136:PRO:O	3:T:126:SER:HB3	1.59	1.02
1:F:331:LEU:H	1:F:331:LEU:HD22	1.19	1.02
1:A:331:LEU:H	1:A:331:LEU:HD22	1.24	1.01
3:R:143:ASP:HA	3:R:176:LYS:HG3	1.36	1.01
4:K:602:NAG:H5	2:7:57:GLN:HE22	1.26	1.00
2:U:136:PRO:O	3:V:126:SER:HB3	1.61	1.00
2:W:33:GLY:HA3	2:W:99:VAL:HG22	1.42	1.00
2:Q:33:GLY:HA3	2:Q:99:VAL:HG22	1.40	1.00
2:7:33:GLY:HA3	2:7:99:VAL:HG22	1.40	0.99
2:Y:33:GLY:HA3	2:Y:99:VAL:HG22	1.40	0.99
2:3:33:GLY:HA3	2:3:99:VAL:HG22	1.43	0.99
2:1:33:GLY:HA3	2:1:99:VAL:HG22	1.42	0.99
2:S:33:GLY:HA3	2:S:99:VAL:HG22	1.41	0.99
2:M:33:GLY:HA3	2:M:99:VAL:HG22	1.42	0.99
1:K:331:LEU:HD22	1:K:331:LEU:H	1.25	0.98
1:H:331:LEU:HD22	1:H:331:LEU:H	1.24	0.98
1:B:331:LEU:HD22	1:B:331:LEU:H	1.24	0.98
1:E:331:LEU:HD22	1:E:331:LEU:H	1.24	0.98
1:I:331:LEU:H	1:I:331:LEU:HD22	1.26	0.98
1:C:331:LEU:HD22	1:C:331:LEU:H	1.27	0.97
2:Q:51:ILE:HD13	2:Q:52:ASN:H	1.30	0.97
2:U:91:THR:HB	2:U:124:VAL:H	1.26	0.97
3:N:11:SER:HB3	3:N:111:LEU:HD11	1.46	0.97
1:J:331:LEU:HD22	1:J:331:LEU:H	1.25	0.96
2:5:33:GLY:HA3	2:5:99:VAL:HG22	1.47	0.96
4:K:602:NAG:H5	2:7:57:GLN:NE2	1.79	0.96
2:U:24:VAL:HG21	2:U:29:LEU:HB3	1.47	0.96
2:W:6:GLN:HE21	2:W:117:GLY:HA3	1.29	0.96
2:W:100:GLU:H	2:W:111:TYR:HB2	1.30	0.96
2:7:51:ILE:HD13	2:7:52:ASN:H	1.31	0.96
2:3:206:THR:HG21	2:3:223:LYS:HE2	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:206:THR:HG21	2:7:223:LYS:HE2	1.48	0.96
2:W:84:LYS:HZ2	2:9:142:LYS:NZ	1.61	0.96
1:F:187:THR:HB	1:F:189:GLN:HE21	1.31	0.96
2:S:51:ILE:HD13	2:S:52:ASN:H	1.31	0.96
2:S:206:THR:HG21	2:S:223:LYS:HE2	1.47	0.95
2:Y:51:ILE:HD13	2:Y:52:ASN:H	1.31	0.95
2:1:206:THR:HG21	2:1:223:LYS:HE2	1.48	0.95
1:L:331:LEU:HD13	1:L:331:LEU:N	1.79	0.95
2:5:206:THR:HG21	2:5:223:LYS:HE2	1.49	0.95
1:H:187:THR:HB	1:H:189:GLN:HE21	1.31	0.95
2:3:24:VAL:HG21	2:3:29:LEU:HB3	1.47	0.95
4:L:602:NAG:H5	2:9:57:GLN:NE2	1.81	0.95
2:O:51:ILE:HD13	2:O:52:ASN:H	1.30	0.95
2:U:51:ILE:HD13	2:U:52:ASN:H	1.32	0.95
2:3:71:THR:HB	2:3:80:TYR:HB2	1.48	0.95
2:9:206:THR:HG21	2:9:223:LYS:HE2	1.48	0.95
2:3:51:ILE:HD13	2:3:52:ASN:H	1.30	0.95
2:W:24:VAL:HG21	2:W:29:LEU:HB3	1.47	0.95
2:Q:24:VAL:HG21	2:Q:29:LEU:HB3	1.50	0.94
1:L:187:THR:HB	1:L:189:GLN:HE21	1.30	0.94
2:M:24:VAL:HG21	2:M:29:LEU:HB3	1.47	0.94
2:3:6:GLN:HE21	2:3:117:GLY:HA3	1.28	0.94
2:9:33:GLY:HA3	2:9:99:VAL:HG22	1.46	0.94
2:5:12:LYS:HD2	2:5:18:VAL:HG22	1.49	0.94
2:O:206:THR:HG21	2:O:223:LYS:HE2	1.49	0.94
2:1:100:GLU:H	2:1:111:TYR:HB2	1.32	0.94
1:I:187:THR:HB	1:I:189:GLN:HE21	1.32	0.94
2:S:100:GLU:H	2:S:111:TYR:HB2	1.32	0.94
2:5:51:ILE:HD13	2:5:52:ASN:H	1.30	0.94
2:7:24:VAL:HG21	2:7:29:LEU:HB3	1.49	0.94
2:W:206:THR:HG21	2:W:223:LYS:HE2	1.49	0.94
2:Y:206:THR:HG21	2:Y:223:LYS:HE2	1.49	0.94
2:O:24:VAL:HG21	2:O:29:LEU:HB3	1.50	0.94
1:D:187:THR:HB	1:D:189:GLN:HE21	1.32	0.93
2:M:206:THR:HG21	2:M:223:LYS:HE2	1.48	0.93
1:E:187:THR:HB	1:E:189:GLN:HE21	1.31	0.93
1:K:187:THR:HB	1:K:189:GLN:HE21	1.32	0.93
2:9:100:GLU:H	2:9:111:TYR:HB2	1.31	0.93
2:9:24:VAL:HG21	2:9:29:LEU:HB3	1.47	0.93
2:U:71:THR:HB	2:U:80:TYR:HB2	1.51	0.93
2:M:51:ILE:HD13	2:M:52:ASN:H	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:331:LEU:HD22	1:L:331:LEU:H	1.34	0.93
2:O:6:GLN:H	2:O:118:GLN:NE2	1.66	0.93
2:S:24:VAL:HG21	2:S:29:LEU:HB3	1.50	0.93
2:W:51:ILE:HD13	2:W:52:ASN:H	1.32	0.93
2:M:12:LYS:HD2	2:M:18:VAL:HG22	1.51	0.93
1:J:187:THR:HB	1:J:189:GLN:HE21	1.31	0.93
2:5:24:VAL:HG21	2:5:29:LEU:HB3	1.49	0.93
2:Q:100:GLU:H	2:Q:111:TYR:HB2	1.34	0.92
2:W:12:LYS:HD2	2:W:18:VAL:HG22	1.50	0.92
3:X:11:SER:HB3	3:X:111:LEU:HD11	1.51	0.92
2:3:91:THR:HB	2:3:124:VAL:H	1.32	0.92
2:U:100:GLU:H	2:U:111:TYR:HB2	1.32	0.92
2:O:6:GLN:H	2:O:118:GLN:HE22	1.07	0.92
2:9:51:ILE:HD13	2:9:52:ASN:H	1.30	0.92
2:Q:71:THR:HB	2:Q:80:TYR:HB2	1.52	0.92
1:A:187:THR:HB	1:A:189:GLN:HE21	1.32	0.92
2:Y:71:THR:HB	2:Y:80:TYR:HB2	1.52	0.92
2:1:24:VAL:HG21	2:1:29:LEU:HB3	1.49	0.92
2:7:71:THR:HB	2:7:80:TYR:HB2	1.51	0.92
2:W:84:LYS:NZ	2:9:142:LYS:HZ1	1.68	0.92
2:Q:206:THR:HG21	2:Q:223:LYS:HE2	1.49	0.92
2:Y:24:VAL:HG21	2:Y:29:LEU:HB3	1.51	0.92
2:M:100:GLU:H	2:M:111:TYR:HB2	1.34	0.92
1:G:187:THR:HB	1:G:189:GLN:HE21	1.31	0.91
2:5:100:GLU:H	2:5:111:TYR:HB2	1.34	0.91
2:O:100:GLU:H	2:O:111:TYR:HB2	1.33	0.91
2:1:51:ILE:HD13	2:1:52:ASN:H	1.32	0.91
2:O:71:THR:HB	2:O:80:TYR:HB2	1.51	0.91
2:3:136:PRO:O	3:4:126:SER:HB3	1.71	0.91
1:C:187:THR:HB	1:C:189:GLN:HE21	1.31	0.91
2:5:71:THR:HB	2:5:80:TYR:HB2	1.52	0.91
2:1:71:THR:HB	2:1:80:TYR:HB2	1.49	0.91
2:U:206:THR:HG21	2:U:223:LYS:HE2	1.50	0.91
2:S:18:VAL:HG23	2:S:86:LEU:HD11	1.53	0.91
2:M:71:THR:HB	2:M:80:TYR:HB2	1.49	0.90
2:7:18:VAL:HG23	2:7:86:LEU:HD11	1.53	0.90
2:7:100:GLU:H	2:7:111:TYR:HB2	1.36	0.90
2:Y:18:VAL:HG23	2:Y:86:LEU:HD11	1.54	0.90
2:Q:12:LYS:HD2	2:Q:18:VAL:HG22	1.52	0.90
2:Q:18:VAL:HG23	2:Q:86:LEU:HD11	1.54	0.90
2:Y:100:GLU:H	2:Y:111:TYR:HB2	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:12:LYS:HD2	2:1:18:VAL:HG22	1.52	0.90
2:5:6:GLN:HE21	2:5:117:GLY:HA3	1.36	0.90
2:9:71:THR:HB	2:9:80:TYR:HB2	1.50	0.90
2:3:12:LYS:HD2	2:3:18:VAL:HG22	1.54	0.90
2:O:18:VAL:HG23	2:O:86:LEU:HD11	1.53	0.89
2:W:71:THR:HB	2:W:80:TYR:HB2	1.52	0.89
2:U:12:LYS:HD2	2:U:18:VAL:HG22	1.52	0.89
1:B:187:THR:HB	1:B:189:GLN:HE21	1.35	0.89
2:3:100:GLU:H	2:3:111:TYR:HB2	1.38	0.89
2:U:18:VAL:HG23	2:U:86:LEU:HD11	1.54	0.88
2:9:18:VAL:HG23	2:9:86:LEU:HD11	1.56	0.88
1:J:463:GLY:HA2	1:K:453:ARG:HD3	1.54	0.88
2:W:18:VAL:HG23	2:W:86:LEU:HD11	1.56	0.87
2:7:6:GLN:HB3	2:7:120:THR:HG23	1.55	0.87
2:M:18:VAL:HG23	2:M:86:LEU:HD11	1.55	0.87
1:B:146:GLY:HA2	1:L:143:PRO:HB3	1.54	0.87
2:5:18:VAL:HG23	2:5:86:LEU:HD11	1.55	0.87
2:9:12:LYS:HD2	2:9:18:VAL:HG22	1.54	0.87
2:1:18:VAL:HG23	2:1:86:LEU:HD11	1.56	0.87
3:N:113:GLN:HG3	3:N:175:ASN:ND2	1.89	0.86
2:W:160:PRO:HD2	2:W:215:PRO:HB3	1.57	0.86
2:7:12:LYS:HD2	2:7:18:VAL:HG22	1.57	0.86
6:C:609:NAG:H3	6:C:610:NAG:H82	1.58	0.86
6:L:609:NAG:H3	6:L:610:NAG:H82	1.57	0.86
1:F:191:GLN:HE21	1:F:217:ILE:HD11	1.40	0.86
1:J:107:SER:HB2	1:L:404:GLY:HA3	1.58	0.86
2:9:6:GLN:HE21	2:9:117:GLY:HA3	1.40	0.86
2:S:71:THR:HB	2:S:80:TYR:HB2	1.56	0.86
2:3:18:VAL:HG23	2:3:86:LEU:HD11	1.56	0.86
2:S:12:LYS:HD2	2:S:18:VAL:HG22	1.56	0.86
2:Y:160:PRO:HD2	2:Y:215:PRO:HB3	1.58	0.85
4:B:602:NAG:H5	2:O:57:GLN:HE22	1.41	0.85
2:O:12:LYS:HD2	2:O:18:VAL:HG22	1.55	0.85
6:D:609:NAG:H3	6:D:610:NAG:H82	1.58	0.85
6:I:609:NAG:H3	6:I:610:NAG:H82	1.58	0.85
2:Y:111:TYR:HE1	2:Y:113:MET:HG2	1.41	0.85
2:Y:12:LYS:HD2	2:Y:18:VAL:HG22	1.55	0.85
2:U:160:PRO:HD2	2:U:215:PRO:HB3	1.59	0.85
1:J:53:ASN:HD21	1:J:276:THR:HA	1.40	0.85
1:E:29:ILE:O	1:F:380:LYS:HG2	1.77	0.85
1:B:326:LYS:HB3	1:B:328:THR:HG23	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:91:THR:HB	2:9:124:VAL:H	1.41	0.84
2:S:160:PRO:HD2	2:S:215:PRO:HB3	1.59	0.84
6:E:609:NAG:H3	6:E:610:NAG:H82	1.59	0.84
2:9:160:PRO:HD2	2:9:215:PRO:HB3	1.59	0.84
2:3:160:PRO:HD2	2:3:215:PRO:HB3	1.59	0.84
2:5:160:PRO:HD2	2:5:215:PRO:HB3	1.58	0.84
1:C:326:LYS:HB3	1:C:328:THR:HG23	1.59	0.84
2:Q:160:PRO:HD2	2:Q:215:PRO:HB3	1.60	0.84
1:I:326:LYS:HB3	1:I:328:THR:HG23	1.58	0.84
1:E:326:LYS:HB3	1:E:328:THR:HG23	1.60	0.83
1:G:326:LYS:HB3	1:G:328:THR:HG23	1.59	0.83
2:W:51:ILE:HG12	2:W:58:THR:HG22	1.60	0.83
2:Y:51:ILE:HG12	2:Y:58:THR:HG22	1.60	0.83
2:Q:6:GLN:HB3	2:Q:120:THR:HG23	1.59	0.83
6:G:609:NAG:H3	6:G:610:NAG:H82	1.60	0.83
2:Q:10:GLU:O	2:Q:122:VAL:HA	1.79	0.83
2:1:160:PRO:HD2	2:1:215:PRO:HB3	1.58	0.83
1:A:326:LYS:HB3	1:A:328:THR:HG23	1.60	0.83
2:M:51:ILE:HG12	2:M:58:THR:HG22	1.61	0.83
2:5:51:ILE:HG12	2:5:58:THR:HG22	1.61	0.83
1:H:326:LYS:HB3	1:H:328:THR:HG23	1.60	0.83
1:K:326:LYS:HB3	1:K:328:THR:HG23	1.60	0.82
6:H:609:NAG:H3	6:H:610:NAG:H82	1.61	0.82
6:J:609:NAG:H3	6:J:610:NAG:H82	1.60	0.82
2:O:160:PRO:HD2	2:O:215:PRO:HB3	1.60	0.82
2:M:160:PRO:HD2	2:M:215:PRO:HB3	1.59	0.82
1:A:463:GLY:HA2	1:B:453:ARG:HD3	1.58	0.82
1:D:326:LYS:HB3	1:D:328:THR:HG23	1.60	0.82
3:N:11:SER:HB3	3:N:111:LEU:CD1	2.09	0.82
2:3:20:VAL:HG13	2:3:120:THR:HG21	1.61	0.82
1:J:326:LYS:HB3	1:J:328:THR:HG23	1.60	0.82
6:K:609:NAG:H3	6:K:610:NAG:H82	1.61	0.82
2:5:6:GLN:HB3	2:5:120:THR:HG23	1.59	0.81
6:A:609:NAG:H3	6:A:610:NAG:H82	1.62	0.81
2:O:6:GLN:HB3	2:O:120:THR:HG23	1.59	0.81
2:O:61:VAL:HG12	2:O:63:LYS:H	1.45	0.81
1:I:53:ASN:HD21	1:I:276:THR:HA	1.46	0.81
2:O:112:PRO:HB2	3:P:51:SER:HB2	1.62	0.81
6:F:609:NAG:H3	6:F:610:NAG:H82	1.62	0.81
2:Q:135:PHE:HB3	3:R:126:SER:OG	1.81	0.81
2:S:6:GLN:HE21	2:S:117:GLY:HA3	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:ASN:ND2	1:F:219:SER:H	1.79	0.81
2:7:160:PRO:HD2	2:7:215:PRO:HB3	1.60	0.81
2:Y:61:VAL:HG12	2:Y:63:LYS:H	1.47	0.80
3:X:11:SER:HB3	3:X:111:LEU:CD1	2.11	0.80
2:M:6:GLN:HE21	2:M:117:GLY:HA3	1.46	0.80
2:W:61:VAL:HG12	2:W:63:LYS:H	1.46	0.80
1:F:53:ASN:HD21	1:F:276:THR:HA	1.44	0.80
6:B:609:NAG:H3	6:B:610:NAG:H82	1.61	0.80
4:B:602:NAG:H5	2:O:57:GLN:NE2	1.96	0.80
2:U:61:VAL:HG12	2:U:63:LYS:H	1.46	0.80
2:3:91:THR:HB	2:3:124:VAL:HG23	1.64	0.80
1:B:191:GLN:HE21	1:B:217:ILE:HD11	1.46	0.80
2:M:91:THR:HB	2:M:124:VAL:H	1.47	0.80
1:F:326:LYS:HB3	1:F:328:THR:HG23	1.62	0.80
2:3:51:ILE:HG12	2:3:58:THR:HG22	1.61	0.80
2:Q:136:PRO:O	3:R:126:SER:HB3	1.81	0.80
4:J:602:NAG:H5	2:5:57:GLN:HE22	1.46	0.79
2:3:61:VAL:HG12	2:3:63:LYS:H	1.47	0.79
2:Q:11:VAL:HG13	2:Q:123:THR:HB	1.64	0.79
2:O:51:ILE:HG12	2:O:58:THR:HG22	1.63	0.79
2:U:51:ILE:HG12	2:U:58:THR:HG22	1.62	0.79
2:M:6:GLN:HB3	2:M:120:THR:HG23	1.63	0.79
1:D:409:LEU:HD11	1:E:413:VAL:HG21	1.64	0.79
3:R:124:PRO:HB3	3:R:211:VAL:HG11	1.65	0.79
2:Y:112:PRO:HB2	3:Z:51:SER:HB2	1.63	0.79
1:D:383:ARG:HD3	1:F:27:LYS:NZ	1.98	0.79
2:M:61:VAL:HG12	2:M:63:LYS:H	1.45	0.79
1:I:191:GLN:HE21	1:I:217:ILE:HD11	1.46	0.79
2:1:61:VAL:HG12	2:1:63:LYS:H	1.47	0.79
1:D:151:LEU:HD22	1:D:252:ILE:HG22	1.63	0.79
2:S:61:VAL:HG12	2:S:63:LYS:H	1.46	0.79
2:9:51:ILE:HG12	2:9:58:THR:HG22	1.64	0.79
2:1:51:ILE:HG12	2:1:58:THR:HG22	1.64	0.79
2:W:84:LYS:HZ2	2:9:142:LYS:HZ1	0.82	0.79
2:5:129:THR:HG22	2:5:160:PRO:HD3	1.65	0.79
1:L:191:GLN:HE21	1:L:217:ILE:HD11	1.48	0.79
1:E:27:LYS:HD3	1:F:383:ARG:CZ	2.13	0.79
2:9:61:VAL:HG12	2:9:63:LYS:H	1.47	0.79
1:K:53:ASN:HD21	1:K:276:THR:HA	1.48	0.79
2:7:51:ILE:HG12	2:7:58:THR:HG22	1.64	0.78
1:L:53:ASN:HD21	1:L:276:THR:HA	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:51:ILE:HG12	2:S:58:THR:HG22	1.65	0.78
2:5:5:VAL:HB	2:5:23:GLN:HB2	1.64	0.78
2:Q:109:HIS:HA	3:R:93:TYR:CG	2.18	0.78
2:7:61:VAL:HG12	2:7:63:LYS:H	1.47	0.78
1:H:53:ASN:HD21	1:H:276:THR:HA	1.49	0.78
2:7:5:VAL:HB	2:7:23:GLN:HB2	1.66	0.78
1:K:140:LYS:HG2	1:K:145:SER:HA	1.66	0.78
2:Y:92:ALA:O	2:Y:122:VAL:HG22	1.83	0.78
2:3:91:THR:CB	2:3:124:VAL:H	1.95	0.78
2:1:136:PRO:O	3:2:126:SER:HB3	1.84	0.78
1:D:53:ASN:HD21	1:D:276:THR:HA	1.47	0.78
2:O:91:THR:HB	2:O:124:VAL:HG23	1.64	0.78
2:Q:61:VAL:HG12	2:Q:63:LYS:H	1.46	0.78
2:W:129:THR:HG22	2:W:160:PRO:HD3	1.66	0.78
1:D:244:VAL:HB	1:F:221:PRO:HD3	1.66	0.78
3:0:124:PRO:HB3	3:0:211:VAL:HG11	1.66	0.78
2:Q:5:VAL:HB	2:Q:23:GLN:HB2	1.65	0.78
2:U:109:HIS:HA	3:V:93:TYR:CG	2.20	0.77
2:Q:51:ILE:HG12	2:Q:58:THR:HG22	1.66	0.77
2:5:48:VAL:O	2:5:61:VAL:HG23	1.85	0.77
2:9:5:VAL:HB	2:9:23:GLN:HB2	1.66	0.77
2:7:6:GLN:HE21	2:7:117:GLY:HA3	1.48	0.77
1:A:272:ALA:HA	2:M:105:VAL:HG22	1.64	0.77
1:K:151:LEU:HD22	1:K:252:ILE:HG22	1.66	0.77
2:3:91:THR:HB	2:3:124:VAL:N	2.00	0.77
2:5:61:VAL:HG12	2:5:63:LYS:H	1.46	0.77
1:E:140:LYS:HG2	1:E:145:SER:HA	1.66	0.77
3:T:124:PRO:HB3	3:T:211:VAL:HG11	1.67	0.77
1:F:272:ALA:HA	2:W:105:VAL:HG22	1.65	0.77
2:S:5:VAL:HB	2:S:23:GLN:HB2	1.67	0.77
2:O:5:VAL:HB	2:O:23:GLN:HB2	1.66	0.77
1:G:191:GLN:HE21	1:G:217:ILE:HD11	1.48	0.77
1:B:140:LYS:HG2	1:B:145:SER:HA	1.64	0.77
2:7:91:THR:HB	2:7:124:VAL:HG23	1.67	0.77
1:A:191:GLN:HE21	1:A:217:ILE:HD11	1.49	0.77
2:1:5:VAL:HB	2:1:23:GLN:HB2	1.67	0.77
1:D:27:LYS:NZ	1:E:383:ARG:HD3	1.98	0.77
1:J:140:LYS:HG2	1:J:145:SER:HA	1.65	0.77
2:5:109:HIS:HA	3:6:93:TYR:CG	2.20	0.77
3:Z:124:PRO:HB3	3:Z:211:VAL:HG11	1.67	0.77
1:B:219:SER:H	1:C:246:ASN:ND2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:124:PRO:HB3	3:N:211:VAL:HG11	1.66	0.77
2:7:112:PRO:HB3	3:8:36:HIS:CE1	2.21	0.76
2:O:129:THR:HG22	2:O:160:PRO:HD3	1.67	0.76
3:6:124:PRO:HB3	3:6:211:VAL:HG11	1.67	0.76
1:B:221:PRO:HD3	1:C:244:VAL:HB	1.68	0.76
1:A:140:LYS:HG2	1:A:145:SER:HA	1.67	0.76
2:W:48:VAL:O	2:W:61:VAL:HG23	1.86	0.76
3:X:124:PRO:HB3	3:X:211:VAL:HG11	1.67	0.76
3:8:124:PRO:HB3	3:8:211:VAL:HG11	1.67	0.76
3:V:143:ASP:HA	3:V:176:LYS:CG	2.15	0.76
2:9:91:THR:HB	2:9:124:VAL:HG23	1.68	0.76
2:3:129:THR:HG22	2:3:160:PRO:HD3	1.68	0.76
1:L:130:VAL:HG11	1:L:164:LEU:HD11	1.68	0.76
2:S:129:THR:HG22	2:S:160:PRO:HD3	1.67	0.76
1:D:191:GLN:HE21	1:D:217:ILE:HD11	1.51	0.76
1:E:401:GLU:HG3	1:F:238:LYS:HE2	1.68	0.76
3:2:143:ASP:HA	3:2:176:LYS:CG	2.15	0.76
1:K:156:LYS:HD2	1:K:196:VAL:HG22	1.67	0.76
1:I:140:LYS:HG2	1:I:145:SER:HA	1.66	0.76
3:X:113:GLN:HG3	3:X:175:ASN:ND2	2.01	0.76
2:U:5:VAL:HB	2:U:23:GLN:HB2	1.66	0.76
3:P:124:PRO:HB3	3:P:211:VAL:HG11	1.68	0.76
2:M:111:TYR:HE1	2:M:113:MET:HG2	1.51	0.75
1:H:191:GLN:HE21	1:H:217:ILE:HD11	1.51	0.75
1:J:191:GLN:HE21	1:J:217:ILE:HD11	1.51	0.75
1:H:130:VAL:HG11	1:H:164:LEU:HD11	1.67	0.75
2:Q:129:THR:HG22	2:Q:160:PRO:HD3	1.68	0.75
1:A:53:ASN:HD21	1:A:276:THR:HA	1.51	0.75
2:Y:6:GLN:HE21	2:Y:117:GLY:HA3	1.50	0.75
1:L:156:LYS:HD2	1:L:196:VAL:HG22	1.68	0.75
1:F:140:LYS:HG2	1:F:145:SER:HA	1.67	0.75
2:Y:5:VAL:HB	2:Y:23:GLN:HB2	1.68	0.75
3:4:124:PRO:HB3	3:4:211:VAL:HG11	1.67	0.75
2:U:91:THR:OG1	2:U:123:THR:HA	1.87	0.75
1:G:140:LYS:HG2	1:G:145:SER:HA	1.68	0.75
2:S:60:TYR:HE1	2:S:70:MET:HG2	1.52	0.75
3:0:143:ASP:CA	3:0:176:LYS:HG3	2.16	0.75
1:J:272:ALA:HA	2:5:105:VAL:HG22	1.68	0.75
1:E:463:GLY:HA2	1:F:453:ARG:HD3	1.68	0.75
1:E:156:LYS:HD2	1:E:196:VAL:HG22	1.69	0.75
3:2:124:PRO:HB3	3:2:211:VAL:HG11	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:156:LYS:HD2	1:H:196:VAL:HG22	1.69	0.75
1:B:156:LYS:HD2	1:B:196:VAL:HG22	1.67	0.75
2:O:60:TYR:HE1	2:O:70:MET:HG2	1.51	0.75
1:G:156:LYS:HD2	1:G:196:VAL:HG22	1.67	0.75
2:M:5:VAL:HB	2:M:23:GLN:HB2	1.68	0.75
2:5:91:THR:OG1	2:5:123:THR:HA	1.87	0.75
1:K:191:GLN:HE21	1:K:217:ILE:HD11	1.52	0.75
1:F:156:LYS:HD2	1:F:196:VAL:HG22	1.67	0.75
3:N:143:ASP:CA	3:N:176:LYS:HG3	2.16	0.75
2:7:113:MET:HG3	3:8:38:TYR:OH	1.86	0.75
1:J:27:LYS:HD3	1:K:383:ARG:NH1	2.02	0.75
1:H:463:GLY:HA2	1:I:453:ARG:HD3	1.69	0.75
2:3:5:VAL:HB	2:3:23:GLN:HB2	1.68	0.75
1:G:151:LEU:HD22	1:G:252:ILE:HG22	1.67	0.75
1:J:29:ILE:O	1:K:380:LYS:HG2	1.86	0.74
2:3:172:LEU:HD21	2:3:195:VAL:HG11	1.69	0.74
3:N:143:ASP:HA	3:N:176:LYS:CG	2.14	0.74
2:9:60:TYR:HE1	2:9:70:MET:HG2	1.53	0.74
3:8:143:ASP:CA	3:8:176:LYS:HG3	2.17	0.74
2:9:129:THR:HG22	2:9:160:PRO:HD3	1.68	0.74
2:M:129:THR:HG22	2:M:160:PRO:HD3	1.68	0.74
1:E:130:VAL:HG11	1:E:164:LEU:HD11	1.68	0.74
2:7:33:GLY:CA	2:7:99:VAL:HG22	2.18	0.74
2:7:6:GLN:HB2	2:7:118:GLN:OE1	1.87	0.74
2:Y:48:VAL:O	2:Y:61:VAL:HG23	1.88	0.74
1:I:272:ALA:HA	2:3:105:VAL:HG22	1.69	0.74
2:S:91:THR:HB	2:S:124:VAL:H	1.50	0.74
1:F:42:LEU:HD11	1:F:316:LEU:HB2	1.69	0.74
1:B:151:LEU:HD22	1:B:252:ILE:HG22	1.68	0.74
1:C:151:LEU:HD22	1:C:252:ILE:HG22	1.66	0.74
2:W:60:TYR:HE1	2:W:70:MET:HG2	1.52	0.74
1:E:27:LYS:HD3	1:F:383:ARG:NH1	2.03	0.74
2:3:60:TYR:HE1	2:3:70:MET:HG2	1.52	0.74
2:U:172:LEU:HD21	2:U:195:VAL:HG11	1.69	0.74
1:J:151:LEU:HD22	1:J:252:ILE:HG22	1.68	0.74
2:7:60:TYR:HE1	2:7:70:MET:HG2	1.52	0.74
3:P:143:ASP:HA	3:P:176:LYS:CG	2.14	0.74
3:X:143:ASP:HA	3:X:176:LYS:CG	2.15	0.74
2:S:6:GLN:HB2	2:S:118:GLN:OE1	1.87	0.74
1:K:130:VAL:HG11	1:K:164:LEU:HD11	1.68	0.74
2:1:172:LEU:HD21	2:1:195:VAL:HG11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:60:TYR:HE1	2:Q:70:MET:HG2	1.51	0.74
3:V:124:PRO:HB3	3:V:211:VAL:HG11	1.69	0.74
3:4:143:ASP:HA	3:4:176:LYS:CG	2.17	0.74
2:Y:33:GLY:CA	2:Y:99:VAL:HG22	2.18	0.74
1:B:146:GLY:HA2	1:L:143:PRO:CB	2.16	0.74
2:O:48:VAL:O	2:O:61:VAL:HG23	1.88	0.74
2:7:48:VAL:O	2:7:61:VAL:HG23	1.87	0.74
1:D:130:VAL:HG11	1:D:164:LEU:HD11	1.70	0.74
2:7:172:LEU:HD21	2:7:195:VAL:HG11	1.69	0.74
1:G:130:VAL:HG11	1:G:164:LEU:HD11	1.69	0.74
1:H:409:LEU:O	1:H:413:VAL:HG23	1.88	0.74
2:O:136:PRO:O	3:P:126:SER:HB3	1.87	0.74
1:C:130:VAL:HG11	1:C:164:LEU:HD11	1.69	0.74
3:0:143:ASP:HA	3:0:176:LYS:CG	2.14	0.74
2:1:48:VAL:O	2:1:61:VAL:HG23	1.88	0.74
2:Q:172:LEU:HD21	2:Q:195:VAL:HG11	1.70	0.74
2:S:52:ASN:HD21	2:S:102:VAL:HA	1.53	0.74
2:O:112:PRO:HB3	3:P:36:HIS:CE1	2.23	0.74
2:M:135:PHE:HB3	3:N:126:SER:OG	1.87	0.74
3:8:143:ASP:HA	3:8:176:LYS:CG	2.15	0.73
1:E:463:GLY:HA3	1:F:453:ARG:HB3	1.70	0.73
1:I:151:LEU:HD22	1:I:252:ILE:HG22	1.69	0.73
1:H:140:LYS:HG2	1:H:145:SER:HA	1.68	0.73
2:W:5:VAL:HB	2:W:23:GLN:HB2	1.69	0.73
2:3:48:VAL:O	2:3:61:VAL:HG23	1.88	0.73
1:E:409:LEU:O	1:E:413:VAL:HG23	1.88	0.73
2:9:48:VAL:O	2:9:61:VAL:HG23	1.88	0.73
2:5:172:LEU:HD21	2:5:195:VAL:HG11	1.70	0.73
1:E:16:GLY:HA2	1:E:338:PHE:HB3	1.70	0.73
3:T:143:ASP:HA	3:T:176:LYS:CG	2.16	0.73
1:F:187:THR:HB	1:F:189:GLN:NE2	2.03	0.73
2:U:129:THR:HG22	2:U:160:PRO:HD3	1.68	0.73
2:1:129:THR:HG22	2:1:160:PRO:HD3	1.69	0.73
1:J:130:VAL:HG11	1:J:164:LEU:HD11	1.70	0.73
2:S:179:PHE:HB3	3:T:180:SER:OG	1.88	0.73
1:D:409:LEU:O	1:D:413:VAL:HG23	1.89	0.73
1:J:16:GLY:HA2	1:J:338:PHE:HB3	1.69	0.73
2:O:172:LEU:HD21	2:O:195:VAL:HG11	1.69	0.73
1:C:79:PHE:O	1:C:82:GLU:HB2	1.88	0.73
1:L:151:LEU:HD22	1:L:252:ILE:HG22	1.70	0.73
2:M:172:LEU:HD21	2:M:195:VAL:HG11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:53:ASN:ND2	1:J:276:THR:HA	2.02	0.73
1:C:53:ASN:HD21	1:C:276:THR:HA	1.52	0.73
1:I:102:VAL:HG22	1:I:232:ILE:HB	1.70	0.73
1:K:102:VAL:HG22	1:K:232:ILE:HB	1.70	0.73
3:2:143:ASP:CA	3:2:176:LYS:HG3	2.17	0.73
1:D:383:ARG:CZ	1:F:27:LYS:HD3	2.19	0.73
1:L:409:LEU:O	1:L:413:VAL:HG23	1.89	0.73
1:D:403:GLU:H	1:D:407:GLN:NE2	1.86	0.73
2:Y:100:GLU:H	2:Y:111:TYR:CB	2.02	0.73
3:Z:143:ASP:CA	3:Z:176:LYS:HG3	2.17	0.73
4:K:602:NAG:C5	2:7:57:GLN:HE22	2.01	0.73
2:7:129:THR:HG22	2:7:160:PRO:HD3	1.70	0.73
2:S:48:VAL:O	2:S:61:VAL:HG23	1.89	0.73
1:D:426:GLU:HG3	1:E:383:ARG:NH2	2.04	0.73
2:5:91:THR:HB	2:5:124:VAL:H	1.54	0.73
2:M:60:TYR:HE1	2:M:70:MET:HG2	1.53	0.73
1:C:191:GLN:HE21	1:C:217:ILE:HD11	1.54	0.73
3:Z:143:ASP:HA	3:Z:176:LYS:CG	2.15	0.73
1:E:222:TRP:CZ3	1:E:225:GLY:HA2	2.24	0.73
2:M:48:VAL:O	2:M:61:VAL:HG23	1.88	0.73
1:D:140:LYS:HG2	1:D:145:SER:HA	1.70	0.73
2:Y:60:TYR:HE1	2:Y:70:MET:HG2	1.52	0.73
2:U:52:ASN:HD21	2:U:102:VAL:HA	1.52	0.73
2:W:52:ASN:HD21	2:W:102:VAL:HA	1.54	0.73
2:Q:33:GLY:CA	2:Q:99:VAL:HG22	2.18	0.73
1:J:331:LEU:CD2	1:J:331:LEU:H	2.00	0.73
1:A:347:ILE:HD13	1:A:347:ILE:H	1.53	0.73
1:G:42:LEU:HD11	1:G:316:LEU:HB2	1.71	0.73
2:Q:48:VAL:O	2:Q:61:VAL:HG23	1.89	0.72
1:A:156:LYS:HD2	1:A:196:VAL:HG22	1.70	0.72
1:G:16:GLY:HA2	1:G:338:PHE:HB3	1.71	0.72
1:H:151:LEU:HD22	1:H:252:ILE:HG22	1.70	0.72
2:U:6:GLN:HB3	2:U:120:THR:HG23	1.71	0.72
1:I:130:VAL:HG11	1:I:164:LEU:HD11	1.72	0.72
1:K:402:VAL:HA	1:K:407:GLN:HE22	1.53	0.72
2:W:172:LEU:HD21	2:W:195:VAL:HG11	1.70	0.72
1:B:130:VAL:HG11	1:B:164:LEU:HD11	1.71	0.72
1:A:42:LEU:HD11	1:A:316:LEU:HB2	1.70	0.72
1:C:140:LYS:HG2	1:C:145:SER:HA	1.70	0.72
1:F:102:VAL:HG22	1:F:232:ILE:HB	1.71	0.72
2:M:179:PHE:CE2	3:N:142:SER:HB3	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:111:TYR:HE1	2:O:113:MET:HG2	1.52	0.72
2:5:60:TYR:HE1	2:5:70:MET:HG2	1.54	0.72
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.69	0.72
1:A:29:ILE:O	1:B:380:LYS:HG2	1.89	0.72
1:A:130:VAL:HG11	1:A:164:LEU:HD11	1.72	0.72
1:J:384:VAL:HG13	1:J:428:LEU:HD21	1.72	0.72
2:1:60:TYR:HE1	2:1:70:MET:HG2	1.52	0.72
2:Q:52:ASN:HD21	2:Q:102:VAL:HA	1.55	0.72
2:5:52:ASN:HD21	2:5:102:VAL:HA	1.54	0.72
1:E:221:PRO:HD3	1:F:244:VAL:HB	1.72	0.72
2:M:109:HIS:HA	3:N:93:TYR:CG	2.24	0.72
2:3:179:PHE:HB3	3:4:180:SER:OG	1.89	0.72
2:Y:179:PHE:CE2	3:Z:142:SER:HB3	2.24	0.72
1:K:404:GLY:HA3	1:L:107:SER:HB2	1.70	0.72
2:O:6:GLN:HE21	2:O:117:GLY:HA3	1.54	0.72
1:H:403:GLU:H	1:H:407:GLN:NE2	1.87	0.72
1:A:16:GLY:HA2	1:A:338:PHE:HB3	1.70	0.72
1:C:187:THR:HB	1:C:189:GLN:NE2	2.05	0.72
1:E:27:LYS:NZ	1:F:383:ARG:HD3	2.04	0.72
1:J:42:LEU:HD11	1:J:316:LEU:HB2	1.70	0.72
1:F:151:LEU:HD22	1:F:252:ILE:HG22	1.72	0.72
1:H:16:GLY:HA2	1:H:338:PHE:HB3	1.71	0.72
3:R:143:ASP:HA	3:R:176:LYS:CG	2.15	0.72
1:I:53:ASN:ND2	1:I:276:THR:HA	2.04	0.72
2:U:48:VAL:O	2:U:61:VAL:HG23	1.90	0.72
1:B:53:ASN:HD21	1:B:276:THR:HA	1.54	0.72
1:J:156:LYS:HD2	1:J:196:VAL:HG22	1.70	0.72
1:I:156:LYS:HD2	1:I:196:VAL:HG22	1.70	0.72
2:Y:52:ASN:HD21	2:Y:102:VAL:HA	1.55	0.71
2:M:52:ASN:HD21	2:M:102:VAL:HA	1.55	0.71
3:T:143:ASP:CA	3:T:176:LYS:HG3	2.17	0.71
4:J:602:NAG:H5	2:5:57:GLN:NE2	2.04	0.71
1:G:347:ILE:H	1:G:347:ILE:HD13	1.55	0.71
3:P:143:ASP:CA	3:P:176:LYS:HG3	2.16	0.71
1:H:187:THR:HB	1:H:189:GLN:NE2	2.05	0.71
2:O:6:GLN:HB2	2:O:118:GLN:OE1	1.90	0.71
2:U:60:TYR:HE1	2:U:70:MET:HG2	1.53	0.71
2:M:112:PRO:HB3	3:N:36:HIS:CE1	2.25	0.71
1:I:42:LEU:HD11	1:I:316:LEU:HB2	1.70	0.71
1:E:53:ASN:HD21	1:E:276:THR:HA	1.54	0.71
2:9:51:ILE:HD13	2:9:52:ASN:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:52:ASN:HD21	2:9:102:VAL:HA	1.55	0.71
4:L:602:NAG:C5	2:9:57:GLN:HE22	2.00	0.71
2:Y:129:THR:HG22	2:Y:160:PRO:HD3	1.71	0.71
1:J:413:VAL:HG21	1:L:409:LEU:HD11	1.69	0.71
1:B:42:LEU:HD11	1:B:316:LEU:HB2	1.72	0.71
2:Y:51:ILE:HD13	2:Y:52:ASN:N	2.06	0.71
2:M:33:GLY:CA	2:M:99:VAL:HG22	2.20	0.71
2:Y:112:PRO:CB	3:Z:51:SER:HB2	2.19	0.71
1:D:16:GLY:HA2	1:D:338:PHE:HB3	1.72	0.71
1:I:347:ILE:H	1:I:347:ILE:HD13	1.54	0.71
1:L:326:LYS:HB3	1:L:328:THR:HG23	1.73	0.71
2:Y:136:PRO:O	3:Z:126:SER:HB3	1.91	0.71
2:Q:44:GLY:HA2	3:R:89:TYR:OH	1.91	0.71
1:K:357:ASN:HD21	1:K:359:GLU:HB2	1.55	0.71
1:F:16:GLY:HA2	1:F:338:PHE:HB3	1.70	0.71
1:D:156:LYS:HD2	1:D:196:VAL:HG22	1.71	0.71
3:X:143:ASP:CA	3:X:176:LYS:HG3	2.17	0.71
2:9:19:THR:HG22	2:9:82:GLU:HG2	1.72	0.71
1:L:16:GLY:HA2	1:L:338:PHE:HB3	1.72	0.71
2:1:44:GLY:HA2	3:2:89:TYR:OH	1.90	0.71
2:Q:148:THR:HB	2:Q:197:VAL:O	1.91	0.71
1:K:403:GLU:H	1:K:407:GLN:NE2	1.89	0.71
1:J:347:ILE:HD13	1:J:347:ILE:H	1.56	0.71
1:H:79:PHE:O	1:H:82:GLU:HB2	1.90	0.71
1:J:102:VAL:HG22	1:J:232:ILE:HB	1.71	0.71
1:A:27:LYS:HD3	1:B:383:ARG:CZ	2.20	0.71
1:J:79:PHE:O	1:J:82:GLU:HB2	1.90	0.71
1:E:187:THR:HB	1:E:189:GLN:NE2	2.05	0.71
1:G:187:THR:HB	1:G:189:GLN:NE2	2.05	0.71
1:I:334:ALA:O	1:I:335:ILE:HG22	1.91	0.71
1:B:102:VAL:HG22	1:B:232:ILE:HB	1.72	0.71
4:E:602:NAG:H81	2:U:55:ASP:OD1	1.90	0.70
1:I:187:THR:HB	1:I:189:GLN:NE2	2.06	0.70
2:O:19:THR:HG22	2:O:82:GLU:HG2	1.73	0.70
1:C:357:ASN:HD21	1:C:359:GLU:HB2	1.56	0.70
1:K:16:GLY:HA2	1:K:338:PHE:HB3	1.72	0.70
1:C:402:VAL:HA	1:C:407:GLN:HE22	1.56	0.70
2:3:111:TYR:HE1	2:3:113:MET:HG2	1.53	0.70
1:C:409:LEU:O	1:C:413:VAL:HG23	1.90	0.70
2:O:33:GLY:CA	2:O:99:VAL:HG22	2.19	0.70
2:7:148:THR:HB	2:7:197:VAL:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ARG:HD3	1:F:27:LYS:HZ2	1.56	0.70
1:C:192:THR:HA	1:C:196:VAL:O	1.91	0.70
1:H:402:VAL:HA	1:H:407:GLN:HE22	1.56	0.70
1:F:347:ILE:H	1:F:347:ILE:HD13	1.56	0.70
1:H:42:LEU:HD11	1:H:316:LEU:HB2	1.73	0.70
2:W:109:HIS:HA	3:X:93:TYR:CG	2.26	0.70
2:3:91:THR:OG1	2:3:123:THR:HA	1.91	0.70
1:K:216:ASN:HB3	1:L:212:THR:HG21	1.74	0.70
1:G:79:PHE:O	1:G:82:GLU:HB2	1.91	0.70
1:A:79:PHE:O	1:A:82:GLU:HB2	1.92	0.70
1:D:102:VAL:HG22	1:D:232:ILE:HB	1.73	0.70
1:E:191:GLN:HE21	1:E:217:ILE:HD11	1.54	0.70
1:B:16:GLY:HA2	1:B:338:PHE:HB3	1.73	0.70
2:9:111:TYR:HE1	2:9:113:MET:HG2	1.56	0.70
2:M:10:GLU:O	2:M:122:VAL:HA	1.92	0.70
1:G:53:ASN:HD21	1:G:276:THR:HA	1.56	0.70
2:O:52:ASN:HD21	2:O:102:VAL:HA	1.56	0.70
2:W:51:ILE:HD13	2:W:52:ASN:N	2.07	0.70
1:I:108:LEU:O	1:I:111:LEU:HG	1.92	0.70
1:A:409:LEU:O	1:A:413:VAL:HG23	1.91	0.70
1:K:221:PRO:HD3	1:L:244:VAL:HB	1.73	0.70
1:I:208:ARG:NH1	1:I:238:LYS:HD2	2.06	0.70
1:J:404:GLY:HA3	1:K:107:SER:HB2	1.73	0.70
2:7:100:GLU:HG2	2:7:110:TYR:OH	1.92	0.70
2:5:19:THR:HG22	2:5:82:GLU:HG2	1.72	0.70
1:A:27:LYS:HD3	1:B:383:ARG:NH1	2.04	0.70
2:Y:172:LEU:HD21	2:Y:195:VAL:HG11	1.72	0.70
1:H:334:ALA:O	1:H:335:ILE:HG22	1.92	0.70
1:F:402:VAL:HA	1:F:407:GLN:HE22	1.57	0.70
2:M:174:SER:HB3	2:7:204:THR:HG21	1.73	0.70
2:W:19:THR:HG22	2:W:82:GLU:HG2	1.72	0.70
1:F:53:ASN:ND2	1:F:276:THR:HA	2.06	0.70
1:C:156:LYS:HD2	1:C:196:VAL:HG22	1.73	0.70
1:B:357:ASN:HD21	1:B:359:GLU:HB2	1.57	0.70
1:E:42:LEU:HD11	1:E:316:LEU:HB2	1.74	0.70
3:6:143:ASP:HA	3:6:176:LYS:CG	2.17	0.70
2:W:160:PRO:HD2	2:W:215:PRO:CB	2.22	0.70
1:F:403:GLU:H	1:F:407:GLN:NE2	1.90	0.70
1:B:426:GLU:HG3	1:C:383:ARG:NH2	2.07	0.70
3:2:163:GLY:O	3:2:183:LEU:HG	1.91	0.70
2:1:11:VAL:HG22	2:1:123:THR:OG1	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ASN:HD21	1:A:359:GLU:HB2	1.57	0.70
3:V:143:ASP:CA	3:V:176:LYS:HG3	2.17	0.70
2:7:19:THR:HG22	2:7:82:GLU:HG2	1.72	0.70
1:G:102:VAL:HG22	1:G:232:ILE:HB	1.73	0.70
3:6:163:GLY:O	3:6:183:LEU:HG	1.91	0.70
1:G:331:LEU:N	1:G:331:LEU:HD22	2.02	0.69
2:O:111:TYR:CE1	2:O:113:MET:HG2	2.27	0.69
2:9:148:THR:HB	2:9:197:VAL:O	1.92	0.69
2:O:20:VAL:HG13	2:O:120:THR:HG21	1.72	0.69
2:3:19:THR:HG22	2:3:82:GLU:HG2	1.72	0.69
1:B:347:ILE:HD13	1:B:347:ILE:H	1.57	0.69
1:I:79:PHE:O	1:I:82:GLU:HB2	1.92	0.69
2:1:109:HIS:HA	3:2:93:TYR:CG	2.27	0.69
3:R:163:GLY:O	3:R:183:LEU:HG	1.92	0.69
1:L:272:ALA:HA	2:9:105:VAL:CG2	2.22	0.69
2:7:100:GLU:H	2:7:111:TYR:CB	2.05	0.69
2:Y:148:THR:HB	2:Y:197:VAL:O	1.92	0.69
1:K:384:VAL:HG13	1:K:428:LEU:HD21	1.74	0.69
1:A:383:ARG:NH2	1:C:426:GLU:HG3	2.07	0.69
1:I:346:MET:HA	1:I:363:GLN:HE22	1.56	0.69
1:C:16:GLY:HA2	1:C:338:PHE:HB3	1.72	0.69
2:W:33:GLY:CA	2:W:99:VAL:HG22	2.21	0.69
2:W:148:THR:HB	2:W:197:VAL:O	1.92	0.69
2:M:148:THR:HB	2:M:197:VAL:O	1.92	0.69
1:L:53:ASN:ND2	1:L:276:THR:HA	2.07	0.69
2:S:172:LEU:HD21	2:S:195:VAL:HG11	1.72	0.69
1:G:404:GLY:HA3	1:H:107:SER:HB2	1.74	0.69
3:6:6:GLN:HG2	3:6:7:PRO:HD2	1.74	0.69
3:R:6:GLN:HG2	3:R:7:PRO:HD2	1.75	0.69
1:H:357:ASN:HD21	1:H:359:GLU:HB2	1.57	0.69
1:G:60:ASP:OD2	1:G:274:ILE:HD11	1.92	0.69
1:K:334:ALA:O	1:K:335:ILE:HG22	1.93	0.69
1:H:347:ILE:H	1:H:347:ILE:HD13	1.56	0.69
1:L:37:THR:HG23	1:L:320:MET:O	1.92	0.69
1:G:107:SER:HB2	1:I:404:GLY:HA3	1.74	0.69
2:U:33:GLY:CA	2:U:99:VAL:HG22	2.19	0.69
2:7:99:VAL:HB	2:7:111:TYR:CE2	2.27	0.69
2:7:99:VAL:HB	2:7:111:TYR:CZ	2.27	0.69
2:5:111:TYR:HE1	2:5:113:MET:HG2	1.57	0.69
2:1:16:ALA:O	2:1:86:LEU:HG	1.92	0.69
2:U:160:PRO:HD2	2:U:215:PRO:CB	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:402:VAL:HA	1:I:407:GLN:HE22	1.58	0.69
2:Q:112:PRO:CB	3:R:51:SER:HB2	2.22	0.69
4:A:602:NAG:H5	2:M:57:GLN:HE22	1.56	0.69
1:K:187:THR:HB	1:K:189:GLN:NE2	2.06	0.69
1:J:403:GLU:H	1:J:407:GLN:NE2	1.89	0.69
3:P:163:GLY:O	3:P:183:LEU:HG	1.93	0.69
1:L:334:ALA:O	1:L:335:ILE:HG22	1.91	0.69
2:3:51:ILE:HD13	2:3:52:ASN:N	2.05	0.69
2:O:17:SER:HB3	2:O:84:LYS:HA	1.73	0.69
2:U:176:VAL:HG22	2:U:195:VAL:HG22	1.75	0.69
1:C:403:GLU:H	1:C:407:GLN:NE2	1.90	0.69
1:H:404:GLY:HA3	1:I:107:SER:HB2	1.74	0.69
1:C:208:ARG:NH1	1:C:238:LYS:HD2	2.07	0.69
3:6:143:ASP:CA	3:6:176:LYS:HG3	2.19	0.69
2:O:51:ILE:HD13	2:O:52:ASN:N	2.06	0.69
1:F:331:LEU:N	1:F:331:LEU:HD13	2.08	0.69
2:7:52:ASN:HD21	2:7:102:VAL:HA	1.55	0.69
2:S:33:GLY:CA	2:S:99:VAL:HG22	2.19	0.69
2:M:51:ILE:HD13	2:M:52:ASN:N	2.07	0.69
2:7:10:GLU:O	2:7:122:VAL:HA	1.91	0.69
1:D:53:ASN:ND2	1:D:276:THR:HA	2.08	0.69
1:I:409:LEU:O	1:I:413:VAL:HG23	1.93	0.69
3:2:93:TYR:CD1	3:2:100:SER:HB3	2.28	0.69
1:B:346:MET:HA	1:B:363:GLN:HE22	1.56	0.69
1:K:79:PHE:O	1:K:82:GLU:HB2	1.93	0.69
1:C:334:ALA:O	1:C:335:ILE:HG22	1.93	0.69
2:9:139:PRO:HD3	2:9:151:LEU:HG	1.74	0.69
1:F:130:VAL:HG11	1:F:164:LEU:HD11	1.72	0.69
2:M:137:LEU:HB3	3:N:123:PHE:CD1	2.28	0.69
2:1:148:THR:HB	2:1:197:VAL:O	1.92	0.69
1:F:192:THR:HA	1:F:196:VAL:O	1.92	0.69
1:B:177:LEU:HB2	1:B:260:MET:SD	2.33	0.69
3:X:167:THR:HG23	3:X:180:SER:H	1.57	0.69
1:I:16:GLY:HA2	1:I:338:PHE:HB3	1.74	0.69
2:O:109:HIS:HA	3:P:93:TYR:CG	2.28	0.69
1:C:347:ILE:HD13	1:C:347:ILE:H	1.56	0.69
1:E:334:ALA:O	1:E:335:ILE:HG22	1.93	0.69
2:Y:19:THR:HG22	2:Y:82:GLU:HG2	1.75	0.68
2:U:10:GLU:O	2:U:122:VAL:HA	1.92	0.68
2:5:160:PRO:HD2	2:5:215:PRO:CB	2.22	0.68
2:U:6:GLN:HB2	2:U:118:GLN:OE1	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:347:ILE:H	1:K:347:ILE:HD13	1.58	0.68
2:M:163:VAL:HG23	2:M:212:ASN:O	1.93	0.68
1:C:384:VAL:HG13	1:C:428:LEU:HD21	1.75	0.68
1:A:402:VAL:HA	1:A:407:GLN:HE22	1.58	0.68
3:4:163:GLY:O	3:4:183:LEU:HG	1.92	0.68
1:F:357:ASN:HD21	1:F:359:GLU:HB2	1.57	0.68
3:T:163:GLY:O	3:T:183:LEU:HG	1.93	0.68
2:5:51:ILE:HD13	2:5:52:ASN:N	2.06	0.68
2:1:19:THR:HG22	2:1:82:GLU:HG2	1.74	0.68
1:E:37:THR:HG23	1:E:320:MET:O	1.93	0.68
1:F:334:ALA:O	1:F:335:ILE:HG22	1.92	0.68
2:S:91:THR:OG1	2:S:123:THR:HA	1.93	0.68
1:K:219:SER:H	1:L:246:ASN:ND2	1.90	0.68
1:G:384:VAL:HG13	1:G:428:LEU:HD21	1.75	0.68
1:L:140:LYS:HG2	1:L:145:SER:HA	1.72	0.68
1:F:409:LEU:O	1:F:413:VAL:HG23	1.92	0.68
1:J:357:ASN:HD21	1:J:359:GLU:HB2	1.56	0.68
2:W:194:VAL:HG21	3:X:140:LEU:CD1	2.24	0.68
3:X:163:GLY:O	3:X:183:LEU:HG	1.93	0.68
1:H:346:MET:HA	1:H:363:GLN:HE22	1.58	0.68
2:1:160:PRO:HD2	2:1:215:PRO:CB	2.23	0.68
1:L:108:LEU:O	1:L:111:LEU:HG	1.94	0.68
3:P:6:GLN:HG2	3:P:7:PRO:HD2	1.75	0.68
2:W:163:VAL:HG23	2:W:212:ASN:O	1.94	0.68
2:Y:99:VAL:HB	2:Y:111:TYR:CE2	2.28	0.68
2:O:148:THR:HB	2:O:197:VAL:O	1.93	0.68
2:M:19:THR:HG22	2:M:82:GLU:HG2	1.74	0.68
1:A:187:THR:HB	1:A:189:GLN:NE2	2.06	0.68
2:Q:19:THR:HG22	2:Q:82:GLU:HG2	1.74	0.68
2:9:16:ALA:O	2:9:86:LEU:HG	1.94	0.68
2:Y:160:PRO:HD2	2:Y:215:PRO:CB	2.23	0.68
2:M:6:GLN:HB3	2:M:120:THR:CG2	2.23	0.68
1:B:384:VAL:HG13	1:B:428:LEU:HD21	1.76	0.68
1:I:403:GLU:H	1:I:407:GLN:NE2	1.92	0.68
1:C:60:ASP:OD2	1:C:274:ILE:HD11	1.94	0.68
1:G:334:ALA:O	1:G:335:ILE:HG22	1.94	0.68
2:Q:100:GLU:HG2	2:Q:110:TYR:OH	1.93	0.68
2:3:148:THR:HB	2:3:197:VAL:O	1.92	0.68
2:S:148:THR:HB	2:S:197:VAL:O	1.93	0.68
1:E:463:GLY:CA	1:F:453:ARG:HB3	2.24	0.68
1:E:192:THR:HA	1:E:196:VAL:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:176:VAL:HG22	2:3:195:VAL:HG22	1.75	0.68
3:T:6:GLN:HG2	3:T:7:PRO:HD2	1.75	0.68
2:9:172:LEU:HD21	2:9:195:VAL:HG11	1.73	0.68
3:X:6:GLN:HG2	3:X:7:PRO:HD2	1.75	0.68
1:L:357:ASN:HD21	1:L:359:GLU:HB2	1.59	0.68
1:B:425:ALA:O	1:B:429:VAL:HG23	1.93	0.68
1:A:334:ALA:O	1:A:335:ILE:HG22	1.92	0.68
2:3:160:PRO:HD2	2:3:215:PRO:CB	2.24	0.68
1:D:27:LYS:HD3	1:E:383:ARG:CZ	2.24	0.68
1:H:192:THR:HA	1:H:196:VAL:O	1.94	0.68
3:0:6:GLN:HG2	3:0:7:PRO:HD2	1.76	0.68
1:L:402:VAL:HA	1:L:407:GLN:HE22	1.58	0.68
3:Z:6:GLN:HG2	3:Z:7:PRO:HD2	1.76	0.68
3:0:93:TYR:CD1	3:0:100:SER:HB3	2.28	0.68
2:U:163:VAL:HG23	2:U:212:ASN:O	1.94	0.68
2:Q:51:ILE:HD13	2:Q:52:ASN:N	2.06	0.68
2:3:52:ASN:HD21	2:3:102:VAL:HA	1.57	0.68
2:S:51:ILE:HD13	2:S:52:ASN:N	2.06	0.68
2:Q:160:PRO:HD2	2:Q:215:PRO:CB	2.24	0.68
2:M:160:PRO:HD2	2:M:215:PRO:CB	2.24	0.68
1:D:192:THR:HA	1:D:196:VAL:O	1.94	0.68
1:F:457:GLU:HG3	1:F:499:ARG:HH12	1.58	0.68
1:A:107:SER:HB2	1:C:404:GLY:HA3	1.74	0.68
2:5:163:VAL:HG23	2:5:212:ASN:O	1.94	0.68
1:H:102:VAL:HG22	1:H:232:ILE:HB	1.76	0.68
1:D:357:ASN:HD21	1:D:359:GLU:HB2	1.58	0.68
1:H:384:VAL:HG13	1:H:428:LEU:HD21	1.75	0.68
3:4:143:ASP:CA	3:4:176:LYS:HG3	2.18	0.68
2:1:52:ASN:HD21	2:1:102:VAL:HA	1.58	0.68
2:5:100:GLU:HG2	2:5:110:TYR:OH	1.93	0.68
1:D:402:VAL:HA	1:D:407:GLN:HE22	1.59	0.68
1:J:108:LEU:O	1:J:111:LEU:HG	1.94	0.68
3:Z:163:GLY:O	3:Z:183:LEU:HG	1.94	0.68
3:N:6:GLN:HG2	3:N:7:PRO:HD2	1.76	0.68
1:L:346:MET:HA	1:L:363:GLN:HE22	1.58	0.68
1:F:346:MET:HA	1:F:363:GLN:HE22	1.58	0.68
1:D:57:ARG:O	1:D:85:ASP:HB2	1.94	0.68
1:G:357:ASN:HD21	1:G:359:GLU:HB2	1.58	0.68
2:7:51:ILE:HD13	2:7:52:ASN:N	2.07	0.68
2:5:148:THR:HB	2:5:197:VAL:O	1.93	0.68
1:B:222:TRP:CZ3	1:B:225:GLY:HA2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:THR:HA	1:G:196:VAL:O	1.94	0.68
2:S:176:VAL:HG22	2:S:195:VAL:HG22	1.76	0.68
2:1:139:PRO:HD3	2:1:151:LEU:HG	1.76	0.68
3:4:6:GLN:HG2	3:4:7:PRO:HD2	1.76	0.68
1:L:79:PHE:O	1:L:82:GLU:HB2	1.93	0.68
3:0:167:THR:HG23	3:0:180:SER:H	1.59	0.68
1:D:346:MET:HA	1:D:363:GLN:HE22	1.58	0.68
1:D:334:ALA:O	1:D:335:ILE:HG22	1.94	0.68
1:A:151:LEU:HD22	1:A:252:ILE:HG22	1.74	0.68
2:M:138:ALA:HB1	2:M:139:PRO:HD2	1.76	0.68
2:W:100:GLU:HG2	2:W:110:TYR:OH	1.94	0.68
1:J:187:THR:HB	1:J:189:GLN:NE2	2.05	0.68
2:7:17:SER:HB3	2:7:84:LYS:HA	1.76	0.68
1:J:192:THR:HA	1:J:196:VAL:O	1.94	0.68
2:1:138:ALA:HB1	2:1:139:PRO:HD2	1.76	0.68
1:B:353:PHE:HE1	1:B:366:ASP:HB2	1.58	0.68
2:3:163:VAL:HG23	2:3:212:ASN:O	1.94	0.68
1:F:37:THR:HG22	1:F:322:ASN:HB2	1.76	0.68
2:7:139:PRO:HD3	2:7:151:LEU:HG	1.76	0.68
2:U:148:THR:HB	2:U:197:VAL:O	1.93	0.67
2:Q:2:VAL:HG23	2:Q:115:VAL:HG11	1.76	0.67
1:F:208:ARG:NH1	1:F:238:LYS:HD2	2.09	0.67
3:N:163:GLY:O	3:N:183:LEU:HG	1.94	0.67
1:E:79:PHE:O	1:E:82:GLU:HB2	1.94	0.67
1:L:57:ARG:O	1:L:85:ASP:HB2	1.94	0.67
3:6:167:THR:HG23	3:6:180:SER:H	1.59	0.67
2:Q:139:PRO:HD3	2:Q:151:LEU:HG	1.76	0.67
2:W:17:SER:HB3	2:W:84:LYS:HA	1.76	0.67
2:1:17:SER:HB3	2:1:84:LYS:HA	1.75	0.67
1:B:192:THR:HA	1:B:196:VAL:O	1.95	0.67
1:E:347:ILE:HD13	1:E:347:ILE:H	1.58	0.67
1:I:177:LEU:HB2	1:I:260:MET:SD	2.34	0.67
1:C:346:MET:HA	1:C:363:GLN:HE22	1.59	0.67
1:A:404:GLY:HA3	1:B:107:SER:HB2	1.75	0.67
2:S:194:VAL:HG21	3:T:140:LEU:CD1	2.24	0.67
1:D:187:THR:HB	1:D:189:GLN:NE2	2.07	0.67
2:U:19:THR:HG22	2:U:82:GLU:HG2	1.74	0.67
2:9:17:SER:HB3	2:9:84:LYS:HA	1.76	0.67
2:9:91:THR:CB	2:9:124:VAL:H	2.07	0.67
2:M:176:VAL:HG22	2:M:195:VAL:HG22	1.75	0.67
2:Q:138:ALA:HB1	2:Q:139:PRO:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:163:GLY:O	3:0:183:LEU:HG	1.95	0.67
1:G:331:LEU:H	1:G:331:LEU:CD2	1.95	0.67
2:O:100:GLU:H	2:O:111:TYR:CB	2.07	0.67
2:3:33:GLY:CA	2:3:99:VAL:HG22	2.21	0.67
2:S:19:THR:HG22	2:S:82:GLU:HG2	1.76	0.67
2:Y:17:SER:HB3	2:Y:84:LYS:HA	1.75	0.67
2:O:176:VAL:HG22	2:O:195:VAL:HG22	1.77	0.67
1:A:192:THR:HA	1:A:196:VAL:O	1.95	0.67
1:I:192:THR:HA	1:I:196:VAL:O	1.94	0.67
1:D:108:LEU:O	1:D:111:LEU:HG	1.95	0.67
1:L:403:GLU:H	1:L:407:GLN:NE2	1.93	0.67
1:B:369:SER:HB3	1:B:447:LEU:HD13	1.76	0.67
1:D:208:ARG:NH1	1:D:238:LYS:HD2	2.09	0.67
1:D:42:LEU:HD11	1:D:316:LEU:HB2	1.76	0.67
1:A:208:ARG:NH1	1:A:238:LYS:HD2	2.09	0.67
1:G:37:THR:HG22	1:G:322:ASN:HB2	1.77	0.67
2:Y:163:VAL:HG23	2:Y:212:ASN:O	1.94	0.67
1:J:331:LEU:N	1:J:331:LEU:HD13	2.09	0.67
1:G:409:LEU:O	1:G:413:VAL:HG23	1.94	0.67
1:K:108:LEU:O	1:K:111:LEU:HG	1.93	0.67
1:B:409:LEU:O	1:B:413:VAL:HG23	1.94	0.67
1:A:403:GLU:H	1:A:407:GLN:NE2	1.93	0.67
1:H:384:VAL:CG1	1:H:428:LEU:HD21	2.24	0.67
1:F:37:THR:HG23	1:F:320:MET:O	1.95	0.67
3:R:15:GLY:HA2	3:R:79:GLY:HA2	1.77	0.67
1:A:384:VAL:HG13	1:A:428:LEU:HD21	1.75	0.67
1:J:57:ARG:O	1:J:85:ASP:HB2	1.95	0.67
1:L:347:ILE:H	1:L:347:ILE:HD13	1.59	0.67
1:A:246:ASN:ND2	1:C:219:SER:H	1.91	0.67
2:1:163:VAL:HG23	2:1:212:ASN:O	1.94	0.67
4:K:602:NAG:H81	2:7:55:ASP:OD1	1.94	0.67
2:S:100:GLU:HG2	2:S:110:TYR:OH	1.94	0.67
1:B:187:THR:HB	1:B:189:GLN:NE2	2.09	0.67
1:J:409:LEU:O	1:J:413:VAL:HG23	1.93	0.67
2:1:91:THR:HB	2:1:124:VAL:HG23	1.75	0.67
1:E:208:ARG:NH1	1:E:238:LYS:HD2	2.10	0.67
1:G:403:GLU:H	1:G:407:GLN:NE2	1.91	0.67
1:H:457:GLU:HG3	1:H:499:ARG:HH12	1.60	0.67
3:8:6:GLN:HG2	3:8:7:PRO:HD2	1.76	0.67
4:A:602:NAG:H81	2:M:55:ASP:OD1	1.94	0.67
2:7:163:VAL:HG23	2:7:212:ASN:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:138:ALA:HB1	2:3:139:PRO:HD2	1.77	0.67
2:3:109:HIS:HA	3:4:93:TYR:CG	2.30	0.67
1:J:346:MET:HA	1:J:363:GLN:HE22	1.59	0.67
1:E:357:ASN:HD21	1:E:359:GLU:HB2	1.59	0.67
1:H:425:ALA:O	1:H:429:VAL:HG23	1.94	0.67
1:L:60:ASP:OD2	1:L:274:ILE:HD11	1.95	0.67
2:Y:139:PRO:HD3	2:Y:151:LEU:HG	1.77	0.67
1:G:353:PHE:HE1	1:G:366:ASP:HB2	1.60	0.67
2:Y:165:VAL:HG12	2:Y:211:VAL:HG22	1.76	0.67
2:Y:138:ALA:HB1	2:Y:139:PRO:HD2	1.77	0.67
1:I:357:ASN:HD21	1:I:359:GLU:HB2	1.59	0.67
1:D:347:ILE:HD13	1:D:347:ILE:H	1.58	0.67
1:E:57:ARG:O	1:E:85:ASP:HB2	1.94	0.67
1:A:212:THR:HG21	1:C:216:ASN:HB3	1.75	0.67
1:B:334:ALA:O	1:B:335:ILE:HG22	1.94	0.67
2:U:100:GLU:N	2:U:111:TYR:HB2	2.08	0.67
1:J:272:ALA:HA	2:5:105:VAL:CG2	2.24	0.67
3:4:93:TYR:CD1	3:4:100:SER:HB3	2.30	0.67
3:2:6:GLN:HG2	3:2:7:PRO:HD2	1.75	0.67
1:G:346:MET:HA	1:G:363:GLN:HE22	1.59	0.67
1:D:79:PHE:O	1:D:82:GLU:HB2	1.94	0.67
1:B:208:ARG:NH1	1:B:238:LYS:HD2	2.09	0.67
2:O:139:PRO:HD3	2:O:151:LEU:HG	1.77	0.67
1:C:57:ARG:O	1:C:85:ASP:HB2	1.94	0.67
1:E:37:THR:HG22	1:E:322:ASN:HB2	1.76	0.67
2:7:160:PRO:HD2	2:7:215:PRO:CB	2.25	0.67
1:K:409:LEU:O	1:K:413:VAL:HG23	1.94	0.67
1:F:108:LEU:O	1:F:111:LEU:HG	1.94	0.67
2:M:139:PRO:HD3	2:M:151:LEU:HG	1.76	0.67
2:S:163:VAL:HG23	2:S:212:ASN:O	1.94	0.67
1:E:384:VAL:HG12	1:E:385:ILE:N	2.10	0.67
1:E:108:LEU:O	1:E:111:LEU:HG	1.94	0.67
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.77	0.67
1:K:63:ASP:HA	1:K:93:ALA:HA	1.77	0.67
3:R:143:ASP:CA	3:R:176:LYS:HG3	2.17	0.66
2:7:112:PRO:HB2	3:8:51:SER:HB2	1.76	0.66
1:L:192:THR:HA	1:L:196:VAL:O	1.95	0.66
3:P:93:TYR:CD1	3:P:100:SER:HB3	2.30	0.66
2:3:165:VAL:HG12	2:3:211:VAL:HG22	1.76	0.66
1:H:177:LEU:HB2	1:H:260:MET:SD	2.35	0.66
1:E:219:SER:H	1:F:246:ASN:ND2	1.91	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:163:VAL:HG23	2:9:212:ASN:O	1.94	0.66
1:J:334:ALA:O	1:J:335:ILE:HG22	1.94	0.66
2:9:100:GLU:HG2	2:9:110:TYR:OH	1.95	0.66
2:U:179:PHE:CE2	3:V:140:LEU:HB3	2.29	0.66
3:X:167:THR:O	3:X:179:ALA:HB1	1.95	0.66
2:1:100:GLU:HG2	2:1:110:TYR:OH	1.95	0.66
2:Q:6:GLN:HB3	2:Q:120:THR:CG2	2.23	0.66
1:J:27:LYS:HD3	1:K:383:ARG:CZ	2.26	0.66
2:W:194:VAL:HG21	3:X:140:LEU:HD13	1.77	0.66
2:7:138:ALA:HB1	2:7:139:PRO:HD2	1.76	0.66
1:C:143:PRO:CG	1:D:155:THR:HB	2.25	0.66
1:L:425:ALA:O	1:L:429:VAL:HG23	1.95	0.66
3:R:167:THR:HG23	3:R:180:SER:H	1.60	0.66
2:5:138:ALA:HB1	2:5:139:PRO:HD2	1.76	0.66
1:B:402:VAL:HA	1:B:407:GLN:HE22	1.61	0.66
2:Y:100:GLU:HG2	2:Y:110:TYR:OH	1.94	0.66
1:J:402:VAL:HA	1:J:407:GLN:HE22	1.60	0.66
2:Q:165:VAL:HG12	2:Q:211:VAL:HG22	1.77	0.66
1:J:327:GLN:HG3	1:J:329:ARG:HE	1.59	0.66
3:8:167:THR:HG23	3:8:180:SER:H	1.60	0.66
1:E:457:GLU:HG3	1:E:499:ARG:HH12	1.59	0.66
2:O:166:SER:OG	2:O:210:ASN:HB2	1.95	0.66
2:5:17:SER:HB3	2:5:84:LYS:HA	1.75	0.66
2:S:160:PRO:HD2	2:S:215:PRO:CB	2.24	0.66
2:Y:176:VAL:HG22	2:Y:195:VAL:HG22	1.77	0.66
3:2:161:LYS:HA	3:2:164:VAL:HG21	1.78	0.66
1:A:384:VAL:CG1	1:A:428:LEU:HD21	2.25	0.66
1:A:346:MET:HA	1:A:363:GLN:HE22	1.59	0.66
2:W:139:PRO:HD3	2:W:151:LEU:HG	1.77	0.66
3:8:163:GLY:O	3:8:183:LEU:HG	1.95	0.66
1:H:57:ARG:O	1:H:85:ASP:HB2	1.96	0.66
1:L:42:LEU:HD11	1:L:316:LEU:HB2	1.75	0.66
1:K:457:GLU:HG3	1:K:499:ARG:HH12	1.58	0.66
1:L:457:GLU:HG3	1:L:499:ARG:HH12	1.61	0.66
1:F:353:PHE:HE1	1:F:366:ASP:HB2	1.60	0.66
3:Z:167:THR:HG23	3:Z:180:SER:H	1.61	0.66
2:Q:16:ALA:O	2:Q:86:LEU:HG	1.96	0.66
2:U:138:ALA:HB1	2:U:139:PRO:HD2	1.77	0.66
2:1:166:SER:OG	2:1:210:ASN:HB2	1.96	0.66
2:1:51:ILE:HD13	2:1:52:ASN:N	2.07	0.66
2:1:33:GLY:CA	2:1:99:VAL:HG22	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:91:THR:HB	2:U:124:VAL:N	2.06	0.66
2:W:6:GLN:HB2	2:W:118:GLN:OE1	1.94	0.66
2:Q:17:SER:HB3	2:Q:84:LYS:HA	1.77	0.66
2:3:17:SER:HB3	2:3:84:LYS:HA	1.75	0.66
2:O:160:PRO:HD2	2:O:215:PRO:CB	2.24	0.66
2:3:194:VAL:HG21	3:4:140:LEU:CD1	2.26	0.66
2:9:138:ALA:HB1	2:9:139:PRO:HD2	1.76	0.66
2:U:165:VAL:HG12	2:U:211:VAL:HG22	1.76	0.66
1:B:403:GLU:H	1:B:407:GLN:NE2	1.94	0.66
2:3:166:SER:OG	2:3:210:ASN:HB2	1.95	0.66
1:D:60:ASP:OD2	1:D:274:ILE:HD11	1.95	0.66
1:L:177:LEU:HB2	1:L:260:MET:SD	2.36	0.66
2:O:163:VAL:HG23	2:O:212:ASN:O	1.94	0.66
2:U:184:GLN:HA	3:V:165:GLU:OE1	1.95	0.66
1:D:212:THR:HG21	1:F:216:ASN:HB3	1.78	0.66
2:W:179:PHE:HB3	3:X:180:SER:OG	1.95	0.66
2:U:100:GLU:HG2	2:U:110:TYR:OH	1.96	0.66
2:Y:16:ALA:O	2:Y:86:LEU:HG	1.96	0.66
2:7:7:SER:O	2:7:120:THR:HG22	1.96	0.66
2:9:160:PRO:HD2	2:9:215:PRO:CB	2.24	0.66
2:Q:176:VAL:HG22	2:Q:195:VAL:HG22	1.77	0.66
1:J:409:LEU:HG	1:L:409:LEU:HD21	1.77	0.66
1:A:108:LEU:O	1:A:111:LEU:HG	1.95	0.66
2:1:6:GLN:HB3	2:1:120:THR:HG23	1.78	0.66
2:7:165:VAL:HG12	2:7:211:VAL:HG22	1.78	0.66
2:5:139:PRO:HD3	2:5:151:LEU:HG	1.77	0.66
3:V:163:GLY:O	3:V:183:LEU:HG	1.95	0.66
2:O:99:VAL:HB	2:O:111:TYR:CE2	2.31	0.66
2:O:112:PRO:CB	3:P:51:SER:HB2	2.25	0.66
1:L:102:VAL:HG22	1:L:232:ILE:HB	1.77	0.66
2:Q:163:VAL:HG23	2:Q:212:ASN:O	1.96	0.66
1:E:402:VAL:HA	1:E:407:GLN:HE22	1.60	0.66
1:J:353:PHE:HE1	1:J:366:ASP:HB2	1.60	0.66
2:U:166:SER:OG	2:U:210:ASN:HB2	1.95	0.66
1:D:331:LEU:N	1:D:331:LEU:HD22	2.06	0.66
1:C:331:LEU:HD13	1:C:331:LEU:N	2.10	0.66
2:W:20:VAL:HG13	2:W:120:THR:HG21	1.75	0.66
2:7:148:THR:HA	2:7:199:SER:H	1.61	0.66
2:M:17:SER:HB3	2:M:84:LYS:HA	1.78	0.66
2:O:10:GLU:O	2:O:122:VAL:HA	1.96	0.66
2:Y:92:ALA:H	2:Y:122:VAL:CG2	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:165:VAL:HG12	2:M:211:VAL:HG22	1.78	0.66
1:L:208:ARG:NH1	1:L:238:LYS:HD2	2.11	0.66
3:2:167:THR:HG23	3:2:180:SER:H	1.59	0.66
2:Y:148:THR:HA	2:Y:199:SER:H	1.60	0.66
2:5:176:VAL:HG22	2:5:195:VAL:HG22	1.76	0.66
1:J:384:VAL:HG12	1:J:385:ILE:N	2.11	0.66
1:G:108:LEU:O	1:G:111:LEU:HG	1.96	0.66
2:1:165:VAL:HG12	2:1:211:VAL:HG22	1.77	0.66
2:W:138:ALA:HB1	2:W:139:PRO:HD2	1.77	0.66
1:E:403:GLU:H	1:E:407:GLN:NE2	1.93	0.66
1:F:79:PHE:O	1:F:82:GLU:HB2	1.95	0.66
1:G:57:ARG:O	1:G:85:ASP:HB2	1.96	0.66
2:W:40:ALA:HB3	2:W:43:GLN:HB3	1.78	0.66
1:A:244:VAL:HB	1:C:221:PRO:HD3	1.77	0.66
1:K:346:MET:HA	1:K:363:GLN:HE22	1.61	0.66
2:3:114:ASP:CG	2:3:115:VAL:HG23	2.17	0.65
1:E:331:LEU:CD2	1:E:331:LEU:H	2.00	0.65
1:K:53:ASN:ND2	1:K:276:THR:HA	2.10	0.65
3:N:7:PRO:O	3:N:106:THR:HG22	1.97	0.65
3:6:167:THR:O	3:6:179:ALA:HB1	1.96	0.65
2:3:139:PRO:HD3	2:3:151:LEU:HG	1.76	0.65
2:Q:87:ARG:HB2	2:Q:90:ASP:OD2	1.97	0.65
2:U:40:ALA:HB3	2:U:43:GLN:HB3	1.79	0.65
1:K:177:LEU:HB2	1:K:260:MET:SD	2.36	0.65
1:C:108:LEU:O	1:C:111:LEU:HG	1.95	0.65
2:M:99:VAL:HB	2:M:111:TYR:CE2	2.30	0.65
2:W:16:ALA:O	2:W:86:LEU:HG	1.96	0.65
2:W:148:THR:HA	2:W:199:SER:H	1.61	0.65
1:D:383:ARG:NH2	1:F:426:GLU:HG3	2.11	0.65
1:H:384:VAL:HG12	1:H:385:ILE:N	2.11	0.65
1:G:463:GLY:HA2	1:H:453:ARG:HD3	1.79	0.65
1:B:79:PHE:O	1:B:82:GLU:HB2	1.96	0.65
2:S:109:HIS:HA	3:T:93:TYR:CG	2.32	0.65
1:K:208:ARG:NH1	1:K:238:LYS:HD2	2.11	0.65
1:E:151:LEU:HD22	1:E:252:ILE:HG22	1.77	0.65
3:V:6:GLN:HG2	3:V:7:PRO:HD2	1.76	0.65
1:L:353:PHE:HE1	1:L:366:ASP:HB2	1.61	0.65
1:E:331:LEU:HD13	1:E:331:LEU:N	2.11	0.65
2:3:148:THR:HA	2:3:199:SER:H	1.61	0.65
1:D:369:SER:HB3	1:D:447:LEU:HD13	1.78	0.65
1:A:73:ASP:OD1	1:A:74:PRO:HD2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:15:GLY:HA2	3:8:79:GLY:HA2	1.79	0.65
1:L:271:ASP:OD2	2:9:103:ARG:HB2	1.96	0.65
1:A:331:LEU:HD13	1:A:331:LEU:N	2.10	0.65
1:H:331:LEU:N	1:H:331:LEU:HD22	2.06	0.65
1:H:331:LEU:N	1:H:331:LEU:HD13	2.11	0.65
3:R:93:TYR:CD1	3:R:100:SER:HB3	2.32	0.65
2:Y:6:GLN:HB3	2:Y:120:THR:HG23	1.78	0.65
1:D:384:VAL:HG13	1:D:428:LEU:HD21	1.76	0.65
2:M:100:GLU:HG2	2:M:110:TYR:OH	1.96	0.65
2:5:108:PHE:HB2	2:5:111:TYR:CE2	2.31	0.65
1:A:413:VAL:HG21	1:C:409:LEU:HD11	1.77	0.65
2:O:138:ALA:HB1	2:O:139:PRO:HD2	1.76	0.65
1:E:293:PRO:HB3	1:E:385:ILE:HD13	1.78	0.65
2:Q:179:PHE:HB3	3:R:180:SER:OG	1.96	0.65
3:6:11:SER:HB3	3:6:111:LEU:CD1	2.25	0.65
1:F:57:ARG:O	1:F:85:ASP:HB2	1.96	0.65
1:L:222:TRP:CZ3	1:L:225:GLY:HA2	2.32	0.65
1:G:177:LEU:HB2	1:G:260:MET:SD	2.36	0.65
2:7:40:ALA:HB3	2:7:43:GLN:HB3	1.79	0.65
2:3:100:GLU:HG2	2:3:110:TYR:OH	1.96	0.65
1:B:331:LEU:HD13	1:B:331:LEU:N	2.12	0.65
1:K:192:THR:HA	1:K:196:VAL:O	1.95	0.65
1:C:384:VAL:HG12	1:C:385:ILE:N	2.12	0.65
2:5:165:VAL:HG12	2:5:211:VAL:HG22	1.76	0.65
1:G:29:ILE:O	1:H:380:LYS:HG2	1.96	0.65
1:A:353:PHE:HE1	1:A:366:ASP:HB2	1.61	0.65
2:S:139:PRO:HD3	2:S:151:LEU:HG	1.77	0.65
1:I:457:GLU:HG3	1:I:499:ARG:HH12	1.61	0.65
3:V:167:THR:HG23	3:V:180:SER:H	1.62	0.65
1:L:187:THR:HB	1:L:189:GLN:NE2	2.06	0.65
2:Q:148:THR:HA	2:Q:199:SER:H	1.62	0.65
2:U:17:SER:HB3	2:U:84:LYS:HA	1.77	0.65
1:J:461:ASP:OD2	1:K:453:ARG:HG2	1.97	0.65
2:1:176:VAL:HG22	2:1:195:VAL:HG22	1.78	0.65
1:J:384:VAL:CG1	1:J:428:LEU:HD21	2.26	0.65
1:B:108:LEU:O	1:B:111:LEU:HG	1.96	0.65
3:4:7:PRO:O	3:4:106:THR:HG22	1.96	0.65
1:G:402:VAL:HA	1:G:407:GLN:HE22	1.60	0.65
2:9:165:VAL:HG12	2:9:211:VAL:HG22	1.79	0.65
2:S:138:ALA:HB1	2:S:139:PRO:HD2	1.77	0.65
1:K:37:THR:HG22	1:K:322:ASN:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:99:VAL:HB	2:U:111:TYR:CE2	2.31	0.65
1:I:331:LEU:N	1:I:331:LEU:HD22	2.07	0.65
2:5:100:GLU:H	2:5:111:TYR:CB	2.08	0.65
2:S:40:ALA:HB3	2:S:43:GLN:HB3	1.79	0.65
1:G:384:VAL:CG1	1:G:428:LEU:HD21	2.27	0.65
2:W:165:VAL:HG12	2:W:211:VAL:HG22	1.79	0.65
3:0:167:THR:O	3:0:179:ALA:HB1	1.96	0.65
2:W:166:SER:OG	2:W:210:ASN:HB2	1.95	0.65
1:J:383:ARG:NH1	1:L:27:LYS:HD3	2.12	0.65
2:Y:180:PRO:HG2	3:Z:170:SER:OG	1.97	0.65
1:K:331:LEU:N	1:K:331:LEU:HD13	2.11	0.65
1:I:331:LEU:N	1:I:331:LEU:HD13	2.11	0.65
1:H:222:TRP:CZ3	1:H:225:GLY:HA2	2.31	0.65
1:A:37:THR:HG22	1:A:322:ASN:HB2	1.79	0.65
3:8:161:LYS:HA	3:8:164:VAL:HG21	1.79	0.65
2:O:165:VAL:HG12	2:O:211:VAL:HG22	1.79	0.65
1:D:384:VAL:HG12	1:D:385:ILE:N	2.12	0.65
1:L:384:VAL:HG12	1:L:385:ILE:N	2.12	0.65
2:O:40:ALA:HB3	2:O:43:GLN:HB3	1.79	0.65
1:I:353:PHE:HE1	1:I:366:ASP:HB2	1.62	0.65
1:D:73:ASP:OD1	1:D:74:PRO:HD2	1.96	0.65
1:D:331:LEU:N	1:D:331:LEU:HD13	2.11	0.65
2:M:148:THR:HA	2:M:199:SER:H	1.62	0.65
1:A:37:THR:HG23	1:A:320:MET:O	1.97	0.65
1:A:272:ALA:HA	2:M:105:VAL:CG2	2.27	0.65
2:W:176:VAL:HG22	2:W:195:VAL:HG22	1.78	0.65
2:S:165:VAL:HG12	2:S:211:VAL:HG22	1.79	0.65
1:G:278:ILE:HD13	3:P:204:GLY:CA	2.27	0.65
1:A:457:GLU:HG3	1:A:499:ARG:HH12	1.62	0.65
2:M:40:ALA:HB3	2:M:43:GLN:HB3	1.79	0.65
3:Z:93:TYR:CD1	3:Z:100:SER:HB3	2.31	0.65
1:C:234:TRP:HE3	1:C:234:TRP:H	1.45	0.65
2:3:39:GLN:HG2	2:3:45:LEU:HD22	1.79	0.65
2:U:51:ILE:HD13	2:U:52:ASN:N	2.07	0.64
2:3:99:VAL:HB	2:3:111:TYR:CE2	2.32	0.64
2:1:148:THR:HA	2:1:199:SER:H	1.60	0.64
1:K:384:VAL:CG1	1:K:428:LEU:HD21	2.27	0.64
2:5:179:PHE:HB3	3:6:180:SER:OG	1.96	0.64
2:Q:166:SER:OG	2:Q:210:ASN:HB2	1.96	0.64
3:P:167:THR:HG23	3:P:180:SER:H	1.62	0.64
1:I:384:VAL:HG12	1:I:385:ILE:N	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:148:THR:HA	2:U:199:SER:H	1.61	0.64
2:O:16:ALA:O	2:O:86:LEU:HG	1.97	0.64
1:F:222:TRP:CZ3	1:F:225:GLY:HA2	2.32	0.64
1:E:346:MET:HA	1:E:363:GLN:HE22	1.62	0.64
2:9:166:SER:OG	2:9:210:ASN:HB2	1.98	0.64
2:1:40:ALA:HB3	2:1:43:GLN:HB3	1.80	0.64
1:A:222:TRP:CZ3	1:A:225:GLY:HA2	2.31	0.64
1:K:272:ALA:HA	2:7:105:VAL:HG22	1.79	0.64
2:5:16:ALA:O	2:5:86:LEU:HG	1.98	0.64
1:E:227:SER:CB	6:F:610:NAG:H83	2.27	0.64
1:D:27:LYS:HZ3	1:E:383:ARG:HD3	1.62	0.64
1:B:457:GLU:HG3	1:B:499:ARG:HH12	1.61	0.64
2:O:100:GLU:HG2	2:O:110:TYR:OH	1.95	0.64
2:Q:99:VAL:HB	2:Q:111:TYR:CE2	2.32	0.64
2:Q:6:GLN:HE21	2:Q:117:GLY:HA3	1.62	0.64
1:A:57:ARG:O	1:A:85:ASP:HB2	1.96	0.64
2:S:166:SER:OG	2:S:210:ASN:HB2	1.98	0.64
1:G:208:ARG:NH1	1:G:238:LYS:HD2	2.12	0.64
2:9:40:ALA:HB3	2:9:43:GLN:HB3	1.79	0.64
3:P:29:ILE:HG21	3:P:71:THR:HG22	1.79	0.64
2:5:92:ALA:O	2:5:122:VAL:HG22	1.97	0.64
2:M:16:ALA:O	2:M:86:LEU:HG	1.96	0.64
3:V:93:TYR:CD1	3:V:100:SER:HB3	2.32	0.64
1:B:384:VAL:HG12	1:B:385:ILE:N	2.13	0.64
3:4:167:THR:HG23	3:4:180:SER:H	1.62	0.64
3:4:161:LYS:HA	3:4:164:VAL:HG21	1.80	0.64
3:Z:161:LYS:HA	3:Z:164:VAL:HG21	1.80	0.64
1:A:384:VAL:HG12	1:A:385:ILE:N	2.11	0.64
3:R:167:THR:O	3:R:179:ALA:HB1	1.98	0.64
1:C:425:ALA:O	1:C:429:VAL:HG23	1.98	0.64
3:Z:167:THR:O	3:Z:179:ALA:HB1	1.98	0.64
2:9:148:THR:HA	2:9:199:SER:H	1.61	0.64
2:S:16:ALA:O	2:S:86:LEU:HG	1.97	0.64
1:A:53:ASN:ND2	1:A:276:THR:HA	2.13	0.64
1:B:384:VAL:CG1	1:B:428:LEU:HD21	2.27	0.64
1:L:272:ALA:HA	2:9:105:VAL:HG22	1.80	0.64
3:X:161:LYS:HA	3:X:164:VAL:HG21	1.80	0.64
3:0:161:LYS:HA	3:0:164:VAL:HG21	1.79	0.64
2:Y:40:ALA:HB3	2:Y:43:GLN:HB3	1.79	0.64
2:W:108:PHE:HB2	2:W:111:TYR:CE2	2.32	0.64
2:1:99:VAL:HB	2:1:111:TYR:CE2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:167:THR:O	3:2:179:ALA:HB1	1.96	0.64
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.79	0.64
1:H:353:PHE:HE1	1:H:366:ASP:HB2	1.63	0.64
3:0:15:GLY:HA2	3:0:79:GLY:HA2	1.79	0.64
1:A:63:ASP:HA	1:A:93:ALA:HA	1.80	0.64
2:5:136:PRO:HD3	2:5:222:LYS:HG2	1.79	0.64
3:T:167:THR:O	3:T:179:ALA:HB1	1.98	0.64
3:T:167:THR:HG23	3:T:180:SER:H	1.61	0.64
2:3:100:GLU:H	2:3:111:TYR:CB	2.08	0.64
1:H:189:GLN:NE2	1:H:189:GLN:H	1.95	0.64
2:S:17:SER:HB3	2:S:84:LYS:HA	1.80	0.64
1:H:53:ASN:ND2	1:H:276:THR:HA	2.12	0.64
2:7:176:VAL:HG22	2:7:195:VAL:HG22	1.79	0.64
1:B:53:ASN:ND2	1:B:276:THR:HA	2.12	0.64
3:P:161:LYS:HA	3:P:164:VAL:HG21	1.79	0.64
1:G:384:VAL:HG12	1:G:385:ILE:N	2.11	0.64
1:B:57:ARG:O	1:B:85:ASP:HB2	1.97	0.64
2:9:87:ARG:HB2	2:9:90:ASP:OD2	1.98	0.64
1:C:222:TRP:CZ3	1:C:225:GLY:HA2	2.32	0.64
1:D:216:ASN:HB3	1:E:212:THR:HG21	1.80	0.64
2:S:148:THR:HA	2:S:199:SER:H	1.62	0.64
2:3:10:GLU:O	2:3:122:VAL:HA	1.98	0.64
1:F:384:VAL:HG13	1:F:428:LEU:HD21	1.80	0.64
1:L:72:GLY:HA3	1:L:149:SER:OG	1.97	0.64
1:K:327:GLN:HG3	1:K:329:ARG:HE	1.63	0.64
1:F:376:GLN:CB	1:F:439:LEU:HD11	2.28	0.64
3:2:15:GLY:HA2	3:2:79:GLY:HA2	1.79	0.64
3:V:167:THR:O	3:V:179:ALA:HB1	1.98	0.64
2:7:33:GLY:HA3	2:7:99:VAL:CG2	2.25	0.64
2:Q:100:GLU:H	2:Q:111:TYR:CB	2.09	0.64
1:J:331:LEU:HD22	1:J:331:LEU:N	2.08	0.64
1:F:384:VAL:HG12	1:F:385:ILE:N	2.13	0.64
1:E:53:ASN:ND2	1:E:276:THR:HA	2.13	0.64
3:0:7:PRO:HG2	3:0:106:THR:HG22	1.80	0.64
2:U:139:PRO:HD3	2:U:151:LEU:HG	1.79	0.64
3:Z:15:GLY:HA2	3:Z:79:GLY:HA2	1.80	0.64
1:E:425:ALA:O	1:E:429:VAL:HG23	1.98	0.64
2:1:136:PRO:HD3	2:1:222:LYS:HG2	1.80	0.63
2:1:91:THR:OG1	2:1:123:THR:HA	1.98	0.63
1:E:111:LEU:HD12	1:E:112:VAL:N	2.13	0.63
1:F:72:GLY:HA3	1:F:149:SER:OG	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:29:ILE:HG21	3:N:71:THR:HG22	1.81	0.63
2:7:166:SER:OG	2:7:210:ASN:HB2	1.98	0.63
1:D:353:PHE:HE1	1:D:366:ASP:HB2	1.63	0.63
1:G:63:ASP:HA	1:G:93:ALA:HA	1.80	0.63
2:5:166:SER:OG	2:5:210:ASN:HB2	1.98	0.63
2:Y:166:SER:OG	2:Y:210:ASN:HB2	1.98	0.63
2:Y:11:VAL:HG22	2:Y:123:THR:OG1	1.98	0.63
1:H:234:TRP:HE3	1:H:234:TRP:H	1.45	0.63
1:G:327:GLN:HG3	1:G:329:ARG:HE	1.63	0.63
1:I:57:ARG:O	1:I:85:ASP:HB2	1.97	0.63
2:O:130:LYS:NZ	2:W:130:LYS:HD3	2.13	0.63
3:T:11:SER:HB3	3:T:111:LEU:CD1	2.28	0.63
1:C:42:LEU:HD11	1:C:316:LEU:HB2	1.80	0.63
3:Z:7:PRO:HG2	3:Z:106:THR:HG22	1.80	0.63
1:H:108:LEU:O	1:H:111:LEU:HG	1.97	0.63
1:K:57:ARG:O	1:K:85:ASP:HB2	1.96	0.63
2:5:40:ALA:HB3	2:5:43:GLN:HB3	1.80	0.63
2:M:166:SER:OG	2:M:210:ASN:HB2	1.99	0.63
3:N:15:GLY:HA2	3:N:79:GLY:HA2	1.80	0.63
2:9:91:THR:OG1	2:9:123:THR:HA	1.98	0.63
3:R:7:PRO:HG2	3:R:106:THR:HG22	1.80	0.63
1:C:384:VAL:CG1	1:C:428:LEU:HD21	2.27	0.63
3:8:7:PRO:HG2	3:8:106:THR:HG22	1.80	0.63
3:8:167:THR:O	3:8:179:ALA:HB1	1.98	0.63
1:I:384:VAL:CG1	1:I:428:LEU:HD21	2.29	0.63
1:J:37:THR:HG22	1:J:322:ASN:HB2	1.80	0.63
1:C:353:PHE:HE1	1:C:366:ASP:HB2	1.63	0.63
1:D:37:THR:HG22	1:D:322:ASN:HB2	1.80	0.63
3:P:15:GLY:HA2	3:P:79:GLY:HA2	1.80	0.63
1:B:331:LEU:HD22	1:B:331:LEU:N	2.06	0.63
1:F:189:GLN:NE2	1:F:189:GLN:H	1.96	0.63
2:3:6:GLN:OE1	2:3:120:THR:HG23	1.97	0.63
2:O:148:THR:HA	2:O:199:SER:H	1.61	0.63
2:9:176:VAL:HG22	2:9:195:VAL:HG22	1.78	0.63
2:U:184:GLN:HG2	3:V:165:GLU:OE1	1.98	0.63
1:K:73:ASP:OD1	1:K:74:PRO:HD2	1.99	0.63
2:U:16:ALA:O	2:U:86:LEU:HG	1.97	0.63
1:C:53:ASN:ND2	1:C:276:THR:HA	2.12	0.63
2:Y:136:PRO:HD3	2:Y:222:LYS:HG2	1.81	0.63
3:X:93:TYR:CD1	3:X:100:SER:HB3	2.33	0.63
3:N:161:LYS:HA	3:N:164:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:430:ALA:HB2	1:I:383:ARG:HH21	1.63	0.63
1:L:295:GLN:NE2	1:L:308:TYR:HB2	2.13	0.63
2:3:40:ALA:HB3	2:3:43:GLN:HB3	1.80	0.63
1:F:384:VAL:CG1	1:F:428:LEU:HD21	2.29	0.63
3:4:167:THR:O	3:4:179:ALA:HB1	1.99	0.63
3:8:7:PRO:O	3:8:106:THR:HG22	1.98	0.63
2:W:135:PHE:HB3	3:X:126:SER:OG	1.98	0.63
1:D:177:LEU:HB2	1:D:260:MET:SD	2.39	0.63
1:A:383:ARG:CZ	1:C:27:LYS:HD3	2.29	0.63
1:L:37:THR:HG22	1:L:322:ASN:HB2	1.81	0.63
3:Z:7:PRO:O	3:Z:106:THR:HG22	1.98	0.63
2:Y:11:VAL:HG13	2:Y:123:THR:HB	1.81	0.63
1:J:208:ARG:NH1	1:J:238:LYS:HD2	2.13	0.63
3:8:93:TYR:CD1	3:8:100:SER:HB3	2.34	0.63
1:K:42:LEU:HD11	1:K:316:LEU:HB2	1.80	0.63
1:A:60:ASP:OD2	1:A:274:ILE:HD11	1.99	0.63
1:H:208:ARG:NH1	1:H:238:LYS:HD2	2.14	0.63
2:9:39:GLN:HG2	2:9:45:LEU:HD22	1.81	0.63
2:9:33:GLY:CA	2:9:99:VAL:HG22	2.23	0.63
2:7:180:PRO:HG2	3:8:170:SER:OG	1.99	0.63
2:5:33:GLY:CA	2:5:99:VAL:HG22	2.24	0.63
2:5:148:THR:HA	2:5:199:SER:H	1.62	0.63
3:6:161:LYS:HA	3:6:164:VAL:HG21	1.81	0.63
3:P:7:PRO:HG2	3:P:106:THR:HG22	1.79	0.63
1:H:37:THR:HG22	1:H:322:ASN:HB2	1.78	0.63
3:T:93:TYR:CD1	3:T:100:SER:HB3	2.34	0.63
1:D:222:TRP:CZ3	1:D:225:GLY:HA2	2.34	0.63
1:G:337:GLY:N	1:G:466:CYS:SG	2.71	0.63
1:K:425:ALA:O	1:K:429:VAL:HG23	1.99	0.63
3:4:29:ILE:HG21	3:4:71:THR:HG22	1.79	0.63
2:7:136:PRO:HD3	2:7:222:LYS:HG2	1.81	0.63
1:B:189:GLN:NE2	1:B:189:GLN:H	1.96	0.63
3:N:7:PRO:HG2	3:N:106:THR:HG22	1.81	0.63
2:Y:91:THR:HB	2:Y:124:VAL:HG23	1.80	0.63
2:7:109:HIS:HA	3:8:93:TYR:CG	2.33	0.63
1:E:73:ASP:OD1	1:E:74:PRO:HD2	1.99	0.63
3:X:15:GLY:HA2	3:X:79:GLY:HA2	1.80	0.63
2:S:154:LEU:HD21	3:T:136:THR:HG21	1.79	0.63
1:K:353:PHE:HE1	1:K:366:ASP:HB2	1.64	0.63
1:A:425:ALA:O	1:A:429:VAL:HG23	1.99	0.63
3:N:167:THR:HG23	3:N:180:SER:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:167:THR:O	3:N:179:ALA:HB1	1.99	0.62
2:U:91:THR:CB	2:U:124:VAL:H	2.06	0.62
2:U:6:GLN:HB3	2:U:120:THR:CG2	2.29	0.62
3:N:93:TYR:CD1	3:N:100:SER:HB3	2.34	0.62
3:X:7:PRO:HG2	3:X:106:THR:HG22	1.81	0.62
1:A:293:PRO:HB3	1:A:385:ILE:HD13	1.81	0.62
3:V:161:LYS:HA	3:V:164:VAL:HG21	1.81	0.62
1:E:404:GLY:HA3	1:F:107:SER:HB2	1.81	0.62
2:5:39:GLN:HG2	2:5:45:LEU:HD22	1.80	0.62
1:J:369:SER:HB3	1:J:447:LEU:HD13	1.81	0.62
3:4:15:GLY:HA2	3:4:79:GLY:HA2	1.79	0.62
2:Q:40:ALA:HB3	2:Q:43:GLN:HB3	1.80	0.62
3:V:15:GLY:HA2	3:V:79:GLY:HA2	1.81	0.62
2:Y:99:VAL:HB	2:Y:111:TYR:CZ	2.34	0.62
2:Q:7:SER:O	2:Q:120:THR:HG22	1.99	0.62
2:Q:136:PRO:HD3	2:Q:222:LYS:HG2	1.81	0.62
3:6:93:TYR:CD1	3:6:100:SER:HB3	2.34	0.62
2:O:22:CYS:HB2	2:O:36:TRP:CH2	2.34	0.62
1:G:380:LYS:NZ	1:G:384:VAL:HG23	2.14	0.62
3:P:7:PRO:O	3:P:106:THR:HG22	1.99	0.62
3:T:7:PRO:HG2	3:T:106:THR:HG22	1.80	0.62
3:4:7:PRO:HG2	3:4:106:THR:HG22	1.81	0.62
3:2:7:PRO:O	3:2:106:THR:HG22	1.98	0.62
1:C:37:THR:HG23	1:C:320:MET:O	1.98	0.62
1:L:73:ASP:OD1	1:L:74:PRO:HD2	1.99	0.62
1:G:73:ASP:OD1	1:G:74:PRO:HD2	1.99	0.62
1:G:331:LEU:N	1:G:331:LEU:HD13	2.14	0.62
2:3:111:TYR:CD1	2:3:111:TYR:C	2.73	0.62
2:5:6:GLN:HB2	2:5:118:GLN:OE1	1.99	0.62
2:3:16:ALA:O	2:3:86:LEU:HG	1.98	0.62
1:A:316:LEU:HD12	1:A:317:ALA:N	2.14	0.62
3:2:7:PRO:HG2	3:2:106:THR:HG22	1.81	0.62
3:V:7:PRO:O	3:V:106:THR:HG22	1.99	0.62
1:D:37:THR:HG23	1:D:320:MET:O	1.99	0.62
2:W:136:PRO:O	3:X:126:SER:HB3	1.99	0.62
2:S:87:ARG:HB2	2:S:90:ASP:OD2	2.00	0.62
3:6:15:GLY:HA2	3:6:79:GLY:HA2	1.80	0.62
1:A:72:GLY:HA3	1:A:149:SER:OG	1.98	0.62
1:E:376:GLN:CB	1:E:439:LEU:HD11	2.29	0.62
1:B:37:THR:HG22	1:B:322:ASN:HB2	1.80	0.62
2:Q:113:MET:HG3	3:R:38:TYR:OH	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:60:ASP:OD2	1:K:274:ILE:HD11	1.99	0.62
2:Y:100:GLU:HB3	2:Y:110:TYR:CE2	2.35	0.62
2:1:100:GLU:H	2:1:111:TYR:CB	2.08	0.62
4:A:602:NAG:H5	2:M:57:GLN:NE2	2.14	0.62
2:3:136:PRO:HD3	2:3:222:LYS:HG2	1.79	0.62
2:Q:109:HIS:HA	3:R:93:TYR:CD1	2.35	0.62
1:J:380:LYS:NZ	1:J:384:VAL:HG23	2.15	0.62
1:E:316:LEU:HD12	1:E:317:ALA:N	2.14	0.62
2:Y:87:ARG:HB2	2:Y:90:ASP:OD2	1.99	0.62
1:L:327:GLN:HG3	1:L:329:ARG:HE	1.63	0.62
3:R:29:ILE:HG21	3:R:71:THR:HG22	1.81	0.62
1:C:331:LEU:HD22	1:C:331:LEU:N	2.09	0.62
2:O:6:GLN:HB3	2:O:120:THR:CG2	2.27	0.62
1:F:191:GLN:NE2	1:F:217:ILE:HD11	2.13	0.62
2:W:105:VAL:O	2:W:106:MET:HB3	2.00	0.62
1:E:384:VAL:CG1	1:E:428:LEU:HD21	2.28	0.62
3:P:167:THR:O	3:P:179:ALA:HB1	1.99	0.62
1:I:37:THR:HG22	1:I:322:ASN:HB2	1.80	0.62
1:G:222:TRP:CZ3	1:G:225:GLY:HA2	2.35	0.62
3:X:29:ILE:HG21	3:X:71:THR:HG22	1.81	0.62
3:V:17:ARG:HH21	3:V:78:THR:CG2	2.13	0.62
1:E:63:ASP:HA	1:E:93:ALA:HA	1.80	0.62
2:Y:109:HIS:HA	3:Z:93:TYR:CG	2.34	0.62
1:I:37:THR:HG23	1:I:320:MET:O	1.99	0.62
1:F:87:PHE:O	1:F:267:ILE:HG13	2.00	0.62
2:U:136:PRO:HD3	2:U:222:LYS:HG2	1.80	0.62
1:B:331:LEU:CD2	1:B:331:LEU:H	2.00	0.62
2:W:6:GLN:OE1	2:W:120:THR:HG23	1.99	0.62
2:7:16:ALA:O	2:7:86:LEU:HG	2.00	0.62
3:R:161:LYS:HA	3:R:164:VAL:HG21	1.81	0.62
3:6:7:PRO:HG2	3:6:106:THR:HG22	1.81	0.62
2:U:163:VAL:HB	2:U:213:HIS:ND1	2.15	0.62
2:3:163:VAL:HB	2:3:213:HIS:ND1	2.15	0.62
1:D:384:VAL:CG1	1:D:428:LEU:HD21	2.29	0.62
1:I:425:ALA:O	1:I:429:VAL:HG23	2.00	0.62
1:I:87:PHE:O	1:I:267:ILE:HG13	2.00	0.62
2:5:87:ARG:HB2	2:5:90:ASP:OD2	1.99	0.62
1:C:457:GLU:HG3	1:C:499:ARG:HH12	1.64	0.62
1:I:222:TRP:CZ3	1:I:225:GLY:HA2	2.35	0.62
1:K:189:GLN:H	1:K:189:GLN:NE2	1.98	0.62
2:M:105:VAL:O	2:M:106:MET:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:GLU:HG3	1:C:238:LYS:HE2	1.82	0.62
2:W:136:PRO:HD3	2:W:222:LYS:HG2	1.82	0.62
3:6:29:ILE:HG21	3:6:71:THR:HG22	1.81	0.62
2:M:87:ARG:HB2	2:M:90:ASP:OD2	2.00	0.62
1:F:369:SER:HB3	1:F:447:LEU:HD13	1.81	0.62
1:A:111:LEU:HD12	1:A:112:VAL:N	2.15	0.62
3:X:7:PRO:O	3:X:106:THR:HG22	2.00	0.62
3:0:7:PRO:O	3:0:106:THR:HG22	2.00	0.62
2:S:163:VAL:HB	2:S:213:HIS:ND1	2.14	0.62
1:F:63:ASP:HA	1:F:93:ALA:HA	1.82	0.62
3:2:29:ILE:HG21	3:2:71:THR:HG22	1.82	0.62
1:D:457:GLU:HG3	1:D:499:ARG:HH12	1.64	0.62
1:H:63:ASP:HA	1:H:93:ALA:HA	1.82	0.62
2:S:136:PRO:HD3	2:S:222:LYS:HG2	1.80	0.62
2:W:100:GLU:HB3	2:W:110:TYR:CE2	2.35	0.62
2:W:148:THR:HG22	2:W:198:PRO:HA	1.82	0.62
2:O:136:PRO:HD3	2:O:222:LYS:HG2	1.82	0.62
1:E:384:VAL:HG13	1:E:428:LEU:HD21	1.82	0.62
3:T:29:ILE:HG21	3:T:71:THR:HG22	1.80	0.62
1:B:73:ASP:OD1	1:B:74:PRO:HD2	1.99	0.62
3:6:130:LEU:HD21	3:6:135:ALA:HB2	1.82	0.62
2:S:100:GLU:H	2:S:111:TYR:CB	2.10	0.61
2:5:105:VAL:O	2:5:106:MET:HB3	2.00	0.61
1:A:383:ARG:HD3	1:C:27:LYS:NZ	2.14	0.61
3:T:161:LYS:HA	3:T:164:VAL:HG21	1.80	0.61
2:M:136:PRO:HD3	2:M:222:LYS:HG2	1.81	0.61
2:U:87:ARG:HB2	2:U:90:ASP:OD2	1.99	0.61
1:I:327:GLN:HG3	1:I:329:ARG:HE	1.65	0.61
2:Q:33:GLY:HA3	2:Q:99:VAL:CG2	2.25	0.61
2:1:94:TYR:HE2	2:1:122:VAL:HG21	1.65	0.61
3:V:7:PRO:HG2	3:V:106:THR:HG22	1.81	0.61
3:6:11:SER:HB3	3:6:111:LEU:HD11	1.82	0.61
1:H:27:LYS:HD3	1:I:383:ARG:NH1	2.15	0.61
1:J:457:GLU:HG3	1:J:499:ARG:HH12	1.64	0.61
2:U:179:PHE:CD2	3:V:140:LEU:HB3	2.35	0.61
1:I:189:GLN:NE2	1:I:189:GLN:H	1.98	0.61
1:K:222:TRP:CZ3	1:K:225:GLY:HA2	2.35	0.61
2:3:22:CYS:HB2	2:3:36:TRP:CH2	2.35	0.61
2:Y:22:CYS:HB2	2:Y:36:TRP:CH2	2.36	0.61
3:6:7:PRO:O	3:6:106:THR:HG22	2.00	0.61
1:K:272:ALA:HA	2:7:105:VAL:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:THR:HG22	1:C:322:ASN:HB2	1.80	0.61
2:3:108:PHE:HB2	2:3:111:TYR:CE2	2.36	0.61
2:9:91:THR:HB	2:9:124:VAL:N	2.12	0.61
1:F:327:GLN:HG3	1:F:329:ARG:HE	1.64	0.61
1:L:326:LYS:HB3	1:L:328:THR:CG2	2.29	0.61
1:A:380:LYS:HG2	1:C:29:ILE:O	2.00	0.61
2:Y:7:SER:HB3	2:Y:21:SER:OG	2.00	0.61
2:9:136:PRO:HD3	2:9:222:LYS:HG2	1.82	0.61
1:K:376:GLN:CB	1:K:439:LEU:HD11	2.31	0.61
2:Y:39:GLN:HG2	2:Y:45:LEU:HD22	1.82	0.61
1:A:189:GLN:H	1:A:189:GLN:NE2	1.99	0.61
2:O:130:LYS:HZ3	2:W:130:LYS:HD3	1.66	0.61
3:0:29:ILE:HG21	3:0:71:THR:HG22	1.81	0.61
1:G:72:GLY:HA3	1:G:149:SER:OG	2.00	0.61
1:E:177:LEU:HB2	1:E:260:MET:SD	2.39	0.61
1:G:425:ALA:O	1:G:429:VAL:HG23	2.01	0.61
1:L:376:GLN:CB	1:L:439:LEU:HD11	2.30	0.61
1:F:189:GLN:CD	1:F:189:GLN:H	2.03	0.61
1:H:189:GLN:H	1:H:189:GLN:CD	2.03	0.61
1:E:463:GLY:O	1:F:453:ARG:HD3	2.01	0.61
1:K:384:VAL:HG12	1:K:385:ILE:N	2.14	0.61
1:A:407:GLN:HG2	1:A:411:LYS:HE3	1.83	0.61
2:1:181:ALA:HB2	2:1:191:LEU:HB3	1.83	0.61
3:R:130:LEU:HD21	3:R:135:ALA:HB2	1.83	0.61
3:T:15:GLY:HA2	3:T:79:GLY:HA2	1.80	0.61
2:U:105:VAL:O	2:U:106:MET:HB3	2.01	0.61
2:5:218:THR:HG22	2:5:220:VAL:HG23	1.82	0.61
2:U:52:ASN:ND2	2:U:102:VAL:HA	2.15	0.61
2:U:99:VAL:HB	2:U:111:TYR:CZ	2.36	0.61
1:D:251:LEU:HD12	1:D:252:ILE:H	1.64	0.61
1:H:14:CYS:SG	1:H:335:ILE:HG23	2.41	0.61
1:F:73:ASP:OD1	1:F:74:PRO:HD2	2.00	0.61
3:X:130:LEU:HD21	3:X:135:ALA:HB2	1.83	0.61
2:U:112:PRO:HB2	3:V:51:SER:HB2	1.83	0.61
1:J:63:ASP:HA	1:J:93:ALA:HA	1.83	0.61
2:Y:218:THR:HG22	2:Y:220:VAL:HG23	1.83	0.61
1:K:87:PHE:O	1:K:267:ILE:HG13	2.01	0.61
2:1:87:ARG:HB2	2:1:90:ASP:OD2	2.00	0.61
2:O:99:VAL:HB	2:O:111:TYR:CZ	2.36	0.61
1:E:189:GLN:NE2	1:E:189:GLN:H	1.99	0.61
1:J:189:GLN:NE2	1:J:189:GLN:H	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:GLN:NE2	1:G:189:GLN:H	1.97	0.61
2:W:218:THR:HG22	2:W:220:VAL:HG23	1.82	0.61
2:Y:105:VAL:O	2:Y:106:MET:HB3	2.01	0.61
1:B:63:ASP:HA	1:B:93:ALA:HA	1.81	0.61
2:O:39:GLN:HG2	2:O:45:LEU:HD22	1.82	0.61
2:W:39:GLN:HG2	2:W:45:LEU:HD22	1.83	0.61
1:J:72:GLY:HA3	1:J:149:SER:OG	2.00	0.61
3:2:113:GLN:HG3	3:2:175:ASN:ND2	2.16	0.61
2:7:98:ARG:O	2:7:113:MET:HA	2.01	0.61
2:Y:148:THR:HG22	2:Y:198:PRO:HA	1.83	0.61
2:O:94:TYR:HE2	2:O:122:VAL:HG21	1.66	0.61
1:B:189:GLN:CD	1:B:189:GLN:H	2.04	0.61
1:K:380:LYS:NZ	1:K:384:VAL:HG23	2.16	0.61
2:9:22:CYS:HB2	2:9:36:TRP:CH2	2.35	0.61
3:P:130:LEU:HD21	3:P:135:ALA:HB2	1.82	0.61
2:3:112:PRO:HB2	3:4:51:SER:HB2	1.82	0.61
1:B:84:TRP:CE2	1:B:116:GLY:HA2	2.36	0.61
1:H:73:ASP:OD1	1:H:74:PRO:HD2	2.01	0.61
1:C:73:ASP:OD1	1:C:74:PRO:HD2	1.99	0.61
1:D:331:LEU:H	1:D:331:LEU:CD2	2.00	0.61
2:M:38:ARG:HD2	2:M:46:GLU:OE1	2.01	0.61
1:D:326:LYS:HB3	1:D:328:THR:CG2	2.31	0.61
1:B:27:LYS:HD3	1:C:383:ARG:CZ	2.31	0.61
1:F:17:HIS:HB2	1:F:320:MET:HE1	1.83	0.61
1:J:453:ARG:HD3	1:L:463:GLY:HA2	1.82	0.61
3:V:29:ILE:HG21	3:V:71:THR:HG22	1.83	0.61
1:L:369:SER:HB3	1:L:447:LEU:HD13	1.82	0.61
1:K:337:GLY:N	1:K:466:CYS:SG	2.74	0.61
1:B:337:GLY:N	1:B:466:CYS:SG	2.74	0.61
1:H:60:ASP:OD2	1:H:274:ILE:HD11	2.00	0.61
2:9:100:GLU:N	2:9:111:TYR:HB2	2.11	0.60
2:Q:22:CYS:HB2	2:Q:36:TRP:CH2	2.35	0.60
1:F:148:PHE:HB2	1:F:151:LEU:HB2	1.83	0.60
1:H:29:ILE:O	1:I:380:LYS:HG2	2.00	0.60
1:I:384:VAL:HG13	1:I:428:LEU:HD21	1.82	0.60
1:I:376:GLN:CB	1:I:439:LEU:HD11	2.30	0.60
1:D:337:GLY:N	1:D:466:CYS:SG	2.74	0.60
1:L:120:PHE:CD2	1:L:150:ARG:HD2	2.36	0.60
1:F:312:ASN:OD1	1:F:313:THR:HG22	2.01	0.60
2:3:7:SER:HB3	2:3:21:SER:OG	2.01	0.60
3:R:113:GLN:HG3	3:R:175:ASN:HD21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:148:THR:HG22	2:S:198:PRO:HA	1.83	0.60
1:C:189:GLN:NE2	1:C:189:GLN:H	1.99	0.60
1:E:222:TRP:HB2	6:F:610:NAG:H62	1.82	0.60
2:3:105:VAL:O	2:3:106:MET:HB3	2.00	0.60
3:R:7:PRO:O	3:R:106:THR:HG22	2.00	0.60
2:M:163:VAL:HB	2:M:213:HIS:ND1	2.17	0.60
2:1:163:VAL:HB	2:1:213:HIS:ND1	2.16	0.60
1:D:221:PRO:HD3	1:E:244:VAL:HB	1.83	0.60
3:P:191:LYS:HD2	3:P:191:LYS:N	2.16	0.60
1:B:234:TRP:H	1:B:234:TRP:HE3	1.47	0.60
3:Z:130:LEU:HD21	3:Z:135:ALA:HB2	1.84	0.60
1:E:353:PHE:HE1	1:E:366:ASP:HB2	1.65	0.60
3:4:11:SER:HB3	3:4:111:LEU:HD11	1.81	0.60
1:J:210:GLN:NE2	1:L:220:ARG:NE	2.48	0.60
2:9:108:PHE:HB2	2:9:111:TYR:CE2	2.36	0.60
2:Y:177:HIS:NE2	3:Z:172:GLN:NE2	2.49	0.60
2:S:34:LEU:HD23	2:S:97:ALA:O	2.02	0.60
1:I:331:LEU:H	1:I:331:LEU:CD2	2.01	0.60
2:W:10:GLU:O	2:W:122:VAL:HA	2.01	0.60
2:1:148:THR:HG22	2:1:198:PRO:HA	1.83	0.60
1:C:243:LEU:HD12	1:C:244:VAL:H	1.66	0.60
2:5:22:CYS:HB2	2:5:36:TRP:CH2	2.36	0.60
1:G:53:ASN:ND2	1:G:276:THR:HA	2.15	0.60
2:Y:163:VAL:HB	2:Y:213:HIS:ND1	2.16	0.60
2:Q:163:VAL:HB	2:Q:213:HIS:ND1	2.16	0.60
1:C:111:LEU:HD12	1:C:112:VAL:N	2.16	0.60
1:A:369:SER:HB3	1:A:447:LEU:HD13	1.83	0.60
1:C:337:GLY:N	1:C:466:CYS:SG	2.74	0.60
1:D:327:GLN:HG3	1:D:329:ARG:HE	1.65	0.60
2:M:218:THR:HG22	2:M:220:VAL:HG23	1.83	0.60
1:D:219:SER:H	1:E:246:ASN:ND2	1.99	0.60
2:9:100:GLU:HB3	2:9:110:TYR:CE2	2.37	0.60
2:S:111:TYR:HE1	2:S:113:MET:HG2	1.67	0.60
1:J:189:GLN:CD	1:J:189:GLN:H	2.05	0.60
2:O:38:ARG:HD2	2:O:46:GLU:OE1	2.00	0.60
2:S:91:THR:HB	2:S:124:VAL:N	2.16	0.60
2:W:163:VAL:HB	2:W:213:HIS:ND1	2.17	0.60
2:Y:181:ALA:HB2	2:Y:191:LEU:HB3	1.82	0.60
1:J:60:ASP:OD2	1:J:274:ILE:HD11	2.01	0.60
2:1:218:THR:HG22	2:1:220:VAL:HG23	1.83	0.60
2:7:87:ARG:HB2	2:7:90:ASP:OD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:148:THR:HG22	2:9:198:PRO:HA	1.83	0.60
1:L:189:GLN:H	1:L:189:GLN:NE2	1.99	0.60
1:I:189:GLN:CD	1:I:189:GLN:H	2.03	0.60
1:A:189:GLN:H	1:A:189:GLN:CD	2.05	0.60
2:5:20:VAL:HG13	2:5:120:THR:HG21	1.82	0.60
2:Q:109:HIS:ND1	3:R:93:TYR:HB3	2.16	0.60
1:L:380:LYS:NZ	1:L:384:VAL:HG23	2.16	0.60
1:A:453:ARG:HD3	1:C:463:GLY:HA2	1.83	0.60
2:1:113:MET:HG3	3:2:38:TYR:OH	2.01	0.60
1:E:331:LEU:HD22	1:E:331:LEU:N	2.06	0.60
1:E:326:LYS:HB3	1:E:328:THR:CG2	2.31	0.60
2:1:39:GLN:HG2	2:1:45:LEU:HD22	1.83	0.60
2:5:163:VAL:HB	2:5:213:HIS:ND1	2.16	0.60
1:A:148:PHE:HB2	1:A:151:LEU:HB2	1.84	0.60
2:Q:218:THR:HG22	2:Q:220:VAL:HG23	1.83	0.60
1:A:331:LEU:CD2	1:A:331:LEU:H	1.99	0.60
2:S:92:ALA:O	2:S:122:VAL:HG22	2.02	0.60
1:E:27:LYS:HZ3	1:F:383:ARG:HD3	1.66	0.60
2:U:6:GLN:HE21	2:U:117:GLY:HA3	1.66	0.60
1:D:403:GLU:HB2	1:D:407:GLN:HB2	1.82	0.60
3:T:57:PRO:HG2	3:T:60:VAL:HB	1.84	0.60
1:F:337:GLY:N	1:F:466:CYS:SG	2.75	0.60
1:A:327:GLN:HG3	1:A:329:ARG:HE	1.66	0.60
1:L:87:PHE:O	1:L:267:ILE:HG13	2.02	0.60
1:F:177:LEU:HB2	1:F:260:MET:SD	2.41	0.60
1:C:327:GLN:HG3	1:C:329:ARG:HE	1.67	0.60
2:7:100:GLU:HB3	2:7:110:TYR:CE2	2.36	0.60
2:7:112:PRO:CB	3:8:51:SER:HB2	2.31	0.60
2:5:100:GLU:HB3	2:5:110:TYR:CE2	2.36	0.60
2:1:7:SER:HB3	2:1:21:SER:OG	2.02	0.60
3:T:7:PRO:O	3:T:106:THR:HG22	2.01	0.60
2:O:163:VAL:HB	2:O:213:HIS:ND1	2.16	0.60
1:B:37:THR:HG23	1:B:320:MET:O	2.01	0.60
1:G:369:SER:HB3	1:G:447:LEU:HD13	1.84	0.60
3:8:191:LYS:N	3:8:191:LYS:HD2	2.16	0.60
1:I:234:TRP:H	1:I:234:TRP:HE3	1.50	0.60
1:E:234:TRP:H	1:E:234:TRP:HE3	1.50	0.60
1:A:337:GLY:N	1:A:466:CYS:SG	2.75	0.60
3:T:151:VAL:HG13	3:T:200:VAL:HG12	1.84	0.60
3:2:151:VAL:HG13	3:2:200:VAL:HG12	1.84	0.60
2:Y:111:TYR:CE1	2:Y:113:MET:HG2	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:100:GLU:HB3	2:S:110:TYR:CE2	2.36	0.60
2:9:6:GLN:HB2	2:9:118:GLN:OE1	2.01	0.60
1:B:380:LYS:NZ	1:B:384:VAL:HG23	2.17	0.60
1:C:357:ASN:ND2	1:C:359:GLU:HB2	2.17	0.60
1:L:343:TRP:HB3	1:L:354:ARG:NH2	2.17	0.60
3:6:147:GLY:O	3:6:169:PRO:HG3	2.02	0.60
2:7:105:VAL:O	2:7:106:MET:HB3	2.02	0.60
3:Z:29:ILE:HG21	3:Z:71:THR:HG22	1.82	0.60
1:H:87:PHE:O	1:H:267:ILE:HG13	2.02	0.60
1:A:376:GLN:CB	1:A:439:LEU:HD11	2.31	0.60
3:0:23:THR:HG22	3:0:72:SER:HB2	1.84	0.60
1:C:177:LEU:HB2	1:C:260:MET:SD	2.41	0.60
1:F:425:ALA:O	1:F:429:VAL:HG23	2.01	0.60
3:X:23:THR:HG22	3:X:72:SER:HB2	1.84	0.60
2:M:39:GLN:HG2	2:M:45:LEU:HD22	1.84	0.60
2:W:52:ASN:ND2	2:W:102:VAL:HA	2.17	0.60
2:Q:100:GLU:HB3	2:Q:110:TYR:CE2	2.37	0.60
2:S:52:ASN:ND2	2:S:102:VAL:HA	2.17	0.60
2:W:84:LYS:NZ	2:9:142:LYS:NZ	2.36	0.60
2:Q:6:GLN:HE22	2:Q:95:TYR:HA	1.66	0.60
1:E:463:GLY:CA	1:F:453:ARG:HD3	2.31	0.60
2:U:181:ALA:HB2	2:U:191:LEU:HB3	1.83	0.60
2:7:181:ALA:HB2	2:7:191:LEU:HB3	1.82	0.60
1:H:37:THR:HG23	1:H:320:MET:O	2.02	0.60
1:B:60:ASP:OD2	1:B:274:ILE:HD11	2.01	0.60
3:P:151:VAL:HG13	3:P:200:VAL:HG12	1.83	0.60
1:H:376:GLN:CB	1:H:439:LEU:HD11	2.32	0.60
1:B:376:GLN:CB	1:B:439:LEU:HD11	2.32	0.60
3:R:191:LYS:HD2	3:R:191:LYS:N	2.16	0.60
3:6:191:LYS:N	3:6:191:LYS:HD2	2.17	0.60
3:P:57:PRO:HG2	3:P:60:VAL:HB	1.84	0.60
3:0:130:LEU:HD21	3:0:135:ALA:HB2	1.84	0.60
3:V:23:THR:HG22	3:V:72:SER:HB2	1.82	0.60
2:Q:105:VAL:O	2:Q:106:MET:HB3	2.01	0.60
2:3:100:GLU:HB3	2:3:110:TYR:CE2	2.37	0.59
2:O:88:SER:O	2:O:91:THR:HG22	2.01	0.59
2:S:22:CYS:HB2	2:S:36:TRP:CH2	2.35	0.59
1:K:108:LEU:O	1:K:112:VAL:HG23	2.02	0.59
1:K:14:CYS:SG	1:K:335:ILE:HG23	2.42	0.59
3:N:7:PRO:HD3	3:N:21:SER:O	2.02	0.59
3:0:139:CYS:HB2	3:0:153:TRP:HZ2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:181:ALA:HB2	2:9:191:LEU:HB3	1.83	0.59
2:Y:88:SER:O	2:Y:91:THR:HG22	2.02	0.59
2:9:218:THR:HG22	2:9:220:VAL:HG23	1.83	0.59
1:J:337:GLY:N	1:J:466:CYS:SG	2.75	0.59
2:5:112:PRO:HB2	3:6:51:SER:HB2	1.82	0.59
2:U:218:THR:HG22	2:U:220:VAL:HG23	1.83	0.59
1:B:72:GLY:HA3	1:B:149:SER:OG	2.02	0.59
1:L:337:GLY:N	1:L:466:CYS:SG	2.75	0.59
2:M:179:PHE:HB3	3:N:180:SER:OG	2.01	0.59
1:F:331:LEU:H	1:F:331:LEU:CD2	1.92	0.59
2:1:100:GLU:HB3	2:1:110:TYR:CE2	2.37	0.59
2:5:52:ASN:ND2	2:5:102:VAL:HA	2.17	0.59
2:3:148:THR:HG22	2:3:198:PRO:HA	1.83	0.59
1:D:189:GLN:H	1:D:189:GLN:NE2	2.00	0.59
1:D:425:ALA:O	1:D:429:VAL:HG23	2.03	0.59
1:J:222:TRP:CZ3	1:J:225:GLY:HA2	2.36	0.59
3:8:29:ILE:HG21	3:8:71:THR:HG22	1.83	0.59
3:2:191:LYS:N	3:2:191:LYS:HD2	2.18	0.59
2:7:218:THR:HG22	2:7:220:VAL:HG23	1.83	0.59
1:A:399:PHE:HE2	1:C:405:ARG:HH21	1.50	0.59
3:Z:147:GLY:O	3:Z:169:PRO:HG3	2.02	0.59
1:G:189:GLN:H	1:G:189:GLN:CD	2.05	0.59
2:U:7:SER:HB3	2:U:21:SER:OG	2.02	0.59
1:L:384:VAL:CG1	1:L:428:LEU:HD21	2.32	0.59
1:C:369:SER:HB3	1:C:447:LEU:HD13	1.84	0.59
1:L:234:TRP:H	1:L:234:TRP:HE3	1.47	0.59
3:V:191:LYS:HD2	3:V:191:LYS:N	2.17	0.59
1:J:73:ASP:OD1	1:J:74:PRO:HD2	2.02	0.59
1:A:331:LEU:N	1:A:331:LEU:HD22	2.06	0.59
4:D:602:NAG:H5	2:S:57:GLN:HE22	1.68	0.59
2:7:148:THR:HG22	2:7:198:PRO:HA	1.83	0.59
2:7:38:ARG:HD2	2:7:46:GLU:OE1	2.01	0.59
2:9:6:GLN:HB3	2:9:120:THR:HG23	1.83	0.59
1:H:326:LYS:HB3	1:H:328:THR:CG2	2.32	0.59
1:G:409:LEU:HD11	1:H:413:VAL:HG21	1.84	0.59
3:T:164:VAL:HG22	3:T:183:LEU:HD21	1.83	0.59
3:P:7:PRO:HD3	3:P:21:SER:O	2.03	0.59
2:3:181:ALA:HB2	2:3:191:LEU:HB3	1.85	0.59
1:L:380:LYS:HZ3	1:L:384:VAL:HG23	1.67	0.59
2:3:218:THR:HG22	2:3:220:VAL:HG23	1.82	0.59
1:G:179:ILE:O	1:G:254:PRO:HB3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:130:LEU:HD21	3:V:135:ALA:HB2	1.84	0.59
2:W:179:PHE:CE2	3:X:142:SER:HB3	2.37	0.59
2:Q:52:ASN:ND2	2:Q:102:VAL:HA	2.18	0.59
2:W:91:THR:OG1	2:W:123:THR:HA	2.03	0.59
2:S:6:GLN:H	2:S:118:GLN:NE2	2.00	0.59
2:M:7:SER:HB3	2:M:21:SER:OG	2.02	0.59
1:K:293:PRO:HB3	1:K:385:ILE:HD13	1.83	0.59
1:J:380:LYS:HG2	1:L:29:ILE:O	2.02	0.59
3:6:164:VAL:HG22	3:6:183:LEU:HD21	1.84	0.59
1:D:238:LYS:HE2	1:F:401:GLU:HG3	1.84	0.59
2:7:163:VAL:HB	2:7:213:HIS:ND1	2.17	0.59
2:S:181:ALA:HB2	2:S:191:LEU:HB3	1.84	0.59
3:8:139:CYS:HB2	3:8:153:TRP:HZ2	1.67	0.59
3:R:23:THR:HG22	3:R:72:SER:HB2	1.83	0.59
1:L:84:TRP:CE2	1:L:116:GLY:HA2	2.37	0.59
1:G:457:GLU:HG3	1:G:499:ARG:HH12	1.66	0.59
1:K:369:SER:HB3	1:K:447:LEU:HD13	1.84	0.59
3:R:57:PRO:HG2	3:R:60:VAL:HB	1.84	0.59
1:E:60:ASP:OD2	1:E:274:ILE:HD11	2.03	0.59
2:W:100:GLU:H	2:W:111:TYR:CB	2.12	0.59
1:C:326:LYS:HB3	1:C:328:THR:CG2	2.31	0.59
1:D:27:LYS:HZ2	1:E:383:ARG:HD3	1.68	0.59
2:W:22:CYS:HB2	2:W:36:TRP:CH2	2.37	0.59
1:E:14:CYS:SG	1:E:335:ILE:HG23	2.43	0.59
1:J:383:ARG:NH2	1:L:426:GLU:HG3	2.17	0.59
1:L:293:PRO:HB3	1:L:385:ILE:HD13	1.85	0.59
3:4:11:SER:HB3	3:4:111:LEU:CD1	2.32	0.59
3:4:191:LYS:HD2	3:4:191:LYS:N	2.18	0.59
3:0:151:VAL:HG13	3:0:200:VAL:HG12	1.85	0.59
2:7:52:ASN:ND2	2:7:102:VAL:HA	2.18	0.59
2:S:7:SER:HB3	2:S:21:SER:OG	2.03	0.59
2:S:2:VAL:HG21	2:S:115:VAL:HG21	1.83	0.59
2:9:105:VAL:O	2:9:106:MET:HB3	2.01	0.59
2:5:181:ALA:HB2	2:5:191:LEU:HB3	1.83	0.59
3:4:7:PRO:HD3	3:4:21:SER:O	2.03	0.59
3:T:23:THR:HG22	3:T:72:SER:HB2	1.84	0.59
1:I:337:GLY:N	1:I:466:CYS:SG	2.76	0.59
2:1:105:VAL:O	2:1:106:MET:HB3	2.01	0.59
3:2:139:CYS:HB2	3:2:153:TRP:HZ2	1.68	0.59
3:T:191:LYS:N	3:T:191:LYS:HD2	2.17	0.59
3:N:151:VAL:HG13	3:N:200:VAL:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:87:ARG:HB2	2:O:90:ASP:OD2	2.02	0.59
2:3:52:ASN:ND2	2:3:102:VAL:HA	2.18	0.59
2:M:100:GLU:HB3	2:M:110:TYR:CE2	2.37	0.59
2:S:6:GLN:HB3	2:S:120:THR:CG2	2.32	0.59
2:7:22:CYS:HB2	2:7:36:TRP:CH2	2.38	0.59
1:B:426:GLU:HG3	1:C:383:ARG:HH22	1.67	0.59
3:P:164:VAL:HG22	3:P:183:LEU:HD21	1.85	0.59
3:T:7:PRO:HD3	3:T:21:SER:O	2.02	0.59
1:G:37:THR:HG23	1:G:320:MET:O	2.02	0.59
1:K:376:GLN:HB3	1:K:439:LEU:HD11	1.85	0.59
1:L:388:THR:CG2	1:L:389:ASN:N	2.65	0.59
1:F:386:GLU:HA	1:F:386:GLU:OE2	2.01	0.59
1:H:295:GLN:NE2	1:H:308:TYR:HB2	2.18	0.59
2:9:52:ASN:ND2	2:9:102:VAL:HA	2.17	0.59
2:S:108:PHE:HB2	2:S:111:TYR:HE2	1.68	0.59
2:M:52:ASN:ND2	2:M:102:VAL:HA	2.18	0.59
2:3:87:ARG:HB2	2:3:90:ASP:OD2	2.02	0.59
2:9:10:GLU:O	2:9:122:VAL:HA	2.03	0.59
2:7:6:GLN:HE22	2:7:95:TYR:HA	1.67	0.59
2:7:88:SER:O	2:7:91:THR:HG22	2.02	0.59
1:K:37:THR:HG23	1:K:320:MET:O	2.02	0.59
1:B:272:ALA:HA	2:O:105:VAL:HG22	1.83	0.59
1:I:369:SER:HB3	1:I:447:LEU:HD13	1.85	0.59
3:N:191:LYS:HD2	3:N:191:LYS:N	2.17	0.59
2:5:97:ALA:HB1	2:5:114:ASP:O	2.03	0.59
1:E:189:GLN:CD	1:E:189:GLN:H	2.05	0.59
1:C:189:GLN:H	1:C:189:GLN:CD	2.06	0.59
1:C:251:LEU:HD12	1:C:252:ILE:H	1.68	0.59
2:1:88:SER:O	2:1:91:THR:HG22	2.03	0.59
3:R:164:VAL:HG22	3:R:183:LEU:HD21	1.85	0.59
3:R:7:PRO:HD3	3:R:21:SER:O	2.03	0.59
1:C:343:TRP:HB3	1:C:354:ARG:NH2	2.18	0.59
2:U:40:ALA:HB3	2:U:43:GLN:CB	2.33	0.59
1:I:380:LYS:NZ	1:I:384:VAL:HG23	2.17	0.59
1:L:99:PRO:HB2	1:L:229:ARG:HD3	1.85	0.59
3:T:49:LEU:O	3:T:57:PRO:HG3	2.03	0.59
1:J:309:VAL:HB	1:J:311:GLN:OE1	2.02	0.59
1:L:96:ASN:HA	1:L:224:ARG:HH11	1.68	0.59
2:S:218:THR:HG22	2:S:220:VAL:HG23	1.83	0.59
2:O:100:GLU:HB3	2:O:110:TYR:CE2	2.37	0.58
2:9:88:SER:O	2:9:91:THR:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:PHE:HB2	1:C:151:LEU:HB2	1.85	0.58
2:3:194:VAL:HG21	3:4:140:LEU:HD13	1.84	0.58
1:A:14:CYS:SG	1:A:335:ILE:HG23	2.42	0.58
1:D:29:ILE:O	1:E:380:LYS:HG2	2.02	0.58
1:E:148:PHE:HB2	1:E:151:LEU:HB2	1.85	0.58
1:H:369:SER:HB3	1:H:447:LEU:HD13	1.84	0.58
3:T:130:LEU:HD21	3:T:135:ALA:HB2	1.84	0.58
1:E:327:GLN:HG3	1:E:329:ARG:HE	1.68	0.58
3:2:23:THR:HG22	3:2:72:SER:HB2	1.84	0.58
2:S:105:VAL:O	2:S:106:MET:HB3	2.03	0.58
3:0:191:LYS:N	3:0:191:LYS:HD2	2.18	0.58
3:N:130:LEU:HD21	3:N:135:ALA:HB2	1.84	0.58
3:8:23:THR:HG22	3:8:72:SER:HB2	1.83	0.58
1:B:179:ILE:O	1:B:254:PRO:HB3	2.02	0.58
2:5:148:THR:HG22	2:5:198:PRO:HA	1.84	0.58
1:J:326:LYS:HB3	1:J:328:THR:CG2	2.31	0.58
3:6:139:CYS:HB2	3:6:153:TRP:HZ2	1.68	0.58
1:K:61:GLY:O	1:K:64:CYS:HB2	2.03	0.58
2:M:181:ALA:HB2	2:M:191:LEU:HB3	1.86	0.58
3:Z:139:CYS:HB2	3:Z:153:TRP:HZ2	1.68	0.58
2:S:39:GLN:HG2	2:S:45:LEU:HD22	1.85	0.58
1:G:87:PHE:O	1:G:267:ILE:HG13	2.02	0.58
3:Z:191:LYS:N	3:Z:191:LYS:HD2	2.18	0.58
1:C:388:THR:CG2	1:C:389:ASN:N	2.65	0.58
3:6:151:VAL:HG13	3:6:200:VAL:HG12	1.85	0.58
1:D:376:GLN:CB	1:D:439:LEU:HD11	2.33	0.58
1:I:72:GLY:HA3	1:I:149:SER:OG	2.02	0.58
1:B:327:GLN:HG3	1:B:329:ARG:HE	1.67	0.58
3:N:147:GLY:O	3:N:169:PRO:HG3	2.03	0.58
2:W:34:LEU:HD23	2:W:97:ALA:O	2.04	0.58
2:Y:52:ASN:ND2	2:Y:102:VAL:HA	2.18	0.58
2:3:88:SER:O	2:3:91:THR:HG22	2.03	0.58
2:Q:148:THR:HG22	2:Q:198:PRO:HA	1.84	0.58
1:K:326:LYS:HB3	1:K:328:THR:CG2	2.32	0.58
1:A:463:GLY:CA	1:B:453:ARG:HD3	2.31	0.58
1:E:222:TRP:CB	6:F:610:NAG:H62	2.33	0.58
2:1:20:VAL:HG13	2:1:120:THR:HG21	1.85	0.58
2:9:163:VAL:HB	2:9:213:HIS:ND1	2.18	0.58
1:J:376:GLN:CB	1:J:439:LEU:HD11	2.33	0.58
3:4:130:LEU:HD21	3:4:135:ALA:HB2	1.85	0.58
1:I:74:PRO:HA	1:I:77:ASP:OD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:7:SER:HB3	2:W:21:SER:OG	2.02	0.58
2:S:108:PHE:HB2	2:S:111:TYR:CE2	2.38	0.58
2:S:99:VAL:HB	2:S:111:TYR:CE2	2.39	0.58
2:M:99:VAL:HB	2:M:111:TYR:CZ	2.39	0.58
2:M:148:THR:HG22	2:M:198:PRO:HA	1.84	0.58
1:B:326:LYS:HB3	1:B:328:THR:CG2	2.31	0.58
2:Q:7:SER:HB3	2:Q:21:SER:OG	2.03	0.58
2:1:22:CYS:HB2	2:1:36:TRP:CH2	2.39	0.58
1:K:357:ASN:ND2	1:K:359:GLU:HB2	2.17	0.58
1:J:406:ILE:HG21	1:L:405:ARG:HD3	1.86	0.58
3:4:93:TYR:HA	3:4:100:SER:HA	1.85	0.58
1:E:120:PHE:CD2	1:E:150:ARG:HD2	2.39	0.58
1:G:388:THR:CG2	1:G:389:ASN:N	2.66	0.58
1:J:425:ALA:O	1:J:429:VAL:HG23	2.03	0.58
3:N:57:PRO:HG2	3:N:60:VAL:HB	1.85	0.58
1:J:177:LEU:HB2	1:J:260:MET:SD	2.42	0.58
1:G:27:LYS:HD3	1:H:383:ARG:NH1	2.18	0.58
2:O:218:THR:HG22	2:O:220:VAL:HG23	1.83	0.58
1:A:179:ILE:O	1:A:254:PRO:HB3	2.04	0.58
3:T:147:GLY:O	3:T:169:PRO:HG3	2.02	0.58
3:V:147:GLY:O	3:V:169:PRO:HG3	2.02	0.58
2:O:34:LEU:HD23	2:O:97:ALA:O	2.03	0.58
1:K:331:LEU:HD22	1:K:331:LEU:N	2.07	0.58
1:G:326:LYS:HB3	1:G:328:THR:CG2	2.33	0.58
1:L:111:LEU:HD12	1:L:112:VAL:N	2.18	0.58
1:L:407:GLN:HG2	1:L:411:LYS:HE3	1.86	0.58
1:H:111:LEU:HD12	1:H:112:VAL:N	2.17	0.58
3:8:7:PRO:HD3	3:8:21:SER:O	2.03	0.58
1:B:74:PRO:HA	1:B:77:ASP:OD2	2.04	0.58
1:D:179:ILE:O	1:D:254:PRO:HB3	2.04	0.58
1:A:386:GLU:HA	1:A:386:GLU:OE2	2.03	0.58
1:A:87:PHE:O	1:A:267:ILE:HG13	2.03	0.58
3:6:57:PRO:HG2	3:6:60:VAL:HB	1.86	0.58
2:9:100:GLU:H	2:9:111:TYR:CB	2.13	0.58
1:E:222:TRP:HB2	6:F:610:NAG:C6	2.33	0.58
1:A:27:LYS:NZ	1:B:383:ARG:HD3	2.19	0.58
1:H:357:ASN:ND2	1:H:359:GLU:HB2	2.19	0.58
1:L:357:ASN:ND2	1:L:359:GLU:HB2	2.18	0.58
3:Z:164:VAL:HG22	3:Z:183:LEU:HD21	1.84	0.58
1:G:357:ASN:ND2	1:G:359:GLU:HB2	2.18	0.58
3:8:147:GLY:O	3:8:169:PRO:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:40:ALA:HB3	2:1:43:GLN:CB	2.34	0.58
1:B:388:THR:CG2	1:B:389:ASN:N	2.66	0.58
1:D:277:CYS:SG	1:D:278:ILE:N	2.77	0.58
2:U:33:GLY:HA3	2:U:99:VAL:CG2	2.26	0.58
2:5:7:SER:O	2:5:120:THR:HG22	2.03	0.58
2:9:7:SER:O	2:9:120:THR:HG22	2.04	0.58
2:5:88:SER:O	2:5:91:THR:HG22	2.04	0.58
1:H:251:LEU:HD12	1:H:252:ILE:H	1.67	0.58
1:K:407:GLN:HG2	1:K:411:LYS:HE3	1.85	0.58
2:Q:40:ALA:HB3	2:Q:43:GLN:CB	2.34	0.58
2:W:87:ARG:HB2	2:W:90:ASP:OD2	2.04	0.58
1:H:277:CYS:SG	1:H:278:ILE:N	2.76	0.58
3:P:23:THR:HG22	3:P:72:SER:HB2	1.86	0.58
3:V:57:PRO:HG2	3:V:60:VAL:HB	1.85	0.58
1:J:388:THR:CG2	1:J:389:ASN:N	2.66	0.58
3:0:128:GLU:O	3:0:131:GLN:HB3	2.04	0.58
3:8:49:LEU:O	3:8:57:PRO:HG3	2.04	0.58
1:D:72:GLY:HA3	1:D:149:SER:OG	2.04	0.58
2:O:108:PHE:HB2	2:O:111:TYR:CE2	2.39	0.58
2:W:111:TYR:C	2:W:111:TYR:CD1	2.77	0.58
1:L:189:GLN:H	1:L:189:GLN:CD	2.07	0.58
3:X:11:SER:CB	3:X:111:LEU:HD11	2.29	0.58
2:U:148:THR:HG22	2:U:198:PRO:HA	1.84	0.58
2:M:6:GLN:HB2	2:M:118:GLN:OE1	2.04	0.58
1:G:316:LEU:HD12	1:G:317:ALA:N	2.18	0.58
3:6:12:GLY:N	3:6:111:LEU:HD13	2.19	0.58
1:C:316:LEU:HD12	1:C:317:ALA:N	2.18	0.58
2:U:112:PRO:CB	3:V:51:SER:HB2	2.34	0.58
1:F:84:TRP:CE2	1:F:116:GLY:HA2	2.38	0.58
1:G:376:GLN:CB	1:G:439:LEU:HD11	2.34	0.58
3:N:113:GLN:CG	3:N:175:ASN:ND2	2.67	0.58
2:O:33:GLY:HA3	2:O:99:VAL:CG2	2.27	0.58
2:O:7:SER:HB3	2:O:21:SER:OG	2.04	0.58
1:E:463:GLY:HA2	1:F:453:ARG:CD	2.33	0.58
2:5:91:THR:HB	2:5:124:VAL:N	2.19	0.58
3:2:164:VAL:HG22	3:2:183:LEU:HD21	1.86	0.58
2:1:11:VAL:HG13	2:1:123:THR:HB	1.86	0.58
1:J:357:ASN:ND2	1:J:359:GLU:HB2	2.19	0.58
3:Z:7:PRO:HD3	3:Z:21:SER:O	2.04	0.58
1:H:293:PRO:HB3	1:H:385:ILE:HD13	1.85	0.58
3:0:139:CYS:HB2	3:0:153:TRP:CZ2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:40:ALA:HB3	2:W:43:GLN:CB	2.33	0.58
2:M:40:ALA:HB3	2:M:43:GLN:CB	2.33	0.58
1:I:293:PRO:HB3	1:I:385:ILE:HD13	1.84	0.58
3:R:49:LEU:O	3:R:57:PRO:HG3	2.04	0.58
2:Q:88:SER:O	2:Q:91:THR:HG22	2.04	0.58
1:B:170:ASN:ND2	1:B:239:PRO:HA	2.19	0.58
3:2:130:LEU:HD21	3:2:135:ALA:HB2	1.86	0.58
2:U:39:GLN:HG2	2:U:45:LEU:HD22	1.85	0.58
1:H:388:THR:CG2	1:H:389:ASN:N	2.66	0.58
1:B:312:ASN:OD1	1:B:313:THR:HG22	2.04	0.58
3:2:57:PRO:HG2	3:2:60:VAL:HB	1.85	0.58
2:U:111:TYR:CD1	2:U:111:TYR:C	2.77	0.58
2:3:37:VAL:HG22	2:3:47:TRP:HA	1.85	0.58
2:M:111:TYR:CE1	2:M:113:MET:HG2	2.36	0.58
2:U:88:SER:O	2:U:91:THR:HG22	2.03	0.58
2:W:88:SER:O	2:W:91:THR:HG22	2.03	0.58
2:3:38:ARG:HD2	2:3:46:GLU:OE1	2.04	0.58
1:D:148:PHE:HB2	1:D:151:LEU:HB2	1.85	0.58
1:D:244:VAL:HG11	1:F:220:ARG:HA	1.86	0.58
1:D:357:ASN:ND2	1:D:359:GLU:HB2	2.19	0.58
1:D:63:ASP:HA	1:D:93:ALA:HA	1.85	0.58
2:O:40:ALA:HB3	2:O:43:GLN:CB	2.34	0.58
3:6:49:LEU:O	3:6:57:PRO:HG3	2.04	0.58
1:I:15:LEU:N	1:I:15:LEU:HD12	2.18	0.58
1:E:96:ASN:HA	1:E:224:ARG:HH11	1.69	0.58
1:I:63:ASP:HA	1:I:93:ALA:HA	1.85	0.58
1:E:369:SER:HB3	1:E:447:LEU:HD13	1.85	0.58
1:D:388:THR:CG2	1:D:389:ASN:N	2.66	0.58
2:S:10:GLU:O	2:S:122:VAL:HA	2.04	0.57
2:O:91:THR:OG1	2:O:123:THR:HA	2.03	0.57
2:7:91:THR:OG1	2:7:123:THR:HA	2.04	0.57
2:Q:39:GLN:HG2	2:Q:45:LEU:HD22	1.86	0.57
1:I:407:GLN:HG2	1:I:411:LYS:HE3	1.86	0.57
3:X:139:CYS:HB2	3:X:153:TRP:HZ2	1.69	0.57
3:V:139:CYS:HB2	3:V:153:TRP:CZ2	2.39	0.57
3:V:7:PRO:HD3	3:V:21:SER:O	2.04	0.57
2:7:40:ALA:HB3	2:7:43:GLN:CB	2.34	0.57
1:I:179:ILE:O	1:I:254:PRO:HB3	2.04	0.57
1:I:386:GLU:HA	1:I:386:GLU:OE2	2.04	0.57
3:P:128:GLU:O	3:P:131:GLN:HB3	2.04	0.57
2:W:111:TYR:HE1	2:W:113:MET:HG2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:99:VAL:HB	2:3:111:TYR:CD2	2.38	0.57
2:O:148:THR:HG22	2:O:198:PRO:HA	1.85	0.57
2:3:94:TYR:HE2	2:3:122:VAL:HG21	1.69	0.57
2:M:88:SER:O	2:M:91:THR:HG22	2.03	0.57
1:F:326:LYS:HD2	1:F:328:THR:H	1.69	0.57
1:B:99:PRO:HB2	1:B:229:ARG:HD3	1.86	0.57
2:U:22:CYS:HB2	2:U:36:TRP:CH2	2.39	0.57
3:P:139:CYS:HB2	3:P:153:TRP:HZ2	1.68	0.57
2:Q:181:ALA:HB2	2:Q:191:LEU:HB3	1.85	0.57
3:2:147:GLY:O	3:2:169:PRO:HG3	2.04	0.57
3:6:29:ILE:HG23	3:6:71:THR:HA	1.86	0.57
2:3:112:PRO:HA	3:4:36:HIS:CD2	2.39	0.57
2:O:105:VAL:O	2:O:106:MET:HB3	2.03	0.57
1:J:312:ASN:OD1	1:J:313:THR:HG22	2.05	0.57
1:H:386:GLU:HA	1:H:386:GLU:OE2	2.04	0.57
2:M:98:ARG:HH11	2:M:98:ARG:HG2	1.69	0.57
1:F:15:LEU:HD12	1:F:15:LEU:N	2.20	0.57
1:I:99:PRO:HB2	1:I:229:ARG:HD3	1.87	0.57
2:5:111:TYR:C	2:5:111:TYR:CD1	2.77	0.57
2:5:38:ARG:HD2	2:5:46:GLU:OE1	2.03	0.57
1:J:463:GLY:CA	1:K:453:ARG:HB3	2.34	0.57
2:7:7:SER:HB3	2:7:21:SER:OG	2.03	0.57
2:S:88:SER:O	2:S:91:THR:HG22	2.03	0.57
3:6:7:PRO:HD3	3:6:21:SER:O	2.04	0.57
3:Z:139:CYS:HB2	3:Z:153:TRP:CZ2	2.39	0.57
3:8:139:CYS:HB2	3:8:153:TRP:CZ2	2.39	0.57
3:P:147:GLY:O	3:P:169:PRO:HG3	2.04	0.57
3:4:29:ILE:HG23	3:4:71:THR:HA	1.86	0.57
1:B:463:GLY:HA2	1:C:453:ARG:HD3	1.86	0.57
3:0:155:ALA:HB1	3:0:193:HIS:CE1	2.39	0.57
1:E:337:GLY:N	1:E:466:CYS:SG	2.78	0.57
1:A:312:ASN:OD1	1:A:313:THR:HG22	2.04	0.57
2:3:168:ASN:HB2	2:3:171:ALA:HB3	1.86	0.57
2:Q:102:VAL:HG12	2:Q:103:ARG:N	2.19	0.57
2:M:100:GLU:H	2:M:111:TYR:CB	2.12	0.57
1:G:380:LYS:HZ3	1:G:384:VAL:HG23	1.69	0.57
3:X:7:PRO:HD3	3:X:21:SER:O	2.04	0.57
2:O:181:ALA:HB2	2:O:191:LEU:HB3	1.84	0.57
1:D:380:LYS:HG2	1:F:29:ILE:O	2.03	0.57
3:8:57:PRO:HG2	3:8:60:VAL:HB	1.85	0.57
1:A:277:CYS:SG	1:A:278:ILE:N	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:277:CYS:SG	1:J:278:ILE:N	2.76	0.57
3:X:191:LYS:N	3:X:191:LYS:HD2	2.18	0.57
2:1:100:GLU:N	2:1:111:TYR:HB2	2.11	0.57
3:4:147:GLY:O	3:4:169:PRO:HG3	2.04	0.57
3:X:164:VAL:HG22	3:X:183:LEU:HD21	1.86	0.57
2:W:181:ALA:HB2	2:W:191:LEU:HB3	1.85	0.57
3:V:139:CYS:HB2	3:V:153:TRP:HZ2	1.68	0.57
2:9:40:ALA:HB3	2:9:43:GLN:CB	2.34	0.57
1:I:73:ASP:OD1	1:I:74:PRO:HD2	2.04	0.57
3:8:130:LEU:HD21	3:8:135:ALA:HB2	1.86	0.57
3:Z:57:PRO:HG2	3:Z:60:VAL:HB	1.85	0.57
3:N:23:THR:HG22	3:N:72:SER:HB2	1.85	0.57
1:F:343:TRP:HB3	1:F:354:ARG:NH2	2.19	0.57
3:0:7:PRO:HD3	3:0:21:SER:O	2.04	0.57
1:E:243:LEU:HD12	1:E:244:VAL:H	1.68	0.57
2:5:40:ALA:HB3	2:5:43:GLN:CB	2.34	0.57
2:3:112:PRO:HB3	3:4:36:HIS:CE1	2.38	0.57
3:X:151:VAL:HG13	3:X:200:VAL:HG12	1.86	0.57
1:H:327:GLN:HG3	1:H:329:ARG:HE	1.70	0.57
3:X:57:PRO:HG2	3:X:60:VAL:HB	1.85	0.57
3:X:147:GLY:O	3:X:169:PRO:HG3	2.04	0.57
2:U:100:GLU:HB3	2:U:110:TYR:CE2	2.40	0.57
2:S:135:PHE:HB3	3:T:126:SER:OG	2.04	0.57
2:1:52:ASN:ND2	2:1:102:VAL:HA	2.19	0.57
2:O:6:GLN:HE22	2:O:95:TYR:HA	1.68	0.57
1:E:227:SER:HB2	6:F:610:NAG:H83	1.87	0.57
2:M:22:CYS:HB2	2:M:36:TRP:CH2	2.40	0.57
3:6:139:CYS:HB2	3:6:153:TRP:CZ2	2.40	0.57
1:L:14:CYS:SG	1:L:335:ILE:HG23	2.45	0.57
3:4:139:CYS:HB2	3:4:153:TRP:HZ2	1.69	0.57
1:E:380:LYS:NZ	1:E:384:VAL:HG23	2.20	0.57
1:D:380:LYS:NZ	1:D:384:VAL:HG23	2.20	0.57
3:N:29:ILE:HG23	3:N:71:THR:HA	1.86	0.57
1:J:37:THR:HG23	1:J:320:MET:O	2.05	0.57
3:0:57:PRO:HG2	3:0:60:VAL:HB	1.86	0.57
1:G:383:ARG:HH21	1:I:430:ALA:HB2	1.69	0.57
2:Y:38:ARG:HD2	2:Y:46:GLU:OE1	2.05	0.57
3:6:128:GLU:O	3:6:131:GLN:HB3	2.04	0.57
1:J:179:ILE:O	1:J:254:PRO:HB3	2.05	0.57
2:M:108:PHE:HB2	2:M:111:TYR:CE2	2.39	0.57
1:J:316:LEU:HD12	1:J:317:ALA:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ILE:HG13	1:B:105:TYR:CE2	2.39	0.57
1:C:403:GLU:HB2	1:C:407:GLN:HB2	1.87	0.57
2:1:6:GLN:HE22	2:1:95:TYR:HA	1.68	0.57
1:H:380:LYS:NZ	1:H:384:VAL:HG23	2.20	0.57
3:2:7:PRO:HD3	3:2:21:SER:O	2.04	0.57
3:V:17:ARG:HH21	3:V:78:THR:HG21	1.70	0.57
1:B:15:LEU:N	1:B:15:LEU:HD12	2.19	0.57
1:F:388:THR:CG2	1:F:389:ASN:N	2.68	0.57
3:4:57:PRO:HG2	3:4:60:VAL:HB	1.85	0.57
1:E:312:ASN:OD1	1:E:313:THR:HG22	2.05	0.57
1:A:388:THR:CG2	1:A:389:ASN:N	2.67	0.57
2:W:38:ARG:HD2	2:W:46:GLU:OE1	2.05	0.57
1:F:277:CYS:SG	1:F:278:ILE:N	2.78	0.57
3:R:113:GLN:HG3	3:R:175:ASN:ND2	2.18	0.57
2:W:99:VAL:HB	2:W:111:TYR:CD2	2.39	0.57
2:1:37:VAL:HG22	2:1:47:TRP:HA	1.87	0.57
2:M:34:LEU:HD23	2:M:97:ALA:O	2.05	0.57
2:5:94:TYR:HE2	2:5:122:VAL:HG21	1.69	0.57
1:F:380:LYS:NZ	1:F:384:VAL:HG23	2.20	0.57
6:H:609:NAG:O3	6:H:610:NAG:H2	2.05	0.57
1:E:222:TRP:CE3	6:F:611:BMA:O2	2.58	0.57
6:F:609:NAG:O3	6:F:610:NAG:H2	2.05	0.57
2:1:7:SER:O	2:1:120:THR:HG22	2.05	0.57
3:4:164:VAL:HG22	3:4:183:LEU:HD21	1.86	0.57
1:K:72:GLY:HA3	1:K:149:SER:OG	2.05	0.57
3:P:155:ALA:HB1	3:P:193:HIS:CE1	2.39	0.57
1:E:386:GLU:OE2	1:E:386:GLU:HA	2.03	0.57
2:9:168:ASN:HB2	2:9:171:ALA:HB3	1.87	0.57
1:E:388:THR:CG2	1:E:389:ASN:N	2.68	0.57
1:H:240:GLY:HA2	2:Y:75:GLY:O	2.05	0.57
2:O:52:ASN:ND2	2:O:102:VAL:HA	2.19	0.57
2:U:99:VAL:HB	2:U:111:TYR:CD2	2.39	0.57
2:9:6:GLN:HE22	2:9:95:TYR:HA	1.70	0.57
1:I:14:CYS:SG	1:I:335:ILE:HG23	2.45	0.57
3:6:20:ILE:CG2	3:6:106:THR:HG21	2.35	0.57
1:B:29:ILE:O	1:C:380:LYS:HG2	2.05	0.57
1:I:380:LYS:HZ3	1:I:384:VAL:HG23	1.69	0.57
1:A:62:ILE:HG13	1:A:63:ASP:N	2.19	0.57
1:F:376:GLN:HB3	1:F:439:LEU:HD11	1.87	0.57
3:6:125:PRO:CG	3:6:135:ALA:HB1	2.35	0.57
3:2:128:GLU:O	3:2:131:GLN:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:151:VAL:HG13	3:4:200:VAL:HG12	1.85	0.57
1:B:386:GLU:HA	1:B:386:GLU:OE2	2.04	0.57
1:G:312:ASN:OD1	1:G:313:THR:HG22	2.05	0.57
1:I:388:THR:CG2	1:I:389:ASN:N	2.67	0.57
1:F:179:ILE:O	1:F:254:PRO:HB3	2.05	0.57
2:1:111:TYR:C	2:1:111:TYR:CD1	2.78	0.56
2:5:99:VAL:HB	2:5:111:TYR:CD2	2.40	0.56
2:W:6:GLN:HE22	2:W:95:TYR:HA	1.69	0.56
2:9:20:VAL:HG13	2:9:120:THR:HG21	1.87	0.56
2:O:112:PRO:HA	3:P:36:HIS:CD2	2.40	0.56
1:B:191:GLN:NE2	1:B:217:ILE:HD11	2.19	0.56
1:K:148:PHE:HB2	1:K:151:LEU:HB2	1.87	0.56
1:K:251:LEU:HD12	1:K:252:ILE:H	1.69	0.56
1:J:29:ILE:HA	1:K:380:LYS:HZ1	1.70	0.56
1:I:251:LEU:HD12	1:I:252:ILE:H	1.69	0.56
3:R:139:CYS:HB2	3:R:153:TRP:HZ2	1.69	0.56
2:3:40:ALA:HB3	2:3:43:GLN:CB	2.34	0.56
3:0:125:PRO:CG	3:0:135:ALA:HB1	2.35	0.56
3:T:125:PRO:CG	3:T:135:ALA:HB1	2.35	0.56
3:8:128:GLU:O	3:8:131:GLN:HB3	2.03	0.56
1:L:63:ASP:HA	1:L:93:ALA:HA	1.86	0.56
2:7:39:GLN:HG2	2:7:45:LEU:HD22	1.86	0.56
3:T:82:ALA:O	3:T:85:GLU:HG2	2.05	0.56
1:C:312:ASN:OD1	1:C:313:THR:HG22	2.05	0.56
3:X:155:ALA:HB1	3:X:193:HIS:CE1	2.40	0.56
1:A:177:LEU:HB2	1:A:260:MET:SD	2.45	0.56
3:8:155:ALA:HB1	3:8:193:HIS:CE1	2.40	0.56
2:O:100:GLU:N	2:O:111:TYR:HB2	2.14	0.56
2:1:108:PHE:HB2	2:1:111:TYR:CE2	2.40	0.56
1:K:189:GLN:CD	1:K:189:GLN:H	2.06	0.56
6:C:609:NAG:O3	6:C:610:NAG:H2	2.05	0.56
1:A:326:LYS:HB3	1:A:328:THR:CG2	2.32	0.56
2:S:6:GLN:HE22	2:S:95:TYR:HA	1.70	0.56
1:D:409:LEU:HD21	1:E:409:LEU:HG	1.86	0.56
2:1:135:PHE:HB3	3:2:126:SER:OG	2.04	0.56
1:D:426:GLU:HG3	1:E:383:ARG:HH22	1.69	0.56
1:B:27:LYS:NZ	1:C:383:ARG:HD3	2.20	0.56
1:F:357:ASN:ND2	1:F:359:GLU:HB2	2.19	0.56
3:0:93:TYR:HA	3:0:100:SER:HA	1.86	0.56
3:Z:93:TYR:HA	3:Z:100:SER:HA	1.88	0.56
2:Y:40:ALA:HB3	2:Y:43:GLN:CB	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:125:PRO:CG	3:N:135:ALA:HB1	2.36	0.56
3:Z:23:THR:HG22	3:Z:72:SER:HB2	1.85	0.56
2:O:168:ASN:HB2	2:O:171:ALA:HB3	1.87	0.56
1:C:459:ALA:HB2	1:C:469:ILE:HA	1.87	0.56
1:L:386:GLU:HA	1:L:386:GLU:OE2	2.05	0.56
2:Y:98:ARG:HH11	2:Y:98:ARG:HG2	1.69	0.56
1:G:120:PHE:O	1:G:121:ILE:HD13	2.05	0.56
2:7:98:ARG:HH11	2:7:98:ARG:HG2	1.69	0.56
2:Q:99:VAL:HB	2:Q:111:TYR:CZ	2.39	0.56
2:1:111:TYR:HE1	2:1:113:MET:HG2	1.70	0.56
2:W:197:VAL:HG21	2:W:207:TYR:CZ	2.41	0.56
2:O:6:GLN:N	2:O:118:GLN:NE2	2.47	0.56
1:F:293:PRO:HB3	1:F:385:ILE:HD13	1.88	0.56
1:C:326:LYS:HZ3	1:C:341:ASN:HD22	1.53	0.56
1:A:347:ILE:HD13	1:A:347:ILE:N	2.20	0.56
1:A:102:VAL:HG11	1:A:108:LEU:HD23	1.87	0.56
1:J:61:GLY:HA2	1:J:79:PHE:CZ	2.39	0.56
1:F:403:GLU:HB2	1:F:407:GLN:HB2	1.87	0.56
3:2:93:TYR:HA	3:2:100:SER:HA	1.87	0.56
3:R:139:CYS:HB2	3:R:153:TRP:CZ2	2.40	0.56
3:T:20:ILE:CG2	3:T:106:THR:HG21	2.35	0.56
1:D:14:CYS:SG	1:D:335:ILE:HG23	2.45	0.56
3:8:20:ILE:CG2	3:8:106:THR:HG21	2.36	0.56
1:C:143:PRO:CD	1:D:155:THR:HB	2.34	0.56
3:P:29:ILE:HG23	3:P:71:THR:HA	1.87	0.56
3:2:29:ILE:HG23	3:2:71:THR:HA	1.88	0.56
3:8:125:PRO:CG	3:8:135:ALA:HB1	2.35	0.56
3:P:196:TYR:O	3:P:210:THR:HG23	2.05	0.56
1:C:120:PHE:CD2	1:C:150:ARG:HD2	2.41	0.56
1:H:337:GLY:N	1:H:466:CYS:SG	2.77	0.56
1:I:60:ASP:OD2	1:I:274:ILE:HD11	2.05	0.56
1:L:459:ALA:HB2	1:L:469:ILE:HA	1.86	0.56
1:H:72:GLY:HA3	1:H:149:SER:OG	2.05	0.56
1:C:96:ASN:HA	1:C:224:ARG:HH11	1.69	0.56
1:A:15:LEU:N	1:A:15:LEU:HD12	2.20	0.56
2:9:111:TYR:CD1	2:9:111:TYR:C	2.78	0.56
4:B:602:NAG:H81	2:O:55:ASP:OD1	2.04	0.56
2:S:37:VAL:HG22	2:S:47:TRP:HA	1.87	0.56
2:M:97:ALA:HB1	2:M:114:ASP:O	2.05	0.56
2:M:99:VAL:HB	2:M:111:TYR:CD2	2.40	0.56
2:W:6:GLN:NE2	2:W:117:GLY:HA3	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:142:LYS:HE2	2:9:144:THR:HG22	1.88	0.56
2:S:197:VAL:HG21	2:S:207:TYR:CZ	2.41	0.56
2:5:10:GLU:O	2:5:122:VAL:HA	2.04	0.56
2:5:7:SER:HB3	2:5:21:SER:OG	2.05	0.56
2:9:7:SER:HB3	2:9:21:SER:OG	2.05	0.56
6:J:609:NAG:O3	6:J:610:NAG:H2	2.06	0.56
2:M:6:GLN:HE22	2:M:95:TYR:HA	1.70	0.56
2:M:11:VAL:HG22	2:M:123:THR:OG1	2.05	0.56
1:C:63:ASP:HA	1:C:93:ALA:HA	1.87	0.56
1:B:357:ASN:ND2	1:B:359:GLU:HB2	2.19	0.56
1:G:14:CYS:SG	1:G:335:ILE:HG23	2.46	0.56
1:J:383:ARG:CZ	1:L:27:LYS:HD3	2.35	0.56
1:D:17:HIS:HB2	1:D:320:MET:HE1	1.88	0.56
3:2:139:CYS:HB2	3:2:153:TRP:CZ2	2.40	0.56
1:K:234:TRP:HE3	1:K:234:TRP:H	1.51	0.56
1:K:179:ILE:O	1:K:254:PRO:HB3	2.05	0.56
1:K:430:ALA:HB2	1:L:383:ARG:HH21	1.71	0.56
2:1:34:LEU:HD23	2:1:97:ALA:O	2.06	0.56
2:5:2:VAL:CG2	2:5:115:VAL:HG21	2.36	0.56
1:E:326:LYS:HZ3	1:E:341:ASN:HD22	1.53	0.56
1:B:293:PRO:HB3	1:B:385:ILE:HD13	1.86	0.56
3:X:139:CYS:HB2	3:X:153:TRP:CZ2	2.41	0.56
1:E:61:GLY:O	1:E:64:CYS:HB2	2.06	0.56
2:U:182:VAL:CG1	3:V:182:TYR:HD2	2.18	0.56
1:D:293:PRO:HB3	1:D:385:ILE:HD13	1.87	0.56
1:G:277:CYS:SG	1:G:278:ILE:N	2.78	0.56
3:0:29:ILE:HG23	3:0:71:THR:HA	1.87	0.56
2:Q:93:VAL:HG22	2:Q:121:MET:HG2	1.88	0.56
1:B:277:CYS:SG	1:B:278:ILE:N	2.78	0.56
1:C:277:CYS:SG	1:C:278:ILE:N	2.79	0.56
1:A:120:PHE:CD2	1:A:150:ARG:HD2	2.40	0.56
3:R:155:ALA:HB1	3:R:193:HIS:CE1	2.40	0.56
3:N:128:GLU:O	3:N:131:GLN:HB3	2.06	0.56
1:C:376:GLN:CB	1:C:439:LEU:HD11	2.35	0.56
2:9:108:PHE:HB2	2:9:111:TYR:HE2	1.70	0.56
2:M:111:TYR:CD1	2:M:111:TYR:C	2.78	0.56
2:Y:197:VAL:HG21	2:Y:207:TYR:CZ	2.41	0.56
1:J:403:GLU:HB2	1:J:407:GLN:HB2	1.87	0.56
1:L:384:VAL:HG12	1:L:385:ILE:HG23	1.88	0.56
3:T:29:ILE:HG23	3:T:71:THR:HA	1.87	0.56
3:2:125:PRO:CG	3:2:135:ALA:HB1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:49:LEU:O	3:2:57:PRO:HG3	2.06	0.56
3:P:50:ILE:HD13	3:P:75:LEU:HD13	1.88	0.56
3:V:151:VAL:HG13	3:V:200:VAL:HG12	1.86	0.56
1:F:96:ASN:HA	1:F:224:ARG:HH11	1.70	0.56
1:D:404:GLY:HA3	1:E:107:SER:HB2	1.85	0.56
2:Y:37:VAL:HG22	2:Y:47:TRP:HA	1.86	0.56
2:S:40:ALA:HB3	2:S:43:GLN:CB	2.34	0.56
2:5:6:GLN:HE22	2:5:95:TYR:HA	1.70	0.56
2:O:17:SER:CB	2:O:84:LYS:HA	2.35	0.56
1:J:430:ALA:HB2	1:K:383:ARG:HH21	1.69	0.56
1:H:148:PHE:HB2	1:H:151:LEU:HB2	1.87	0.56
2:1:6:GLN:HE21	2:1:117:GLY:HA3	1.70	0.56
1:D:316:LEU:HD12	1:D:317:ALA:N	2.21	0.56
3:T:11:SER:HB3	3:T:111:LEU:HD12	1.88	0.56
1:B:87:PHE:O	1:B:267:ILE:HG13	2.05	0.56
1:F:60:ASP:OD2	1:F:274:ILE:HD11	2.06	0.56
1:G:386:GLU:HA	1:G:386:GLU:OE2	2.06	0.56
2:S:98:ARG:HH11	2:S:98:ARG:HG2	1.70	0.56
2:W:168:ASN:HB2	2:W:171:ALA:HB3	1.88	0.56
1:L:277:CYS:SG	1:L:278:ILE:N	2.79	0.56
1:K:388:THR:CG2	1:K:389:ASN:N	2.68	0.56
3:6:155:ALA:HB1	3:6:193:HIS:CE1	2.40	0.56
2:M:50:TRP:HE1	2:M:99:VAL:HG21	1.71	0.56
2:W:84:LYS:NZ	2:9:142:LYS:CE	2.69	0.56
1:D:189:GLN:CD	1:D:189:GLN:H	2.07	0.56
2:U:38:ARG:HD2	2:U:46:GLU:OE1	2.05	0.56
6:I:609:NAG:O3	6:I:610:NAG:H2	2.06	0.56
2:Q:6:GLN:HB2	2:Q:118:GLN:OE1	2.05	0.56
1:A:326:LYS:HZ3	1:A:341:ASN:HD22	1.53	0.56
2:O:11:VAL:HG13	2:O:123:THR:HB	1.87	0.56
2:7:11:VAL:HG22	2:7:123:THR:OG1	2.06	0.56
2:U:4:LEU:HD11	2:U:115:VAL:O	2.05	0.56
2:S:91:THR:CB	2:S:124:VAL:H	2.18	0.56
1:H:403:GLU:HB2	1:H:407:GLN:HB2	1.88	0.56
1:D:213:ILE:HG13	1:D:233:TYR:CE2	2.41	0.56
2:1:38:ARG:HD2	2:1:46:GLU:OE1	2.05	0.56
1:G:108:LEU:O	1:G:112:VAL:HG23	2.06	0.56
1:I:403:GLU:HB2	1:I:407:GLN:HB2	1.87	0.56
3:P:139:CYS:HB2	3:P:153:TRP:CZ2	2.40	0.56
3:8:164:VAL:HG22	3:8:183:LEU:HD21	1.88	0.56
3:X:49:LEU:O	3:X:57:PRO:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:30:THR:HG22	2:M:74:THR:HG22	1.88	0.56
4:G:601:NAG:HB1	4:G:602:NAG:O7	2.06	0.56
2:7:197:VAL:HG21	2:7:207:TYR:CZ	2.41	0.56
2:5:6:GLN:HB3	2:5:120:THR:CG2	2.35	0.56
1:I:326:LYS:HB3	1:I:328:THR:CG2	2.31	0.56
1:I:191:GLN:NE2	1:I:217:ILE:HD11	2.20	0.56
1:A:161:TYR:HB2	1:A:196:VAL:CG2	2.36	0.56
1:A:357:ASN:ND2	1:A:359:GLU:HB2	2.20	0.56
1:A:383:ARG:HH22	1:C:426:GLU:HG3	1.70	0.56
1:E:335:ILE:HG23	1:E:335:ILE:O	2.06	0.56
3:T:139:CYS:HB2	3:T:153:TRP:CZ2	2.41	0.56
1:G:384:VAL:HG12	1:G:385:ILE:HG23	1.88	0.56
1:A:343:TRP:HB3	1:A:354:ARG:NH2	2.21	0.56
1:A:208:ARG:CZ	1:A:238:LYS:HD2	2.36	0.56
2:1:133:SER:O	2:1:155:VAL:HA	2.06	0.56
3:X:125:PRO:CG	3:X:135:ALA:HB1	2.35	0.56
2:7:168:ASN:HB2	2:7:171:ALA:HB3	1.88	0.56
1:I:277:CYS:SG	1:I:278:ILE:N	2.78	0.56
1:K:386:GLU:HA	1:K:386:GLU:OE2	2.05	0.56
2:Y:168:ASN:HB2	2:Y:171:ALA:HB3	1.88	0.56
1:I:312:ASN:OD1	1:I:313:THR:HG22	2.05	0.56
2:Y:108:PHE:HB2	2:Y:111:TYR:CE2	2.41	0.56
2:3:34:LEU:HD23	2:3:97:ALA:O	2.06	0.56
2:U:197:VAL:HG21	2:U:207:TYR:CZ	2.41	0.56
1:D:383:ARG:HH22	1:F:426:GLU:HG3	1.70	0.56
1:I:148:PHE:HB2	1:I:151:LEU:HB2	1.88	0.56
1:K:335:ILE:HG23	1:K:335:ILE:O	2.06	0.56
1:K:426:GLU:HG3	1:L:383:ARG:NH2	2.21	0.56
3:Z:155:ALA:HB1	3:Z:193:HIS:CE1	2.41	0.56
3:Z:128:GLU:O	3:Z:131:GLN:HB3	2.06	0.56
3:6:23:THR:HG22	3:6:72:SER:HB2	1.88	0.56
3:T:155:ALA:HB1	3:T:193:HIS:CE1	2.41	0.56
3:V:128:GLU:O	3:V:131:GLN:HB3	2.05	0.56
2:U:179:PHE:HB3	3:V:180:SER:OG	2.05	0.55
2:O:98:ARG:HH11	2:O:98:ARG:HG2	1.71	0.55
2:W:99:VAL:HB	2:W:111:TYR:CE2	2.40	0.55
2:S:99:VAL:HB	2:S:111:TYR:CD2	2.41	0.55
2:5:102:VAL:HG12	2:5:103:ARG:N	2.22	0.55
2:9:197:VAL:HG21	2:9:207:TYR:CZ	2.42	0.55
2:1:17:SER:CB	2:1:84:LYS:HA	2.36	0.55
2:9:94:TYR:HE2	2:9:122:VAL:HG21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:609:NAG:O3	6:E:610:NAG:H2	2.05	0.55
1:F:326:LYS:NZ	1:F:341:ASN:HD22	2.04	0.55
1:B:148:PHE:HB2	1:B:151:LEU:HB2	1.88	0.55
1:I:111:LEU:HD12	1:I:112:VAL:N	2.21	0.55
1:H:407:GLN:HG2	1:H:411:LYS:HE3	1.86	0.55
3:P:93:TYR:HA	3:P:100:SER:HA	1.88	0.55
3:T:139:CYS:HB2	3:T:153:TRP:HZ2	1.71	0.55
1:L:403:GLU:HB2	1:L:407:GLN:HB2	1.88	0.55
3:N:20:ILE:CG2	3:N:106:THR:HG21	2.36	0.55
2:Y:133:SER:O	2:Y:155:VAL:HA	2.06	0.55
1:G:278:ILE:HD13	3:P:204:GLY:HA2	1.87	0.55
1:J:210:GLN:HE21	1:L:220:ARG:NE	2.03	0.55
3:8:29:ILE:HG23	3:8:71:THR:HA	1.88	0.55
3:4:125:PRO:CG	3:4:135:ALA:HB1	2.36	0.55
1:K:277:CYS:SG	1:K:278:ILE:N	2.78	0.55
1:G:453:ARG:HD3	1:I:463:GLY:HA2	1.87	0.55
3:T:172:GLN:HB2	3:T:176:LYS:O	2.07	0.55
3:R:172:GLN:HB2	3:R:176:LYS:O	2.06	0.55
2:Q:99:VAL:HB	2:Q:111:TYR:CD2	2.42	0.55
2:1:50:TRP:HE1	2:1:99:VAL:HG21	1.70	0.55
2:S:102:VAL:HG12	2:S:103:ARG:N	2.22	0.55
2:5:37:VAL:HG22	2:5:47:TRP:HA	1.87	0.55
1:G:148:PHE:HB2	1:G:151:LEU:HB2	1.87	0.55
1:H:316:LEU:HD12	1:H:317:ALA:N	2.21	0.55
3:2:161:LYS:HA	3:2:164:VAL:CG2	2.36	0.55
1:K:61:GLY:HA2	1:K:79:PHE:CZ	2.41	0.55
3:Z:20:ILE:CG2	3:Z:106:THR:HG21	2.37	0.55
1:A:251:LEU:HD12	1:A:252:ILE:H	1.71	0.55
3:V:164:VAL:HG22	3:V:183:LEU:HD21	1.87	0.55
3:X:26:SER:HA	3:X:29:ILE:HB	1.89	0.55
3:R:125:PRO:CG	3:R:135:ALA:HB1	2.36	0.55
2:3:98:ARG:HG2	2:3:98:ARG:HH11	1.71	0.55
3:R:151:VAL:HG13	3:R:200:VAL:HG12	1.88	0.55
1:A:234:TRP:H	1:A:234:TRP:HE3	1.54	0.55
1:H:312:ASN:OD1	1:H:313:THR:HG22	2.05	0.55
3:6:82:ALA:O	3:6:85:GLU:HG2	2.06	0.55
1:D:15:LEU:HD12	1:D:15:LEU:N	2.22	0.55
3:N:155:ALA:HB1	3:N:193:HIS:CE1	2.41	0.55
2:O:99:VAL:HB	2:O:111:TYR:CD2	2.42	0.55
2:3:50:TRP:HE1	2:3:99:VAL:HG21	1.71	0.55
2:Y:17:SER:CB	2:Y:84:LYS:HA	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:609:NAG:O3	6:B:610:NAG:H2	2.06	0.55
1:L:191:GLN:NE2	1:L:217:ILE:HD11	2.21	0.55
2:U:6:GLN:HE22	2:U:95:TYR:HA	1.71	0.55
1:J:293:PRO:HB3	1:J:385:ILE:HD13	1.88	0.55
3:P:20:ILE:CG2	3:P:106:THR:HG21	2.36	0.55
3:O:147:GLY:O	3:O:169:PRO:HG3	2.06	0.55
2:3:133:SER:O	2:3:155:VAL:HA	2.06	0.55
3:X:29:ILE:HG23	3:X:71:THR:HA	1.87	0.55
3:V:125:PRO:CG	3:V:135:ALA:HB1	2.36	0.55
2:7:30:THR:HG22	2:7:74:THR:HG22	1.88	0.55
1:K:96:ASN:HA	1:K:224:ARG:HH11	1.71	0.55
1:B:459:ALA:HB2	1:B:469:ILE:HA	1.89	0.55
1:G:84:TRP:CE2	1:G:116:GLY:HA2	2.42	0.55
2:Q:168:ASN:HB2	2:Q:171:ALA:HB3	1.88	0.55
2:9:37:VAL:HG22	2:9:47:TRP:HA	1.87	0.55
3:N:113:GLN:HG3	3:N:175:ASN:HD21	1.69	0.55
3:N:172:GLN:HB2	3:N:176:LYS:O	2.07	0.55
3:V:172:GLN:HB2	3:V:176:LYS:O	2.07	0.55
2:Q:37:VAL:HG22	2:Q:47:TRP:HA	1.89	0.55
2:1:99:VAL:HB	2:1:111:TYR:CZ	2.40	0.55
2:S:38:ARG:HD2	2:S:46:GLU:OE1	2.05	0.55
2:S:6:GLN:HB3	2:S:120:THR:HG23	1.88	0.55
2:Q:4:LEU:HD11	2:Q:115:VAL:O	2.06	0.55
1:J:384:VAL:CG1	1:J:385:ILE:N	2.70	0.55
1:I:316:LEU:HD12	1:I:317:ALA:N	2.21	0.55
2:U:133:SER:O	2:U:155:VAL:HA	2.07	0.55
1:I:357:ASN:ND2	1:I:359:GLU:HB2	2.19	0.55
2:S:133:SER:O	2:S:155:VAL:HA	2.07	0.55
1:C:99:PRO:HB2	1:C:229:ARG:HD3	1.88	0.55
1:J:99:PRO:HB2	1:J:229:ARG:HD3	1.89	0.55
3:Z:82:ALA:O	3:Z:85:GLU:HG2	2.07	0.55
1:E:277:CYS:SG	1:E:278:ILE:N	2.79	0.55
2:5:154:LEU:HD23	3:6:129:GLU:OE2	2.06	0.55
2:9:34:LEU:HD23	2:9:97:ALA:O	2.06	0.55
2:7:179:PHE:HE2	3:8:142:SER:HB3	1.72	0.55
3:X:172:GLN:HB2	3:X:176:LYS:O	2.06	0.55
2:7:99:VAL:HB	2:7:111:TYR:CD2	2.42	0.55
2:Q:100:GLU:N	2:Q:111:TYR:HB2	2.14	0.55
2:Y:102:VAL:HG12	2:Y:103:ARG:N	2.22	0.55
1:K:331:LEU:H	1:K:331:LEU:CD2	2.00	0.55
2:5:50:TRP:HE1	2:5:99:VAL:HG21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:197:VAL:HG21	2:5:207:TYR:CZ	2.41	0.55
2:5:17:SER:CB	2:5:84:LYS:HA	2.37	0.55
3:V:93:TYR:HA	3:V:100:SER:HA	1.88	0.55
1:B:216:ASN:HB3	1:C:212:THR:HG21	1.87	0.55
1:J:251:LEU:HD12	1:J:252:ILE:H	1.72	0.55
2:U:112:PRO:HB3	3:V:36:HIS:CE1	2.41	0.55
1:I:376:GLN:HB3	1:I:439:LEU:HD11	1.89	0.55
3:4:49:LEU:O	3:4:57:PRO:HG3	2.07	0.55
1:C:15:LEU:HD12	1:C:15:LEU:N	2.20	0.55
3:T:128:GLU:O	3:T:131:GLN:HB3	2.07	0.55
1:H:309:VAL:HB	1:H:311:GLN:OE1	2.06	0.55
4:B:601:NAG:H61	4:B:602:NAG:O7	2.07	0.55
3:X:169:PRO:HA	3:X:179:ALA:HB2	1.89	0.55
2:Y:33:GLY:HA3	2:Y:99:VAL:CG2	2.25	0.55
2:3:102:VAL:HG12	2:3:103:ARG:N	2.22	0.55
1:B:227:SER:CB	6:C:610:NAG:H83	2.37	0.55
1:A:463:GLY:HA3	1:B:453:ARG:HB3	1.89	0.55
2:S:2:VAL:CG2	2:S:115:VAL:HG21	2.37	0.55
1:D:309:VAL:HB	1:D:311:GLN:OE1	2.06	0.55
1:B:99:PRO:HB2	1:B:229:ARG:CD	2.37	0.55
2:1:92:ALA:H	2:1:122:VAL:HG22	1.71	0.55
1:C:293:PRO:HB3	1:C:385:ILE:HD13	1.88	0.55
1:A:403:GLU:HB2	1:A:407:GLN:HB2	1.88	0.55
2:W:133:SER:O	2:W:155:VAL:HA	2.07	0.55
3:4:20:ILE:CG2	3:4:106:THR:HG21	2.37	0.55
3:0:164:VAL:HG22	3:0:183:LEU:HD21	1.87	0.55
3:R:29:ILE:HG23	3:R:71:THR:HA	1.87	0.55
2:S:44:GLY:HA2	3:T:89:TYR:OH	2.07	0.55
1:K:120:PHE:O	1:K:121:ILE:HD13	2.07	0.55
1:I:96:ASN:HA	1:I:224:ARG:HH11	1.71	0.55
2:M:37:VAL:HG22	2:M:47:TRP:HA	1.88	0.55
1:H:331:LEU:CD2	1:H:331:LEU:H	1.99	0.55
1:B:326:LYS:HZ3	1:B:341:ASN:HD22	1.55	0.55
1:B:220:ARG:HA	1:C:244:VAL:HG11	1.87	0.55
1:I:61:GLY:HA2	1:I:79:PHE:CZ	2.42	0.55
3:N:139:CYS:HB2	3:N:153:TRP:CZ2	2.41	0.55
3:N:139:CYS:HB2	3:N:153:TRP:HZ2	1.71	0.55
3:4:139:CYS:HB2	3:4:153:TRP:CZ2	2.40	0.55
1:H:384:VAL:CG1	1:H:385:ILE:N	2.70	0.55
1:J:14:CYS:SG	1:J:335:ILE:HG23	2.46	0.55
1:L:384:VAL:HG13	1:L:428:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:26:SER:HA	3:N:29:ILE:HB	1.89	0.55
1:L:376:GLN:HB3	1:L:439:LEU:HD11	1.88	0.55
1:G:376:GLN:HB3	1:G:439:LEU:HD11	1.88	0.55
1:F:295:GLN:NE2	1:F:308:TYR:HB2	2.22	0.55
1:I:459:ALA:HB2	1:I:469:ILE:HA	1.88	0.55
1:G:15:LEU:N	1:G:15:LEU:HD12	2.22	0.55
2:1:52:ASN:CG	2:1:55:ASP:HB3	2.27	0.55
2:M:197:VAL:HG21	2:M:207:TYR:CZ	2.42	0.55
1:F:335:ILE:O	1:F:335:ILE:HG23	2.07	0.55
2:Q:112:PRO:HB3	3:R:51:SER:HB2	1.89	0.55
1:G:335:ILE:HG23	1:G:335:ILE:O	2.06	0.55
3:0:161:LYS:HA	3:0:164:VAL:CG2	2.36	0.55
1:B:407:GLN:HG2	1:B:411:LYS:HE3	1.89	0.55
1:D:384:VAL:CG1	1:D:385:ILE:N	2.70	0.55
3:2:125:PRO:HG2	3:2:135:ALA:HB1	1.89	0.55
1:D:84:TRP:CE2	1:D:116:GLY:HA2	2.42	0.55
1:C:87:PHE:O	1:C:267:ILE:HG13	2.07	0.55
3:2:155:ALA:HB1	3:2:193:HIS:CE1	2.42	0.55
1:L:312:ASN:OD1	1:L:313:THR:HG22	2.07	0.55
1:D:459:ALA:HB2	1:D:469:ILE:HA	1.86	0.55
1:D:386:GLU:HA	1:D:386:GLU:OE2	2.04	0.55
2:W:112:PRO:HB3	3:X:36:HIS:CE1	2.42	0.55
2:M:177:HIS:NE2	3:N:172:GLN:CD	2.61	0.55
2:W:50:TRP:HE1	2:W:99:VAL:HG21	1.71	0.55
2:Y:35:SER:HB2	2:Y:47:TRP:HE1	1.72	0.55
2:5:99:VAL:HB	2:5:111:TYR:CE2	2.41	0.55
2:5:34:LEU:HD23	2:5:97:ALA:O	2.07	0.55
6:L:609:NAG:O3	6:L:610:NAG:H2	2.07	0.55
6:D:609:NAG:O3	6:D:610:NAG:H2	2.06	0.55
3:N:93:TYR:HA	3:N:100:SER:HA	1.88	0.55
1:F:347:ILE:N	1:F:347:ILE:HD13	2.22	0.55
1:A:61:GLY:O	1:A:64:CYS:HB2	2.07	0.55
2:M:174:SER:HB3	2:7:204:THR:CG2	2.36	0.55
1:A:383:ARG:NH1	1:C:27:LYS:HD3	2.21	0.55
1:H:347:ILE:N	1:H:347:ILE:HD13	2.22	0.55
1:C:14:CYS:SG	1:C:335:ILE:HG23	2.47	0.55
1:E:357:ASN:ND2	1:E:359:GLU:HB2	2.21	0.55
3:R:169:PRO:HA	3:R:179:ALA:HB2	1.89	0.55
3:R:147:GLY:O	3:R:169:PRO:HG3	2.07	0.55
1:J:383:ARG:HH22	1:L:426:GLU:HG3	1.72	0.55
1:E:376:GLN:HB3	1:E:439:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:29:ILE:HG23	3:V:71:THR:HA	1.89	0.55
3:V:155:ALA:HB1	3:V:193:HIS:CE1	2.41	0.55
3:R:82:ALA:O	3:R:85:GLU:HG2	2.06	0.55
1:A:96:ASN:HA	1:A:224:ARG:HH11	1.71	0.55
1:E:15:LEU:N	1:E:15:LEU:HD12	2.22	0.55
1:L:15:LEU:N	1:L:15:LEU:HD12	2.21	0.55
1:J:84:TRP:CE2	1:J:116:GLY:HA2	2.41	0.55
3:8:151:VAL:HG13	3:8:200:VAL:HG12	1.87	0.55
3:P:82:ALA:O	3:P:85:GLU:HG2	2.07	0.55
1:D:120:PHE:CD2	1:D:150:ARG:HD2	2.41	0.55
4:D:602:NAG:H81	2:S:55:ASP:OD1	2.07	0.55
1:B:251:LEU:HD12	1:B:252:ILE:H	1.71	0.55
1:K:111:LEU:HD12	1:K:112:VAL:N	2.21	0.55
1:I:347:ILE:HD13	1:I:347:ILE:N	2.21	0.55
3:X:20:ILE:CG2	3:X:106:THR:HG21	2.37	0.55
1:A:384:VAL:CG1	1:A:385:ILE:N	2.70	0.55
3:V:125:PRO:HG2	3:V:135:ALA:HB1	1.89	0.55
1:H:431:LEU:O	1:H:435:HIS:HB2	2.07	0.55
1:A:431:LEU:O	1:A:435:HIS:HB2	2.07	0.55
2:U:179:PHE:CG	3:V:140:LEU:HD22	2.43	0.54
2:O:52:ASN:CG	2:O:55:ASP:HB3	2.27	0.54
2:1:102:VAL:HG12	2:1:103:ARG:N	2.21	0.54
1:D:243:LEU:HD12	1:D:244:VAL:H	1.71	0.54
1:L:161:TYR:HB2	1:L:196:VAL:CG2	2.37	0.54
1:K:384:VAL:HG12	1:K:385:ILE:HG23	1.89	0.54
1:H:335:ILE:HG23	1:H:335:ILE:O	2.07	0.54
3:P:161:LYS:HA	3:P:164:VAL:CG2	2.37	0.54
1:C:380:LYS:NZ	1:C:384:VAL:HG23	2.21	0.54
1:D:74:PRO:HA	1:D:77:ASP:OD2	2.07	0.54
2:M:210:ASN:HA	2:M:221:ASP:OD1	2.07	0.54
3:P:125:PRO:CG	3:P:135:ALA:HB1	2.36	0.54
3:Z:125:PRO:CG	3:Z:135:ALA:HB1	2.36	0.54
3:Z:26:SER:HA	3:Z:29:ILE:HB	1.89	0.54
1:D:272:ALA:HA	2:S:105:VAL:HG22	1.89	0.54
1:D:312:ASN:OD1	1:D:313:THR:HG22	2.06	0.54
3:4:23:THR:HG22	3:4:72:SER:HB2	1.88	0.54
2:1:168:ASN:HB2	2:1:171:ALA:HB3	1.90	0.54
1:L:170:ASN:ND2	1:L:239:PRO:HA	2.22	0.54
2:5:168:ASN:HB2	2:5:171:ALA:HB3	1.89	0.54
2:U:37:VAL:HG22	2:U:47:TRP:HA	1.89	0.54
2:7:99:VAL:HB	2:7:111:TYR:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:197:VAL:HG21	2:1:207:TYR:CZ	2.42	0.54
2:U:94:TYR:HE2	2:U:122:VAL:HG21	1.71	0.54
2:Y:92:ALA:H	2:Y:122:VAL:HG22	1.71	0.54
1:G:161:TYR:HB2	1:G:196:VAL:CG2	2.38	0.54
2:5:91:THR:CB	2:5:124:VAL:H	2.19	0.54
3:X:93:TYR:HA	3:X:100:SER:HA	1.89	0.54
1:D:335:ILE:HG23	1:D:335:ILE:O	2.06	0.54
2:7:133:SER:O	2:7:155:VAL:HA	2.07	0.54
1:B:14:CYS:SG	1:B:335:ILE:HG23	2.46	0.54
1:B:335:ILE:O	1:B:335:ILE:HG23	2.06	0.54
1:E:407:GLN:HG2	1:E:411:LYS:HE3	1.90	0.54
1:K:316:LEU:HD12	1:K:317:ALA:N	2.22	0.54
1:G:74:PRO:HA	1:G:77:ASP:OD2	2.06	0.54
3:V:49:LEU:O	3:V:57:PRO:HG3	2.07	0.54
2:Q:38:ARG:HD2	2:Q:46:GLU:OE1	2.07	0.54
3:Z:151:VAL:HG13	3:Z:200:VAL:HG12	1.88	0.54
1:H:80:GLN:HB3	1:H:150:ARG:NH2	2.22	0.54
1:J:87:PHE:O	1:J:267:ILE:HG13	2.07	0.54
2:9:100:GLU:HG2	2:9:110:TYR:HH	1.73	0.54
2:9:111:TYR:CE1	2:9:113:MET:HG2	2.40	0.54
3:6:172:GLN:HB2	3:6:176:LYS:O	2.07	0.54
2:3:197:VAL:HG21	2:3:207:TYR:CZ	2.41	0.54
2:W:17:SER:CB	2:W:84:LYS:HA	2.38	0.54
1:A:321:ARG:HD2	1:A:437:ILE:HG23	1.90	0.54
2:Q:60:TYR:CE1	2:Q:70:MET:HG2	2.39	0.54
1:L:326:LYS:HZ3	1:L:341:ASN:HD22	1.55	0.54
1:K:99:PRO:HB2	1:K:229:ARG:CD	2.37	0.54
1:D:111:LEU:HD12	1:D:112:VAL:N	2.22	0.54
1:C:335:ILE:O	1:C:335:ILE:HG23	2.06	0.54
1:C:74:PRO:HA	1:C:77:ASP:OD2	2.07	0.54
1:J:74:PRO:HA	1:J:77:ASP:OD2	2.07	0.54
1:G:426:GLU:HG3	1:H:383:ARG:NH2	2.22	0.54
1:D:278:ILE:HD13	3:0:204:GLY:CA	2.37	0.54
3:0:49:LEU:O	3:0:57:PRO:HG3	2.07	0.54
1:C:431:LEU:O	1:C:435:HIS:HB2	2.07	0.54
3:X:82:ALA:O	3:X:85:GLU:HG2	2.08	0.54
3:0:196:TYR:O	3:0:210:THR:HG23	2.08	0.54
1:B:134:GLY:HA3	1:B:153:TRP:HB3	1.88	0.54
3:0:113:GLN:HG3	3:0:175:ASN:ND2	2.22	0.54
2:U:11:VAL:HG22	2:U:123:THR:OG1	2.08	0.54
2:5:108:PHE:CB	2:5:111:TYR:HE2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:6:GLN:HE22	2:3:95:TYR:HA	1.71	0.54
2:O:197:VAL:HG21	2:O:207:TYR:CZ	2.42	0.54
2:Q:197:VAL:HG21	2:Q:207:TYR:CZ	2.42	0.54
1:H:401:GLU:HG3	1:I:238:LYS:HE2	1.89	0.54
3:R:20:ILE:CG2	3:R:106:THR:HG21	2.38	0.54
3:N:164:VAL:HG22	3:N:183:LEU:HD21	1.88	0.54
3:Z:137:LEU:HB3	3:Z:153:TRP:CH2	2.43	0.54
1:E:384:VAL:CG1	1:E:385:ILE:N	2.69	0.54
3:8:161:LYS:HA	3:8:164:VAL:CG2	2.37	0.54
1:E:403:GLU:HB2	1:E:407:GLN:HB2	1.88	0.54
1:I:384:VAL:CG1	1:I:385:ILE:N	2.70	0.54
3:Z:125:PRO:HG2	3:Z:135:ALA:HB1	1.90	0.54
3:Z:49:LEU:O	3:Z:57:PRO:HG3	2.07	0.54
1:K:27:LYS:HD3	1:L:383:ARG:NH1	2.22	0.54
1:J:96:ASN:HA	1:J:224:ARG:HH11	1.73	0.54
2:U:168:ASN:HB2	2:U:171:ALA:HB3	1.89	0.54
1:E:431:LEU:O	1:E:435:HIS:HB2	2.08	0.54
1:B:96:ASN:HA	1:B:224:ARG:HH11	1.72	0.54
1:E:87:PHE:O	1:E:267:ILE:HG13	2.08	0.54
2:O:102:VAL:HG12	2:O:103:ARG:N	2.22	0.54
2:U:34:LEU:HD23	2:U:97:ALA:O	2.08	0.54
2:9:38:ARG:HD2	2:9:46:GLU:OE1	2.07	0.54
2:9:17:SER:CB	2:9:84:LYS:HA	2.36	0.54
6:K:609:NAG:O3	6:K:610:NAG:H2	2.07	0.54
3:6:93:TYR:HA	3:6:100:SER:HA	1.89	0.54
1:G:251:LEU:HD12	1:G:252:ILE:H	1.72	0.54
1:C:61:GLY:O	1:C:64:CYS:HB2	2.07	0.54
1:F:148:PHE:CB	1:F:151:LEU:HB2	2.37	0.54
1:H:343:TRP:HB3	1:H:354:ARG:NH2	2.21	0.54
3:4:161:LYS:HA	3:4:164:VAL:CG2	2.37	0.54
3:X:161:LYS:HA	3:X:164:VAL:CG2	2.37	0.54
2:9:133:SER:O	2:9:155:VAL:HA	2.08	0.54
1:J:335:ILE:HG23	1:J:335:ILE:O	2.07	0.54
1:L:431:LEU:O	1:L:435:HIS:HB2	2.08	0.54
3:4:155:ALA:HB1	3:4:193:HIS:CE1	2.41	0.54
1:I:84:TRP:CE2	1:I:116:GLY:HA2	2.43	0.54
1:E:459:ALA:HB2	1:E:469:ILE:HA	1.89	0.54
1:H:220:ARG:HB2	1:H:221:PRO:HD2	1.89	0.54
2:S:168:ASN:HB2	2:S:171:ALA:HB3	1.88	0.54
2:O:179:PHE:CE2	3:P:142:SER:HB3	2.42	0.54
2:O:111:TYR:CD1	2:O:111:TYR:C	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:33:GLY:HA3	2:M:99:VAL:CG2	2.28	0.54
3:4:126:SER:OG	3:4:129:GLU:HB2	2.08	0.54
6:G:609:NAG:O3	6:G:610:NAG:H2	2.07	0.54
2:M:91:THR:CB	2:M:124:VAL:H	2.18	0.54
1:L:148:PHE:HB2	1:L:151:LEU:HB2	1.88	0.54
2:1:6:GLN:HB3	2:1:120:THR:CG2	2.38	0.54
1:L:17:HIS:HB2	1:L:320:MET:HE1	1.90	0.54
3:T:161:LYS:HA	3:T:164:VAL:CG2	2.38	0.54
1:B:343:TRP:HB3	1:B:354:ARG:NH2	2.23	0.54
1:C:99:PRO:HB2	1:C:229:ARG:CD	2.38	0.54
3:T:93:TYR:HA	3:T:100:SER:HA	1.89	0.54
1:K:29:ILE:O	1:L:380:LYS:HG2	2.08	0.54
1:H:272:ALA:HA	2:1:105:VAL:CG2	2.37	0.54
3:T:125:PRO:HG2	3:T:135:ALA:HB1	1.89	0.54
1:I:243:LEU:HD12	1:I:244:VAL:H	1.71	0.54
2:Q:98:ARG:HH11	2:Q:98:ARG:HG2	1.72	0.54
1:J:386:GLU:HA	1:J:386:GLU:OE2	2.06	0.54
3:0:82:ALA:O	3:0:85:GLU:HG2	2.08	0.54
1:G:459:ALA:HB2	1:G:469:ILE:HA	1.90	0.54
2:9:99:VAL:HB	2:9:111:TYR:CE2	2.42	0.54
3:4:172:GLN:HB2	3:4:176:LYS:O	2.07	0.54
2:U:111:TYR:HE1	2:U:113:MET:HG2	1.72	0.54
3:V:126:SER:OG	3:V:129:GLU:HB2	2.08	0.54
2:7:17:SER:CB	2:7:84:LYS:HA	2.38	0.54
2:9:18:VAL:HG12	2:9:19:THR:N	2.23	0.54
2:Y:112:PRO:HB3	3:Z:36:HIS:CE1	2.43	0.54
2:Y:20:VAL:HG13	2:Y:120:THR:HG21	1.90	0.54
1:K:67:ILE:HG13	1:K:105:TYR:CE2	2.43	0.54
1:G:347:ILE:N	1:G:347:ILE:HD13	2.21	0.54
2:1:6:GLN:HB2	2:1:118:GLN:OE1	2.07	0.54
1:A:335:ILE:HD11	1:A:354:ARG:HB3	1.90	0.54
1:E:384:VAL:HG12	1:E:385:ILE:HG23	1.90	0.54
1:C:321:ARG:HD2	1:C:437:ILE:HG23	1.89	0.54
3:Z:29:ILE:HG23	3:Z:71:THR:HA	1.88	0.54
3:8:26:SER:HA	3:8:29:ILE:HB	1.89	0.54
3:N:49:LEU:O	3:N:57:PRO:HG3	2.07	0.54
1:H:120:PHE:CD2	1:H:150:ARG:HD2	2.42	0.54
1:H:99:PRO:HB2	1:H:229:ARG:HD3	1.89	0.54
1:A:183:HIS:HA	1:A:230:ILE:HD13	1.88	0.54
2:Y:52:ASN:CG	2:Y:55:ASP:HB3	2.28	0.54
2:W:18:VAL:HG12	2:W:19:THR:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:18:VAL:HG12	2:Y:19:THR:N	2.23	0.54
1:L:167:THR:HB	6:L:609:NAG:H61	1.90	0.54
1:F:167:THR:HB	6:F:609:NAG:H61	1.90	0.54
2:M:91:THR:HB	2:M:124:VAL:N	2.20	0.54
1:F:326:LYS:NZ	1:F:341:ASN:ND2	2.55	0.54
2:U:2:VAL:HG21	2:U:115:VAL:HG21	1.89	0.54
1:H:61:GLY:O	1:H:64:CYS:HB2	2.08	0.54
1:J:61:GLY:O	1:J:64:CYS:HB2	2.07	0.54
1:C:384:VAL:CG1	1:C:385:ILE:N	2.70	0.54
3:0:169:PRO:HA	3:0:179:ALA:HB2	1.90	0.54
1:D:99:PRO:HB2	1:D:229:ARG:HD3	1.90	0.54
1:D:61:GLY:O	1:D:64:CYS:HB2	2.08	0.54
1:I:384:VAL:HG12	1:I:385:ILE:HG23	1.90	0.54
3:4:50:ILE:HD13	3:4:75:LEU:HD13	1.90	0.54
1:B:182:VAL:HG22	1:B:202:VAL:HG21	1.90	0.54
1:I:80:GLN:HB3	1:I:150:ARG:NH2	2.23	0.54
1:H:179:ILE:O	1:H:254:PRO:HB3	2.07	0.54
2:7:29:LEU:HD23	2:7:29:LEU:N	2.23	0.54
1:D:403:GLU:H	1:D:407:GLN:HE21	1.56	0.54
1:J:380:LYS:HZ3	1:J:384:VAL:HG23	1.72	0.54
2:9:109:HIS:HA	3:0:93:TYR:CG	2.43	0.54
1:H:384:VAL:HG12	1:H:385:ILE:HG23	1.90	0.54
1:G:403:GLU:HB2	1:G:407:GLN:HB2	1.90	0.54
3:2:169:PRO:HA	3:2:179:ALA:HB2	1.89	0.54
1:A:74:PRO:HA	1:A:77:ASP:OD2	2.08	0.54
1:G:62:ILE:HG13	1:G:63:ASP:N	2.23	0.54
3:R:125:PRO:HG2	3:R:135:ALA:HB1	1.90	0.54
1:B:376:GLN:HB3	1:B:439:LEU:HD11	1.90	0.54
3:0:125:PRO:HG2	3:0:135:ALA:HB1	1.88	0.54
3:2:82:ALA:O	3:2:85:GLU:HG2	2.08	0.54
1:J:436:THR:O	1:J:440:THR:HG23	2.07	0.54
1:C:386:GLU:OE2	1:C:386:GLU:HA	2.06	0.54
1:G:99:PRO:HB2	1:G:229:ARG:HD3	1.89	0.54
1:D:170:ASN:ND2	1:D:239:PRO:HA	2.23	0.54
3:N:196:TYR:O	3:N:210:THR:HG23	2.08	0.54
1:C:173:ASN:HA	2:O:75:GLY:HA3	1.90	0.54
3:T:169:PRO:HA	3:T:179:ALA:HB2	1.90	0.54
2:9:52:ASN:CG	2:9:55:ASP:HB3	2.28	0.54
2:7:111:TYR:C	2:7:111:TYR:CD1	2.81	0.54
2:W:102:VAL:HG12	2:W:103:ARG:N	2.23	0.54
1:B:227:SER:HB2	6:C:610:NAG:H83	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:326:LYS:HZ3	1:I:341:ASN:HD22	1.56	0.54
1:J:148:PHE:HB2	1:J:151:LEU:HB2	1.89	0.54
1:K:403:GLU:H	1:K:407:GLN:HE21	1.55	0.54
1:D:161:TYR:HB2	1:D:196:VAL:CG2	2.38	0.54
1:I:208:ARG:CZ	1:I:238:LYS:HD2	2.37	0.54
1:F:403:GLU:H	1:F:407:GLN:HE21	1.56	0.54
1:A:335:ILE:O	1:A:335:ILE:HG23	2.07	0.54
1:G:407:GLN:HG2	1:G:411:LYS:HE3	1.89	0.54
3:4:26:SER:HA	3:4:29:ILE:HB	1.89	0.54
3:X:125:PRO:HG2	3:X:135:ALA:HB1	1.89	0.54
1:L:99:PRO:HB2	1:L:229:ARG:CD	2.38	0.54
2:9:102:VAL:HG12	2:9:103:ARG:N	2.23	0.53
2:Y:50:TRP:HE1	2:Y:99:VAL:HG21	1.73	0.53
2:1:108:PHE:O	2:1:111:TYR:CD2	2.61	0.53
2:W:6:GLN:HB3	2:W:120:THR:CG2	2.38	0.53
2:Y:29:LEU:HD23	2:Y:29:LEU:N	2.23	0.53
2:O:18:VAL:HG12	2:O:19:THR:N	2.22	0.53
2:7:2:VAL:CG2	2:7:115:VAL:HG21	2.37	0.53
1:J:384:VAL:HG12	1:J:385:ILE:HG23	1.90	0.53
1:K:99:PRO:HB2	1:K:229:ARG:HD3	1.88	0.53
1:B:403:GLU:HB2	1:B:407:GLN:HB2	1.90	0.53
1:L:321:ARG:HD2	1:L:437:ILE:HG23	1.90	0.53
1:E:251:LEU:HD12	1:E:252:ILE:H	1.73	0.53
1:B:17:HIS:HB2	1:B:320:MET:HE1	1.90	0.53
3:R:26:SER:HA	3:R:29:ILE:HB	1.89	0.53
1:J:431:LEU:O	1:J:435:HIS:HB2	2.08	0.53
1:J:234:TRP:HE3	1:J:234:TRP:H	1.52	0.53
1:F:431:LEU:O	1:F:435:HIS:HB2	2.08	0.53
2:5:98:ARG:HH11	2:5:98:ARG:HG2	1.72	0.53
3:Z:172:GLN:HB2	3:Z:176:LYS:O	2.07	0.53
2:Y:179:PHE:HB3	3:Z:180:SER:OG	2.07	0.53
2:U:50:TRP:HE1	2:U:99:VAL:HG21	1.73	0.53
2:Q:34:LEU:CD2	2:Q:35:SER:H	2.21	0.53
2:3:206:THR:HG21	2:3:223:LYS:CE	2.31	0.53
2:1:18:VAL:HG12	2:1:19:THR:N	2.23	0.53
1:K:227:SER:HB2	6:L:610:NAG:H83	1.90	0.53
1:G:67:ILE:HG13	1:G:105:TYR:CE2	2.43	0.53
1:K:347:ILE:N	1:K:347:ILE:HD13	2.23	0.53
1:G:384:VAL:CG1	1:G:385:ILE:N	2.71	0.53
3:Z:7:PRO:HG2	3:Z:106:THR:CG2	2.38	0.53
2:5:133:SER:O	2:5:155:VAL:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:HIS:HB2	1:H:320:MET:HE1	1.90	0.53
3:P:49:LEU:O	3:P:57:PRO:HG3	2.07	0.53
1:F:170:ASN:ND2	1:F:239:PRO:HA	2.23	0.53
1:F:298:ASN:OD1	1:F:300:ILE:N	2.36	0.53
2:M:93:VAL:HG22	2:M:121:MET:SD	2.48	0.53
2:W:30:THR:HG22	2:W:74:THR:HG22	1.90	0.53
1:K:459:ALA:HB2	1:K:469:ILE:HA	1.90	0.53
3:R:50:ILE:HD13	3:R:75:LEU:HD13	1.90	0.53
2:9:99:VAL:HB	2:9:111:TYR:CD2	2.42	0.53
2:7:52:ASN:CG	2:7:55:ASP:HB3	2.29	0.53
2:W:108:PHE:HB2	2:W:111:TYR:HE2	1.71	0.53
2:W:37:VAL:HG22	2:W:47:TRP:HA	1.89	0.53
2:W:52:ASN:CG	2:W:55:ASP:HB3	2.29	0.53
2:Y:34:LEU:HD21	2:Y:96:CYS:HB2	1.90	0.53
2:S:52:ASN:CG	2:S:55:ASP:HB3	2.29	0.53
2:M:35:SER:HB2	2:M:47:TRP:HE1	1.73	0.53
6:D:610:NAG:H83	1:F:227:SER:CB	2.39	0.53
1:F:384:VAL:CG1	1:F:385:ILE:N	2.72	0.53
1:F:14:CYS:SG	1:F:335:ILE:HG23	2.48	0.53
1:D:148:PHE:CB	1:D:151:LEU:HB2	2.38	0.53
2:Y:6:GLN:HE22	2:Y:95:TYR:HA	1.72	0.53
1:K:384:VAL:CG1	1:K:385:ILE:HG23	2.39	0.53
1:K:403:GLU:HB2	1:K:407:GLN:HB2	1.91	0.53
1:C:407:GLN:HG2	1:C:411:LYS:HE3	1.90	0.53
2:1:91:THR:HB	2:1:124:VAL:H	1.73	0.53
1:L:335:ILE:O	1:L:335:ILE:HG23	2.07	0.53
1:E:335:ILE:HD11	1:E:354:ARG:HB3	1.91	0.53
1:A:380:LYS:NZ	1:A:384:VAL:HG23	2.23	0.53
1:K:457:GLU:HG3	1:K:499:ARG:NH1	2.23	0.53
1:L:384:VAL:CG1	1:L:385:ILE:N	2.71	0.53
1:F:62:ILE:HG13	1:F:63:ASP:N	2.21	0.53
3:2:26:SER:HA	3:2:29:ILE:HB	1.90	0.53
1:J:421:TRP:HA	1:J:424:ASN:HD22	1.74	0.53
1:B:183:HIS:HA	1:B:230:ILE:HD13	1.90	0.53
2:U:30:THR:HG22	2:U:74:THR:HG22	1.89	0.53
3:4:128:GLU:O	3:4:131:GLN:HB3	2.07	0.53
3:R:35:VAL:HG13	3:R:92:SER:HB2	1.91	0.53
1:G:96:ASN:HA	1:G:224:ARG:HH11	1.73	0.53
1:B:169:PRO:HA	1:B:242:VAL:HG23	1.90	0.53
2:3:154:LEU:HD21	3:4:136:THR:HG21	1.89	0.53
1:G:321:ARG:HD2	1:G:437:ILE:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:172:GLN:HB2	3:0:176:LYS:O	2.08	0.53
2:U:108:PHE:HB2	2:U:111:TYR:CE2	2.43	0.53
2:Y:99:VAL:HB	2:Y:111:TYR:CD2	2.43	0.53
2:3:97:ALA:HA	2:3:115:VAL:O	2.08	0.53
2:7:29:LEU:CD2	2:7:77:ASN:HA	2.38	0.53
2:7:94:TYR:HE2	2:7:122:VAL:HG21	1.73	0.53
2:U:18:VAL:HG12	2:U:19:THR:N	2.23	0.53
6:A:609:NAG:O3	6:A:610:NAG:H2	2.07	0.53
2:5:91:THR:HG1	2:5:123:THR:HA	1.73	0.53
3:P:7:PRO:HG2	3:P:106:THR:CG2	2.38	0.53
3:8:169:PRO:HA	3:8:179:ALA:HB2	1.91	0.53
1:L:316:LEU:HD12	1:L:317:ALA:N	2.23	0.53
3:P:26:SER:HA	3:P:29:ILE:HB	1.89	0.53
1:H:376:GLN:HB3	1:H:439:LEU:HD11	1.90	0.53
1:B:272:ALA:HA	2:O:105:VAL:CG2	2.39	0.53
1:E:109:ARG:NH2	1:E:267:ILE:HD13	2.23	0.53
3:R:17:ARG:HH21	3:R:78:THR:CG2	2.21	0.53
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.90	0.53
1:E:321:ARG:HD2	1:E:437:ILE:HG23	1.90	0.53
2:9:50:TRP:HE1	2:9:99:VAL:HG21	1.72	0.53
3:8:172:GLN:HB2	3:8:176:LYS:O	2.08	0.53
2:W:113:MET:HB2	3:X:38:TYR:OH	2.09	0.53
2:W:29:LEU:CD2	2:W:77:ASN:HA	2.39	0.53
2:5:18:VAL:HG12	2:5:19:THR:N	2.23	0.53
2:3:17:SER:CB	2:3:84:LYS:HA	2.37	0.53
2:3:18:VAL:HG12	2:3:19:THR:N	2.23	0.53
2:M:7:SER:O	2:M:120:THR:HG22	2.09	0.53
1:F:220:ARG:HB2	1:F:221:PRO:HD2	1.91	0.53
1:K:384:VAL:CG1	1:K:385:ILE:N	2.72	0.53
1:F:111:LEU:HD12	1:F:112:VAL:N	2.24	0.53
1:G:61:GLY:O	1:G:64:CYS:HB2	2.09	0.53
1:J:407:GLN:HG2	1:J:411:LYS:HE3	1.89	0.53
3:N:161:LYS:HA	3:N:164:VAL:CG2	2.38	0.53
3:6:169:PRO:HA	3:6:179:ALA:HB2	1.90	0.53
2:O:133:SER:O	2:O:155:VAL:HA	2.08	0.53
3:V:161:LYS:HA	3:V:164:VAL:CG2	2.38	0.53
1:J:353:PHE:CE1	1:J:366:ASP:HB2	2.43	0.53
3:8:126:SER:OG	3:8:129:GLU:HB2	2.08	0.53
1:F:74:PRO:HA	1:F:77:ASP:OD2	2.07	0.53
1:J:376:GLN:HB3	1:J:439:LEU:HD11	1.90	0.53
3:N:138:VAL:HG13	3:N:182:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:309:VAL:HB	1:E:311:GLN:OE1	2.08	0.53
1:H:84:TRP:CE2	1:H:116:GLY:HA2	2.44	0.53
1:I:134:GLY:HA3	1:I:153:TRP:HB3	1.90	0.53
2:M:168:ASN:HB2	2:M:171:ALA:HB3	1.89	0.53
3:V:82:ALA:O	3:V:85:GLU:HG2	2.09	0.53
3:P:172:GLN:HB2	3:P:176:LYS:O	2.08	0.53
3:R:142:SER:O	3:R:143:ASP:HB2	2.09	0.53
2:Q:111:TYR:CD1	2:Q:111:TYR:C	2.82	0.53
2:Q:17:SER:CB	2:Q:84:LYS:HA	2.39	0.53
2:U:7:SER:O	2:U:120:THR:HG22	2.08	0.53
1:B:103:PRO:HD2	1:B:232:ILE:O	2.08	0.53
1:C:347:ILE:HD13	1:C:347:ILE:N	2.22	0.53
1:C:384:VAL:HG12	1:C:385:ILE:HG23	1.90	0.53
3:Z:161:LYS:HA	3:Z:164:VAL:CG2	2.37	0.53
1:I:495:ALA:O	1:I:499:ARG:HG3	2.09	0.53
2:O:44:GLY:C	2:O:45:LEU:HD23	2.28	0.53
3:6:196:TYR:O	3:6:210:THR:HG23	2.08	0.53
1:A:220:ARG:HB2	1:A:221:PRO:HD2	1.90	0.53
2:M:194:VAL:HG21	3:N:140:LEU:CD1	2.39	0.53
1:K:15:LEU:N	1:K:15:LEU:HD12	2.23	0.53
1:D:321:ARG:HD2	1:D:437:ILE:HG23	1.90	0.53
1:G:431:LEU:O	1:G:435:HIS:HB2	2.08	0.53
2:M:179:PHE:HE2	3:N:142:SER:HB3	1.73	0.53
3:Z:169:PRO:HA	3:Z:179:ALA:HB2	1.90	0.53
3:6:172:GLN:CB	3:6:176:LYS:HD2	2.39	0.53
2:O:113:MET:HG3	3:P:38:TYR:OH	2.08	0.53
2:Q:52:ASN:CG	2:Q:55:ASP:HB3	2.29	0.53
2:Y:111:TYR:C	2:Y:111:TYR:CD1	2.81	0.53
2:U:91:THR:HG1	2:U:123:THR:HA	1.73	0.53
2:S:29:LEU:HD21	2:S:77:ASN:HA	1.90	0.53
2:U:17:SER:CB	2:U:84:LYS:HA	2.39	0.53
1:J:463:GLY:HA2	1:K:453:ARG:HB3	1.90	0.53
1:G:183:HIS:HA	1:G:230:ILE:HD13	1.91	0.53
2:M:133:SER:O	2:M:155:VAL:HA	2.09	0.53
2:U:182:VAL:HG11	3:V:182:TYR:HD2	1.74	0.53
3:V:20:ILE:CG2	3:V:106:THR:HG21	2.39	0.53
3:8:125:PRO:HG2	3:8:135:ALA:HB1	1.90	0.53
1:I:120:PHE:O	1:I:121:ILE:HD13	2.09	0.53
2:W:98:ARG:HH11	2:W:98:ARG:HG2	1.73	0.53
1:E:72:GLY:HA3	1:E:149:SER:OG	2.08	0.53
2:Y:30:THR:HG22	2:Y:74:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:44:GLY:HA2	3:0:89:TYR:OH	2.09	0.53
2:W:108:PHE:N	2:W:108:PHE:CD2	2.74	0.53
2:3:52:ASN:CG	2:3:55:ASP:HB3	2.29	0.53
2:9:29:LEU:CD2	2:9:77:ASN:HA	2.39	0.53
1:J:463:GLY:CA	1:K:453:ARG:HD3	2.36	0.53
1:I:335:ILE:O	1:I:335:ILE:HG23	2.07	0.53
1:G:324:PRO:O	1:G:325:GLU:HB3	2.09	0.53
3:R:128:GLU:O	3:R:131:GLN:HB3	2.09	0.53
3:R:93:TYR:HA	3:R:100:SER:HA	1.90	0.53
1:J:111:LEU:HD12	1:J:112:VAL:N	2.23	0.53
1:L:169:PRO:HA	1:L:242:VAL:HG23	1.90	0.53
3:R:161:LYS:HA	3:R:164:VAL:CG2	2.39	0.53
3:N:7:PRO:HG2	3:N:106:THR:CG2	2.39	0.53
3:6:125:PRO:HG2	3:6:135:ALA:HB1	1.90	0.53
3:V:26:SER:HA	3:V:29:ILE:HB	1.89	0.53
2:W:112:PRO:HB2	3:X:51:SER:HB2	1.90	0.53
1:A:459:ALA:HB2	1:A:469:ILE:HA	1.91	0.53
1:K:309:VAL:HB	1:K:311:GLN:OE1	2.08	0.53
2:9:30:THR:HG22	2:9:74:THR:HG22	1.91	0.53
1:F:459:ALA:HB2	1:F:469:ILE:HA	1.90	0.53
3:N:169:PRO:HA	3:N:179:ALA:HB2	1.91	0.53
3:4:172:GLN:CB	3:4:176:LYS:HD2	2.38	0.53
2:7:102:VAL:HG12	2:7:103:ARG:N	2.24	0.53
2:7:37:VAL:HG22	2:7:47:TRP:HA	1.90	0.53
2:1:99:VAL:HB	2:1:111:TYR:CD2	2.44	0.53
2:M:108:PHE:CZ	3:N:99:GLY:HA2	2.44	0.53
4:J:602:NAG:H81	2:5:55:ASP:OD1	2.08	0.53
2:5:29:LEU:CD2	2:5:77:ASN:HA	2.39	0.53
2:S:18:VAL:HG12	2:S:19:THR:N	2.22	0.53
1:F:67:ILE:HG13	1:F:105:TYR:CE2	2.44	0.53
1:B:384:VAL:CG1	1:B:385:ILE:N	2.71	0.53
1:G:213:ILE:HG13	1:G:233:TYR:CE2	2.44	0.53
1:K:343:TRP:HB3	1:K:354:ARG:NH2	2.24	0.53
1:G:293:PRO:HB3	1:G:385:ILE:HD13	1.90	0.53
1:A:384:VAL:HG12	1:A:385:ILE:HG23	1.90	0.53
3:8:137:LEU:HB3	3:8:153:TRP:CH2	2.44	0.53
3:P:125:PRO:HG2	3:P:135:ALA:HB1	1.90	0.53
1:A:376:GLN:HB3	1:A:439:LEU:HD11	1.90	0.53
3:8:196:TYR:O	3:8:210:THR:HG23	2.09	0.53
3:8:17:ARG:HH21	3:8:78:THR:CG2	2.21	0.53
1:F:120:PHE:O	1:F:121:ILE:HD13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:GLN:HB3	1:B:150:ARG:NH2	2.23	0.53
1:L:352:GLY:HA2	1:L:365:ALA:HA	1.91	0.53
3:V:142:SER:O	3:V:143:ASP:HB2	2.09	0.53
3:6:142:SER:O	3:6:143:ASP:HB2	2.09	0.53
2:Q:29:LEU:N	2:Q:29:LEU:HD23	2.23	0.53
1:F:384:VAL:HG12	1:F:385:ILE:HG23	1.89	0.53
1:B:156:LYS:HD2	1:B:196:VAL:CG2	2.39	0.53
1:F:251:LEU:HD12	1:F:252:ILE:H	1.73	0.53
1:F:407:GLN:HG2	1:F:411:LYS:HE3	1.91	0.53
3:0:20:ILE:CG2	3:0:106:THR:HG21	2.39	0.53
3:4:6:GLN:CG	3:4:7:PRO:HD2	2.39	0.53
3:8:7:PRO:HG2	3:8:106:THR:CG2	2.39	0.53
3:V:138:VAL:HG13	3:V:182:TYR:CE1	2.44	0.53
3:0:26:SER:HA	3:0:29:ILE:HB	1.90	0.53
3:4:125:PRO:HG2	3:4:135:ALA:HB1	1.90	0.53
1:L:62:ILE:HG13	1:L:63:ASP:N	2.22	0.53
1:K:120:PHE:CD2	1:K:150:ARG:HD2	2.44	0.53
1:D:96:ASN:HA	1:D:224:ARG:HH11	1.73	0.53
3:Z:50:ILE:HD13	3:Z:75:LEU:HD13	1.91	0.53
1:J:15:LEU:HD12	1:J:15:LEU:N	2.23	0.53
1:F:134:GLY:HA3	1:F:153:TRP:HB3	1.91	0.53
2:9:35:SER:HB2	2:9:47:TRP:HE1	1.74	0.52
2:7:34:LEU:HD21	2:7:96:CYS:HB2	1.91	0.52
2:W:100:GLU:N	2:W:111:TYR:HB2	2.11	0.52
2:W:35:SER:HB2	2:W:47:TRP:HE1	1.74	0.52
2:Q:102:VAL:HG12	2:Q:103:ARG:H	1.73	0.52
2:S:35:SER:HB2	2:S:47:TRP:HE1	1.73	0.52
2:M:52:ASN:CG	2:M:55:ASP:HB3	2.29	0.52
2:S:29:LEU:CD2	2:S:77:ASN:HA	2.39	0.52
2:S:29:LEU:N	2:S:29:LEU:HD23	2.24	0.52
2:7:18:VAL:HG12	2:7:19:THR:N	2.24	0.52
3:2:126:SER:OG	3:2:129:GLU:HB2	2.10	0.52
1:J:27:LYS:NZ	1:K:383:ARG:HD3	2.24	0.52
3:4:169:PRO:HA	3:4:179:ALA:HB2	1.90	0.52
1:C:309:VAL:HB	1:C:311:GLN:OE1	2.09	0.52
3:X:137:LEU:HB3	3:X:153:TRP:CH2	2.44	0.52
1:G:220:ARG:HB2	1:G:221:PRO:HD2	1.91	0.52
3:8:17:ARG:HH21	3:8:78:THR:HG21	1.74	0.52
1:H:219:SER:H	1:I:246:ASN:ND2	2.07	0.52
3:4:82:ALA:O	3:4:85:GLU:HG2	2.08	0.52
1:C:170:ASN:ND2	1:C:239:PRO:HA	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:17:ARG:HH21	3:2:78:THR:CG2	2.22	0.52
3:N:82:ALA:O	3:N:85:GLU:HG2	2.10	0.52
1:A:309:VAL:HB	1:A:311:GLN:OE1	2.09	0.52
2:7:179:PHE:CE2	3:8:142:SER:HB3	2.44	0.52
3:8:142:SER:O	3:8:143:ASP:HB2	2.09	0.52
3:V:169:PRO:HA	3:V:179:ALA:HB2	1.90	0.52
3:4:142:SER:O	3:4:143:ASP:HB2	2.08	0.52
2:O:35:SER:HB2	2:O:47:TRP:HE1	1.74	0.52
2:M:102:VAL:HG12	2:M:103:ARG:N	2.24	0.52
2:U:29:LEU:CD2	2:U:77:ASN:HA	2.39	0.52
2:3:29:LEU:CD2	2:3:77:ASN:HA	2.39	0.52
2:M:18:VAL:HG12	2:M:19:THR:N	2.24	0.52
1:G:167:THR:HB	6:G:609:NAG:H61	1.92	0.52
2:M:91:THR:OG1	2:M:123:THR:HA	2.09	0.52
1:F:161:TYR:HB2	1:F:196:VAL:CG2	2.39	0.52
1:J:247:SER:HB3	1:J:251:LEU:HD22	1.91	0.52
1:B:27:LYS:HD3	1:C:383:ARG:NH1	2.24	0.52
1:C:169:PRO:HA	1:C:242:VAL:HG23	1.90	0.52
1:L:347:ILE:N	1:L:347:ILE:HD13	2.24	0.52
1:E:457:GLU:HG3	1:E:499:ARG:NH1	2.24	0.52
1:L:74:PRO:HA	1:L:77:ASP:OD2	2.10	0.52
3:T:26:SER:HA	3:T:29:ILE:HB	1.90	0.52
1:J:220:ARG:HB2	1:J:221:PRO:HD2	1.91	0.52
1:H:99:PRO:HB2	1:H:229:ARG:CD	2.39	0.52
2:5:30:THR:HG22	2:5:74:THR:HG22	1.91	0.52
1:K:312:ASN:OD1	1:K:313:THR:HG22	2.09	0.52
2:S:30:THR:HG22	2:S:74:THR:HG22	1.91	0.52
3:Z:196:TYR:O	3:Z:210:THR:HG23	2.09	0.52
1:I:220:ARG:HB2	1:I:221:PRO:HD2	1.90	0.52
1:C:123:GLU:OE1	1:C:168:MET:HG2	2.09	0.52
1:J:120:PHE:O	1:J:121:ILE:HD13	2.10	0.52
3:T:172:GLN:CB	3:T:176:LYS:HD2	2.39	0.52
2:S:111:TYR:C	2:S:111:TYR:CD1	2.83	0.52
2:5:52:ASN:CG	2:5:55:ASP:HB3	2.29	0.52
2:9:142:LYS:CE	2:9:144:THR:HG22	2.38	0.52
2:7:38:ARG:HB3	2:7:94:TYR:CE1	2.45	0.52
2:Q:159:PHE:HB2	2:Q:188:LEU:HD22	1.92	0.52
1:I:343:TRP:HB3	1:I:354:ARG:NH2	2.23	0.52
1:K:161:TYR:HB2	1:K:196:VAL:CG2	2.40	0.52
1:J:161:TYR:HB2	1:J:196:VAL:CG2	2.40	0.52
1:B:213:ILE:HG13	1:B:233:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:137:LEU:HB3	3:6:153:TRP:CH2	2.44	0.52
1:B:347:ILE:HD13	1:B:347:ILE:N	2.23	0.52
1:I:61:GLY:O	1:I:64:CYS:HB2	2.08	0.52
3:X:6:GLN:CG	3:X:7:PRO:HD2	2.40	0.52
1:D:347:ILE:N	1:D:347:ILE:HD13	2.24	0.52
3:V:6:GLN:CG	3:V:7:PRO:HD2	2.40	0.52
3:6:26:SER:HA	3:6:29:ILE:HB	1.91	0.52
1:I:295:GLN:NE2	1:I:308:TYR:HB2	2.24	0.52
2:9:44:GLY:C	2:9:45:LEU:HD23	2.29	0.52
4:L:602:NAG:H81	2:9:55:ASP:OD1	2.09	0.52
2:Y:179:PHE:HE2	3:Z:142:SER:HB3	1.68	0.52
2:U:102:VAL:HG12	2:U:103:ARG:N	2.24	0.52
2:1:148:THR:C	2:1:199:SER:HB2	2.29	0.52
2:7:29:LEU:HD21	2:7:77:ASN:HA	1.91	0.52
2:M:17:SER:CB	2:M:84:LYS:HA	2.39	0.52
2:O:83:MET:HB3	2:O:86:LEU:CD2	2.40	0.52
1:A:463:GLY:CA	1:B:453:ARG:HB3	2.38	0.52
1:D:191:GLN:NE2	1:D:217:ILE:HD11	2.24	0.52
3:R:7:PRO:HG2	3:R:106:THR:CG2	2.40	0.52
1:J:403:GLU:H	1:J:407:GLN:HE21	1.57	0.52
1:C:335:ILE:HD11	1:C:354:ARG:HB3	1.91	0.52
3:4:137:LEU:HB3	3:4:153:TRP:CH2	2.44	0.52
3:0:6:GLN:CG	3:0:7:PRO:HD2	2.39	0.52
1:G:17:HIS:HB2	1:G:320:MET:HE1	1.92	0.52
3:2:20:ILE:CG2	3:2:106:THR:HG21	2.40	0.52
1:D:384:VAL:HG12	1:D:385:ILE:HG23	1.90	0.52
2:9:210:ASN:HA	2:9:221:ASP:OD1	2.10	0.52
2:M:44:GLY:HA2	3:N:89:TYR:OH	2.10	0.52
1:D:80:GLN:HB3	1:D:150:ARG:NH2	2.24	0.52
1:J:80:GLN:HB3	1:J:150:ARG:NH2	2.24	0.52
1:D:134:GLY:HA3	1:D:153:TRP:HB3	1.91	0.52
1:H:15:LEU:HD12	1:H:15:LEU:N	2.24	0.52
1:E:295:GLN:NE2	1:E:308:TYR:HB2	2.24	0.52
3:2:172:GLN:HB2	3:2:176:LYS:O	2.08	0.52
3:X:142:SER:O	3:X:143:ASP:HB2	2.10	0.52
2:U:52:ASN:CG	2:U:55:ASP:HB3	2.29	0.52
1:F:187:THR:CB	1:F:189:GLN:HE21	2.14	0.52
1:D:167:THR:HB	6:D:609:NAG:H61	1.91	0.52
2:S:159:PHE:HB2	2:S:188:LEU:HD22	1.92	0.52
1:B:190:GLU:O	1:B:194:LEU:HD13	2.10	0.52
1:F:272:ALA:HA	2:W:105:VAL:CG2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:22:CYS:HB2	2:9:36:TRP:HH2	1.74	0.52
3:P:137:LEU:HB3	3:P:153:TRP:CH2	2.44	0.52
3:2:6:GLN:CG	3:2:7:PRO:HD2	2.39	0.52
3:N:125:PRO:HG2	3:N:135:ALA:HB1	1.90	0.52
1:G:383:ARG:NH2	1:I:426:GLU:HG3	2.24	0.52
3:6:197:SER:HB3	3:6:210:THR:OG1	2.09	0.52
2:1:98:ARG:HH11	2:1:98:ARG:HG2	1.74	0.52
1:H:459:ALA:HB2	1:H:469:ILE:HA	1.92	0.52
2:O:30:THR:HG22	2:O:74:THR:HG22	1.91	0.52
3:X:118:PRO:HB3	3:X:141:ILE:HG23	1.92	0.52
1:A:214:ILE:N	1:A:214:ILE:HD12	2.24	0.52
1:B:214:ILE:N	1:B:214:ILE:HD12	2.25	0.52
1:G:234:TRP:HE3	1:G:234:TRP:H	1.54	0.52
1:L:179:ILE:O	1:L:254:PRO:HB3	2.09	0.52
1:E:183:HIS:HA	1:E:230:ILE:HD13	1.92	0.52
3:T:113:GLN:HG3	3:T:175:ASN:ND2	2.25	0.52
3:T:142:SER:O	3:T:143:ASP:HB2	2.08	0.52
4:K:601:NAG:H61	4:K:602:NAG:O7	2.09	0.52
2:3:108:PHE:CB	2:3:111:TYR:CE2	2.91	0.52
2:1:101:GLY:H	2:1:111:TYR:HB3	1.75	0.52
2:M:29:LEU:CD2	2:M:77:ASN:HA	2.40	0.52
1:H:161:TYR:HB2	1:H:196:VAL:CG2	2.40	0.52
2:3:152:GLY:HA2	2:3:167:TRP:CH2	2.45	0.52
1:H:403:GLU:H	1:H:407:GLN:HE21	1.56	0.52
3:6:161:LYS:HA	3:6:164:VAL:CG2	2.39	0.52
3:N:6:GLN:CG	3:N:7:PRO:HD2	2.39	0.52
1:D:384:VAL:CG1	1:D:385:ILE:HG23	2.40	0.52
1:L:295:GLN:HE22	1:L:308:TYR:HB2	1.74	0.52
1:J:62:ILE:HG13	1:J:63:ASP:N	2.25	0.52
1:G:309:VAL:HB	1:G:311:GLN:OE1	2.10	0.52
1:J:183:HIS:HA	1:J:230:ILE:HD13	1.92	0.52
1:I:183:HIS:HA	1:I:230:ILE:HD13	1.91	0.52
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.44	0.52
2:S:137:LEU:HD11	3:T:138:VAL:HG21	1.92	0.52
1:C:295:GLN:NE2	1:C:308:TYR:HB2	2.24	0.52
2:U:98:ARG:HH11	2:U:98:ARG:HG2	1.75	0.52
2:S:50:TRP:HE1	2:S:99:VAL:HG21	1.74	0.52
2:7:148:THR:C	2:7:199:SER:HB2	2.30	0.52
2:7:83:MET:HB3	2:7:86:LEU:CD2	2.39	0.52
1:D:383:ARG:NH1	1:F:27:LYS:HD3	2.24	0.52
1:G:156:LYS:HD2	1:G:196:VAL:CG2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:126:SER:OG	3:P:129:GLU:HB2	2.09	0.52
2:1:44:GLY:C	2:1:45:LEU:HD23	2.30	0.52
1:L:243:LEU:HD12	1:L:244:VAL:H	1.73	0.52
1:A:61:GLY:HA2	1:A:79:PHE:CZ	2.45	0.52
3:T:6:GLN:CG	3:T:7:PRO:HD2	2.39	0.52
1:A:384:VAL:CG1	1:A:385:ILE:HG23	2.40	0.52
2:U:112:PRO:HA	3:V:36:HIS:CD2	2.45	0.52
1:G:430:ALA:HB2	1:H:383:ARG:HH21	1.75	0.52
1:B:352:GLY:HA2	1:B:365:ALA:HA	1.91	0.52
3:X:50:ILE:HD13	3:X:75:LEU:HD13	1.92	0.52
3:R:196:TYR:O	3:R:210:THR:HG23	2.10	0.52
1:D:234:TRP:HE3	1:D:234:TRP:H	1.52	0.52
3:T:17:ARG:HH21	3:T:78:THR:CG2	2.23	0.52
1:G:295:GLN:NE2	1:G:308:TYR:HB2	2.24	0.52
1:A:213:ILE:HG13	1:A:233:TYR:CE2	2.44	0.52
2:Q:108:PHE:HB2	2:Q:111:TYR:CE2	2.45	0.52
1:C:331:LEU:H	1:C:331:LEU:CD2	2.02	0.52
2:5:33:GLY:HA3	2:5:99:VAL:CG2	2.32	0.52
2:5:35:SER:HB2	2:5:47:TRP:HE1	1.75	0.52
2:Q:148:THR:C	2:Q:199:SER:HB2	2.30	0.52
1:A:17:HIS:HB2	1:A:320:MET:HE1	1.92	0.52
2:Q:152:GLY:HA2	2:Q:167:TRP:CH2	2.45	0.52
2:5:152:GLY:HA2	2:5:167:TRP:CH2	2.45	0.52
1:H:148:PHE:CB	1:H:151:LEU:HB2	2.40	0.52
1:B:384:VAL:HG12	1:B:385:ILE:HG23	1.90	0.52
3:T:7:PRO:HG2	3:T:106:THR:CG2	2.39	0.52
3:Z:6:GLN:CG	3:Z:7:PRO:HD2	2.40	0.52
1:G:353:PHE:CE1	1:G:366:ASP:HB2	2.43	0.52
1:D:62:ILE:HG13	1:D:63:ASP:N	2.23	0.52
2:Y:44:GLY:C	2:Y:45:LEU:HD23	2.30	0.52
1:L:220:ARG:HB2	1:L:221:PRO:HD2	1.92	0.52
1:C:427:LEU:O	1:C:431:LEU:HD12	2.10	0.52
1:E:182:VAL:HG22	1:E:202:VAL:HG21	1.91	0.52
1:L:309:VAL:HB	1:L:311:GLN:OE1	2.10	0.52
3:4:120:VAL:O	3:4:209:LYS:HG3	2.10	0.52
3:6:50:ILE:HD13	3:6:75:LEU:HD13	1.92	0.52
1:D:87:PHE:O	1:D:267:ILE:HG13	2.10	0.52
3:2:172:GLN:CB	3:2:176:LYS:HD2	2.40	0.52
2:S:194:VAL:HG21	3:T:140:LEU:HD13	1.88	0.52
3:V:172:GLN:CB	3:V:176:LYS:HD2	2.40	0.52
2:Y:34:LEU:HD23	2:Y:97:ALA:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:601:NAG:H61	4:D:602:NAG:O7	2.10	0.52
2:S:50:TRP:CH2	2:S:52:ASN:HB2	2.44	0.52
2:O:29:LEU:CD2	2:O:77:ASN:HA	2.40	0.52
2:Q:18:VAL:HG12	2:Q:19:THR:N	2.24	0.52
1:C:167:THR:HB	6:C:609:NAG:H61	1.92	0.52
1:F:384:VAL:CG1	1:F:385:ILE:HG23	2.40	0.52
1:H:326:LYS:HZ3	1:H:341:ASN:HD22	1.58	0.52
1:E:222:TRP:CZ3	6:F:611:BMA:O2	2.62	0.52
1:B:167:THR:HB	6:B:609:NAG:H61	1.92	0.52
1:E:161:TYR:HB2	1:E:196:VAL:CG2	2.40	0.52
1:E:99:PRO:HB2	1:E:229:ARG:HD3	1.91	0.52
3:6:6:GLN:CG	3:6:7:PRO:HD2	2.39	0.52
3:T:137:LEU:HB3	3:T:153:TRP:CH2	2.45	0.52
3:Z:137:LEU:HB3	3:Z:153:TRP:HH2	1.75	0.52
1:E:384:VAL:CG1	1:E:385:ILE:HG23	2.40	0.52
2:Q:194:VAL:HG21	3:R:140:LEU:CD1	2.40	0.52
3:V:137:LEU:HD11	3:V:190:TRP:HZ3	1.75	0.52
1:L:384:VAL:CG1	1:L:385:ILE:HG23	2.40	0.52
2:S:210:ASN:HA	2:S:221:ASP:OD1	2.10	0.52
1:C:495:ALA:O	1:C:499:ARG:HG3	2.09	0.52
1:G:383:ARG:NH1	1:I:27:LYS:HD3	2.25	0.52
3:T:50:ILE:HD13	3:T:75:LEU:HD13	1.92	0.52
1:D:424:ASN:HB3	1:F:423:TYR:CE2	2.45	0.52
2:S:112:PRO:HB2	3:T:51:SER:HB2	1.92	0.52
3:8:50:ILE:HD13	3:8:75:LEU:HD13	1.92	0.52
3:X:41:LEU:HB3	3:X:42:PRO:HD2	1.92	0.52
2:W:34:LEU:HD21	2:W:96:CYS:HB2	1.92	0.52
2:U:29:LEU:N	2:U:29:LEU:HD23	2.25	0.52
2:M:29:LEU:HD23	2:M:29:LEU:N	2.25	0.52
1:A:463:GLY:HA2	1:B:453:ARG:CD	2.35	0.52
1:F:326:LYS:HB3	1:F:328:THR:CG2	2.34	0.52
1:F:326:LYS:HZ1	1:F:341:ASN:ND2	2.08	0.52
2:3:22:CYS:HB2	2:3:36:TRP:HH2	1.74	0.52
1:D:407:GLN:HG2	1:D:411:LYS:HE3	1.90	0.52
1:F:247:SER:HB3	1:F:251:LEU:HD22	1.92	0.52
1:J:213:ILE:HG13	1:J:233:TYR:CE2	2.45	0.52
1:E:347:ILE:HD13	1:E:347:ILE:N	2.24	0.52
3:V:7:PRO:HG2	3:V:106:THR:CG2	2.40	0.52
2:9:136:PRO:O	3:0:126:SER:HB3	2.10	0.52
1:C:80:GLN:HB3	1:C:150:ARG:NH2	2.24	0.52
1:H:221:PRO:HD3	1:I:244:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:169:PRO:HA	1:I:242:VAL:HG23	1.92	0.52
3:4:41:LEU:HB3	3:4:42:PRO:HD2	1.92	0.52
3:8:82:ALA:O	3:8:85:GLU:HG2	2.10	0.52
1:D:431:LEU:O	1:D:435:HIS:HB2	2.10	0.52
3:Z:165:GLU:HG2	3:Z:182:TYR:O	2.09	0.52
1:H:169:PRO:HA	1:H:242:VAL:HG23	1.92	0.52
2:O:34:LEU:HD21	2:O:96:CYS:HB2	1.91	0.51
2:U:34:LEU:CD2	2:U:35:SER:H	2.23	0.51
2:1:108:PHE:HB2	2:1:111:TYR:HE2	1.74	0.51
2:5:34:LEU:HD21	2:5:96:CYS:HB2	1.91	0.51
2:3:29:LEU:N	2:3:29:LEU:HD23	2.25	0.51
2:M:83:MET:HB3	2:M:86:LEU:CD2	2.40	0.51
2:5:29:LEU:N	2:5:29:LEU:HD23	2.25	0.51
2:7:20:VAL:HG13	2:7:120:THR:HG21	1.92	0.51
2:5:159:PHE:HB2	2:5:188:LEU:HD22	1.91	0.51
1:L:183:HIS:HA	1:L:230:ILE:HD13	1.92	0.51
1:K:156:LYS:HD2	1:K:196:VAL:CG2	2.39	0.51
1:J:103:PRO:HD2	1:J:232:ILE:O	2.10	0.51
3:6:137:LEU:HD11	3:6:190:TRP:HZ3	1.75	0.51
3:N:137:LEU:HB3	3:N:153:TRP:CH2	2.45	0.51
3:4:137:LEU:HD11	3:4:190:TRP:HZ3	1.75	0.51
1:G:335:ILE:HD11	1:G:354:ARG:HB3	1.91	0.51
1:H:384:VAL:CG1	1:H:385:ILE:HG23	2.40	0.51
1:I:353:PHE:CE1	1:I:366:ASP:HB2	2.45	0.51
1:J:17:HIS:HB2	1:J:320:MET:HE1	1.92	0.51
1:K:74:PRO:HA	1:K:77:ASP:OD2	2.09	0.51
2:O:44:GLY:HA2	3:P:89:TYR:OH	2.10	0.51
1:B:120:PHE:CD2	1:B:150:ARG:HD2	2.45	0.51
1:C:155:THR:HB	1:D:143:PRO:CG	2.40	0.51
1:J:459:ALA:HB2	1:J:469:ILE:HA	1.92	0.51
1:K:134:GLY:HA3	1:K:153:TRP:HB3	1.92	0.51
1:E:179:ILE:O	1:E:254:PRO:HB3	2.10	0.51
3:6:17:ARG:HH21	3:6:78:THR:CG2	2.23	0.51
3:0:142:SER:O	3:0:143:ASP:HB2	2.10	0.51
3:Z:142:SER:O	3:Z:143:ASP:HB2	2.10	0.51
2:7:108:PHE:HB2	2:7:111:TYR:CE2	2.44	0.51
2:3:35:SER:HB2	2:3:47:TRP:HE1	1.74	0.51
2:5:108:PHE:HB2	2:5:111:TYR:HE2	1.71	0.51
2:Y:159:PHE:HB2	2:Y:188:LEU:HD22	1.92	0.51
1:K:326:LYS:HZ3	1:K:341:ASN:HD22	1.56	0.51
1:F:208:ARG:CZ	1:F:238:LYS:HD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:22:CYS:HB2	2:O:36:TRP:HH2	1.74	0.51
2:U:152:GLY:HA2	2:U:167:TRP:CH2	2.45	0.51
1:L:247:SER:HB3	1:L:251:LEU:HD22	1.93	0.51
1:F:102:VAL:HG11	1:F:108:LEU:HD23	1.91	0.51
3:N:137:LEU:HD11	3:N:190:TRP:HZ3	1.75	0.51
1:C:384:VAL:CG1	1:C:385:ILE:HG23	2.40	0.51
3:O:93:TYR:HD1	3:O:100:SER:HB3	1.75	0.51
2:O:210:ASN:HA	2:O:221:ASP:OD1	2.10	0.51
2:3:44:GLY:C	2:3:45:LEU:HD23	2.29	0.51
1:B:470:TYR:CG	1:B:499:ARG:HG2	2.45	0.51
2:7:210:ASN:HA	2:7:221:ASP:OD1	2.09	0.51
1:I:99:PRO:HB2	1:I:229:ARG:CD	2.41	0.51
1:G:80:GLN:HB3	1:G:150:ARG:NH2	2.25	0.51
1:G:99:PRO:HB2	1:G:229:ARG:CD	2.41	0.51
1:A:99:PRO:HB2	1:A:229:ARG:HD3	1.91	0.51
1:B:120:PHE:O	1:B:121:ILE:HD13	2.10	0.51
3:Z:138:VAL:HG13	3:Z:182:TYR:CE1	2.45	0.51
1:I:421:TRP:HA	1:I:424:ASN:HD22	1.75	0.51
3:X:128:GLU:O	3:X:131:GLN:HB3	2.09	0.51
1:J:321:ARG:HD2	1:J:437:ILE:HG23	1.92	0.51
1:I:214:ILE:N	1:I:214:ILE:HD12	2.25	0.51
1:L:214:ILE:HD12	1:L:214:ILE:N	2.25	0.51
1:K:321:ARG:HD2	1:K:437:ILE:HG23	1.92	0.51
3:2:196:TYR:O	3:2:210:THR:HG23	2.09	0.51
3:6:126:SER:OG	3:6:129:GLU:HB2	2.10	0.51
3:Z:172:GLN:CB	3:Z:176:LYS:HD2	2.40	0.51
3:8:172:GLN:CB	3:8:176:LYS:HD2	2.40	0.51
2:1:35:SER:HB2	2:1:47:TRP:HE1	1.75	0.51
1:J:190:GLU:O	1:J:194:LEU:HD13	2.11	0.51
1:B:161:TYR:HB2	1:B:196:VAL:CG2	2.40	0.51
1:G:247:SER:HB3	1:G:251:LEU:HD22	1.92	0.51
1:C:148:PHE:CB	1:C:151:LEU:HB2	2.40	0.51
1:C:161:TYR:HB2	1:C:196:VAL:CG2	2.40	0.51
1:B:384:VAL:CG1	1:B:385:ILE:HG23	2.41	0.51
1:J:347:ILE:HD13	1:J:347:ILE:N	2.22	0.51
1:G:111:LEU:HD12	1:G:112:VAL:N	2.24	0.51
1:D:220:ARG:HB2	1:D:221:PRO:HD2	1.93	0.51
1:E:169:PRO:HA	1:E:242:VAL:HG23	1.93	0.51
3:8:6:GLN:CG	3:8:7:PRO:HD2	2.41	0.51
1:G:461:ASP:OD2	1:H:453:ARG:HG2	2.09	0.51
1:L:353:PHE:CE1	1:L:366:ASP:HB2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:210:ASN:HA	2:W:221:ASP:OD1	2.10	0.51
2:5:210:ASN:HA	2:5:221:ASP:OD1	2.10	0.51
1:E:74:PRO:HA	1:E:77:ASP:OD2	2.10	0.51
1:B:62:ILE:HG13	1:B:63:ASP:N	2.25	0.51
2:5:112:PRO:CB	3:6:51:SER:HB2	2.40	0.51
2:Y:27:TYR:O	2:Y:98:ARG:NH2	2.43	0.51
3:0:197:SER:HB3	3:0:210:THR:OG1	2.09	0.51
1:I:431:LEU:O	1:I:435:HIS:HB2	2.11	0.51
3:8:138:VAL:HG13	3:8:182:TYR:CE1	2.46	0.51
1:H:123:GLU:OE1	1:H:168:MET:HG2	2.10	0.51
2:9:34:LEU:HD21	2:9:96:CYS:HB2	1.93	0.51
2:W:101:GLY:H	2:W:111:TYR:HB3	1.76	0.51
2:M:108:PHE:O	2:M:111:TYR:CD2	2.64	0.51
2:3:148:THR:C	2:3:199:SER:HB2	2.30	0.51
2:Q:29:LEU:HD21	2:Q:77:ASN:HA	1.93	0.51
1:D:326:LYS:HZ3	1:D:341:ASN:HD22	1.57	0.51
2:M:117:GLY:C	2:M:119:GLY:H	2.14	0.51
1:F:335:ILE:HD11	1:F:354:ARG:HB3	1.91	0.51
1:D:169:PRO:HA	1:D:242:VAL:HG23	1.92	0.51
1:F:103:PRO:HD2	1:F:232:ILE:O	2.10	0.51
1:D:108:LEU:O	1:D:112:VAL:HG23	2.10	0.51
2:S:152:GLY:HA2	2:S:167:TRP:CH2	2.46	0.51
1:G:381:LEU:O	1:G:385:ILE:HG13	2.09	0.51
1:F:457:GLU:HG3	1:F:499:ARG:NH1	2.23	0.51
2:Q:133:SER:O	2:Q:155:VAL:HA	2.09	0.51
3:8:137:LEU:HB3	3:8:153:TRP:HH2	1.76	0.51
3:X:126:SER:OG	3:X:129:GLU:HB2	2.11	0.51
3:8:93:TYR:HA	3:8:100:SER:HA	1.91	0.51
2:5:44:GLY:HA2	3:6:89:TYR:OH	2.11	0.51
2:5:44:GLY:C	2:5:45:LEU:HD23	2.31	0.51
3:0:126:SER:OG	3:0:129:GLU:HB2	2.10	0.51
2:7:44:GLY:HA2	3:8:89:TYR:OH	2.10	0.51
1:G:120:PHE:CD2	1:G:150:ARG:HD2	2.46	0.51
1:K:213:ILE:HG13	1:K:233:TYR:CE2	2.46	0.51
1:C:214:ILE:HD12	1:C:214:ILE:N	2.24	0.51
1:H:421:TRP:HA	1:H:424:ASN:HD22	1.75	0.51
2:5:108:PHE:O	2:5:111:TYR:CD2	2.63	0.51
2:S:17:SER:CB	2:S:84:LYS:HA	2.40	0.51
2:3:83:MET:HB3	2:3:86:LEU:CD2	2.41	0.51
1:B:220:ARG:HB2	1:B:221:PRO:HD2	1.90	0.51
2:W:152:GLY:HA2	2:W:167:TRP:CH2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:325:GLU:HG2	1:L:326:LYS:N	2.25	0.51
1:B:111:LEU:HD12	1:B:112:VAL:N	2.25	0.51
1:C:403:GLU:H	1:C:407:GLN:HE21	1.58	0.51
1:K:220:ARG:HB2	1:K:221:PRO:HD2	1.91	0.51
1:H:335:ILE:HD11	1:H:354:ARG:HB3	1.93	0.51
1:E:343:TRP:HB3	1:E:354:ARG:NH2	2.25	0.51
3:4:7:PRO:HG2	3:4:106:THR:CG2	2.39	0.51
1:B:353:PHE:CE1	1:B:366:ASP:HB2	2.42	0.51
3:2:7:PRO:HG2	3:2:106:THR:CG2	2.40	0.51
3:P:169:PRO:HA	3:P:179:ALA:HB2	1.91	0.51
1:A:421:TRP:HA	1:A:424:ASN:HD22	1.75	0.51
1:E:214:ILE:N	1:E:214:ILE:HD12	2.25	0.51
3:N:64:PHE:CD1	3:N:77:ILE:HG12	2.46	0.51
1:J:298:ASN:OD1	1:J:300:ILE:N	2.40	0.51
1:C:180:TRP:CD2	1:C:204:VAL:HG21	2.46	0.51
3:R:172:GLN:CB	3:R:176:LYS:HD2	2.40	0.51
2:Q:50:TRP:HE1	2:Q:99:VAL:HG21	1.74	0.51
2:M:4:LEU:HD11	2:M:115:VAL:O	2.10	0.51
2:5:108:PHE:CD2	2:5:108:PHE:N	2.75	0.51
2:9:29:LEU:N	2:9:29:LEU:HD23	2.25	0.51
1:I:213:ILE:HG13	1:I:233:TYR:CE2	2.46	0.51
1:B:316:LEU:HD12	1:B:317:ALA:N	2.24	0.51
1:B:103:PRO:HG2	1:B:233:TYR:CE1	2.46	0.51
2:1:38:ARG:HB3	2:1:94:TYR:CE1	2.45	0.51
2:1:92:ALA:O	2:1:122:VAL:HG22	2.10	0.51
1:J:399:PHE:HE2	1:L:405:ARG:HH21	1.58	0.51
1:L:102:VAL:O	1:L:105:TYR:HB2	2.11	0.51
3:0:7:PRO:HG2	3:0:106:THR:CG2	2.39	0.51
1:E:62:ILE:HG13	1:E:63:ASP:N	2.26	0.51
2:Y:210:ASN:HA	2:Y:221:ASP:OD1	2.11	0.51
2:Q:91:THR:HB	2:Q:124:VAL:H	1.76	0.51
1:I:309:VAL:HB	1:I:311:GLN:OE1	2.11	0.51
3:0:64:PHE:CD1	3:0:77:ILE:HG12	2.45	0.51
2:3:30:THR:HG22	2:3:74:THR:HG22	1.91	0.51
1:G:214:ILE:N	1:G:214:ILE:HD12	2.26	0.51
2:1:30:THR:HG22	2:1:74:THR:HG22	1.91	0.51
3:4:17:ARG:HH21	3:4:78:THR:CG2	2.24	0.51
3:N:142:SER:O	3:N:143:ASP:HB2	2.09	0.51
2:O:50:TRP:HE1	2:O:99:VAL:HG21	1.75	0.51
3:R:113:GLN:CG	3:R:175:ASN:ND2	2.74	0.51
2:S:34:LEU:HD21	2:S:96:CYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:108:PHE:CZ	3:6:99:GLY:HA2	2.45	0.51
2:O:148:THR:C	2:O:199:SER:HB2	2.31	0.51
2:W:148:THR:C	2:W:199:SER:HB2	2.31	0.51
2:9:29:LEU:HD21	2:9:77:ASN:HA	1.92	0.51
2:1:29:LEU:N	2:1:29:LEU:HD23	2.25	0.51
2:U:83:MET:HB3	2:U:86:LEU:CD2	2.41	0.51
2:U:159:PHE:HB2	2:U:188:LEU:HD22	1.92	0.51
1:K:324:PRO:O	1:K:325:GLU:HB3	2.10	0.51
3:R:126:SER:OG	3:R:129:GLU:HB2	2.11	0.51
1:B:381:LEU:O	1:B:385:ILE:HG13	2.11	0.51
1:A:383:ARG:HD3	1:C:27:LYS:HZ3	1.74	0.51
1:A:403:GLU:H	1:A:407:GLN:HE21	1.58	0.51
1:H:380:LYS:HZ3	1:H:384:VAL:HG23	1.76	0.51
3:0:137:LEU:HD11	3:0:190:TRP:HZ3	1.75	0.51
1:D:99:PRO:HB2	1:D:229:ARG:CD	2.40	0.51
1:J:343:TRP:HB3	1:J:354:ARG:NH2	2.26	0.51
3:V:137:LEU:HB3	3:V:153:TRP:CH2	2.45	0.51
1:E:272:ALA:HA	2:U:105:VAL:HG22	1.93	0.51
1:J:99:PRO:HB2	1:J:229:ARG:CD	2.40	0.51
1:J:424:ASN:HB3	1:L:423:TYR:CE2	2.46	0.51
1:F:120:PHE:CD2	1:F:150:ARG:HD2	2.46	0.51
1:D:405:ARG:HD3	1:E:406:ILE:HG21	1.93	0.51
1:F:182:VAL:HG22	1:F:202:VAL:HG21	1.93	0.51
3:T:197:SER:HB3	3:T:210:THR:OG1	2.11	0.51
3:N:41:LEU:HB3	3:N:42:PRO:HD2	1.93	0.51
1:B:309:VAL:HB	1:B:311:GLN:OE1	2.11	0.51
2:Q:62:LYS:CE	3:R:97:LEU:HD13	2.41	0.51
2:9:100:GLU:O	2:9:102:VAL:N	2.44	0.51
2:3:33:GLY:HA3	2:3:99:VAL:CG2	2.28	0.51
2:9:148:THR:C	2:9:199:SER:HB2	2.31	0.51
2:9:206:THR:HG22	2:9:207:TYR:N	2.26	0.51
1:I:167:THR:HB	6:I:609:NAG:H61	1.93	0.51
2:M:159:PHE:HB2	2:M:188:LEU:HD22	1.93	0.51
2:Q:22:CYS:HB2	2:Q:36:TRP:HH2	1.75	0.51
1:G:413:VAL:HG21	1:I:409:LEU:HD11	1.92	0.51
2:Y:60:TYR:CE1	2:Y:70:MET:HG2	2.40	0.51
1:E:99:PRO:HB2	1:E:229:ARG:CD	2.41	0.51
1:B:321:ARG:HD2	1:B:437:ILE:HG23	1.93	0.51
1:B:102:VAL:HG11	1:B:108:LEU:HD23	1.92	0.51
3:R:137:LEU:HB3	3:R:153:TRP:CH2	2.45	0.51
3:R:6:GLN:CG	3:R:7:PRO:HD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:137:LEU:HB3	3:0:153:TRP:CH2	2.46	0.51
1:I:384:VAL:CG1	1:I:385:ILE:HG23	2.40	0.51
2:S:44:GLY:C	2:S:45:LEU:HD23	2.31	0.51
1:I:62:ILE:HG13	1:I:63:ASP:N	2.26	0.51
1:I:120:PHE:CD2	1:I:150:ARG:HD2	2.45	0.51
1:D:421:TRP:HA	1:D:424:ASN:HD22	1.76	0.51
3:6:17:ARG:HH21	3:6:78:THR:HG21	1.76	0.51
1:K:183:HIS:HA	1:K:230:ILE:HD13	1.91	0.51
1:K:170:ASN:ND2	1:K:239:PRO:HA	2.25	0.51
2:9:98:ARG:HH11	2:9:98:ARG:HG2	1.74	0.51
1:D:214:ILE:HD12	1:D:214:ILE:N	2.26	0.51
2:O:68:VAL:O	2:O:69:THR:HG23	2.11	0.51
2:Q:30:THR:HG22	2:Q:74:THR:HG22	1.93	0.51
3:8:41:LEU:HB3	3:8:42:PRO:HD2	1.93	0.51
3:R:41:LEU:HB3	3:R:42:PRO:HD2	1.93	0.51
3:Z:64:PHE:CD1	3:Z:77:ILE:HG12	2.46	0.51
2:Q:35:SER:HB2	2:Q:47:TRP:HE1	1.76	0.51
2:1:34:LEU:HD21	2:1:96:CYS:HB2	1.93	0.51
2:5:83:MET:HB3	2:5:86:LEU:CD2	2.40	0.51
2:1:83:MET:HB3	2:1:86:LEU:CD2	2.41	0.51
2:9:83:MET:HB3	2:9:86:LEU:CD2	2.41	0.51
2:3:159:PHE:HB2	2:3:188:LEU:HD22	1.93	0.51
1:E:324:PRO:O	1:E:325:GLU:HB3	2.10	0.51
1:A:324:PRO:O	1:A:325:GLU:HB3	2.11	0.51
1:F:326:LYS:NZ	1:F:343:TRP:CD1	2.78	0.51
1:L:156:LYS:HD2	1:L:196:VAL:CG2	2.41	0.51
2:S:22:CYS:HB2	2:S:36:TRP:HH2	1.76	0.51
2:1:152:GLY:HA2	2:1:167:TRP:CH2	2.46	0.51
2:Y:135:PHE:HB3	3:Z:126:SER:OG	2.10	0.51
3:4:137:LEU:HB3	3:4:153:TRP:HH2	1.76	0.51
3:T:137:LEU:HD11	3:T:190:TRP:HZ3	1.75	0.51
3:P:6:GLN:CG	3:P:7:PRO:HD2	2.39	0.51
1:C:59:LEU:HD12	1:C:60:ASP:N	2.26	0.51
1:F:37:THR:CG2	1:F:322:ASN:HB2	2.40	0.51
1:E:108:LEU:O	1:E:112:VAL:HG23	2.11	0.51
2:Q:210:ASN:HA	2:Q:221:ASP:OD1	2.11	0.51
1:H:426:GLU:HG3	1:I:383:ARG:NH2	2.26	0.51
1:I:321:ARG:HD2	1:I:437:ILE:HG23	1.93	0.51
3:V:64:PHE:CD1	3:V:77:ILE:HG12	2.45	0.51
3:8:197:SER:HB3	3:8:210:THR:OG1	2.11	0.51
1:B:243:LEU:HD12	1:B:244:VAL:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:17:ARG:HH21	3:Z:78:THR:CG2	2.23	0.51
1:D:18:HIS:H	1:D:18:HIS:CD2	2.29	0.51
7:H:616:NAG:H61	7:H:617:BMA:H2	1.93	0.51
2:1:179:PHE:HE2	3:2:142:SER:HB3	1.75	0.51
3:0:172:GLN:CB	3:0:176:LYS:HD2	2.40	0.51
3:P:142:SER:O	3:P:143:ASP:HB2	2.10	0.51
3:P:172:GLN:CB	3:P:176:LYS:HD2	2.41	0.51
2:Q:108:PHE:HB2	2:Q:111:TYR:HE2	1.76	0.51
2:Q:34:LEU:HD21	2:Q:96:CYS:HB2	1.92	0.51
2:S:148:THR:C	2:S:199:SER:HB2	2.32	0.51
2:3:6:GLN:HE21	2:3:117:GLY:CA	2.13	0.51
2:Y:148:THR:C	2:Y:199:SER:HB2	2.30	0.51
2:Y:29:LEU:CD2	2:Y:77:ASN:HA	2.41	0.51
2:Y:83:MET:HB3	2:Y:86:LEU:CD2	2.41	0.51
2:W:159:PHE:HB2	2:W:188:LEU:HD22	1.93	0.51
1:F:326:LYS:HZ2	1:F:341:ASN:HD22	1.58	0.51
1:C:247:SER:HB3	1:C:251:LEU:HD22	1.93	0.51
2:7:60:TYR:CE1	2:7:70:MET:HG2	2.40	0.51
3:N:126:SER:OG	3:N:129:GLU:HB2	2.11	0.51
1:I:403:GLU:H	1:I:407:GLN:HE21	1.59	0.51
3:X:138:VAL:HG13	3:X:182:TYR:CE1	2.47	0.51
3:X:137:LEU:HD11	3:X:190:TRP:HZ3	1.75	0.51
1:H:321:ARG:HD2	1:H:437:ILE:HG23	1.93	0.51
3:8:137:LEU:HD11	3:8:190:TRP:HZ3	1.76	0.51
1:L:470:TYR:CG	1:L:499:ARG:HG2	2.46	0.51
3:6:135:ALA:O	3:6:184:SER:HB2	2.10	0.51
1:H:74:PRO:HA	1:H:77:ASP:OD2	2.10	0.51
1:J:453:ARG:HG2	1:L:461:ASP:OD2	2.10	0.51
3:V:135:ALA:O	3:V:184:SER:HB2	2.11	0.51
1:G:495:ALA:O	1:G:499:ARG:HG3	2.11	0.51
1:D:376:GLN:HB3	1:D:439:LEU:HD11	1.92	0.51
1:G:27:LYS:HD3	1:H:383:ARG:CZ	2.40	0.51
3:T:17:ARG:HH21	3:T:78:THR:HG21	1.76	0.51
1:K:169:PRO:HA	1:K:242:VAL:HG23	1.93	0.51
1:E:170:ASN:ND2	1:E:239:PRO:HA	2.25	0.51
3:V:196:TYR:O	3:V:210:THR:HG23	2.11	0.51
3:P:17:ARG:HH21	3:P:78:THR:CG2	2.23	0.51
3:X:172:GLN:CB	3:X:176:LYS:HD2	2.41	0.50
2:U:34:LEU:HD21	2:U:96:CYS:HB2	1.93	0.50
2:7:50:TRP:HE1	2:7:99:VAL:HG21	1.76	0.50
2:Y:100:GLU:N	2:Y:111:TYR:HB2	2.17	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:2:VAL:HG21	2:5:115:VAL:HG21	1.92	0.50
2:3:29:LEU:HD21	2:3:77:ASN:HA	1.93	0.50
1:I:335:ILE:HD11	1:I:354:ARG:HB3	1.92	0.50
1:J:326:LYS:HZ3	1:J:341:ASN:HD22	1.59	0.50
1:B:380:LYS:HZ3	1:B:384:VAL:HG23	1.76	0.50
1:J:381:LEU:O	1:J:385:ILE:HG13	2.12	0.50
1:J:384:VAL:CG1	1:J:385:ILE:HG23	2.40	0.50
1:F:243:LEU:HD12	1:F:244:VAL:H	1.76	0.50
1:L:335:ILE:HD11	1:L:354:ARG:HB3	1.92	0.50
1:C:208:ARG:CZ	1:C:238:LYS:HD2	2.40	0.50
1:G:37:THR:CG2	1:G:322:ASN:HB2	2.40	0.50
1:A:380:LYS:HZ3	1:A:384:VAL:HG23	1.76	0.50
1:A:401:GLU:HG3	1:B:238:LYS:HE2	1.91	0.50
1:C:220:ARG:HB2	1:C:221:PRO:HD2	1.91	0.50
1:B:61:GLY:O	1:B:64:CYS:HB2	2.10	0.50
3:P:135:ALA:O	3:P:184:SER:HB2	2.10	0.50
3:P:197:SER:HB3	3:P:210:THR:OG1	2.11	0.50
1:D:120:PHE:O	1:D:121:ILE:HD13	2.11	0.50
1:A:99:PRO:HB2	1:A:229:ARG:CD	2.42	0.50
3:R:17:ARG:HH21	3:R:78:THR:HG21	1.75	0.50
2:M:194:VAL:HG21	3:N:140:LEU:HD13	1.92	0.50
3:P:165:GLU:HG2	3:P:182:TYR:O	2.11	0.50
1:J:352:GLY:HA2	1:J:365:ALA:HA	1.93	0.50
3:2:50:ILE:HD13	3:2:75:LEU:HD13	1.92	0.50
1:H:183:HIS:HA	1:H:230:ILE:HD13	1.93	0.50
1:B:18:HIS:H	1:B:18:HIS:CD2	2.29	0.50
3:P:41:LEU:HB3	3:P:42:PRO:HD2	1.93	0.50
1:F:436:THR:O	1:F:440:THR:HG23	2.11	0.50
3:V:120:VAL:O	3:V:209:LYS:HG3	2.11	0.50
1:D:295:GLN:NE2	1:D:308:TYR:HB2	2.26	0.50
2:U:180:PRO:O	3:V:167:THR:HG21	2.11	0.50
2:O:50:TRP:CH2	2:O:52:ASN:HB2	2.46	0.50
2:W:108:PHE:CB	2:W:111:TYR:HE2	2.24	0.50
2:W:34:LEU:CD2	2:W:35:SER:H	2.24	0.50
2:W:29:LEU:N	2:W:29:LEU:HD23	2.26	0.50
2:5:29:LEU:HD21	2:5:77:ASN:HA	1.92	0.50
1:A:325:GLU:HG2	1:A:326:LYS:N	2.26	0.50
1:D:325:GLU:HG2	1:D:326:LYS:N	2.26	0.50
2:1:60:TYR:CE1	2:1:70:MET:HG2	2.40	0.50
2:1:91:THR:HB	2:1:124:VAL:N	2.26	0.50
1:G:380:LYS:HG2	1:I:29:ILE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:ILE:CD1	1:G:354:ARG:HB3	2.41	0.50
1:D:208:ARG:CZ	1:D:238:LYS:HD2	2.42	0.50
2:M:44:GLY:C	2:M:45:LEU:HD23	2.30	0.50
3:0:135:ALA:O	3:0:184:SER:HB2	2.11	0.50
3:2:137:LEU:HD11	3:2:190:TRP:HZ3	1.76	0.50
1:C:376:GLN:HB3	1:C:439:LEU:HD11	1.93	0.50
3:8:17:ARG:HA	3:8:77:ILE:O	2.11	0.50
3:2:17:ARG:HH21	3:2:78:THR:HG21	1.75	0.50
3:2:197:SER:HB3	3:2:210:THR:OG1	2.11	0.50
3:T:196:TYR:O	3:T:210:THR:HG23	2.11	0.50
3:Z:17:ARG:HH21	3:Z:78:THR:HG21	1.75	0.50
3:P:17:ARG:HH21	3:P:78:THR:HG21	1.76	0.50
1:C:179:ILE:O	1:C:254:PRO:HB3	2.12	0.50
1:E:280:GLU:HB2	1:E:290:ASN:ND2	2.26	0.50
2:U:179:PHE:CD1	3:V:140:LEU:HD22	2.46	0.50
2:U:99:VAL:HA	2:U:111:TYR:CD1	2.46	0.50
2:1:100:GLU:O	2:1:102:VAL:N	2.44	0.50
2:M:100:GLU:N	2:M:111:TYR:HB2	2.14	0.50
2:3:206:THR:HG22	2:3:207:TYR:N	2.26	0.50
2:5:148:THR:C	2:5:199:SER:HB2	2.32	0.50
2:S:83:MET:HB3	2:S:86:LEU:CD2	2.42	0.50
2:9:159:PHE:HB2	2:9:188:LEU:HD22	1.94	0.50
2:Y:112:PRO:HA	3:Z:36:HIS:CD2	2.46	0.50
1:A:190:GLU:O	1:A:194:LEU:HD13	2.12	0.50
3:6:7:PRO:HG2	3:6:106:THR:CG2	2.41	0.50
2:Q:112:PRO:HB2	3:R:51:SER:HB2	1.92	0.50
2:9:151:LEU:HB3	2:9:224:VAL:HG11	1.94	0.50
2:1:151:LEU:HB3	2:1:224:VAL:HG11	1.94	0.50
1:A:148:PHE:CB	1:A:151:LEU:HB2	2.40	0.50
1:H:457:GLU:HG3	1:H:499:ARG:NH1	2.25	0.50
1:E:102:VAL:HG11	1:E:108:LEU:HD23	1.93	0.50
1:A:85:ASP:O	1:A:265:SER:HA	2.12	0.50
1:K:27:LYS:HD3	1:L:383:ARG:CZ	2.42	0.50
2:S:27:TYR:O	2:S:98:ARG:NH2	2.44	0.50
3:0:17:ARG:HH21	3:0:78:THR:CG2	2.24	0.50
3:8:35:VAL:HG13	3:8:92:SER:HB2	1.93	0.50
3:4:118:PRO:HB3	3:4:141:ILE:HG23	1.93	0.50
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.46	0.50
3:0:138:VAL:HG13	3:0:182:TYR:CE1	2.46	0.50
3:0:50:ILE:HD13	3:0:75:LEU:HD13	1.93	0.50
3:2:142:SER:O	3:2:143:ASP:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:100:GLU:N	2:7:111:TYR:HB2	2.16	0.50
2:5:34:LEU:CD2	2:5:35:SER:H	2.24	0.50
2:M:148:THR:C	2:M:199:SER:HB2	2.31	0.50
2:9:11:VAL:HG22	2:9:123:THR:OG1	2.11	0.50
1:A:108:LEU:O	1:A:112:VAL:HG23	2.11	0.50
3:Z:126:SER:OG	3:Z:129:GLU:HB2	2.12	0.50
1:L:457:GLU:HG3	1:L:499:ARG:NH1	2.27	0.50
1:L:495:ALA:O	1:L:499:ARG:HG3	2.12	0.50
1:I:85:ASP:O	1:I:265:SER:HA	2.11	0.50
2:U:44:GLY:C	2:U:45:LEU:HD23	2.31	0.50
3:R:138:VAL:HG13	3:R:182:TYR:CE1	2.47	0.50
3:6:41:LEU:HB3	3:6:42:PRO:HD2	1.92	0.50
1:B:298:ASN:OD1	1:B:300:ILE:N	2.37	0.50
3:6:118:PRO:HB3	3:6:141:ILE:HG23	1.94	0.50
1:K:463:GLY:HA2	1:L:453:ARG:HD3	1.93	0.50
1:A:123:GLU:OE1	1:A:168:MET:HG2	2.11	0.50
3:T:120:VAL:O	3:T:209:LYS:HG3	2.12	0.50
2:W:83:MET:HB3	2:W:86:LEU:CD2	2.41	0.50
3:X:12:GLY:N	3:X:111:LEU:HD13	2.26	0.50
2:7:38:ARG:HB3	2:7:94:TYR:HE1	1.77	0.50
2:7:4:LEU:HD11	2:7:115:VAL:O	2.11	0.50
1:K:247:SER:HB3	1:K:251:LEU:HD22	1.93	0.50
1:A:191:GLN:NE2	1:A:217:ILE:HD11	2.22	0.50
1:F:192:THR:HG22	1:F:198:ALA:HB2	1.93	0.50
1:K:381:LEU:O	1:K:385:ILE:HG13	2.11	0.50
2:Q:36:TRP:NE1	2:Q:70:MET:HE1	2.27	0.50
1:L:251:LEU:HD12	1:L:252:ILE:H	1.76	0.50
2:Q:44:GLY:C	2:Q:45:LEU:HD23	2.32	0.50
1:G:384:VAL:CG1	1:G:385:ILE:HG23	2.40	0.50
3:X:7:PRO:HG2	3:X:106:THR:CG2	2.40	0.50
3:Z:137:LEU:HD11	3:Z:190:TRP:HZ3	1.77	0.50
2:3:151:LEU:HB3	2:3:224:VAL:HG11	1.94	0.50
1:F:61:GLY:O	1:F:64:CYS:HB2	2.12	0.50
3:Z:135:ALA:O	3:Z:184:SER:HB2	2.11	0.50
3:2:137:LEU:HB3	3:2:153:TRP:CH2	2.46	0.50
2:W:27:TYR:O	2:W:98:ARG:NH2	2.45	0.50
3:T:64:PHE:CD1	3:T:77:ILE:HG12	2.47	0.50
3:0:165:GLU:HG2	3:0:182:TYR:O	2.12	0.50
3:X:64:PHE:CD1	3:X:77:ILE:HG12	2.47	0.50
1:D:436:THR:O	1:D:440:THR:HG23	2.10	0.50
1:K:431:LEU:O	1:K:435:HIS:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:HIS:H	1:F:18:HIS:CD2	2.29	0.50
1:D:463:GLY:HA2	1:E:453:ARG:HD3	1.94	0.50
2:W:68:VAL:O	2:W:69:THR:HG23	2.12	0.50
2:O:142:LYS:HE2	2:O:144:THR:HG22	1.94	0.50
2:O:37:VAL:HG22	2:O:47:TRP:HA	1.94	0.50
2:Q:50:TRP:CH2	2:Q:52:ASN:HB2	2.47	0.50
2:1:33:GLY:HA3	2:1:99:VAL:CG2	2.28	0.50
4:H:601:NAG:H61	4:H:602:NAG:O7	2.12	0.50
2:S:100:GLU:O	2:S:102:VAL:N	2.45	0.50
2:Q:83:MET:HB3	2:Q:86:LEU:CD2	2.41	0.50
1:E:326:LYS:NZ	1:E:341:ASN:HD22	2.10	0.50
2:1:159:PHE:HB2	2:1:188:LEU:HD22	1.94	0.50
2:7:159:PHE:HB2	2:7:188:LEU:HD22	1.94	0.50
1:K:409:LEU:HD11	1:L:413:VAL:HG21	1.92	0.50
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.46	0.50
1:E:208:ARG:CZ	1:E:238:LYS:HD2	2.41	0.50
2:1:210:ASN:HA	2:1:221:ASP:OD1	2.12	0.50
3:V:165:GLU:HG2	3:V:182:TYR:O	2.11	0.50
1:H:353:PHE:CE1	1:H:366:ASP:HB2	2.46	0.50
3:4:135:ALA:O	3:4:184:SER:HB2	2.11	0.50
3:2:135:ALA:O	3:2:184:SER:HB2	2.12	0.50
2:W:112:PRO:HA	3:X:36:HIS:CD2	2.45	0.50
3:8:165:GLU:HG2	3:8:182:TYR:O	2.11	0.50
1:H:170:ASN:ND2	1:H:239:PRO:HA	2.27	0.50
3:4:196:TYR:O	3:4:210:THR:HG23	2.12	0.50
1:B:295:GLN:NE2	1:B:308:TYR:HB2	2.26	0.50
1:G:170:ASN:ND2	1:G:239:PRO:HA	2.26	0.50
1:L:123:GLU:OE1	1:L:168:MET:HG2	2.12	0.50
3:V:50:ILE:HD13	3:V:75:LEU:HD13	1.92	0.50
3:T:35:VAL:HG13	3:T:92:SER:HB2	1.93	0.50
1:H:138:ALA:HB2	1:H:226:LEU:HD12	1.94	0.50
2:3:137:LEU:HD11	3:4:138:VAL:HG21	1.93	0.50
1:B:423:TYR:CZ	1:B:427:LEU:HD22	2.47	0.50
2:9:108:PHE:CD2	2:9:108:PHE:N	2.73	0.50
2:O:98:ARG:O	2:O:113:MET:HA	2.11	0.50
2:O:27:TYR:O	2:O:98:ARG:NH2	2.44	0.50
2:Y:108:PHE:CB	2:Y:111:TYR:HE2	2.24	0.50
2:O:29:LEU:HD23	2:O:29:LEU:N	2.25	0.50
2:3:10:GLU:OE1	2:3:18:VAL:HG13	2.11	0.50
1:A:326:LYS:NZ	1:A:341:ASN:ND2	2.60	0.50
2:O:159:PHE:HB2	2:O:188:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:6:GLN:HE21	2:M:117:GLY:CA	2.22	0.50
2:S:60:TYR:CE1	2:S:70:MET:HG2	2.40	0.50
1:E:156:LYS:HD2	1:E:196:VAL:CG2	2.40	0.50
1:F:316:LEU:HD12	1:F:317:ALA:N	2.26	0.50
1:K:338:PHE:CG	1:K:339:ILE:N	2.80	0.50
3:P:137:LEU:HB3	3:P:153:TRP:HH2	1.76	0.50
2:Y:151:LEU:HB3	2:Y:224:VAL:HG11	1.94	0.50
2:3:210:ASN:HA	2:3:221:ASP:OD1	2.11	0.50
1:I:470:TYR:CG	1:I:499:ARG:HG2	2.46	0.50
1:L:327:GLN:HG3	1:L:329:ARG:NE	2.26	0.50
1:K:426:GLU:HG3	1:L:383:ARG:HH22	1.77	0.50
3:4:35:VAL:HG13	3:4:92:SER:HB2	1.94	0.50
7:D:616:NAG:H61	7:D:617:BMA:H2	1.94	0.50
1:H:298:ASN:OD1	1:H:300:ILE:N	2.40	0.50
1:H:214:ILE:HD12	1:H:214:ILE:N	2.27	0.50
1:D:268:MET:HE1	1:D:282:ILE:HG22	1.94	0.50
1:H:96:ASN:HA	1:H:224:ARG:HH11	1.75	0.50
1:B:133:ASN:HB3	1:L:142:GLY:HA3	1.94	0.50
2:O:100:GLU:O	2:O:102:VAL:N	2.45	0.50
2:O:6:GLN:OE1	2:O:120:THR:HG23	2.11	0.50
2:1:29:LEU:CD2	2:1:77:ASN:HA	2.41	0.50
2:S:38:ARG:HB3	2:S:94:TYR:CE1	2.47	0.50
1:E:325:GLU:HG2	1:E:326:LYS:N	2.27	0.50
1:A:326:LYS:NZ	1:A:341:ASN:HD22	2.09	0.50
1:J:325:GLU:HG2	1:J:326:LYS:N	2.26	0.50
1:H:156:LYS:HD2	1:H:196:VAL:CG2	2.40	0.50
1:K:190:GLU:O	1:K:194:LEU:HD13	2.11	0.50
1:A:67:ILE:HG13	1:A:105:TYR:CE2	2.47	0.50
2:1:44:GLY:HA2	3:2:89:TYR:CZ	2.47	0.50
1:E:190:GLU:O	1:E:194:LEU:HD13	2.11	0.50
2:1:142:LYS:CE	2:1:144:THR:HG22	2.42	0.50
2:S:151:LEU:HB3	2:S:224:VAL:HG11	1.93	0.50
2:Y:38:ARG:HB3	2:Y:94:TYR:CE1	2.46	0.50
1:E:109:ARG:CZ	1:E:267:ILE:HD13	2.42	0.50
3:T:165:GLU:HG2	3:T:182:TYR:O	2.12	0.50
3:4:64:PHE:CD1	3:4:77:ILE:HG12	2.47	0.50
1:B:431:LEU:O	1:B:435:HIS:HB2	2.12	0.50
3:X:120:VAL:O	3:X:209:LYS:HG3	2.11	0.50
7:G:616:NAG:H61	7:G:617:BMA:H2	1.94	0.50
1:F:352:GLY:HA2	1:F:365:ALA:HA	1.94	0.50
1:F:414:GLU:O	1:F:418:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:33:GLY:HA3	2:9:99:VAL:CG2	2.31	0.50
3:4:172:GLN:HB2	3:4:176:LYS:HD2	1.93	0.50
2:O:108:PHE:CB	2:O:111:TYR:HE2	2.25	0.50
3:X:167:THR:HG22	3:X:180:SER:O	2.12	0.50
3:T:126:SER:OG	3:T:129:GLU:HB2	2.11	0.50
2:Q:108:PHE:CD2	2:Q:108:PHE:N	2.74	0.50
2:3:102:VAL:HG12	2:3:103:ARG:H	1.77	0.50
2:O:38:ARG:HB3	2:O:94:TYR:CE1	2.47	0.50
2:7:6:GLN:HB3	2:7:120:THR:CG2	2.33	0.50
1:E:167:THR:HB	6:E:609:NAG:H61	1.93	0.50
1:E:17:HIS:HB2	1:E:320:MET:HE1	1.94	0.50
1:D:383:ARG:HD3	1:F:27:LYS:HZ3	1.72	0.50
2:O:60:TYR:CE1	2:O:70:MET:HG2	2.39	0.50
2:W:22:CYS:HB2	2:W:36:TRP:HH2	1.76	0.50
1:D:338:PHE:CG	1:D:339:ILE:N	2.79	0.50
1:L:324:PRO:O	1:L:325:GLU:HB3	2.11	0.50
1:L:326:LYS:NZ	1:L:341:ASN:ND2	2.60	0.50
1:A:430:ALA:HB2	1:B:383:ARG:HH21	1.77	0.50
1:G:61:GLY:HA2	1:G:79:PHE:CZ	2.47	0.50
3:6:137:LEU:HB3	3:6:153:TRP:HH2	1.76	0.50
1:H:470:TYR:CG	1:H:499:ARG:HG2	2.47	0.50
1:B:208:ARG:CZ	1:B:238:LYS:HD2	2.42	0.50
3:V:164:VAL:HG12	3:V:164:VAL:O	2.12	0.50
1:C:99:PRO:HB3	1:C:223:VAL:HG21	1.94	0.50
1:A:495:ALA:O	1:A:499:ARG:HG3	2.12	0.50
1:B:457:GLU:HG3	1:B:499:ARG:NH1	2.27	0.50
3:X:135:ALA:O	3:X:184:SER:HB2	2.11	0.50
1:D:327:GLN:HG3	1:D:329:ARG:NE	2.27	0.50
1:H:120:PHE:O	1:H:121:ILE:HD13	2.12	0.50
1:F:421:TRP:HA	1:F:424:ASN:HD22	1.77	0.50
3:P:64:PHE:CD1	3:P:77:ILE:HG12	2.46	0.50
3:4:138:VAL:HG13	3:4:182:TYR:CE1	2.47	0.50
2:W:180:PRO:HG2	3:X:170:SER:OG	2.12	0.50
2:W:33:GLY:HA3	2:W:99:VAL:CG2	2.28	0.49
2:S:99:VAL:HB	2:S:111:TYR:CZ	2.47	0.49
2:O:29:LEU:HD21	2:O:77:ASN:HA	1.94	0.49
2:U:2:VAL:HG23	2:U:115:VAL:HG11	1.93	0.49
2:Y:6:GLN:HB2	2:Y:118:GLN:OE1	2.11	0.49
2:O:152:GLY:HA2	2:O:167:TRP:CH2	2.47	0.49
1:I:156:LYS:HD2	1:I:196:VAL:CG2	2.42	0.49
1:J:102:VAL:HG11	1:J:108:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:17:HIS:HA	1:L:350:TRP:O	2.12	0.49
3:T:137:LEU:HB3	3:T:153:TRP:HH2	1.77	0.49
3:X:137:LEU:HB3	3:X:153:TRP:HH2	1.76	0.49
1:A:335:ILE:CD1	1:A:354:ARG:HB3	2.42	0.49
1:B:335:ILE:HD11	1:B:354:ARG:HB3	1.92	0.49
1:I:457:GLU:HG3	1:I:499:ARG:NH1	2.27	0.49
1:L:427:LEU:O	1:L:431:LEU:HD12	2.12	0.49
1:H:99:PRO:HB3	1:H:223:VAL:HG21	1.94	0.49
3:N:17:ARG:HH21	3:N:78:THR:CG2	2.25	0.49
2:7:142:LYS:CE	2:7:144:THR:HG22	2.42	0.49
1:J:243:LEU:HD12	1:J:244:VAL:H	1.77	0.49
3:0:41:LEU:HB3	3:0:42:PRO:HD2	1.94	0.49
7:F:616:NAG:H61	7:F:617:BMA:H2	1.94	0.49
1:F:173:ASN:HA	2:U:75:GLY:HA3	1.94	0.49
3:2:118:PRO:HB3	3:2:141:ILE:HG23	1.94	0.49
1:D:123:GLU:OE1	1:D:168:MET:HG2	2.11	0.49
2:3:6:GLN:HB3	2:3:120:THR:HG23	1.94	0.49
2:O:7:SER:O	2:O:120:THR:HG22	2.12	0.49
2:U:148:THR:C	2:U:199:SER:HB2	2.32	0.49
1:E:426:GLU:HG3	1:F:383:ARG:NH2	2.27	0.49
2:S:4:LEU:HD11	2:S:115:VAL:O	2.12	0.49
1:I:103:PRO:HD2	1:I:232:ILE:O	2.13	0.49
1:H:61:GLY:HA2	1:H:79:PHE:CZ	2.46	0.49
1:C:381:LEU:O	1:C:385:ILE:HG13	2.11	0.49
2:7:151:LEU:HB3	2:7:224:VAL:HG11	1.94	0.49
1:H:495:ALA:O	1:H:499:ARG:HG3	2.11	0.49
2:O:151:LEU:HB3	2:O:224:VAL:HG11	1.95	0.49
1:A:120:PHE:O	1:A:121:ILE:HD13	2.11	0.49
3:N:197:SER:HB3	3:N:210:THR:OG1	2.11	0.49
2:Y:184:GLN:HA	3:Z:165:GLU:OE1	2.12	0.49
3:4:197:SER:HB3	3:4:210:THR:OG1	2.12	0.49
1:J:170:ASN:ND2	1:J:239:PRO:HA	2.26	0.49
3:Z:38:TYR:HE2	3:Z:48:LEU:HD13	1.77	0.49
1:I:280:GLU:HB2	1:I:290:ASN:ND2	2.27	0.49
3:V:41:LEU:HB3	3:V:42:PRO:HD2	1.95	0.49
1:G:169:PRO:HA	1:G:242:VAL:HG23	1.93	0.49
2:U:142:LYS:CE	2:U:144:THR:HG22	2.42	0.49
3:N:172:GLN:CB	3:N:176:LYS:HD2	2.41	0.49
2:O:102:VAL:HG12	2:O:103:ARG:H	1.77	0.49
2:Y:102:VAL:HG12	2:Y:103:ARG:H	1.76	0.49
2:3:34:LEU:CD2	2:3:35:SER:H	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:102:VAL:HG12	2:1:103:ARG:H	1.77	0.49
1:L:331:LEU:CD2	1:L:331:LEU:H	2.07	0.49
1:D:324:PRO:O	1:D:325:GLU:HB3	2.11	0.49
1:I:161:TYR:HB2	1:I:196:VAL:CG2	2.41	0.49
1:C:338:PHE:CG	1:C:339:ILE:N	2.80	0.49
1:K:37:THR:CG2	1:K:322:ASN:HB2	2.42	0.49
1:J:208:ARG:CZ	1:J:238:LYS:HD2	2.43	0.49
3:V:64:PHE:HD1	3:V:77:ILE:HG12	1.78	0.49
1:A:99:PRO:HB3	1:A:223:VAL:HG21	1.95	0.49
3:V:197:SER:HB3	3:V:210:THR:OG1	2.12	0.49
3:P:138:VAL:HG13	3:P:182:TYR:CE1	2.47	0.49
2:7:142:LYS:HE2	2:7:144:THR:HG22	1.94	0.49
1:E:152:ASN:HB2	1:E:255:ARG:NH1	2.27	0.49
3:Z:41:LEU:HB3	3:Z:42:PRO:HD2	1.94	0.49
7:J:616:NAG:H61	7:J:617:BMA:H2	1.94	0.49
1:L:134:GLY:HA3	1:L:153:TRP:HB3	1.94	0.49
3:6:120:VAL:O	3:6:209:LYS:HG3	2.12	0.49
1:D:298:ASN:OD1	1:D:300:ILE:N	2.39	0.49
1:G:212:THR:HG21	1:I:216:ASN:HB3	1.94	0.49
7:A:616:NAG:H61	7:A:617:BMA:H2	1.94	0.49
2:9:44:GLY:HA2	3:0:89:TYR:CZ	2.47	0.49
2:O:34:LEU:CD2	2:O:35:SER:H	2.25	0.49
2:U:50:TRP:CH2	2:U:52:ASN:HB2	2.47	0.49
2:7:108:PHE:O	2:7:111:TYR:CD2	2.65	0.49
2:W:34:LEU:HD22	2:W:35:SER:N	2.27	0.49
2:3:100:GLU:O	2:3:102:VAL:N	2.45	0.49
2:5:108:PHE:CB	2:5:111:TYR:CE2	2.95	0.49
2:S:206:THR:HG21	2:S:223:LYS:CE	2.33	0.49
2:Q:29:LEU:CD2	2:Q:77:ASN:HA	2.42	0.49
1:B:325:GLU:HG2	1:B:326:LYS:N	2.26	0.49
1:D:247:SER:HB3	1:D:251:LEU:HD22	1.94	0.49
1:K:191:GLN:NE2	1:K:217:ILE:HD11	2.24	0.49
1:E:220:ARG:HB2	1:E:221:PRO:HD2	1.92	0.49
1:L:67:ILE:HG13	1:L:105:TYR:CE2	2.47	0.49
1:D:221:PRO:HG2	1:E:206:THR:C	2.32	0.49
1:E:67:ILE:HG13	1:E:105:TYR:CE2	2.48	0.49
3:N:26:SER:N	3:N:29:ILE:HD12	2.28	0.49
1:J:470:TYR:CG	1:J:499:ARG:HG2	2.48	0.49
3:R:135:ALA:O	3:R:184:SER:HB2	2.13	0.49
3:8:64:PHE:CD1	3:8:77:ILE:HG12	2.47	0.49
3:2:64:PHE:CD1	3:2:77:ILE:HG12	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:17:ARG:HA	3:2:77:ILE:O	2.13	0.49
1:I:427:LEU:O	1:I:431:LEU:HD12	2.12	0.49
1:C:180:TRP:CE2	1:C:204:VAL:HG21	2.48	0.49
3:P:35:VAL:HG13	3:P:92:SER:HB2	1.93	0.49
3:N:118:PRO:HB3	3:N:141:ILE:HG23	1.94	0.49
3:8:91:GLN:HB2	3:8:102:PHE:HE2	1.78	0.49
1:K:138:ALA:HB2	1:K:226:LEU:HD12	1.93	0.49
3:T:41:LEU:HB3	3:T:42:PRO:HD2	1.93	0.49
2:O:180:PRO:HG2	3:P:170:SER:OG	2.12	0.49
2:Y:142:LYS:HE2	2:Y:144:THR:HG22	1.94	0.49
1:C:138:ALA:HB2	1:C:226:LEU:HD12	1.92	0.49
2:S:179:PHE:CD1	3:T:140:LEU:HD22	2.47	0.49
2:7:50:TRP:CH2	2:7:52:ASN:HB2	2.48	0.49
2:Q:34:LEU:HD22	2:Q:35:SER:N	2.27	0.49
2:U:29:LEU:HD21	2:U:77:ASN:HA	1.94	0.49
2:O:206:THR:HG22	2:O:207:TYR:N	2.27	0.49
2:3:91:THR:CG2	2:3:124:VAL:H	2.26	0.49
2:1:10:GLU:OE1	2:1:18:VAL:HG13	2.12	0.49
1:H:324:PRO:O	1:H:325:GLU:HB3	2.12	0.49
1:G:191:GLN:NE2	1:G:217:ILE:HD11	2.23	0.49
1:E:401:GLU:HG3	1:F:238:LYS:CE	2.41	0.49
1:J:185:PRO:HA	1:J:190:GLU:OE2	2.13	0.49
2:M:152:GLY:HA2	2:M:167:TRP:CH2	2.48	0.49
1:I:102:VAL:HG11	1:I:108:LEU:HD23	1.93	0.49
2:1:36:TRP:NE1	2:1:70:MET:HE1	2.27	0.49
3:R:137:LEU:HD11	3:R:190:TRP:HZ3	1.77	0.49
2:Q:151:LEU:HB3	2:Q:224:VAL:HG11	1.94	0.49
1:K:62:ILE:HG13	1:K:63:ASP:N	2.26	0.49
1:K:470:TYR:CG	1:K:499:ARG:HG2	2.47	0.49
1:K:208:ARG:CZ	1:K:238:LYS:HD2	2.41	0.49
1:E:148:PHE:CB	1:E:151:LEU:HB2	2.42	0.49
1:K:327:GLN:HG3	1:K:329:ARG:NE	2.27	0.49
1:C:17:HIS:HB2	1:C:320:MET:HE1	1.94	0.49
1:B:37:THR:CG2	1:B:322:ASN:HB2	2.42	0.49
1:G:243:LEU:HD12	1:G:244:VAL:H	1.77	0.49
1:J:120:PHE:CD2	1:J:150:ARG:HD2	2.47	0.49
3:R:91:GLN:HB2	3:R:102:PHE:HE2	1.77	0.49
2:S:179:PHE:CZ	3:T:140:LEU:HB3	2.48	0.49
2:9:101:GLY:H	2:9:111:TYR:HB3	1.77	0.49
3:R:174:ASN:HD21	3:R:176:LYS:HB3	1.78	0.49
2:Q:34:LEU:HD23	2:Q:97:ALA:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:91:THR:HB	2:W:124:VAL:N	2.28	0.49
2:M:29:LEU:HD21	2:M:77:ASN:HA	1.94	0.49
2:Y:29:LEU:HD21	2:Y:77:ASN:HA	1.94	0.49
1:F:381:LEU:O	1:F:385:ILE:HG13	2.13	0.49
2:O:159:PHE:CD1	2:O:160:PRO:HA	2.48	0.49
2:Q:114:ASP:OD2	2:Q:115:VAL:HG23	2.13	0.49
2:Y:93:VAL:HA	2:Y:120:THR:O	2.12	0.49
1:E:197:GLN:CD	1:E:197:GLN:H	2.16	0.49
2:9:36:TRP:NE1	2:9:70:MET:HE1	2.27	0.49
1:F:321:ARG:HD2	1:F:437:ILE:HG23	1.94	0.49
1:I:338:PHE:CG	1:I:339:ILE:N	2.81	0.49
3:4:164:VAL:O	3:4:164:VAL:HG12	2.12	0.49
2:M:151:LEU:HB3	2:M:224:VAL:HG11	1.94	0.49
3:0:164:VAL:O	3:0:164:VAL:HG12	2.13	0.49
1:J:335:ILE:CD1	1:J:354:ARG:HB3	2.42	0.49
2:U:151:LEU:HB3	2:U:224:VAL:HG11	1.94	0.49
1:D:212:THR:HG21	1:F:216:ASN:CB	2.42	0.49
1:K:353:PHE:CE1	1:K:366:ASP:HB2	2.46	0.49
1:D:470:TYR:CG	1:D:499:ARG:HG2	2.48	0.49
3:Z:118:PRO:HB3	3:Z:141:ILE:HG23	1.94	0.49
2:5:142:LYS:CE	2:5:144:THR:HG22	2.42	0.49
7:K:616:NAG:H61	7:K:617:BMA:H2	1.94	0.49
1:L:471:HIS:HB2	1:L:494:GLU:OE1	2.12	0.49
2:U:99:VAL:HB	2:U:111:TYR:CE1	2.48	0.49
2:Y:97:ALA:HB1	2:Y:114:ASP:O	2.12	0.49
2:3:34:LEU:HD22	2:3:35:SER:N	2.28	0.49
2:M:108:PHE:CD2	2:M:108:PHE:N	2.74	0.49
2:7:206:THR:HG22	2:7:207:TYR:N	2.28	0.49
2:W:29:LEU:HD21	2:W:77:ASN:HA	1.93	0.49
2:W:206:THR:HG22	2:W:207:TYR:N	2.28	0.49
2:3:91:THR:CB	2:3:124:VAL:HG23	2.39	0.49
2:U:206:THR:HG22	2:U:207:TYR:N	2.28	0.49
2:1:159:PHE:CD1	2:1:160:PRO:HA	2.48	0.49
2:M:117:GLY:C	2:M:119:GLY:N	2.66	0.49
3:R:93:TYR:HD1	3:R:100:SER:HB3	1.78	0.49
1:F:99:PRO:HB3	1:F:223:VAL:HG21	1.95	0.49
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.48	0.49
1:G:148:PHE:CB	1:G:151:LEU:HB2	2.43	0.49
1:H:338:PHE:CG	1:H:339:ILE:N	2.81	0.49
1:H:108:LEU:O	1:H:112:VAL:HG23	2.11	0.49
2:1:142:LYS:HE2	2:1:144:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:THR:CG2	1:H:322:ASN:HB2	2.43	0.49
2:5:151:LEU:HB3	2:5:224:VAL:HG11	1.94	0.49
2:O:158:TYR:OH	2:O:191:LEU:HD23	2.13	0.49
2:U:210:ASN:HA	2:U:221:ASP:OD1	2.12	0.49
1:L:382:ASN:O	1:L:385:ILE:O	2.30	0.49
1:I:17:HIS:HA	1:I:350:TRP:O	2.13	0.49
3:N:165:GLU:HG2	3:N:182:TYR:O	2.13	0.49
3:Z:197:SER:HB3	3:Z:210:THR:OG1	2.12	0.49
2:Y:142:LYS:CE	2:Y:144:THR:HG22	2.42	0.49
7:I:616:NAG:H61	7:I:617:BMA:H2	1.95	0.49
3:R:118:PRO:HB3	3:R:141:ILE:HG23	1.93	0.49
1:C:436:THR:O	1:C:440:THR:HG23	2.13	0.49
3:N:50:ILE:HD13	3:N:75:LEU:HD13	1.95	0.49
1:E:84:TRP:CE2	1:E:116:GLY:HA2	2.47	0.49
3:R:120:VAL:O	3:R:209:LYS:HG3	2.13	0.49
1:A:197:GLN:CD	1:A:197:GLN:H	2.16	0.49
7:L:616:NAG:H61	7:L:617:BMA:H2	1.94	0.49
2:7:68:VAL:O	2:7:69:THR:HG23	2.11	0.49
1:G:134:GLY:HA3	1:G:153:TRP:HB3	1.93	0.49
1:G:123:GLU:OE1	1:G:168:MET:HG2	2.13	0.49
3:8:172:GLN:HB2	3:8:176:LYS:HD2	1.95	0.49
2:U:180:PRO:HG2	3:V:170:SER:OG	2.12	0.49
3:X:172:GLN:HB2	3:X:176:LYS:HD2	1.94	0.49
2:3:34:LEU:HD21	2:3:96:CYS:HB2	1.94	0.49
2:S:206:THR:HG22	2:S:207:TYR:N	2.28	0.49
2:Y:206:THR:HG22	2:Y:207:TYR:N	2.27	0.49
1:I:324:PRO:O	1:I:325:GLU:HB3	2.12	0.49
2:7:159:PHE:CD1	2:7:160:PRO:HA	2.48	0.49
1:F:335:ILE:CD1	1:F:354:ARG:HB3	2.42	0.49
1:A:338:PHE:CG	1:A:339:ILE:N	2.81	0.49
2:Y:152:GLY:HA2	2:Y:167:TRP:CH2	2.48	0.49
3:P:164:VAL:O	3:P:164:VAL:HG12	2.13	0.49
3:X:164:VAL:O	3:X:164:VAL:HG12	2.12	0.49
3:8:164:VAL:HG12	3:8:164:VAL:O	2.13	0.49
2:Y:91:THR:OG1	2:Y:123:THR:HA	2.13	0.49
1:D:37:THR:CG2	1:D:322:ASN:HB2	2.42	0.49
1:C:470:TYR:CG	1:C:499:ARG:HG2	2.48	0.49
3:6:26:SER:N	3:6:29:ILE:HD12	2.28	0.49
3:R:17:ARG:HA	3:R:77:ILE:O	2.13	0.49
3:N:17:ARG:HH21	3:N:78:THR:HG21	1.78	0.49
2:O:142:LYS:CE	2:O:144:THR:HG22	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:112:PRO:HB2	3:0:51:SER:HB2	1.93	0.49
1:H:352:GLY:HA2	1:H:365:ALA:HA	1.94	0.49
3:0:35:VAL:HG13	3:0:92:SER:HB2	1.94	0.49
1:F:234:TRP:HE3	1:F:234:TRP:H	1.55	0.49
1:I:18:HIS:CD2	1:I:18:HIS:H	2.30	0.49
3:2:113:GLN:HG3	3:2:175:ASN:HD21	1.76	0.49
4:L:601:NAG:H61	4:L:602:NAG:O7	2.13	0.49
2:O:108:PHE:O	2:O:111:TYR:CD2	2.66	0.49
2:U:35:SER:HB2	2:U:47:TRP:HE1	1.77	0.49
2:Q:108:PHE:O	2:Q:111:TYR:CD2	2.66	0.49
2:M:34:LEU:HD21	2:M:96:CYS:HB2	1.94	0.49
2:1:206:THR:HG22	2:1:207:TYR:N	2.28	0.49
2:M:10:GLU:OE1	2:M:18:VAL:HG13	2.13	0.49
1:C:325:GLU:HG2	1:C:326:LYS:N	2.26	0.49
1:H:326:LYS:NZ	1:H:341:ASN:ND2	2.61	0.49
2:Y:6:GLN:H	2:Y:118:GLN:HE22	1.60	0.49
1:I:271:ASP:C	2:3:105:VAL:HG23	2.32	0.49
1:J:148:PHE:CB	1:J:151:LEU:HB2	2.42	0.49
1:I:108:LEU:O	1:I:112:VAL:HG23	2.13	0.49
1:H:247:SER:HB3	1:H:251:LEU:HD22	1.94	0.49
2:M:112:PRO:HA	3:N:36:HIS:CD2	2.48	0.49
1:K:335:ILE:HD11	1:K:354:ARG:HB3	1.94	0.49
3:P:137:LEU:HD11	3:P:190:TRP:HZ3	1.77	0.49
2:9:152:GLY:HA2	2:9:167:TRP:CH2	2.47	0.49
1:E:61:GLY:HA2	1:E:79:PHE:CZ	2.47	0.49
1:E:102:VAL:O	1:E:105:TYR:HB2	2.13	0.49
1:J:335:ILE:HD11	1:J:354:ARG:HB3	1.93	0.49
2:5:139:PRO:HB2	2:5:141:SER:O	2.13	0.49
3:T:135:ALA:O	3:T:184:SER:HB2	2.13	0.49
2:W:142:LYS:CE	2:W:144:THR:HG22	2.43	0.49
2:Q:154:LEU:HD21	3:R:136:THR:HG21	1.93	0.49
1:L:138:ALA:HB2	1:L:226:LEU:HD12	1.94	0.49
1:B:123:GLU:OE1	1:B:168:MET:HG2	2.12	0.49
3:2:165:GLU:HG2	3:2:182:TYR:O	2.13	0.49
3:2:41:LEU:HB3	3:2:42:PRO:HD2	1.93	0.49
1:C:72:GLY:HA3	1:C:149:SER:OG	2.12	0.49
1:L:280:GLU:HB2	1:L:290:ASN:ND2	2.27	0.49
2:W:100:GLU:O	2:W:102:VAL:N	2.46	0.49
2:W:108:PHE:O	2:W:111:TYR:CD2	2.65	0.49
2:Y:100:GLU:O	2:Y:102:VAL:N	2.46	0.49
2:3:114:ASP:OD2	2:3:115:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:102:VAL:HG12	2:S:103:ARG:H	1.77	0.49
2:M:34:LEU:CD2	2:M:35:SER:H	2.26	0.49
2:M:206:THR:HG22	2:M:207:TYR:N	2.28	0.49
2:Q:206:THR:HG22	2:Q:207:TYR:N	2.27	0.49
2:3:92:ALA:O	2:3:122:VAL:HG22	2.13	0.49
1:E:326:LYS:NZ	1:E:341:ASN:ND2	2.60	0.49
1:G:325:GLU:HG2	1:G:326:LYS:N	2.28	0.49
1:I:148:PHE:CB	1:I:151:LEU:HB2	2.42	0.49
1:C:183:HIS:HA	1:C:230:ILE:HD13	1.95	0.49
1:J:161:TYR:CZ	1:J:249:GLY:HA2	2.48	0.49
2:1:91:THR:HA	2:1:122:VAL:HG23	1.95	0.49
2:W:44:GLY:C	2:W:45:LEU:HD23	2.32	0.49
3:8:135:ALA:O	3:8:184:SER:HB2	2.13	0.49
3:Z:37:TRP:HB2	3:Z:50:ILE:HG13	1.95	0.49
1:D:405:ARG:HH21	1:E:399:PHE:HE2	1.60	0.49
2:U:142:LYS:HE2	2:U:144:THR:HG22	1.94	0.49
3:2:138:VAL:HG13	3:2:182:TYR:CE1	2.48	0.49
2:3:142:LYS:HE2	2:3:144:THR:HG22	1.95	0.49
3:0:38:TYR:HE2	3:0:48:LEU:HD13	1.77	0.49
1:G:138:ALA:HB2	1:G:226:LEU:HD12	1.95	0.49
2:1:179:PHE:CE2	3:2:142:SER:HB3	2.48	0.48
3:0:172:GLN:HB2	3:0:176:LYS:HD2	1.94	0.48
2:Q:100:GLU:O	2:Q:102:VAL:N	2.46	0.48
2:Y:2:VAL:HG21	2:Y:115:VAL:HG21	1.95	0.48
2:S:108:PHE:O	2:S:111:TYR:CD2	2.66	0.48
2:S:33:GLY:HA3	2:S:99:VAL:CG2	2.27	0.48
1:J:187:THR:CB	1:J:189:GLN:HE21	2.16	0.48
6:D:610:NAG:H62	1:F:222:TRP:HB2	1.94	0.48
1:K:326:LYS:NZ	1:K:341:ASN:HD22	2.11	0.48
1:F:326:LYS:CD	1:F:328:THR:H	2.25	0.48
1:B:99:PRO:HB3	1:B:223:VAL:HG21	1.94	0.48
1:F:213:ILE:HG13	1:F:233:TYR:CE2	2.48	0.48
2:M:109:HIS:HA	3:N:93:TYR:CD1	2.48	0.48
3:R:164:VAL:O	3:R:164:VAL:HG12	2.13	0.48
3:N:137:LEU:HB3	3:N:153:TRP:HH2	1.78	0.48
3:4:93:TYR:HD1	3:4:100:SER:HB3	1.76	0.48
2:W:151:LEU:HB3	2:W:224:VAL:HG11	1.95	0.48
1:C:102:VAL:O	1:C:105:TYR:HB2	2.12	0.48
1:E:247:SER:HB3	1:E:251:LEU:HD22	1.93	0.48
1:J:37:THR:CG2	1:J:322:ASN:HB2	2.43	0.48
1:G:272:ALA:HA	2:Y:105:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:120:PHE:O	1:L:121:ILE:HD13	2.13	0.48
3:T:138:VAL:HG13	3:T:182:TYR:CE1	2.48	0.48
3:X:17:ARG:HH21	3:X:78:THR:CG2	2.26	0.48
1:B:487:ASP:OD2	1:B:490:VAL:HG23	2.13	0.48
1:D:352:GLY:HA2	1:D:365:ALA:HA	1.95	0.48
1:G:352:GLY:HA2	1:G:365:ALA:HA	1.95	0.48
3:T:172:GLN:HB2	3:T:176:LYS:HD2	1.94	0.48
3:O:174:ASN:HD21	3:O:176:LYS:HB3	1.78	0.48
2:9:108:PHE:O	2:9:111:TYR:CD2	2.65	0.48
3:V:172:GLN:HB2	3:V:176:LYS:HD2	1.94	0.48
2:7:27:TYR:O	2:7:98:ARG:NH2	2.46	0.48
2:Y:108:PHE:O	2:Y:111:TYR:CD2	2.66	0.48
2:5:102:VAL:HG12	2:5:103:ARG:H	1.77	0.48
2:Y:17:SER:HA	2:Y:86:LEU:HG	1.95	0.48
2:1:17:SER:HA	2:1:86:LEU:HG	1.95	0.48
1:I:335:ILE:HG12	1:I:354:ARG:HB3	1.94	0.48
1:F:327:GLN:HG3	1:F:329:ARG:NE	2.28	0.48
1:F:99:PRO:HB2	1:F:229:ARG:HD3	1.95	0.48
1:J:338:PHE:CG	1:J:339:ILE:N	2.81	0.48
1:J:409:LEU:HD11	1:K:413:VAL:HG21	1.95	0.48
1:J:405:ARG:HD3	1:K:406:ILE:HG21	1.95	0.48
1:F:338:PHE:CG	1:F:339:ILE:N	2.81	0.48
1:D:197:GLN:CD	1:D:197:GLN:H	2.16	0.48
1:G:103:PRO:HD2	1:G:232:ILE:O	2.13	0.48
3:R:137:LEU:HB3	3:R:153:TRP:HH2	1.77	0.48
2:Y:158:TYR:OH	2:Y:191:LEU:HD23	2.13	0.48
1:C:102:VAL:HG11	1:C:108:LEU:HD23	1.95	0.48
1:H:62:ILE:HG13	1:H:63:ASP:N	2.27	0.48
3:2:137:LEU:HB3	3:2:153:TRP:HH2	1.78	0.48
3:R:64:PHE:CD1	3:R:77:ILE:HG12	2.48	0.48
1:K:243:LEU:HD12	1:K:244:VAL:H	1.77	0.48
3:6:35:VAL:HG13	3:6:92:SER:HB2	1.95	0.48
2:U:179:PHE:CE2	3:V:142:SER:HB3	2.48	0.48
3:6:172:GLN:HB2	3:6:176:LYS:HD2	1.95	0.48
3:X:167:THR:CG2	3:X:180:SER:H	2.26	0.48
2:7:34:LEU:HD23	2:7:97:ALA:O	2.14	0.48
2:7:35:SER:HB2	2:7:47:TRP:HE1	1.77	0.48
4:F:601:NAG:H61	4:F:602:NAG:O7	2.13	0.48
3:X:38:TYR:HE2	3:X:48:LEU:HD13	1.78	0.48
2:5:100:GLU:O	2:5:102:VAL:N	2.46	0.48
2:S:94:TYR:HE2	2:S:122:VAL:HG21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:159:PHE:CD1	2:S:160:PRO:HA	2.49	0.48
1:I:335:ILE:CD1	1:I:354:ARG:HB3	2.42	0.48
1:H:326:LYS:NZ	1:H:341:ASN:HD22	2.11	0.48
1:K:325:GLU:HG2	1:K:326:LYS:N	2.28	0.48
1:C:62:ILE:HG13	1:C:63:ASP:N	2.27	0.48
2:Y:22:CYS:HB2	2:Y:36:TRP:HH2	1.76	0.48
1:A:161:TYR:HB2	1:A:196:VAL:HG21	1.95	0.48
3:Z:164:VAL:O	3:Z:164:VAL:HG12	2.12	0.48
1:L:114:SER:HA	1:L:265:SER:O	2.13	0.48
1:B:335:ILE:CD1	1:B:354:ARG:HB3	2.42	0.48
3:R:167:THR:HG22	3:R:180:SER:O	2.13	0.48
3:8:167:THR:HG22	3:8:180:SER:O	2.13	0.48
1:D:381:LEU:O	1:D:385:ILE:HG13	2.13	0.48
1:L:423:TYR:CZ	1:L:427:LEU:HD22	2.47	0.48
2:3:68:VAL:O	2:3:69:THR:HG23	2.12	0.48
3:0:11:SER:HB3	3:0:111:LEU:CD1	2.43	0.48
1:G:44:GLN:OE1	1:G:289:PRO:HG2	2.14	0.48
3:8:118:PRO:HB3	3:8:141:ILE:HG23	1.95	0.48
1:E:138:ALA:HB2	1:E:226:LEU:HD12	1.94	0.48
2:Y:68:VAL:O	2:Y:69:THR:HG23	2.13	0.48
3:X:91:GLN:HB2	3:X:102:PHE:HE2	1.77	0.48
3:6:138:VAL:HG13	3:6:182:TYR:CE1	2.48	0.48
3:6:165:GLU:HG2	3:6:182:TYR:O	2.13	0.48
2:9:45:LEU:HB2	3:0:102:PHE:CE1	2.48	0.48
3:P:174:ASN:HD21	3:P:176:LYS:HB3	1.77	0.48
2:U:108:PHE:HB2	2:U:111:TYR:HE2	1.77	0.48
2:1:50:TRP:CH2	2:1:52:ASN:HB2	2.48	0.48
2:M:101:GLY:H	2:M:111:TYR:HB3	1.79	0.48
2:W:148:THR:HA	2:W:199:SER:N	2.27	0.48
2:Y:159:PHE:CD1	2:Y:160:PRO:HA	2.48	0.48
1:A:167:THR:HB	6:A:609:NAG:H61	1.94	0.48
2:M:91:THR:HB	2:M:124:VAL:HG23	1.95	0.48
1:D:251:LEU:HD12	1:D:252:ILE:N	2.28	0.48
2:W:36:TRP:NE1	2:W:70:MET:HE1	2.28	0.48
2:5:22:CYS:HB2	2:5:36:TRP:HH2	1.77	0.48
2:W:137:LEU:HB3	3:X:123:PHE:CD1	2.48	0.48
1:H:102:VAL:O	1:H:105:TYR:HB2	2.12	0.48
1:H:384:VAL:HG21	1:H:428:LEU:HD11	1.96	0.48
3:V:137:LEU:HB3	3:V:153:TRP:HH2	1.77	0.48
1:F:85:ASP:O	1:F:265:SER:HA	2.14	0.48
1:A:353:PHE:CE1	1:A:366:ASP:HB2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:381:LEU:O	1:L:385:ILE:HG13	2.13	0.48
2:7:44:GLY:C	2:7:45:LEU:HD23	2.33	0.48
1:H:423:TYR:CZ	1:H:427:LEU:HD22	2.47	0.48
3:R:197:SER:HB3	3:R:210:THR:OG1	2.14	0.48
3:6:64:PHE:CD1	3:6:77:ILE:HG12	2.47	0.48
3:P:64:PHE:HD1	3:P:77:ILE:HG12	1.79	0.48
1:H:180:TRP:CD2	1:H:204:VAL:HG21	2.49	0.48
2:1:62:LYS:CE	3:2:97:LEU:HD13	2.43	0.48
2:M:142:LYS:CE	2:M:144:THR:HG22	2.43	0.48
2:Q:68:VAL:O	2:Q:69:THR:HG23	2.13	0.48
2:O:101:GLY:H	2:O:111:TYR:HB3	1.77	0.48
2:Q:101:GLY:H	2:Q:111:TYR:HB3	1.79	0.48
2:Y:50:TRP:CH2	2:Y:52:ASN:HB2	2.48	0.48
2:1:206:THR:HG21	2:1:223:LYS:CE	2.33	0.48
6:D:610:NAG:H83	1:F:227:SER:HB2	1.94	0.48
1:H:325:GLU:HG2	1:H:326:LYS:N	2.27	0.48
1:I:190:GLU:O	1:I:194:LEU:HD13	2.13	0.48
1:E:27:LYS:HZ2	1:F:383:ARG:HD3	1.77	0.48
3:V:93:TYR:HD1	3:V:100:SER:HB3	1.78	0.48
1:H:190:GLU:O	1:H:194:LEU:HD13	2.14	0.48
1:G:197:GLN:H	1:G:197:GLN:CD	2.17	0.48
1:I:271:ASP:C	2:3:105:VAL:CG2	2.81	0.48
1:L:335:ILE:CD1	1:L:354:ARG:HB3	2.43	0.48
2:5:179:PHE:CD1	3:6:140:LEU:HD22	2.49	0.48
3:0:137:LEU:HB3	3:0:153:TRP:HH2	1.78	0.48
1:B:403:GLU:H	1:B:407:GLN:HE21	1.59	0.48
1:A:169:PRO:HA	1:A:242:VAL:HG23	1.94	0.48
1:I:382:ASN:O	1:I:385:ILE:O	2.32	0.48
1:H:427:LEU:O	1:H:431:LEU:HD12	2.13	0.48
2:U:27:TYR:O	2:U:98:ARG:NH2	2.46	0.48
3:4:17:ARG:HH21	3:4:78:THR:HG21	1.77	0.48
3:Z:17:ARG:HA	3:Z:77:ILE:O	2.14	0.48
2:3:142:LYS:CE	2:3:144:THR:HG22	2.43	0.48
1:A:44:GLN:OE1	1:A:289:PRO:HG2	2.13	0.48
1:C:352:GLY:HA2	1:C:365:ALA:HA	1.93	0.48
2:Q:142:LYS:HE2	2:Q:144:THR:HG22	1.96	0.48
1:I:352:GLY:HA2	1:I:365:ALA:HA	1.95	0.48
2:5:68:VAL:O	2:5:69:THR:HG23	2.13	0.48
3:Z:120:VAL:O	3:Z:209:LYS:HG3	2.14	0.48
2:1:68:VAL:O	2:1:69:THR:HG23	2.13	0.48
1:J:295:GLN:NE2	1:J:308:TYR:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:34:LEU:HD22	2:O:35:SER:N	2.28	0.48
2:W:177:HIS:NE2	3:X:172:GLN:CD	2.67	0.48
2:S:111:TYR:CE1	2:S:113:MET:HG2	2.46	0.48
2:M:100:GLU:O	2:M:102:VAL:N	2.46	0.48
2:5:206:THR:HG22	2:5:207:TYR:N	2.28	0.48
2:3:6:GLN:HB3	2:3:120:THR:CG2	2.44	0.48
2:9:17:SER:HA	2:9:86:LEU:HG	1.96	0.48
1:B:324:PRO:O	1:B:325:GLU:HB3	2.12	0.48
2:3:159:PHE:CD1	2:3:160:PRO:HA	2.49	0.48
1:C:324:PRO:O	1:C:325:GLU:HB3	2.12	0.48
1:J:324:PRO:O	1:J:325:GLU:HB3	2.12	0.48
1:E:222:TRP:CG	6:F:610:NAG:H5	2.48	0.48
2:Q:114:ASP:CG	2:Q:115:VAL:HG23	2.33	0.48
1:A:185:PRO:HA	1:A:190:GLU:OE2	2.12	0.48
1:D:27:LYS:HD3	1:E:383:ARG:NH1	2.29	0.48
1:K:380:LYS:HZ2	1:K:384:VAL:HG23	1.78	0.48
1:B:148:PHE:CB	1:B:151:LEU:HB2	2.44	0.48
3:2:164:VAL:HG12	3:2:164:VAL:O	2.13	0.48
1:J:403:GLU:CD	1:L:405:ARG:HH22	2.17	0.48
1:C:335:ILE:CD1	1:C:354:ARG:HB3	2.43	0.48
1:F:470:TYR:CG	1:F:499:ARG:HG2	2.48	0.48
1:C:37:THR:CG2	1:C:322:ASN:HB2	2.44	0.48
1:A:372:ALA:O	1:A:376:GLN:HG3	2.14	0.48
1:G:470:TYR:CG	1:G:499:ARG:HG2	2.48	0.48
2:Y:38:ARG:HB3	2:Y:94:TYR:HE1	1.78	0.48
2:5:142:LYS:HE2	2:5:144:THR:HG22	1.94	0.48
2:1:62:LYS:HE3	3:2:97:LEU:HD13	1.96	0.48
1:G:405:ARG:HD3	1:H:406:ILE:HG21	1.96	0.48
3:0:118:PRO:HB3	3:0:141:ILE:HG23	1.95	0.48
3:Z:35:VAL:HG13	3:Z:92:SER:HB2	1.94	0.48
3:V:118:PRO:HB3	3:V:141:ILE:HG23	1.96	0.48
1:F:183:HIS:HA	1:F:230:ILE:HD13	1.96	0.48
3:2:172:GLN:HB2	3:2:176:LYS:HD2	1.95	0.48
2:O:32:TYR:CD1	2:O:98:ARG:HD3	2.49	0.48
3:X:174:ASN:HD21	3:X:176:LYS:HB3	1.77	0.48
4:F:602:NAG:H81	2:W:55:ASP:OD1	2.13	0.48
2:3:108:PHE:O	2:3:111:TYR:CD2	2.67	0.48
4:D:602:NAG:H5	2:S:57:GLN:NE2	2.28	0.48
1:L:330:GLY:C	1:L:331:LEU:HD13	2.32	0.48
2:Q:148:THR:HA	2:Q:199:SER:N	2.29	0.48
2:Q:17:SER:HA	2:Q:86:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:38:ARG:HB3	2:9:94:TYR:CE1	2.49	0.48
1:F:190:GLU:O	1:F:194:LEU:HD13	2.14	0.48
1:C:326:LYS:NZ	1:C:341:ASN:HD22	2.11	0.48
1:I:325:GLU:HG2	1:I:326:LYS:N	2.29	0.48
1:L:190:GLU:O	1:L:194:LEU:HD13	2.13	0.48
2:7:152:GLY:HA2	2:7:167:TRP:CH2	2.49	0.48
1:I:192:THR:HG22	1:I:198:ALA:HB2	1.95	0.48
2:M:112:PRO:HB2	3:N:51:SER:HB2	1.96	0.48
1:J:103:PRO:HG2	1:J:233:TYR:CE1	2.48	0.48
3:N:164:VAL:O	3:N:164:VAL:HG12	2.14	0.48
3:P:93:TYR:HD1	3:P:100:SER:HB3	1.76	0.48
1:H:381:LEU:O	1:H:385:ILE:HG13	2.13	0.48
1:D:343:TRP:HB3	1:D:354:ARG:NH2	2.28	0.48
3:6:147:GLY:HA3	3:6:177:TYR:CG	2.49	0.48
1:A:457:GLU:HG3	1:A:499:ARG:NH1	2.28	0.48
1:H:234:TRP:N	1:H:234:TRP:CE3	2.78	0.48
3:X:196:TYR:O	3:X:210:THR:HG23	2.12	0.48
2:Q:38:ARG:HB3	2:Q:94:TYR:CE1	2.48	0.48
2:Q:27:TYR:O	2:Q:98:ARG:NH2	2.46	0.48
2:9:27:TYR:O	2:9:98:ARG:NH2	2.46	0.48
4:I:601:NAG:H61	4:I:602:NAG:O7	2.13	0.48
2:9:68:VAL:O	2:9:69:THR:HG23	2.14	0.48
3:T:38:TYR:HE2	3:T:48:LEU:HD13	1.79	0.48
1:E:18:HIS:H	1:E:18:HIS:CD2	2.31	0.48
1:L:18:HIS:CD2	1:L:18:HIS:H	2.32	0.48
2:1:116:TRP:CD1	2:1:116:TRP:N	2.81	0.48
2:U:68:VAL:O	2:U:69:THR:HG23	2.13	0.48
3:N:174:ASN:HD21	3:N:176:LYS:HB3	1.79	0.48
4:B:602:NAG:C5	2:O:57:GLN:HE22	2.19	0.48
2:U:108:PHE:O	2:U:111:TYR:CD2	2.66	0.48
2:Y:34:LEU:CD2	2:Y:35:SER:H	2.27	0.48
2:5:34:LEU:HD22	2:5:35:SER:N	2.28	0.48
1:F:380:LYS:HZ3	1:F:384:VAL:HG23	1.77	0.48
1:K:326:LYS:NZ	1:K:341:ASN:ND2	2.62	0.48
1:F:325:GLU:HG2	1:F:326:LYS:N	2.28	0.48
1:B:247:SER:HB3	1:B:251:LEU:HD22	1.96	0.48
1:E:338:PHE:CG	1:E:339:ILE:N	2.82	0.48
1:E:339:ILE:HG22	1:E:340:GLU:N	2.29	0.48
1:I:103:PRO:HG2	1:I:233:TYR:CE1	2.48	0.48
1:F:169:PRO:HA	1:F:242:VAL:HG23	1.94	0.48
1:B:108:LEU:O	1:B:112:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:167:THR:HG22	3:6:180:SER:O	2.14	0.48
1:G:403:GLU:H	1:G:407:GLN:HE21	1.58	0.48
2:S:158:TYR:OH	2:S:191:LEU:HD23	2.14	0.48
1:G:208:ARG:CZ	1:G:238:LYS:HD2	2.42	0.48
1:H:27:LYS:HD3	1:I:383:ARG:CZ	2.43	0.48
1:H:208:ARG:CZ	1:H:238:LYS:HD2	2.43	0.48
1:I:99:PRO:HB3	1:I:223:VAL:HG21	1.96	0.48
1:K:423:TYR:CZ	1:K:427:LEU:HD22	2.48	0.48
2:W:142:LYS:HE2	2:W:144:THR:HG22	1.95	0.48
1:L:280:GLU:HB2	1:L:290:ASN:HD21	1.78	0.48
3:2:120:VAL:O	3:2:209:LYS:HG3	2.13	0.48
3:V:35:VAL:HG13	3:V:92:SER:HB2	1.95	0.48
2:M:68:VAL:O	2:M:69:THR:HG23	2.13	0.48
1:D:453:ARG:HD3	1:F:463:GLY:HA2	1.96	0.48
1:E:352:GLY:HA2	1:E:365:ALA:HA	1.95	0.48
3:P:118:PRO:HB3	3:P:141:ILE:HG23	1.95	0.48
1:H:134:GLY:HA3	1:H:153:TRP:HB3	1.95	0.48
1:A:436:THR:O	1:A:440:THR:HG23	2.14	0.48
2:5:154:LEU:HD21	3:6:136:THR:HG21	1.96	0.48
3:Z:174:ASN:HD21	3:Z:176:LYS:HB3	1.78	0.48
2:O:108:PHE:H	2:O:108:PHE:HD2	1.58	0.48
2:Y:114:ASP:OD2	2:Y:115:VAL:HG23	2.14	0.48
2:1:148:THR:HA	2:1:199:SER:N	2.28	0.48
1:C:326:LYS:NZ	1:C:341:ASN:ND2	2.61	0.48
1:E:335:ILE:CD1	1:E:354:ARG:HB3	2.43	0.48
1:L:96:ASN:CA	1:L:224:ARG:HH11	2.26	0.48
1:E:120:PHE:O	1:E:121:ILE:HD13	2.13	0.48
2:W:32:TYR:CD1	2:W:98:ARG:HD3	2.48	0.48
2:1:27:TYR:O	2:1:98:ARG:NH2	2.46	0.48
3:0:17:ARG:HH21	3:0:78:THR:HG21	1.78	0.48
3:4:38:TYR:HE2	3:4:48:LEU:HD13	1.78	0.48
1:G:268:MET:CE	1:G:282:ILE:HG22	2.44	0.48
1:K:182:VAL:HG22	1:K:202:VAL:HG21	1.96	0.48
3:R:172:GLN:HB2	3:R:176:LYS:HD2	1.94	0.48
2:7:99:VAL:HA	2:7:111:TYR:CD1	2.49	0.48
2:M:2:VAL:HG21	2:M:115:VAL:HG21	1.96	0.48
2:W:82:GLU:OE2	2:W:84:LYS:HE2	2.14	0.48
2:5:10:GLU:OE1	2:5:18:VAL:HG13	2.13	0.48
2:5:17:SER:HA	2:5:86:LEU:HG	1.95	0.48
2:O:18:VAL:HG12	2:O:19:THR:H	1.79	0.48
2:U:10:GLU:OE1	2:U:18:VAL:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:11:VAL:HG13	2:M:123:THR:O	2.14	0.48
1:L:185:PRO:O	1:L:217:ILE:HA	2.14	0.48
2:3:60:TYR:CE1	2:3:70:MET:HG2	2.40	0.48
2:M:60:TYR:CE1	2:M:70:MET:HG2	2.41	0.48
1:G:338:PHE:CG	1:G:339:ILE:N	2.82	0.48
2:9:139:PRO:HB2	2:9:141:SER:O	2.14	0.48
3:T:163:GLY:O	3:T:183:LEU:HA	2.14	0.48
1:G:335:ILE:HG12	1:G:354:ARG:HB3	1.96	0.48
1:D:335:ILE:HD11	1:D:354:ARG:HB3	1.96	0.48
2:3:158:TYR:OH	2:3:191:LEU:HD23	2.14	0.48
3:R:147:GLY:HA3	3:R:177:TYR:CG	2.49	0.48
1:A:243:LEU:HD12	1:A:244:VAL:H	1.76	0.48
3:R:26:SER:N	3:R:29:ILE:HD12	2.29	0.48
1:I:327:GLN:HG3	1:I:329:ARG:NE	2.28	0.48
1:L:372:ALA:O	1:L:376:GLN:HG3	2.13	0.48
1:C:388:THR:HG23	1:C:389:ASN:N	2.29	0.48
1:G:423:TYR:CZ	1:G:427:LEU:HD22	2.49	0.48
3:T:17:ARG:HA	3:T:77:ILE:O	2.13	0.48
3:N:17:ARG:HA	3:N:77:ILE:O	2.14	0.48
2:Q:142:LYS:CE	2:Q:144:THR:HG22	2.44	0.48
3:2:145:TYR:HA	3:2:146:PRO:C	2.34	0.48
1:B:44:GLN:OE1	1:B:289:PRO:HG2	2.13	0.48
2:9:14:PRO:HD2	2:9:126:SER:HA	1.96	0.48
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.95	0.48
1:A:352:GLY:HA2	1:A:365:ALA:HA	1.96	0.48
1:J:123:GLU:OE1	1:J:168:MET:HG2	2.14	0.48
2:M:180:PRO:HG2	3:N:170:SER:OG	2.14	0.48
3:N:147:GLY:HA3	3:N:177:TYR:CG	2.50	0.47
3:N:172:GLN:HB2	3:N:176:LYS:HD2	1.96	0.47
2:W:111:TYR:HE1	2:W:113:MET:CG	2.27	0.47
3:6:38:TYR:HE2	3:6:48:LEU:HD13	1.77	0.47
1:E:29:ILE:HA	1:F:380:LYS:HZ1	1.77	0.47
2:Q:11:VAL:HG22	2:Q:123:THR:OG1	2.15	0.47
1:I:102:VAL:O	1:I:105:TYR:HB2	2.14	0.47
1:J:384:VAL:HG21	1:J:428:LEU:HD11	1.96	0.47
3:R:51:SER:OG	3:R:55:ASN:HB3	2.14	0.47
1:E:345:GLY:O	1:E:347:ILE:HG23	2.13	0.47
3:0:167:THR:HG22	3:0:180:SER:O	2.14	0.47
2:M:139:PRO:HB2	2:M:141:SER:O	2.14	0.47
1:D:208:ARG:HG3	1:D:241:ASP:OD2	2.14	0.47
1:D:61:GLY:HA2	1:D:79:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:158:TYR:OH	2:Q:191:LEU:HD23	2.14	0.47
1:H:426:GLU:HG3	1:I:383:ARG:HH22	1.79	0.47
1:A:15:LEU:HB3	1:A:444:MET:HE1	1.96	0.47
3:N:64:PHE:HD1	3:N:77:ILE:HG12	1.79	0.47
3:4:17:ARG:HA	3:4:77:ILE:O	2.14	0.47
3:4:165:GLU:HG2	3:4:182:TYR:O	2.14	0.47
1:H:352:GLY:CA	1:H:365:ALA:HA	2.44	0.47
1:F:50:LYS:HD3	1:F:275:ASP:HB2	1.95	0.47
1:K:123:GLU:OE1	1:K:168:MET:HG2	2.14	0.47
1:A:280:GLU:HB2	1:A:290:ASN:ND2	2.29	0.47
2:S:68:VAL:O	2:S:69:THR:HG23	2.14	0.47
1:H:497:ASN:HD22	1:H:497:ASN:HA	1.53	0.47
1:A:18:HIS:H	1:A:18:HIS:CD2	2.32	0.47
3:6:145:TYR:HA	3:6:146:PRO:C	2.34	0.47
3:T:91:GLN:HB2	3:T:102:PHE:HE2	1.79	0.47
1:J:182:VAL:HG22	1:J:202:VAL:HG21	1.94	0.47
1:A:295:GLN:NE2	1:A:308:TYR:HB2	2.28	0.47
2:M:177:HIS:NE2	3:N:172:GLN:NE2	2.62	0.47
2:U:154:LEU:HD21	3:V:136:THR:HG21	1.95	0.47
2:M:38:ARG:HB3	2:M:94:TYR:CE1	2.49	0.47
2:1:29:LEU:HD21	2:1:77:ASN:HA	1.95	0.47
2:U:38:ARG:HB3	2:U:94:TYR:CE1	2.49	0.47
2:5:159:PHE:CD1	2:5:160:PRO:HA	2.49	0.47
1:J:167:THR:HB	6:J:609:NAG:H61	1.95	0.47
1:B:338:PHE:CG	1:B:339:ILE:N	2.81	0.47
3:6:164:VAL:O	3:6:164:VAL:HG12	2.12	0.47
1:L:335:ILE:HG12	1:L:354:ARG:HB3	1.96	0.47
2:M:137:LEU:HD22	3:N:123:PHE:HB3	1.94	0.47
3:Z:163:GLY:O	3:Z:183:LEU:HA	2.14	0.47
1:K:495:ALA:O	1:K:499:ARG:HG3	2.14	0.47
1:C:120:PHE:O	1:C:121:ILE:HD13	2.14	0.47
1:D:15:LEU:HB3	1:D:444:MET:HE1	1.96	0.47
2:5:32:TYR:CD1	2:5:98:ARG:HD3	2.49	0.47
1:L:61:GLY:O	1:L:64:CYS:HB2	2.14	0.47
3:4:91:GLN:HB2	3:4:102:PHE:HE2	1.79	0.47
3:R:146:PRO:HD2	3:R:203:GLU:OE1	2.13	0.47
1:K:352:GLY:HA2	1:K:365:ALA:HA	1.95	0.47
3:N:120:VAL:O	3:N:209:LYS:HG3	2.14	0.47
2:O:179:PHE:HE2	3:P:142:SER:HB3	1.79	0.47
2:U:101:GLY:H	2:U:111:TYR:HB3	1.79	0.47
2:3:108:PHE:CB	2:3:111:TYR:HE2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:331:LEU:CD2	1:J:331:LEU:N	2.75	0.47
2:3:17:SER:HA	2:3:86:LEU:HG	1.96	0.47
1:E:222:TRP:CH2	1:E:225:GLY:HA2	2.48	0.47
1:E:99:PRO:HB3	1:E:223:VAL:HG21	1.95	0.47
1:I:161:TYR:CZ	1:I:249:GLY:HA2	2.48	0.47
2:U:212:ASN:HB2	2:U:219:LYS:HD3	1.96	0.47
1:C:353:PHE:CE1	1:C:366:ASP:HB2	2.47	0.47
1:L:99:PRO:HB3	1:L:223:VAL:HG21	1.96	0.47
1:B:307:LYS:HE2	1:B:421:TRP:CZ2	2.49	0.47
1:E:134:GLY:CA	1:E:153:TRP:HB3	2.45	0.47
1:L:352:GLY:CA	1:L:365:ALA:HA	2.44	0.47
1:E:414:GLU:O	1:E:418:ILE:HG13	2.14	0.47
2:Q:116:TRP:CD1	2:Q:116:TRP:N	2.81	0.47
1:C:280:GLU:HB2	1:C:290:ASN:ND2	2.30	0.47
1:J:280:GLU:HB2	1:J:290:ASN:ND2	2.29	0.47
2:U:100:GLU:H	2:U:111:TYR:CB	2.14	0.47
2:Y:108:PHE:N	2:Y:108:PHE:CD2	2.75	0.47
2:M:34:LEU:HD22	2:M:35:SER:N	2.30	0.47
2:M:50:TRP:CH2	2:M:52:ASN:HB2	2.50	0.47
2:9:92:ALA:O	2:9:122:VAL:HG22	2.14	0.47
1:K:148:PHE:CB	1:K:151:LEU:HB2	2.44	0.47
1:L:148:PHE:CB	1:L:151:LEU:HB2	2.43	0.47
1:A:29:ILE:HA	1:B:380:LYS:HZ1	1.78	0.47
1:H:335:ILE:CD1	1:H:354:ARG:HB3	2.45	0.47
3:R:163:GLY:O	3:R:183:LEU:HA	2.14	0.47
1:F:346:MET:HE3	1:F:349:GLY:O	2.13	0.47
1:B:208:ARG:HG3	1:B:241:ASP:OD2	2.15	0.47
1:C:143:PRO:HD2	1:D:155:THR:HB	1.95	0.47
1:E:403:GLU:H	1:E:407:GLN:HE21	1.62	0.47
1:J:383:ARG:HH21	1:L:430:ALA:HB2	1.79	0.47
3:P:26:SER:N	3:P:29:ILE:HD12	2.30	0.47
1:C:321:ARG:HD2	1:C:437:ILE:CG2	2.45	0.47
3:6:25:SER:O	3:6:29:ILE:HG13	2.15	0.47
2:3:112:PRO:CB	3:4:51:SER:HB2	2.42	0.47
1:B:372:ALA:O	1:B:376:GLN:HG3	2.14	0.47
3:X:197:SER:HB3	3:X:210:THR:OG1	2.14	0.47
1:D:321:ARG:HD2	1:D:437:ILE:CG2	2.44	0.47
1:B:352:GLY:CA	1:B:365:ALA:HA	2.44	0.47
1:I:280:GLU:HB2	1:I:290:ASN:HD21	1.80	0.47
1:F:214:ILE:N	1:F:214:ILE:HD12	2.29	0.47
1:I:298:ASN:OD1	1:I:300:ILE:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:GLU:OE1	1:I:168:MET:HG2	2.14	0.47
3:2:174:ASN:HD21	3:2:176:LYS:HB3	1.80	0.47
3:V:147:GLY:HA3	3:V:177:TYR:CG	2.50	0.47
2:S:108:PHE:N	2:S:108:PHE:CD2	2.75	0.47
2:5:114:ASP:O	2:5:115:VAL:O	2.33	0.47
2:Y:148:THR:HA	2:Y:199:SER:N	2.28	0.47
2:Y:18:VAL:HG12	2:Y:19:THR:H	1.79	0.47
2:Q:159:PHE:CD1	2:Q:160:PRO:HA	2.50	0.47
1:K:167:THR:HB	6:K:609:NAG:H61	1.97	0.47
1:J:27:LYS:HZ3	1:K:383:ARG:HD3	1.79	0.47
1:E:220:ARG:HA	1:F:244:VAL:HG11	1.95	0.47
2:1:94:TYR:O	2:1:119:GLY:HA2	2.15	0.47
1:G:343:TRP:HB3	1:G:354:ARG:NH2	2.30	0.47
3:0:6:GLN:NE2	3:0:105:GLY:H	2.12	0.47
1:L:403:GLU:H	1:L:407:GLN:HE21	1.61	0.47
1:E:470:TYR:CG	1:E:499:ARG:HG2	2.49	0.47
2:U:139:PRO:HB2	2:U:141:SER:O	2.14	0.47
3:4:26:SER:N	3:4:29:ILE:HD12	2.29	0.47
3:2:26:SER:N	3:2:29:ILE:HD12	2.30	0.47
3:V:26:SER:N	3:V:29:ILE:HD12	2.30	0.47
1:E:80:GLN:HB3	1:E:150:ARG:NH2	2.29	0.47
2:W:38:ARG:HB3	2:W:94:TYR:CE1	2.50	0.47
2:Y:32:TYR:CD1	2:Y:98:ARG:HD3	2.49	0.47
1:B:134:GLY:CA	1:B:153:TRP:HB3	2.44	0.47
3:4:38:TYR:HD2	3:4:48:LEU:HA	1.79	0.47
1:E:497:ASN:HD22	1:E:497:ASN:HA	1.53	0.47
1:F:44:GLN:OE1	1:F:289:PRO:HG2	2.13	0.47
7:B:616:NAG:H61	7:B:617:BMA:H2	1.96	0.47
1:B:436:THR:O	1:B:440:THR:HG23	2.14	0.47
3:Z:172:GLN:HB2	3:Z:176:LYS:HD2	1.95	0.47
3:V:174:ASN:HD21	3:V:176:LYS:HB3	1.80	0.47
2:7:108:PHE:HB2	2:7:111:TYR:HE2	1.80	0.47
2:3:148:THR:HA	2:3:199:SER:N	2.28	0.47
2:O:148:THR:HA	2:O:199:SER:N	2.29	0.47
1:B:222:TRP:HB2	6:C:610:NAG:H62	1.95	0.47
2:Q:214:LYS:HB2	2:Q:215:PRO:HD3	1.97	0.47
1:K:185:PRO:HA	1:K:190:GLU:OE2	2.14	0.47
1:A:102:VAL:HG22	1:A:232:ILE:CB	2.44	0.47
1:L:338:PHE:CG	1:L:339:ILE:N	2.82	0.47
3:2:163:GLY:O	3:2:183:LEU:HA	2.14	0.47
1:A:384:VAL:HG21	1:A:428:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:26:SER:N	3:T:29:ILE:HD12	2.29	0.47
1:J:205:SER:OG	1:L:221:PRO:HD3	2.13	0.47
1:H:388:THR:HG23	1:H:389:ASN:N	2.30	0.47
1:E:423:TYR:CZ	1:E:427:LEU:HD22	2.50	0.47
3:P:17:ARG:HA	3:P:77:ILE:O	2.14	0.47
3:X:17:ARG:HA	3:X:77:ILE:O	2.15	0.47
2:S:142:LYS:HE2	2:S:144:THR:HG22	1.96	0.47
1:K:268:MET:CE	1:K:282:ILE:HG22	2.45	0.47
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.95	0.47
2:9:50:TRP:CH2	2:9:52:ASN:HB2	2.50	0.47
3:P:172:GLN:HB2	3:P:176:LYS:HD2	1.96	0.47
2:7:34:LEU:CD2	2:7:35:SER:H	2.27	0.47
2:W:102:VAL:HG12	2:W:103:ARG:H	1.79	0.47
2:3:2:VAL:HG21	2:3:115:VAL:HG21	1.96	0.47
1:D:271:ASP:OD2	2:S:103:ARG:HB2	2.14	0.47
4:J:601:NAG:H61	4:J:602:NAG:O7	2.15	0.47
2:M:94:TYR:HE2	2:M:122:VAL:HG21	1.80	0.47
2:O:17:SER:HA	2:O:86:LEU:HG	1.96	0.47
1:J:463:GLY:HA3	1:K:453:ARG:HB3	1.96	0.47
1:A:37:THR:CG2	1:A:322:ASN:HB2	2.45	0.47
2:M:214:LYS:HB2	2:M:215:PRO:HD3	1.97	0.47
1:C:61:GLY:HA2	1:C:79:PHE:CZ	2.50	0.47
1:L:326:LYS:NZ	1:L:341:ASN:HD22	2.12	0.47
3:4:163:GLY:O	3:4:183:LEU:HA	2.14	0.47
3:T:164:VAL:O	3:T:164:VAL:HG12	2.13	0.47
3:X:165:GLU:HG2	3:X:182:TYR:O	2.14	0.47
1:G:382:ASN:O	1:G:385:ILE:O	2.33	0.47
3:P:20:ILE:HG23	3:P:106:THR:HG21	1.97	0.47
2:W:158:TYR:OH	2:W:191:LEU:HD23	2.14	0.47
3:T:20:ILE:HG23	3:T:106:THR:HG21	1.96	0.47
2:5:158:TYR:OH	2:5:191:LEU:HD23	2.15	0.47
2:3:155:VAL:HG11	2:3:211:VAL:HG11	1.97	0.47
1:D:221:PRO:HG2	1:E:206:THR:CA	2.45	0.47
1:E:380:LYS:HZ3	1:E:384:VAL:HG23	1.79	0.47
2:Q:179:PHE:CD1	3:R:140:LEU:HD22	2.50	0.47
1:K:401:GLU:HG3	1:L:238:LYS:HE2	1.95	0.47
3:2:167:THR:HG22	3:2:180:SER:O	2.14	0.47
1:C:103:PRO:HD2	1:C:232:ILE:O	2.14	0.47
2:S:139:PRO:HB2	2:S:141:SER:O	2.15	0.47
1:J:383:ARG:HD3	1:L:27:LYS:NZ	2.29	0.47
1:I:17:HIS:HB2	1:I:320:MET:HE1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:ALA:O	1:C:376:GLN:HG3	2.14	0.47
1:C:109:ARG:NH2	1:C:267:ILE:HD13	2.30	0.47
3:Z:37:TRP:CZ3	3:Z:90:CYS:HB3	2.49	0.47
2:U:32:TYR:CD1	2:U:98:ARG:HD3	2.50	0.47
1:I:421:TRP:CE3	1:I:421:TRP:HA	2.50	0.47
3:O:64:PHE:HD1	3:O:77:ILE:HG12	1.78	0.47
1:H:183:HIS:ND1	1:H:184:HIS:N	2.63	0.47
1:E:84:TRP:HZ2	1:E:113:ALA:HA	1.79	0.47
1:K:352:GLY:CA	1:K:365:ALA:HA	2.45	0.47
2:S:142:LYS:CE	2:S:144:THR:HG22	2.44	0.47
1:K:84:TRP:CE2	1:K:116:GLY:HA2	2.49	0.47
1:C:200:GLY:HA3	1:C:250:ASN:OD1	2.14	0.47
3:R:67:SER:O	3:R:73:ALA:HB1	2.15	0.47
3:8:145:TYR:HA	3:8:146:PRO:C	2.35	0.47
1:K:214:ILE:HD12	1:K:214:ILE:N	2.29	0.47
1:H:487:ASP:OD2	1:H:490:VAL:HG23	2.15	0.47
3:8:120:VAL:O	3:8:209:LYS:HG3	2.14	0.47
1:J:134:GLY:HA3	1:J:153:TRP:HB3	1.97	0.47
1:F:323:VAL:O	1:F:323:VAL:HG23	2.15	0.47
3:T:145:TYR:HA	3:T:146:PRO:C	2.35	0.47
3:T:118:PRO:HB3	3:T:141:ILE:HG23	1.95	0.47
2:9:194:VAL:HG21	3:O:140:LEU:HD13	1.97	0.47
3:2:11:SER:HB3	3:2:111:LEU:HD12	1.97	0.47
2:U:102:VAL:HG12	2:U:103:ARG:H	1.80	0.47
2:7:100:GLU:O	2:7:102:VAL:N	2.47	0.47
2:Y:108:PHE:CB	2:Y:111:TYR:CE2	2.97	0.47
2:1:108:PHE:CB	2:1:111:TYR:HE2	2.28	0.47
2:S:38:ARG:HB3	2:S:94:TYR:HE1	1.80	0.47
1:G:161:TYR:CZ	1:G:249:GLY:HA2	2.50	0.47
2:3:36:TRP:NE1	2:3:70:MET:HE1	2.29	0.47
3:4:147:GLY:HA3	3:4:177:TYR:CG	2.50	0.47
1:G:102:VAL:O	1:G:105:TYR:HB2	2.15	0.47
3:X:163:GLY:O	3:X:183:LEU:HA	2.15	0.47
1:H:103:PRO:HD2	1:H:232:ILE:O	2.15	0.47
3:2:167:THR:CG2	3:2:180:SER:H	2.27	0.47
3:Z:93:TYR:HD1	3:Z:100:SER:HB3	1.76	0.47
1:I:381:LEU:O	1:I:385:ILE:HG13	2.13	0.47
3:V:17:ARG:HA	3:V:77:ILE:O	2.15	0.47
3:O:26:SER:N	3:O:29:ILE:HD12	2.29	0.47
3:Z:26:SER:N	3:Z:29:ILE:HD12	2.29	0.47
3:8:26:SER:N	3:8:29:ILE:HD12	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:423:TYR:CZ	1:I:427:LEU:HD22	2.50	0.47
3:R:165:GLU:HG2	3:R:182:TYR:O	2.13	0.47
1:J:176:LYS:HD3	1:J:178:TYR:OH	2.14	0.47
3:P:145:TYR:HA	3:P:146:PRO:C	2.35	0.47
7:C:616:NAG:H61	7:C:617:BMA:H2	1.96	0.47
3:X:35:VAL:HG13	3:X:92:SER:HB2	1.96	0.47
1:C:18:HIS:H	1:C:18:HIS:CD2	2.33	0.47
1:J:44:GLN:OE1	1:J:289:PRO:HG2	2.15	0.47
1:L:436:THR:O	1:L:440:THR:HG23	2.15	0.47
3:T:167:THR:HG22	3:T:180:SER:O	2.15	0.47
3:T:174:ASN:HD21	3:T:176:LYS:HE3	1.80	0.47
2:O:108:PHE:HB2	2:O:111:TYR:HE2	1.76	0.47
2:Q:47:TRP:HZ2	2:Q:50:TRP:HB2	1.80	0.47
2:3:111:TYR:CD1	2:3:111:TYR:O	2.68	0.47
2:W:18:VAL:HG12	2:W:19:THR:H	1.80	0.47
2:W:214:LYS:HB2	2:W:215:PRO:HD3	1.97	0.47
2:O:214:LYS:HB2	2:O:215:PRO:HD3	1.96	0.47
2:5:36:TRP:NE1	2:5:70:MET:HE1	2.30	0.47
1:C:382:ASN:O	1:C:385:ILE:O	2.32	0.47
3:0:20:ILE:HG23	3:0:106:THR:HG21	1.97	0.47
2:Q:139:PRO:HB2	2:Q:141:SER:O	2.13	0.47
1:J:335:ILE:HG12	1:J:354:ARG:HB3	1.96	0.47
1:D:495:ALA:O	1:D:499:ARG:HG3	2.15	0.47
1:J:495:ALA:O	1:J:499:ARG:HG3	2.14	0.47
3:N:135:ALA:O	3:N:184:SER:HB2	2.15	0.47
1:G:27:LYS:NZ	1:H:383:ARG:HD3	2.30	0.47
1:F:421:TRP:CE3	1:F:421:TRP:HA	2.49	0.47
3:R:64:PHE:HD1	3:R:77:ILE:HG12	1.79	0.47
1:H:15:LEU:HB3	1:H:444:MET:HE1	1.97	0.47
3:T:64:PHE:HD1	3:T:77:ILE:HG12	1.79	0.47
2:M:142:LYS:HE2	2:M:144:THR:HG22	1.96	0.47
7:E:616:NAG:H61	7:E:617:BMA:H2	1.96	0.47
1:J:138:ALA:HB2	1:J:226:LEU:HD12	1.97	0.47
1:G:49:GLY:HA2	1:G:285:ASN:O	2.15	0.47
1:B:280:GLU:HB2	1:B:290:ASN:ND2	2.30	0.47
1:D:183:HIS:HA	1:D:230:ILE:HD13	1.96	0.47
3:P:120:VAL:O	3:P:209:LYS:HG3	2.15	0.47
2:U:34:LEU:HD22	2:U:35:SER:N	2.29	0.47
1:K:331:LEU:N	1:K:331:LEU:CD2	2.74	0.47
2:O:117:GLY:O	2:O:118:GLN:C	2.54	0.47
2:Y:10:GLU:OE1	2:Y:18:VAL:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:214:LYS:HB2	2:S:215:PRO:HD3	1.97	0.47
2:7:22:CYS:HB2	2:7:36:TRP:HH2	1.79	0.47
1:J:156:LYS:HD2	1:J:196:VAL:CG2	2.41	0.47
1:J:197:GLN:CD	1:J:197:GLN:H	2.18	0.47
1:E:185:PRO:O	1:E:217:ILE:HA	2.15	0.47
1:C:384:VAL:HG21	1:C:428:LEU:HD11	1.96	0.47
2:7:139:PRO:HB2	2:7:141:SER:O	2.14	0.47
2:W:139:PRO:HB2	2:W:141:SER:O	2.15	0.47
1:C:101:ASP:O	1:C:103:PRO:HD3	2.15	0.47
3:P:147:GLY:HA3	3:P:177:TYR:CG	2.49	0.47
3:X:26:SER:N	3:X:29:ILE:HD12	2.30	0.47
1:A:327:GLN:HG3	1:A:329:ARG:NE	2.28	0.47
1:B:15:LEU:HD22	1:B:448:PHE:HA	1.96	0.47
1:K:80:GLN:HB3	1:K:150:ARG:NH2	2.30	0.47
2:Q:32:TYR:CD1	2:Q:98:ARG:HD3	2.49	0.47
1:J:321:ARG:O	1:J:321:ARG:HG2	2.15	0.47
3:T:38:TYR:HD2	3:T:48:LEU:HA	1.80	0.47
3:V:145:TYR:HA	3:V:146:PRO:C	2.35	0.47
2:O:2:VAL:HG23	2:O:115:VAL:HG11	1.97	0.47
1:B:323:VAL:HG23	1:B:323:VAL:O	2.15	0.47
3:N:67:SER:O	3:N:73:ALA:HB1	2.15	0.47
3:T:147:GLY:HA3	3:T:177:TYR:CG	2.50	0.46
2:9:179:PHE:CE2	3:0:142:SER:HB3	2.50	0.46
2:9:102:VAL:HG12	2:9:103:ARG:H	1.78	0.46
2:7:108:PHE:CB	2:7:111:TYR:HE2	2.28	0.46
2:W:108:PHE:CB	2:W:111:TYR:CE2	2.98	0.46
3:6:38:TYR:HD2	3:6:48:LEU:HA	1.80	0.46
2:M:17:SER:HA	2:M:86:LEU:HG	1.96	0.46
2:S:17:SER:HA	2:S:86:LEU:HG	1.97	0.46
2:7:17:SER:HA	2:7:86:LEU:HG	1.97	0.46
1:F:324:PRO:O	1:F:325:GLU:HB3	2.15	0.46
1:I:185:PRO:HA	1:I:190:GLU:OE2	2.14	0.46
1:J:102:VAL:HG22	1:J:232:ILE:CB	2.44	0.46
1:D:101:ASP:O	1:D:103:PRO:HD3	2.16	0.46
3:P:163:GLY:O	3:P:183:LEU:HA	2.15	0.46
3:N:163:GLY:O	3:N:183:LEU:HA	2.15	0.46
1:H:101:ASP:O	1:H:103:PRO:HD3	2.15	0.46
2:7:158:TYR:OH	2:7:191:LEU:HD23	2.14	0.46
2:3:139:PRO:HB2	2:3:141:SER:O	2.14	0.46
3:2:147:GLY:HA3	3:2:177:TYR:CG	2.50	0.46
1:A:470:TYR:CG	1:A:499:ARG:HG2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:39:GLN:HE21	2:3:45:LEU:HD23	1.80	0.46
2:M:98:ARG:NH1	2:M:98:ARG:HG2	2.30	0.46
3:T:155:ALA:N	3:T:158:SER:O	2.47	0.46
1:E:321:ARG:HD2	1:E:437:ILE:CG2	2.45	0.46
1:E:352:GLY:CA	1:E:365:ALA:HA	2.45	0.46
3:R:145:TYR:HA	3:R:146:PRO:C	2.34	0.46
1:E:123:GLU:OE1	1:E:168:MET:HG2	2.15	0.46
1:I:170:ASN:ND2	1:I:239:PRO:HA	2.30	0.46
1:H:280:GLU:HB2	1:H:290:ASN:HD21	1.80	0.46
1:D:107:SER:HB2	1:F:404:GLY:HA3	1.97	0.46
1:F:138:ALA:HB2	1:F:226:LEU:HD12	1.97	0.46
3:T:67:SER:O	3:T:73:ALA:HB1	2.14	0.46
1:D:487:ASP:OD2	1:D:490:VAL:HG23	2.15	0.46
2:O:47:TRP:HZ2	2:O:50:TRP:HB2	1.80	0.46
2:U:111:TYR:CE1	2:U:113:MET:HG2	2.49	0.46
1:H:331:LEU:CD2	1:H:331:LEU:N	2.73	0.46
3:N:11:SER:CB	3:N:111:LEU:HD11	2.31	0.46
2:5:38:ARG:HB3	2:5:94:TYR:CE1	2.49	0.46
2:9:10:GLU:OE1	2:9:18:VAL:HG13	2.15	0.46
2:W:159:PHE:CD1	2:W:160:PRO:HA	2.50	0.46
2:M:159:PHE:CD1	2:M:160:PRO:HA	2.49	0.46
1:B:220:ARG:HD2	1:B:229:ARG:HG2	1.98	0.46
1:H:191:GLN:NE2	1:H:217:ILE:HD11	2.25	0.46
1:L:197:GLN:H	1:L:197:GLN:CD	2.18	0.46
1:C:185:PRO:HA	1:C:190:GLU:OE2	2.15	0.46
1:K:99:PRO:HB3	1:K:223:VAL:HG21	1.96	0.46
3:R:53:ASN:O	3:R:54:SER:CB	2.64	0.46
2:Y:155:VAL:HG11	2:Y:211:VAL:HG11	1.97	0.46
1:E:101:ASP:O	1:E:103:PRO:HD3	2.15	0.46
3:8:147:GLY:HA3	3:8:177:TYR:CG	2.50	0.46
3:T:25:SER:O	3:T:29:ILE:HG13	2.16	0.46
1:B:427:LEU:O	1:B:431:LEU:HD12	2.15	0.46
2:S:142:LYS:O	2:S:144:THR:HG23	2.16	0.46
1:D:138:ALA:HB2	1:D:226:LEU:HD12	1.96	0.46
3:4:145:TYR:HA	3:4:146:PRO:C	2.34	0.46
1:F:123:GLU:OE1	1:F:168:MET:HG2	2.15	0.46
1:B:138:ALA:HB2	1:B:226:LEU:HD12	1.98	0.46
2:1:112:PRO:HB2	3:2:51:SER:HB2	1.96	0.46
3:2:51:SER:OG	3:2:55:ASN:HB3	2.15	0.46
3:4:174:ASN:HD21	3:4:176:LYS:HB3	1.81	0.46
3:4:174:ASN:HD21	3:4:176:LYS:HE3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:174:ASN:HD21	3:6:176:LYS:HB3	1.80	0.46
3:P:38:TYR:HE2	3:P:48:LEU:HD13	1.80	0.46
2:M:102:VAL:HG12	2:M:103:ARG:H	1.80	0.46
2:5:101:GLY:H	2:5:111:TYR:HB3	1.80	0.46
2:W:17:SER:HA	2:W:86:LEU:HG	1.97	0.46
1:F:382:ASN:O	1:F:385:ILE:O	2.33	0.46
1:I:326:LYS:NZ	1:I:341:ASN:ND2	2.63	0.46
2:1:214:LYS:HB2	2:1:215:PRO:HD3	1.98	0.46
2:7:214:LYS:HB2	2:7:215:PRO:HD3	1.97	0.46
2:Y:61:VAL:HG12	2:Y:63:LYS:N	2.25	0.46
1:D:190:GLU:O	1:D:194:LEU:HD13	2.16	0.46
1:K:197:GLN:H	1:K:197:GLN:CD	2.17	0.46
3:6:163:GLY:O	3:6:183:LEU:HA	2.14	0.46
2:1:109:HIS:HA	3:2:93:TYR:CD1	2.50	0.46
3:P:6:GLN:NE2	3:P:105:GLY:H	2.13	0.46
3:X:6:GLN:NE2	3:X:105:GLY:H	2.13	0.46
1:H:382:ASN:O	1:H:385:ILE:O	2.33	0.46
2:1:155:VAL:HG11	2:1:211:VAL:HG11	1.98	0.46
2:O:139:PRO:HB2	2:O:141:SER:O	2.14	0.46
1:C:114:SER:HA	1:C:265:SER:O	2.15	0.46
1:I:372:ALA:O	1:I:376:GLN:HG3	2.15	0.46
3:8:155:ALA:N	3:8:158:SER:O	2.48	0.46
2:3:32:TYR:CD1	2:3:98:ARG:HD3	2.50	0.46
3:V:155:ALA:N	3:V:158:SER:O	2.48	0.46
1:A:423:TYR:CZ	1:A:427:LEU:HD22	2.50	0.46
2:5:27:TYR:O	2:5:98:ARG:NH2	2.48	0.46
3:X:118:PRO:HB3	3:X:141:ILE:CG2	2.45	0.46
2:Y:182:VAL:HG11	3:Z:182:TYR:HD2	1.80	0.46
3:Z:64:PHE:HD1	3:Z:77:ILE:HG12	1.78	0.46
2:O:194:VAL:HG21	3:P:140:LEU:CD1	2.45	0.46
3:N:35:VAL:HG13	3:N:92:SER:HB2	1.97	0.46
1:A:471:HIS:HB2	1:A:494:GLU:OE1	2.15	0.46
1:A:141:ARG:NH1	1:A:141:ARG:HB2	2.30	0.46
1:I:323:VAL:O	1:I:323:VAL:HG23	2.15	0.46
1:F:497:ASN:HA	1:F:497:ASN:HD22	1.53	0.46
1:F:355:HIS:NE2	1:F:362:GLY:HA3	2.31	0.46
2:1:34:LEU:CD2	2:1:35:SER:H	2.28	0.46
2:M:108:PHE:CB	2:M:111:TYR:HE2	2.28	0.46
2:M:4:LEU:HA	2:M:23:GLN:O	2.16	0.46
2:Y:214:LYS:HB2	2:Y:215:PRO:HD3	1.98	0.46
2:U:159:PHE:CD1	2:U:160:PRO:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:LYS:NZ	1:B:341:ASN:ND2	2.64	0.46
2:9:214:LYS:HB2	2:9:215:PRO:HD3	1.97	0.46
2:M:20:VAL:HG13	2:M:120:THR:HG21	1.97	0.46
1:B:185:PRO:O	1:B:217:ILE:HA	2.16	0.46
1:H:185:PRO:O	1:H:217:ILE:HA	2.15	0.46
1:H:197:GLN:CD	1:H:197:GLN:H	2.17	0.46
1:A:29:ILE:H	1:A:434:GLN:HB2	1.80	0.46
2:1:38:ARG:HB3	2:1:94:TYR:HE1	1.80	0.46
1:G:101:ASP:O	1:G:103:PRO:HD3	2.15	0.46
3:T:93:TYR:HD1	3:T:100:SER:HB3	1.80	0.46
3:X:24:GLY:O	3:X:29:ILE:HD11	2.16	0.46
1:K:372:ALA:O	1:K:376:GLN:HG3	2.15	0.46
3:R:155:ALA:N	3:R:158:SER:O	2.47	0.46
3:2:64:PHE:HD1	3:2:77:ILE:HG12	1.81	0.46
3:T:51:SER:OG	3:T:55:ASN:HB3	2.15	0.46
3:X:17:ARG:HH21	3:X:78:THR:HG21	1.80	0.46
2:M:142:LYS:O	2:M:144:THR:HG23	2.15	0.46
1:C:352:GLY:CA	1:C:365:ALA:HA	2.45	0.46
3:8:146:PRO:HD2	3:8:203:GLU:OE1	2.16	0.46
1:C:421:TRP:HA	1:C:424:ASN:HD22	1.80	0.46
3:X:145:TYR:HA	3:X:146:PRO:C	2.35	0.46
1:K:18:HIS:CD2	1:K:18:HIS:H	2.32	0.46
1:G:18:HIS:CD2	1:G:18:HIS:H	2.31	0.46
1:K:436:THR:O	1:K:440:THR:HG23	2.16	0.46
3:0:145:TYR:HA	3:0:146:PRO:C	2.35	0.46
1:A:414:GLU:O	1:A:418:ILE:HG13	2.15	0.46
3:T:174:ASN:HD21	3:T:176:LYS:HB3	1.81	0.46
3:Z:147:GLY:HA3	3:Z:177:TYR:CG	2.50	0.46
2:W:108:PHE:H	2:W:108:PHE:HD2	1.59	0.46
2:W:50:TRP:CH2	2:W:52:ASN:HB2	2.51	0.46
2:S:34:LEU:CD2	2:S:35:SER:H	2.28	0.46
2:U:17:SER:HA	2:U:86:LEU:HG	1.96	0.46
1:A:321:ARG:HD2	1:A:437:ILE:CG2	2.46	0.46
3:P:53:ASN:O	3:P:54:SER:CB	2.64	0.46
1:D:185:PRO:HA	1:D:190:GLU:OE2	2.16	0.46
1:K:192:THR:HG22	1:K:198:ALA:HB2	1.96	0.46
1:E:192:THR:HG22	1:E:198:ALA:HB2	1.96	0.46
2:9:60:TYR:CE1	2:9:70:MET:HG2	2.41	0.46
1:F:108:LEU:O	1:F:112:VAL:HG23	2.15	0.46
2:1:92:ALA:H	2:1:122:VAL:CG2	2.29	0.46
1:B:401:GLU:N	1:B:401:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:20:ILE:HG23	3:X:106:THR:HG21	1.97	0.46
1:H:102:VAL:HG11	1:H:108:LEU:HD23	1.97	0.46
1:H:213:ILE:HG13	1:H:233:TYR:CE2	2.51	0.46
1:H:29:ILE:H	1:H:434:GLN:HB2	1.81	0.46
1:J:208:ARG:HG3	1:J:241:ASP:OD2	2.16	0.46
2:3:27:TYR:O	2:3:98:ARG:NH2	2.48	0.46
1:A:427:LEU:O	1:A:431:LEU:HD12	2.15	0.46
1:B:421:TRP:HA	1:B:424:ASN:HD22	1.80	0.46
3:6:17:ARG:HA	3:6:77:ILE:O	2.14	0.46
1:H:323:VAL:O	1:H:323:VAL:HG23	2.16	0.46
1:A:138:ALA:HB2	1:A:226:LEU:HD12	1.96	0.46
3:Z:146:PRO:HD2	3:Z:203:GLU:OE1	2.16	0.46
3:V:167:THR:CG2	3:V:180:SER:H	2.29	0.46
2:O:99:VAL:HB	2:O:111:TYR:CE1	2.51	0.46
3:8:38:TYR:HD2	3:8:48:LEU:HA	1.80	0.46
2:5:100:GLU:N	2:5:111:TYR:HB2	2.17	0.46
2:S:18:VAL:HG12	2:S:19:THR:H	1.79	0.46
2:9:95:TYR:CE1	2:9:119:GLY:HA3	2.50	0.46
1:H:326:LYS:HD3	1:H:328:THR:H	1.80	0.46
1:G:185:PRO:HA	1:G:190:GLU:OE2	2.16	0.46
1:K:102:VAL:O	1:K:105:TYR:HB2	2.15	0.46
2:1:22:CYS:HB2	2:1:36:TRP:HH2	1.79	0.46
1:J:102:VAL:O	1:J:105:TYR:HB2	2.15	0.46
1:D:103:PRO:HD2	1:D:232:ILE:O	2.16	0.46
3:0:167:THR:CG2	3:0:180:SER:H	2.27	0.46
3:0:163:GLY:O	3:0:183:LEU:HA	2.16	0.46
1:L:208:ARG:CZ	1:L:238:LYS:HD2	2.45	0.46
1:F:376:GLN:HB2	1:F:439:LEU:HD11	1.98	0.46
1:E:280:GLU:HB2	1:E:290:ASN:HD21	1.80	0.46
3:0:38:TYR:HD2	3:0:48:LEU:HA	1.80	0.46
3:Z:145:TYR:HA	3:Z:146:PRO:C	2.35	0.46
1:F:280:GLU:HB2	1:F:290:ASN:ND2	2.30	0.46
1:J:323:VAL:HG23	1:J:323:VAL:O	2.16	0.46
3:6:67:SER:O	3:6:73:ALA:HB1	2.15	0.46
3:Z:91:GLN:HB2	3:Z:102:PHE:HE2	1.80	0.46
3:0:120:VAL:O	3:0:209:LYS:HG3	2.16	0.46
3:N:145:TYR:HA	3:N:146:PRO:C	2.35	0.46
1:C:414:GLU:O	1:C:418:ILE:HG13	2.16	0.46
3:2:67:SER:O	3:2:73:ALA:HB1	2.15	0.46
3:X:147:GLY:HA3	3:X:177:TYR:CG	2.50	0.46
2:M:114:ASP:OD1	2:M:115:VAL:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:18:VAL:HG12	2:5:19:THR:H	1.81	0.46
1:B:146:GLY:CA	1:L:143:PRO:HB3	2.37	0.46
1:F:185:PRO:HA	1:F:190:GLU:OE2	2.16	0.46
2:U:214:LYS:HB2	2:U:215:PRO:HD3	1.97	0.46
1:H:167:THR:HB	6:H:609:NAG:H61	1.96	0.46
2:Q:2:VAL:HG21	2:Q:115:VAL:HG21	1.97	0.46
1:C:197:GLN:CD	1:C:197:GLN:H	2.19	0.46
1:A:409:LEU:HG	1:C:409:LEU:HD21	1.98	0.46
3:R:139:CYS:CB	3:R:153:TRP:HZ2	2.29	0.46
2:W:155:VAL:HG11	2:W:211:VAL:HG11	1.98	0.46
1:H:67:ILE:HG13	1:H:105:TYR:CE2	2.51	0.46
3:8:163:GLY:O	3:8:183:LEU:HA	2.16	0.46
1:F:61:GLY:HA2	1:F:79:PHE:CZ	2.51	0.46
1:K:208:ARG:HG3	1:K:241:ASP:OD2	2.16	0.46
3:P:167:THR:HG22	3:P:180:SER:O	2.14	0.46
1:G:327:GLN:HG3	1:G:329:ARG:NE	2.27	0.46
1:E:353:PHE:CE1	1:E:366:ASP:HB2	2.48	0.46
1:B:327:GLN:HG3	1:B:329:ARG:NE	2.29	0.46
2:W:112:PRO:CB	3:X:51:SER:HB2	2.46	0.46
1:B:183:HIS:ND1	1:B:184:HIS:N	2.64	0.46
3:X:37:TRP:HB2	3:X:50:ILE:HG13	1.98	0.46
2:S:112:PRO:CB	3:T:51:SER:HB2	2.46	0.46
1:D:423:TYR:CE2	1:E:424:ASN:HB3	2.51	0.46
1:J:433:ASN:O	1:J:437:ILE:HG13	2.16	0.46
3:8:188:GLU:H	3:8:188:GLU:CD	2.18	0.46
1:C:323:VAL:O	1:C:323:VAL:HG23	2.16	0.46
1:H:18:HIS:H	1:H:18:HIS:CD2	2.33	0.46
3:2:35:VAL:HG13	3:2:92:SER:HB2	1.98	0.46
1:L:414:GLU:O	1:L:418:ILE:HG13	2.16	0.46
1:I:487:ASP:OD2	1:I:490:VAL:HG23	2.15	0.46
1:E:471:HIS:HB2	1:E:494:GLU:OE1	2.15	0.46
2:9:34:LEU:CD2	2:9:35:SER:H	2.29	0.46
2:7:98:ARG:NH1	2:7:98:ARG:HG2	2.31	0.46
2:W:47:TRP:HZ2	2:W:50:TRP:HB2	1.80	0.46
2:3:34:LEU:HD22	2:3:35:SER:H	1.80	0.46
2:9:142:LYS:O	2:9:144:THR:HG23	2.16	0.46
2:7:18:VAL:HG12	2:7:19:THR:H	1.81	0.46
2:O:38:ARG:HB3	2:O:94:TYR:HE1	1.79	0.46
1:F:309:VAL:HB	1:F:311:GLN:OE1	2.15	0.46
1:K:137:ASN:O	1:K:140:LYS:HG3	2.16	0.46
1:H:161:TYR:CZ	1:H:249:GLY:HA2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:ASP:O	1:F:103:PRO:HD3	2.16	0.46
1:B:382:ASN:O	1:B:385:ILE:O	2.32	0.46
1:I:208:ARG:HG3	1:I:241:ASP:OD2	2.16	0.46
3:P:6:GLN:HG2	3:P:106:THR:HG23	1.98	0.46
2:U:155:VAL:HG11	2:U:211:VAL:HG11	1.97	0.46
2:1:139:PRO:HB2	2:1:141:SER:O	2.16	0.46
2:Y:212:ASN:HB2	2:Y:219:LYS:HD3	1.98	0.46
1:B:335:ILE:HG12	1:B:354:ARG:HB3	1.98	0.46
1:I:384:VAL:HG11	1:I:428:LEU:HD11	1.97	0.46
3:V:53:ASN:O	3:V:54:SER:CB	2.64	0.46
1:J:210:GLN:HE21	1:L:220:ARG:HE	1.62	0.46
1:J:388:THR:HG23	1:J:389:ASN:N	2.31	0.46
2:S:32:TYR:CD1	2:S:98:ARG:HD3	2.51	0.46
1:D:84:TRP:HZ2	1:D:113:ALA:HA	1.81	0.46
1:G:321:ARG:HD2	1:G:437:ILE:CG2	2.45	0.46
3:6:64:PHE:HD1	3:6:77:ILE:HG12	1.80	0.46
1:J:321:ARG:HD2	1:J:437:ILE:CG2	2.45	0.46
3:2:37:TRP:CZ3	3:2:90:CYS:HB3	2.50	0.46
1:F:352:GLY:CA	1:F:365:ALA:HA	2.46	0.46
3:P:146:PRO:HD2	3:P:203:GLU:OE1	2.15	0.46
1:A:323:VAL:O	1:A:323:VAL:HG23	2.16	0.46
1:I:182:VAL:HG22	1:I:202:VAL:HG21	1.98	0.46
1:H:91:SER:O	2:1:31:SER:HB2	2.16	0.46
1:H:98:TYR:OH	1:H:228:SER:HB2	2.16	0.46
2:7:32:TYR:CD1	2:7:98:ARG:HD3	2.51	0.46
2:W:97:ALA:HA	2:W:115:VAL:O	2.15	0.46
3:X:38:TYR:HD2	3:X:48:LEU:HA	1.81	0.46
2:3:101:GLY:H	2:3:111:TYR:HB3	1.81	0.46
1:F:220:ARG:HD2	1:F:229:ARG:HG2	1.97	0.46
1:F:208:ARG:HG3	1:F:241:ASP:OD2	2.16	0.46
1:G:196:VAL:O	1:G:197:GLN:C	2.54	0.46
1:H:137:ASN:O	1:H:140:LYS:HG3	2.16	0.46
1:C:192:THR:HG22	1:C:198:ALA:HB2	1.96	0.46
1:F:102:VAL:O	1:F:105:TYR:HB2	2.16	0.46
1:J:192:THR:HG22	1:J:198:ALA:HB2	1.98	0.46
1:J:101:ASP:O	1:J:103:PRO:HD3	2.16	0.46
1:E:185:PRO:HA	1:E:190:GLU:OE2	2.16	0.46
1:K:335:ILE:CD1	1:K:354:ARG:HB3	2.46	0.46
2:M:158:TYR:OH	2:M:191:LEU:HD23	2.16	0.46
1:L:346:MET:HE3	1:L:349:GLY:O	2.16	0.46
2:1:158:TYR:OH	2:1:191:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:155:VAL:HG11	2:S:211:VAL:HG11	1.98	0.46
1:D:382:ASN:O	1:D:385:ILE:O	2.34	0.46
2:S:151:LEU:HB3	2:S:224:VAL:CG1	2.46	0.46
1:K:17:HIS:HA	1:K:350:TRP:O	2.16	0.46
1:L:384:VAL:HG11	1:L:428:LEU:HD11	1.97	0.46
3:8:93:TYR:HD1	3:8:100:SER:HB3	1.79	0.46
3:4:25:SER:O	3:4:29:ILE:HG13	2.16	0.46
1:B:17:HIS:HA	1:B:350:TRP:O	2.16	0.46
1:I:388:THR:HG23	1:I:389:ASN:N	2.31	0.46
2:S:98:ARG:NH1	2:S:98:ARG:HG2	2.31	0.46
3:4:37:TRP:HB2	3:4:50:ILE:HG13	1.97	0.46
3:R:37:TRP:HB2	3:R:50:ILE:HG13	1.97	0.46
1:D:427:LEU:O	1:D:431:LEU:HD12	2.16	0.46
2:Y:184:GLN:HG2	3:Z:165:GLU:OE1	2.16	0.46
1:F:141:ARG:NH1	1:F:141:ARG:HB2	2.31	0.46
1:J:214:ILE:N	1:J:214:ILE:HD12	2.30	0.46
3:Z:188:GLU:H	3:Z:188:GLU:CD	2.19	0.46
1:L:421:TRP:HA	1:L:424:ASN:HD22	1.80	0.46
2:9:180:PRO:HG2	3:0:170:SER:OG	2.15	0.46
1:G:436:THR:O	1:G:440:THR:HG23	2.15	0.46
2:9:47:TRP:HZ2	2:9:50:TRP:HB2	1.81	0.46
2:7:112:PRO:HA	3:8:36:HIS:CD2	2.51	0.46
2:W:6:GLN:HB3	2:W:120:THR:HG22	1.97	0.46
2:7:148:THR:HA	2:7:199:SER:N	2.28	0.46
2:9:206:THR:HG21	2:9:223:LYS:CE	2.34	0.46
2:3:20:VAL:CG1	2:3:120:THR:HG21	2.40	0.46
2:S:214:LYS:N	2:S:215:PRO:CD	2.79	0.46
1:I:326:LYS:NZ	1:I:341:ASN:HD22	2.14	0.46
1:H:461:ASP:OD2	1:I:453:ARG:HG2	2.16	0.46
1:K:103:PRO:HD2	1:K:232:ILE:O	2.16	0.46
1:D:102:VAL:O	1:D:105:TYR:HB2	2.15	0.46
3:2:93:TYR:HD1	3:2:100:SER:HB3	1.76	0.46
2:Q:212:ASN:HB2	2:Q:219:LYS:HD3	1.97	0.46
3:V:139:CYS:CB	3:V:153:TRP:HZ2	2.29	0.46
1:G:208:ARG:HG3	1:G:241:ASP:OD2	2.16	0.46
1:I:37:THR:CG2	1:I:322:ASN:HB2	2.44	0.46
1:C:457:GLU:HG3	1:C:499:ARG:NH1	2.29	0.46
3:4:53:ASN:O	3:4:54:SER:CB	2.64	0.46
1:J:210:GLN:NE2	1:L:220:ARG:CZ	2.79	0.46
1:L:388:THR:HG23	1:L:389:ASN:N	2.30	0.46
1:G:99:PRO:HB3	1:G:223:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:321:ARG:O	1:G:321:ARG:HG2	2.14	0.46
1:I:134:GLY:CA	1:I:153:TRP:HB3	2.46	0.46
1:J:352:GLY:CA	1:J:365:ALA:HA	2.45	0.46
2:W:142:LYS:O	2:W:144:THR:HG23	2.16	0.46
3:T:115:LYS:HG2	3:T:146:PRO:HD3	1.97	0.46
1:H:436:THR:O	1:H:440:THR:HG23	2.16	0.46
3:O:188:GLU:H	3:O:188:GLU:CD	2.18	0.46
1:J:18:HIS:CD2	1:J:18:HIS:H	2.33	0.46
1:A:170:ASN:ND2	1:A:239:PRO:HA	2.30	0.46
1:A:152:ASN:HB2	1:A:255:ARG:NH1	2.31	0.46
1:D:182:VAL:HG22	1:D:202:VAL:HG21	1.98	0.46
3:8:174:ASN:HD21	3:8:176:LYS:HB3	1.81	0.45
2:S:47:TRP:HZ2	2:S:50:TRP:HB2	1.81	0.45
2:S:10:GLU:OE1	2:S:18:VAL:HG13	2.16	0.45
2:O:10:GLU:OE1	2:O:18:VAL:HG13	2.16	0.45
2:9:11:VAL:HG13	2:9:123:THR:O	2.16	0.45
1:A:463:GLY:C	1:A:465:GLY:H	2.18	0.45
1:K:380:LYS:HZ3	1:K:384:VAL:HG23	1.81	0.45
1:F:316:LEU:HD12	1:F:433:ASN:OD1	2.16	0.45
2:M:22:CYS:HB2	2:M:36:TRP:HH2	1.81	0.45
1:K:357:ASN:HB2	1:K:473:CYS:O	2.16	0.45
1:D:102:VAL:HG11	1:D:108:LEU:HD23	1.97	0.45
1:L:137:ASN:O	1:L:140:LYS:HG3	2.16	0.45
1:L:101:ASP:O	1:L:103:PRO:HD3	2.16	0.45
3:4:20:ILE:HG23	3:4:106:THR:HG21	1.98	0.45
3:O:147:GLY:HA3	3:O:177:TYR:CG	2.50	0.45
1:D:335:ILE:HG12	1:D:354:ARG:HB3	1.98	0.45
1:F:17:HIS:HA	1:F:350:TRP:O	2.16	0.45
1:G:17:HIS:HA	1:G:350:TRP:O	2.16	0.45
1:A:381:LEU:O	1:A:385:ILE:HG13	2.15	0.45
3:V:163:GLY:O	3:V:183:LEU:HA	2.17	0.45
1:D:17:HIS:HA	1:D:350:TRP:O	2.16	0.45
3:6:24:GLY:O	3:6:29:ILE:HD11	2.16	0.45
1:G:426:GLU:HG3	1:H:383:ARG:HH22	1.80	0.45
1:I:59:LEU:HD12	1:I:60:ASP:N	2.30	0.45
1:C:109:ARG:CZ	1:C:267:ILE:HD13	2.47	0.45
1:K:321:ARG:HG2	1:K:321:ARG:O	2.16	0.45
1:J:169:PRO:HA	1:J:242:VAL:HG23	1.98	0.45
3:T:146:PRO:HD2	3:T:203:GLU:OE1	2.16	0.45
3:X:67:SER:O	3:X:73:ALA:HB1	2.16	0.45
3:N:38:TYR:HE2	3:N:48:LEU:HD13	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:ARG:NH1	1:I:141:ARG:HB2	2.31	0.45
3:0:67:SER:O	3:0:73:ALA:HB1	2.16	0.45
2:5:161:GLU:HA	2:5:162:PRO:HA	1.77	0.45
2:Y:34:LEU:HD22	2:Y:35:SER:N	2.31	0.45
2:5:50:TRP:CH2	2:5:52:ASN:HB2	2.52	0.45
2:3:87:ARG:C	2:3:124:VAL:HG11	2.36	0.45
1:B:326:LYS:NZ	1:B:341:ASN:HD22	2.14	0.45
1:D:326:LYS:NZ	1:D:341:ASN:HD22	2.14	0.45
1:B:196:VAL:O	1:B:197:GLN:C	2.55	0.45
2:S:11:VAL:HG13	2:S:123:THR:HB	1.97	0.45
1:A:335:ILE:HG12	1:A:354:ARG:HB3	1.98	0.45
1:E:381:LEU:O	1:E:385:ILE:HG13	2.16	0.45
1:L:321:ARG:O	1:L:321:ARG:HG2	2.15	0.45
3:V:25:SER:O	3:V:29:ILE:HG13	2.16	0.45
3:P:37:TRP:CZ3	3:P:90:CYS:HB3	2.51	0.45
3:2:53:ASN:O	3:2:54:SER:CB	2.64	0.45
1:L:487:ASP:OD2	1:L:490:VAL:HG23	2.16	0.45
1:I:152:ASN:HB2	1:I:255:ARG:NH1	2.31	0.45
3:P:188:GLU:H	3:P:188:GLU:CD	2.20	0.45
1:J:497:ASN:HD22	1:J:497:ASN:HA	1.53	0.45
1:D:323:VAL:O	1:D:323:VAL:HG23	2.16	0.45
1:A:91:SER:O	2:M:31:SER:HB2	2.15	0.45
1:E:50:LYS:HD3	1:E:275:ASP:HB2	1.99	0.45
3:Z:167:THR:HG22	3:Z:180:SER:O	2.16	0.45
3:V:167:THR:HG22	3:V:180:SER:O	2.15	0.45
3:8:53:ASN:O	3:8:54:SER:CB	2.64	0.45
2:1:18:VAL:HG12	2:1:19:THR:H	1.81	0.45
2:3:18:VAL:HG12	2:3:19:THR:H	1.82	0.45
2:9:18:VAL:HG12	2:9:19:THR:H	1.81	0.45
1:F:185:PRO:O	1:F:217:ILE:HA	2.16	0.45
1:F:384:VAL:HG21	1:F:428:LEU:HD11	1.98	0.45
2:5:214:LYS:HB2	2:5:215:PRO:HD3	1.97	0.45
1:I:272:ALA:HA	2:3:105:VAL:CG2	2.44	0.45
1:F:321:ARG:HG2	1:F:321:ARG:O	2.14	0.45
1:A:102:VAL:O	1:A:105:TYR:HB2	2.15	0.45
1:E:220:ARG:HD2	1:E:229:ARG:HG2	1.98	0.45
2:W:194:VAL:CG2	3:X:140:LEU:HD13	2.44	0.45
1:D:85:ASP:O	1:D:265:SER:HA	2.16	0.45
3:0:139:CYS:CB	3:0:153:TRP:HZ2	2.28	0.45
1:B:61:GLY:HA2	1:B:79:PHE:CZ	2.51	0.45
3:V:6:GLN:HG2	3:V:106:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:20:ILE:HG23	3:V:106:THR:HG21	1.98	0.45
3:0:25:SER:O	3:0:29:ILE:HG13	2.16	0.45
3:N:155:ALA:N	3:N:158:SER:O	2.46	0.45
3:8:64:PHE:HD1	3:8:77:ILE:HG12	1.80	0.45
3:X:64:PHE:HD1	3:X:77:ILE:HG12	1.81	0.45
2:U:142:LYS:O	2:U:144:THR:HG23	2.17	0.45
2:1:112:PRO:CB	3:2:51:SER:HB2	2.46	0.45
3:N:146:PRO:HD2	3:N:203:GLU:OE1	2.16	0.45
1:H:182:VAL:HG22	1:H:202:VAL:HG21	1.98	0.45
1:F:203:THR:HG23	1:F:212:THR:OG1	2.16	0.45
3:R:188:GLU:CD	3:R:188:GLU:H	2.20	0.45
1:B:404:GLY:HA3	1:C:107:SER:HB2	1.98	0.45
3:V:38:TYR:HE2	3:V:48:LEU:HD13	1.81	0.45
2:S:34:LEU:HD22	2:S:35:SER:N	2.32	0.45
2:W:11:VAL:HG22	2:W:123:THR:HB	1.98	0.45
2:3:38:ARG:HB3	2:3:94:TYR:CE1	2.51	0.45
2:U:18:VAL:HG12	2:U:19:THR:H	1.81	0.45
2:Y:214:LYS:N	2:Y:215:PRO:CD	2.79	0.45
1:E:37:THR:CG2	1:E:322:ASN:HB2	2.43	0.45
1:B:185:PRO:HA	1:B:190:GLU:OE2	2.16	0.45
1:C:191:GLN:NE2	1:C:217:ILE:HD11	2.26	0.45
3:P:139:CYS:CB	3:P:153:TRP:HZ2	2.29	0.45
1:D:346:MET:HE3	1:D:349:GLY:O	2.17	0.45
1:L:85:ASP:O	1:L:265:SER:HA	2.16	0.45
1:E:384:VAL:HG11	1:E:428:LEU:HD11	1.98	0.45
2:U:182:VAL:HG12	3:V:182:TYR:CD2	2.52	0.45
1:J:17:HIS:HA	1:J:350:TRP:O	2.16	0.45
1:E:376:GLN:HB2	1:E:439:LEU:HD11	1.96	0.45
2:M:184:GLN:HA	3:N:165:GLU:OE1	2.15	0.45
1:E:183:HIS:ND1	1:E:184:HIS:N	2.64	0.45
3:0:53:ASN:O	3:0:54:SER:CB	2.64	0.45
1:H:280:GLU:HB2	1:H:290:ASN:ND2	2.30	0.45
3:X:115:LYS:HG2	3:X:146:PRO:HD3	1.98	0.45
1:G:323:VAL:O	1:G:323:VAL:HG23	2.17	0.45
1:K:323:VAL:O	1:K:323:VAL:HG23	2.16	0.45
2:Y:34:LEU:N	2:Y:99:VAL:HG13	2.32	0.45
2:1:108:PHE:H	2:1:108:PHE:HD2	1.59	0.45
2:5:83:MET:HB3	2:5:86:LEU:HD21	1.97	0.45
2:3:214:LYS:HB2	2:3:215:PRO:HD3	1.97	0.45
2:7:4:LEU:HA	2:7:23:GLN:O	2.16	0.45
1:E:191:GLN:NE2	1:E:217:ILE:HD11	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:29:ILE:H	1:I:434:GLN:HB2	1.82	0.45
1:F:495:ALA:O	1:F:499:ARG:HG3	2.17	0.45
3:N:20:ILE:HG23	3:N:106:THR:HG21	1.99	0.45
1:A:405:ARG:HD3	1:B:406:ILE:HG21	1.99	0.45
1:H:321:ARG:HG2	1:H:321:ARG:O	2.15	0.45
2:Y:139:PRO:HB2	2:Y:141:SER:O	2.16	0.45
2:5:151:LEU:HB3	2:5:224:VAL:CG1	2.47	0.45
1:I:376:GLN:HB2	1:I:439:LEU:HD11	1.98	0.45
1:C:327:GLN:HG3	1:C:329:ARG:NE	2.30	0.45
1:H:372:ALA:O	1:H:376:GLN:HG3	2.16	0.45
3:6:53:ASN:O	3:6:54:SER:CB	2.65	0.45
3:8:25:SER:O	3:8:29:ILE:HG13	2.17	0.45
1:I:463:GLY:C	1:I:465:GLY:H	2.20	0.45
1:A:421:TRP:HA	1:A:421:TRP:CE3	2.51	0.45
3:Z:37:TRP:HB2	3:Z:50:ILE:CG1	2.46	0.45
3:Z:38:TYR:HD2	3:Z:48:LEU:HA	1.81	0.45
1:G:352:GLY:CA	1:G:365:ALA:HA	2.46	0.45
1:J:423:TYR:CE2	1:K:424:ASN:HB3	2.51	0.45
1:K:487:ASP:OD2	1:K:490:VAL:HG23	2.17	0.45
2:O:34:LEU:N	2:O:99:VAL:HG13	2.31	0.45
3:8:38:TYR:HE2	3:8:48:LEU:HD13	1.81	0.45
2:W:34:LEU:HD22	2:W:35:SER:H	1.80	0.45
2:U:91:THR:CB	2:U:123:THR:HA	2.47	0.45
2:5:148:THR:HA	2:5:199:SER:N	2.29	0.45
2:M:83:MET:HB3	2:M:86:LEU:HD21	1.99	0.45
1:H:227:SER:HB2	6:I:610:NAG:H83	1.97	0.45
2:9:159:PHE:CD1	2:9:160:PRO:HA	2.52	0.45
3:P:51:SER:OG	3:P:55:ASN:HB3	2.16	0.45
2:M:6:GLN:OE1	2:M:120:THR:HG23	2.17	0.45
1:F:156:LYS:HD2	1:F:196:VAL:CG2	2.40	0.45
2:3:195:VAL:HG12	2:3:196:THR:N	2.32	0.45
2:3:179:PHE:CZ	3:4:140:LEU:HB3	2.52	0.45
2:M:112:PRO:HB3	3:N:36:HIS:NE2	2.32	0.45
2:Y:195:VAL:HG12	2:Y:196:THR:N	2.31	0.45
2:W:155:VAL:CG2	2:W:191:LEU:HG	2.47	0.45
3:X:6:GLN:HG2	3:X:106:THR:HG23	1.99	0.45
2:9:158:TYR:OH	2:9:191:LEU:HD23	2.17	0.45
2:9:212:ASN:HB2	2:9:219:LYS:HD3	1.99	0.45
1:K:346:MET:HE3	1:K:349:GLY:O	2.17	0.45
1:B:85:ASP:O	1:B:265:SER:HA	2.17	0.45
1:D:457:GLU:HG3	1:D:499:ARG:NH1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:25:SER:O	3:Z:29:ILE:HG13	2.17	0.45
3:2:139:CYS:CB	3:2:153:TRP:HZ2	2.30	0.45
2:M:32:TYR:CD1	2:M:98:ARG:HD3	2.52	0.45
3:P:37:TRP:HB2	3:P:50:ILE:HG13	1.98	0.45
1:I:96:ASN:CA	1:I:224:ARG:HH11	2.30	0.45
2:Q:38:ARG:HB3	2:Q:94:TYR:HE1	1.82	0.45
3:4:155:ALA:N	3:4:158:SER:O	2.48	0.45
3:R:37:TRP:HB2	3:R:50:ILE:CG1	2.47	0.45
1:E:421:TRP:HA	1:E:424:ASN:HD22	1.81	0.45
1:E:213:ILE:HG13	1:E:233:TYR:CE2	2.52	0.45
3:T:53:ASN:O	3:T:54:SER:CB	2.64	0.45
1:I:50:LYS:HD3	1:I:275:ASP:HB2	1.98	0.45
1:E:49:GLY:HA2	1:E:285:ASN:O	2.16	0.45
4:A:601:NAG:H61	4:A:602:NAG:O7	2.16	0.45
2:W:10:GLU:OE1	2:W:18:VAL:HG13	2.16	0.45
2:7:83:MET:HB3	2:7:86:LEU:HD21	1.97	0.45
3:Z:53:ASN:O	3:Z:54:SER:CB	2.64	0.45
1:F:99:PRO:HB2	1:F:229:ARG:CD	2.47	0.45
1:B:197:GLN:CD	1:B:197:GLN:H	2.20	0.45
1:F:197:GLN:CD	1:F:197:GLN:H	2.18	0.45
2:Y:36:TRP:NE1	2:Y:70:MET:HE1	2.32	0.45
1:B:321:ARG:HG2	1:B:321:ARG:O	2.15	0.45
1:F:339:ILE:HG22	1:F:340:GLU:N	2.30	0.45
1:D:161:TYR:HB2	1:D:196:VAL:HG21	1.99	0.45
1:G:102:VAL:HG11	1:G:108:LEU:HD23	1.97	0.45
2:S:167:TRP:CB	2:S:172:LEU:HB3	2.47	0.45
1:K:335:ILE:HG12	1:K:354:ARG:HB3	1.98	0.45
1:C:208:ARG:HG3	1:C:241:ASP:OD2	2.16	0.45
3:X:139:CYS:CB	3:X:153:TRP:HZ2	2.30	0.45
1:L:102:VAL:HG11	1:L:108:LEU:HD23	1.98	0.45
2:1:151:LEU:HB3	2:1:224:VAL:CG1	2.47	0.45
1:D:335:ILE:CD1	1:D:354:ARG:HB3	2.46	0.45
2:Q:151:LEU:HB3	2:Q:224:VAL:CG1	2.47	0.45
1:J:114:SER:HA	1:J:265:SER:O	2.17	0.45
3:8:6:GLN:NE2	3:8:105:GLY:H	2.15	0.45
1:H:321:ARG:HD2	1:H:437:ILE:CG2	2.47	0.45
2:O:155:VAL:HG11	2:O:211:VAL:HG11	1.98	0.45
2:U:182:VAL:CG1	3:V:182:TYR:CD2	2.98	0.45
2:5:39:GLN:HE21	2:5:45:LEU:HD23	1.81	0.45
1:D:388:THR:HG23	1:D:389:ASN:N	2.31	0.45
1:A:388:THR:HG23	1:A:389:ASN:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.81	0.45
2:1:32:TYR:CD1	2:1:98:ARG:HD3	2.52	0.45
3:8:37:TRP:CZ3	3:8:90:CYS:HB3	2.51	0.45
3:0:17:ARG:HA	3:0:77:ILE:O	2.16	0.45
1:E:66:LEU:HD11	1:E:84:TRP:CH2	2.52	0.45
1:H:180:TRP:CE2	1:H:204:VAL:HG21	2.52	0.45
1:I:416:THR:HG22	1:I:420:LEU:HD11	1.99	0.45
3:4:67:SER:O	3:4:73:ALA:HB1	2.16	0.45
3:2:188:GLU:H	3:2:188:GLU:CD	2.19	0.45
1:J:268:MET:HE1	1:J:282:ILE:HG22	1.98	0.45
1:I:138:ALA:HB2	1:I:226:LEU:HD12	1.98	0.45
3:T:167:THR:CG2	3:T:180:SER:H	2.29	0.45
3:Z:172:GLN:HE21	3:Z:176:LYS:NZ	2.15	0.45
2:7:102:VAL:HG12	2:7:103:ARG:H	1.80	0.45
2:Q:34:LEU:N	2:Q:99:VAL:HG13	2.32	0.45
2:S:101:GLY:H	2:S:111:TYR:HB3	1.81	0.45
2:M:108:PHE:HZ	3:N:99:GLY:HA2	1.80	0.45
2:S:83:MET:HB3	2:S:86:LEU:HD21	1.99	0.45
2:7:10:GLU:OE1	2:7:18:VAL:HG13	2.17	0.45
2:Q:10:GLU:OE1	2:Q:18:VAL:HG13	2.17	0.45
1:J:463:GLY:HA2	1:K:453:ARG:CD	2.38	0.45
2:Q:214:LYS:N	2:Q:215:PRO:CD	2.80	0.45
2:7:214:LYS:N	2:7:215:PRO:CD	2.79	0.45
1:B:98:TYR:OH	1:B:228:SER:HB2	2.16	0.45
1:D:185:PRO:O	1:D:217:ILE:HA	2.17	0.45
1:H:192:THR:HG22	1:H:198:ALA:HB2	1.99	0.45
2:O:36:TRP:NE1	2:O:70:MET:HE1	2.32	0.45
1:K:382:ASN:O	1:K:385:ILE:O	2.34	0.45
1:F:103:PRO:HG2	1:F:233:TYR:CE1	2.51	0.45
1:I:197:GLN:CD	1:I:197:GLN:H	2.20	0.45
2:U:22:CYS:HB2	2:U:36:TRP:HH2	1.80	0.45
1:G:182:VAL:HG22	1:G:202:VAL:HG21	1.99	0.45
3:4:6:GLN:HG2	3:4:106:THR:HG23	1.99	0.45
1:A:247:SER:HB3	1:A:251:LEU:HD22	1.99	0.45
1:I:384:VAL:HG21	1:I:428:LEU:HD11	1.99	0.45
1:B:470:TYR:CE2	1:B:499:ARG:HA	2.52	0.45
1:C:321:ARG:HG2	1:C:321:ARG:O	2.16	0.45
3:X:25:SER:O	3:X:29:ILE:HG13	2.15	0.45
2:5:112:PRO:HA	3:6:36:HIS:CD2	2.52	0.45
1:G:457:GLU:HG3	1:G:499:ARG:NH1	2.30	0.45
1:C:96:ASN:CA	1:C:224:ARG:HH11	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:155:ALA:N	3:2:158:SER:O	2.47	0.45
1:E:15:LEU:HD22	1:E:448:PHE:HA	1.99	0.45
3:R:91:GLN:HB2	3:R:102:PHE:CE2	2.52	0.45
2:5:142:LYS:O	2:5:144:THR:HG23	2.16	0.45
2:3:142:LYS:O	2:3:144:THR:HG23	2.17	0.45
1:C:280:GLU:HB2	1:C:290:ASN:HD21	1.82	0.45
1:D:54:ASN:OD1	3:0:203:GLU:HB3	2.17	0.45
1:E:436:THR:O	1:E:440:THR:HG23	2.16	0.45
1:L:180:TRP:CD2	1:L:204:VAL:HG21	2.51	0.45
3:2:91:GLN:HB2	3:2:102:PHE:HE2	1.82	0.45
1:L:213:ILE:HG13	1:L:233:TYR:CE2	2.51	0.45
2:W:154:LEU:HD21	3:X:136:THR:HG21	1.99	0.45
1:A:487:ASP:OD2	1:A:490:VAL:HG23	2.16	0.45
1:A:416:THR:HG22	1:A:420:LEU:CD1	2.47	0.45
3:P:38:TYR:HD2	3:P:48:LEU:HA	1.81	0.45
1:D:331:LEU:N	1:D:331:LEU:CD2	2.74	0.45
3:8:51:SER:OG	3:8:55:ASN:HB3	2.17	0.45
2:3:34:LEU:N	2:3:99:VAL:HG13	2.32	0.45
2:5:111:TYR:HE1	2:5:113:MET:CG	2.28	0.45
2:W:83:MET:HB3	2:W:86:LEU:HD21	1.99	0.45
2:W:206:THR:HG21	2:W:223:LYS:CE	2.34	0.45
2:7:19:THR:HG22	2:7:82:GLU:CG	2.44	0.45
1:L:143:PRO:HG2	1:L:144:GLY:H	1.82	0.45
1:B:222:TRP:CB	6:C:610:NAG:H62	2.46	0.45
2:5:214:LYS:N	2:5:215:PRO:CD	2.79	0.45
1:E:326:LYS:HD3	1:E:328:THR:H	1.82	0.45
1:G:326:LYS:HZ3	1:G:341:ASN:HD22	1.65	0.45
1:A:17:HIS:HA	1:A:350:TRP:O	2.17	0.45
2:O:214:LYS:N	2:O:215:PRO:CD	2.80	0.45
2:M:95:TYR:CE1	2:M:119:GLY:HA3	2.52	0.45
1:D:203:THR:HG21	1:F:220:ARG:HH21	1.81	0.45
1:A:272:ALA:N	2:M:105:VAL:HG23	2.32	0.45
1:L:161:TYR:HB2	1:L:196:VAL:HG21	1.98	0.45
2:S:195:VAL:HG12	2:S:196:THR:N	2.32	0.45
3:N:153:TRP:CD2	3:N:183:LEU:HD13	2.52	0.45
2:9:167:TRP:CB	2:9:172:LEU:HB3	2.47	0.45
3:Z:6:GLN:NE2	3:Z:105:GLY:H	2.15	0.45
3:2:6:GLN:HG2	3:2:106:THR:HG23	1.98	0.45
1:C:108:LEU:O	1:C:112:VAL:HG23	2.17	0.45
1:C:17:HIS:HA	1:C:350:TRP:O	2.17	0.45
1:I:321:ARG:O	1:I:321:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:51:SER:OG	3:X:55:ASN:HB3	2.17	0.45
2:Y:142:LYS:O	2:Y:144:THR:HG23	2.16	0.45
1:A:352:GLY:CA	1:A:365:ALA:HA	2.47	0.45
3:4:146:PRO:HD2	3:4:203:GLU:OE1	2.17	0.45
3:0:115:LYS:HG2	3:0:146:PRO:HD3	1.98	0.45
3:Z:115:LYS:HG2	3:Z:146:PRO:HD3	1.98	0.45
1:H:471:HIS:HB2	1:H:494:GLU:OE1	2.17	0.45
3:V:91:GLN:HB2	3:V:102:PHE:HE2	1.81	0.45
3:N:113:GLN:HA	3:N:114:PRO:HD3	1.72	0.45
2:O:37:VAL:HG11	3:P:102:PHE:HE1	1.82	0.45
2:U:108:PHE:CD2	2:U:108:PHE:N	2.75	0.45
2:U:34:LEU:HD22	2:U:35:SER:H	1.82	0.45
2:S:34:LEU:N	2:S:99:VAL:HG13	2.32	0.45
1:J:463:GLY:C	1:J:465:GLY:H	2.19	0.45
2:U:214:LYS:N	2:U:215:PRO:CD	2.80	0.45
1:E:326:LYS:CD	1:E:328:THR:H	2.30	0.45
2:S:6:GLN:H	2:S:118:GLN:HE22	1.63	0.45
2:M:117:GLY:O	2:M:119:GLY:N	2.50	0.45
2:M:11:VAL:HG13	2:M:123:THR:HB	1.99	0.45
1:G:185:PRO:O	1:G:217:ILE:HA	2.17	0.45
1:G:137:ASN:O	1:G:140:LYS:HG3	2.17	0.45
1:B:192:THR:HG22	1:B:198:ALA:HB2	1.99	0.45
1:F:161:TYR:CZ	1:F:249:GLY:HA2	2.52	0.45
1:A:192:THR:HG22	1:A:198:ALA:HB2	1.98	0.45
1:D:192:THR:HG22	1:D:198:ALA:HB2	1.99	0.45
1:J:67:ILE:HG13	1:J:105:TYR:CE2	2.52	0.45
2:U:151:LEU:HB3	2:U:224:VAL:CG1	2.47	0.45
1:G:114:SER:O	1:G:265:SER:HB2	2.17	0.45
1:K:17:HIS:HB2	1:K:320:MET:HE1	1.98	0.45
3:4:24:GLY:O	3:4:29:ILE:HD11	2.17	0.45
1:D:272:ALA:HA	2:S:105:VAL:CG2	2.47	0.45
1:G:383:ARG:HH22	1:I:426:GLU:HG3	1.81	0.45
3:P:155:ALA:N	3:P:158:SER:O	2.48	0.45
3:P:37:TRP:HB2	3:P:50:ILE:CG1	2.47	0.45
1:I:183:HIS:ND1	1:I:184:HIS:N	2.65	0.45
1:K:321:ARG:HD2	1:K:437:ILE:CG2	2.47	0.45
1:B:44:GLN:HG2	1:B:288:ILE:HD12	1.98	0.45
3:6:146:PRO:HD2	3:6:203:GLU:OE1	2.17	0.45
3:0:146:PRO:HD2	3:0:203:GLU:OE1	2.17	0.45
3:N:188:GLU:H	3:N:188:GLU:CD	2.20	0.45
1:K:141:ARG:HB2	1:K:141:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:280:GLU:HB2	1:K:290:ASN:ND2	2.32	0.45
1:G:152:ASN:HB2	1:G:255:ARG:NH1	2.31	0.45
2:Y:55:ASP:OD2	2:Y:57:GLN:HB2	2.17	0.44
2:3:55:ASP:OD2	2:3:57:GLN:HB2	2.17	0.44
2:5:47:TRP:HZ2	2:5:50:TRP:HB2	1.83	0.44
2:Y:83:MET:HB3	2:Y:86:LEU:HD21	1.99	0.44
2:9:214:LYS:N	2:9:215:PRO:CD	2.79	0.44
2:M:214:LYS:N	2:M:215:PRO:CD	2.80	0.44
1:K:101:ASP:O	1:K:103:PRO:HD3	2.16	0.44
1:L:29:ILE:H	1:L:434:GLN:HB2	1.82	0.44
3:N:53:ASN:O	3:N:54:SER:CB	2.64	0.44
3:6:20:ILE:HG23	3:6:106:THR:HG21	1.98	0.44
2:9:195:VAL:HG12	2:9:196:THR:N	2.32	0.44
2:3:212:ASN:HB2	2:3:219:LYS:HD3	1.99	0.44
3:P:25:SER:O	3:P:29:ILE:HG13	2.18	0.44
3:6:130:LEU:CD2	3:6:135:ALA:HB2	2.46	0.44
3:Z:5:THR:HB	3:Z:23:THR:OG1	2.17	0.44
1:K:96:ASN:CA	1:K:224:ARG:HH11	2.30	0.44
1:D:134:GLY:CA	1:D:153:TRP:HB3	2.47	0.44
1:J:183:HIS:ND1	1:J:184:HIS:N	2.65	0.44
1:D:463:GLY:C	1:D:465:GLY:H	2.20	0.44
3:V:37:TRP:CZ3	3:V:90:CYS:HB3	2.52	0.44
1:E:255:ARG:HG2	1:E:255:ARG:HH11	1.82	0.44
1:D:453:ARG:HD3	1:F:463:GLY:O	2.17	0.44
3:P:115:LYS:HG2	3:P:146:PRO:HD3	1.99	0.44
3:N:38:TYR:HD2	3:N:48:LEU:HA	1.81	0.44
1:K:421:TRP:HA	1:K:424:ASN:HD22	1.81	0.44
3:N:91:GLN:HB2	3:N:102:PHE:HE2	1.81	0.44
3:Z:67:SER:O	3:Z:73:ALA:HB1	2.16	0.44
3:P:83:GLU:H	3:P:83:GLU:CD	2.21	0.44
3:T:188:GLU:H	3:T:188:GLU:CD	2.21	0.44
1:J:50:LYS:HD3	1:J:275:ASP:HB2	1.98	0.44
1:I:414:GLU:O	1:I:418:ILE:HG13	2.18	0.44
3:X:53:ASN:O	3:X:54:SER:CB	2.64	0.44
2:O:55:ASP:OD2	2:O:57:GLN:HB2	2.17	0.44
2:Y:47:TRP:HZ2	2:Y:50:TRP:HB2	1.82	0.44
2:3:50:TRP:CH2	2:3:52:ASN:HB2	2.51	0.44
2:9:148:THR:HA	2:9:199:SER:N	2.29	0.44
1:D:326:LYS:NZ	1:D:341:ASN:ND2	2.64	0.44
1:G:190:GLU:O	1:G:194:LEU:HD13	2.16	0.44
3:6:93:TYR:HD1	3:6:100:SER:HB3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:463:GLY:C	1:E:465:GLY:H	2.19	0.44
1:E:463:GLY:HA2	1:F:453:ARG:HB3	1.97	0.44
1:L:37:THR:CG2	1:L:322:ASN:HB2	2.46	0.44
3:T:139:CYS:CB	3:T:153:TRP:HZ2	2.30	0.44
2:W:212:ASN:HB2	2:W:219:LYS:HD3	1.99	0.44
2:O:212:ASN:HB2	2:O:219:LYS:HD3	1.98	0.44
1:I:470:TYR:CE2	1:I:499:ARG:HA	2.52	0.44
1:H:208:ARG:HG3	1:H:241:ASP:OD2	2.17	0.44
1:I:234:TRP:N	1:I:234:TRP:CE3	2.81	0.44
1:L:234:TRP:HE3	1:L:234:TRP:N	2.15	0.44
3:N:130:LEU:CD2	3:N:135:ALA:HB2	2.47	0.44
1:E:388:THR:HG23	1:E:389:ASN:N	2.32	0.44
1:A:80:GLN:HB3	1:A:150:ARG:NH2	2.32	0.44
1:G:220:ARG:HD2	1:G:229:ARG:HG2	1.98	0.44
1:K:183:HIS:ND1	1:K:184:HIS:N	2.65	0.44
3:8:91:GLN:HB2	3:8:102:PHE:CE2	2.52	0.44
1:G:280:GLU:HB2	1:G:290:ASN:ND2	2.32	0.44
1:K:98:TYR:OH	1:K:228:SER:HB2	2.17	0.44
1:D:152:ASN:HB2	1:D:255:ARG:NH1	2.32	0.44
2:O:34:LEU:HD22	2:O:35:SER:H	1.82	0.44
2:3:108:PHE:CZ	3:4:99:GLY:HA2	2.52	0.44
2:1:100:GLU:CB	2:1:111:TYR:HB2	2.48	0.44
2:U:148:THR:HA	2:U:199:SER:N	2.29	0.44
2:O:83:MET:HB3	2:O:86:LEU:HD21	1.98	0.44
2:W:214:LYS:N	2:W:215:PRO:CD	2.79	0.44
2:1:214:LYS:N	2:1:215:PRO:CD	2.79	0.44
2:9:4:LEU:HA	2:9:23:GLN:O	2.18	0.44
2:1:4:LEU:HD11	2:1:115:VAL:O	2.16	0.44
1:H:463:GLY:C	1:H:465:GLY:H	2.21	0.44
2:W:60:TYR:CE1	2:W:70:MET:HG2	2.41	0.44
2:1:195:VAL:HG12	2:1:196:THR:N	2.32	0.44
3:N:139:CYS:CB	3:N:153:TRP:HZ2	2.30	0.44
1:E:335:ILE:HG12	1:E:354:ARG:HB3	2.00	0.44
1:J:357:ASN:HB2	1:J:473:CYS:O	2.18	0.44
3:Z:20:ILE:HG23	3:Z:106:THR:HG21	1.99	0.44
2:U:158:TYR:OH	2:U:191:LEU:HD23	2.16	0.44
3:8:6:GLN:HG2	3:8:106:THR:HG23	1.99	0.44
1:H:114:SER:HA	1:H:265:SER:O	2.18	0.44
1:C:222:TRP:CH2	1:C:225:GLY:HA2	2.53	0.44
3:N:25:SER:O	3:N:29:ILE:HG13	2.16	0.44
1:D:353:PHE:CE1	1:D:366:ASP:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:59:LEU:HD12	1:J:60:ASP:N	2.33	0.44
3:V:130:LEU:CD2	3:V:135:ALA:HB2	2.47	0.44
2:U:44:GLY:HA2	3:V:89:TYR:OH	2.17	0.44
3:P:37:TRP:CH2	3:P:90:CYS:HB3	2.52	0.44
1:K:388:THR:HG23	1:K:389:ASN:N	2.32	0.44
1:H:243:LEU:HD12	1:H:244:VAL:H	1.81	0.44
3:X:146:PRO:HD2	3:X:203:GLU:OE1	2.17	0.44
1:L:421:TRP:HA	1:L:421:TRP:CE3	2.52	0.44
1:G:471:HIS:HB2	1:G:494:GLU:OE1	2.17	0.44
2:7:161:GLU:HA	2:7:162:PRO:HA	1.77	0.44
1:B:268:MET:CE	1:B:282:ILE:HG22	2.48	0.44
1:L:323:VAL:HG23	1:L:323:VAL:O	2.16	0.44
1:I:44:GLN:OE1	1:I:289:PRO:HG2	2.17	0.44
1:K:50:LYS:HA	1:K:273:PRO:HG2	2.00	0.44
2:O:32:TYR:CG	2:O:98:ARG:HD3	2.53	0.44
2:U:34:LEU:N	2:U:99:VAL:HG13	2.32	0.44
2:7:101:GLY:H	2:7:111:TYR:HB3	1.83	0.44
2:5:113:MET:HB2	3:6:38:TYR:OH	2.17	0.44
2:3:214:LYS:N	2:3:215:PRO:CD	2.79	0.44
1:K:196:VAL:O	1:K:197:GLN:C	2.56	0.44
1:J:185:PRO:O	1:J:217:ILE:HA	2.18	0.44
1:K:384:VAL:HG21	1:K:428:LEU:HD11	2.00	0.44
3:6:6:GLN:HG2	3:6:106:THR:HG23	1.99	0.44
3:4:139:CYS:CB	3:4:153:TRP:HZ2	2.30	0.44
3:Z:6:GLN:HG2	3:Z:106:THR:HG23	1.98	0.44
1:E:384:VAL:HG21	1:E:428:LEU:HD11	2.00	0.44
1:L:321:ARG:HD2	1:L:437:ILE:CG2	2.47	0.44
1:L:470:TYR:CE2	1:L:499:ARG:HA	2.53	0.44
2:O:158:TYR:CE2	2:O:163:VAL:HG12	2.52	0.44
3:P:167:THR:CG2	3:P:180:SER:H	2.30	0.44
3:Z:130:LEU:CD2	3:Z:135:ALA:HB2	2.47	0.44
1:H:109:ARG:NH2	1:H:267:ILE:HD13	2.32	0.44
1:H:272:ALA:HA	2:1:105:VAL:HG22	1.98	0.44
1:A:424:ASN:HB3	1:C:423:TYR:CE2	2.52	0.44
2:9:32:TYR:CD1	2:9:98:ARG:HD3	2.52	0.44
3:6:118:PRO:HB3	3:6:141:ILE:CG2	2.48	0.44
1:D:352:GLY:CA	1:D:365:ALA:HA	2.48	0.44
3:2:146:PRO:HD2	3:2:203:GLU:OE1	2.17	0.44
1:A:280:GLU:HB2	1:A:290:ASN:HD21	1.82	0.44
1:B:49:GLY:HA2	1:B:285:ASN:O	2.16	0.44
3:4:188:GLU:CD	3:4:188:GLU:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:414:GLU:O	1:G:418:ILE:HG13	2.18	0.44
1:C:213:ILE:HG13	1:C:233:TYR:CE2	2.53	0.44
3:T:81:GLN:O	3:T:110:VAL:HG11	2.17	0.44
2:S:179:PHE:CE2	3:T:142:SER:HB3	2.53	0.44
2:9:39:GLN:HE21	2:9:45:LEU:HD23	1.83	0.44
2:7:35:SER:OG	2:7:113:MET:CE	2.65	0.44
2:1:47:TRP:HZ2	2:1:50:TRP:HB2	1.83	0.44
2:O:206:THR:HG21	2:O:223:LYS:CE	2.34	0.44
2:3:83:MET:HB3	2:3:86:LEU:HD21	1.98	0.44
1:K:222:TRP:CH2	1:K:225:GLY:HA2	2.53	0.44
1:A:350:TRP:HB2	1:A:370:THR:HG23	2.00	0.44
2:7:2:VAL:HG21	2:7:115:VAL:HG21	1.99	0.44
1:E:137:ASN:O	1:E:140:LYS:HG3	2.17	0.44
1:B:98:TYR:CD1	1:B:99:PRO:HD2	2.53	0.44
1:G:161:TYR:HB2	1:G:196:VAL:HG21	1.99	0.44
1:C:137:ASN:O	1:C:140:LYS:HG3	2.17	0.44
1:A:339:ILE:HG22	1:A:340:GLU:N	2.32	0.44
1:F:147:PHE:CG	1:F:148:PHE:N	2.86	0.44
1:D:156:LYS:HD2	1:D:196:VAL:CG2	2.44	0.44
3:R:6:GLN:HG2	3:R:106:THR:HG23	1.99	0.44
2:M:151:LEU:HB3	2:M:224:VAL:CG1	2.48	0.44
2:1:212:ASN:HB2	2:1:219:LYS:HD3	1.99	0.44
2:3:151:LEU:HB3	2:3:224:VAL:CG1	2.47	0.44
1:E:382:ASN:O	1:E:385:ILE:O	2.35	0.44
3:6:12:GLY:CA	3:6:111:LEU:HD13	2.48	0.44
3:X:130:LEU:CD2	3:X:135:ALA:HB2	2.47	0.44
3:0:130:LEU:CD2	3:0:135:ALA:HB2	2.46	0.44
2:M:27:TYR:O	2:M:98:ARG:NH2	2.50	0.44
1:A:15:LEU:HD22	1:A:448:PHE:HA	1.99	0.44
1:F:134:GLY:CA	1:F:153:TRP:HB3	2.46	0.44
1:J:423:TYR:CZ	1:J:427:LEU:HD22	2.53	0.44
1:A:416:THR:HG22	1:A:420:LEU:HD11	1.98	0.44
3:R:122:LEU:HD13	3:R:198:CYS:HB2	1.98	0.44
1:K:416:THR:HG22	1:K:420:LEU:HD11	2.00	0.44
1:G:141:ARG:HB2	1:G:141:ARG:NH1	2.32	0.44
1:D:141:ARG:NH1	1:D:141:ARG:HB2	2.33	0.44
1:L:497:ASN:HA	1:L:497:ASN:HD22	1.53	0.44
3:8:195:SER:HB3	3:8:212:ALA:HB2	2.00	0.44
1:G:421:TRP:HA	1:G:424:ASN:HD22	1.81	0.44
2:1:182:VAL:O	2:1:189:TYR:HA	2.18	0.44
3:V:67:SER:O	3:V:73:ALA:HB1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:177:HIS:NE2	3:N:172:GLN:OE1	2.51	0.44
2:O:108:PHE:CB	2:O:111:TYR:CE2	3.01	0.44
2:W:34:LEU:N	2:W:99:VAL:HG13	2.32	0.44
2:Y:101:GLY:H	2:Y:111:TYR:HB3	1.81	0.44
2:1:34:LEU:HD22	2:1:35:SER:N	2.32	0.44
2:S:206:THR:CG2	2:S:223:LYS:HG2	2.48	0.44
2:O:198:PRO:HG2	2:O:201:SER:OG	2.18	0.44
2:3:135:PHE:HB3	3:4:126:SER:OG	2.18	0.44
2:1:19:THR:HG22	2:1:82:GLU:CG	2.46	0.44
2:U:83:MET:HB3	2:U:86:LEU:HD21	1.99	0.44
1:H:222:TRP:CH2	1:H:225:GLY:HA2	2.52	0.44
1:F:335:ILE:HG12	1:F:354:ARG:HB3	2.00	0.44
1:J:29:ILE:H	1:J:434:GLN:HB2	1.83	0.44
2:5:195:VAL:HG12	2:5:196:THR:N	2.33	0.44
1:B:384:VAL:HG21	1:B:428:LEU:HD11	2.00	0.44
1:A:27:LYS:HZ2	1:B:383:ARG:HD3	1.83	0.44
1:D:67:ILE:HG13	1:D:105:TYR:CE2	2.52	0.44
1:B:27:LYS:HZ3	1:C:383:ARG:HD3	1.82	0.44
2:W:137:LEU:HD11	3:X:138:VAL:HG21	1.99	0.44
3:N:6:GLN:HG2	3:N:106:THR:HG23	1.99	0.44
2:5:179:PHE:CZ	3:6:140:LEU:HB3	2.52	0.44
1:D:99:PRO:HB3	1:D:223:VAL:HG21	1.99	0.44
2:7:212:ASN:HB2	2:7:219:LYS:HD3	1.98	0.44
2:Q:155:VAL:HG11	2:Q:211:VAL:HG11	1.99	0.44
1:B:495:ALA:O	1:B:499:ARG:HG3	2.17	0.44
1:B:114:SER:HA	1:B:265:SER:O	2.17	0.44
3:N:24:GLY:O	3:N:29:ILE:HD11	2.18	0.44
3:R:38:TYR:HE2	3:R:48:LEU:HD13	1.82	0.44
1:J:470:TYR:CE2	1:J:499:ARG:HA	2.52	0.44
1:L:80:GLN:HB3	1:L:150:ARG:NH2	2.32	0.44
1:H:295:GLN:HE22	1:H:308:TYR:HB2	1.80	0.44
1:F:388:THR:HG23	1:F:389:ASN:N	2.33	0.44
1:F:96:ASN:CA	1:F:224:ARG:HH11	2.30	0.44
1:F:80:GLN:HB3	1:F:150:ARG:NH2	2.33	0.44
3:Z:37:TRP:CH2	3:Z:90:CYS:HB3	2.52	0.44
1:I:220:ARG:HB2	1:I:221:PRO:CD	2.48	0.44
3:T:37:TRP:HB2	3:T:50:ILE:HG13	2.00	0.44
1:K:134:GLY:CA	1:K:153:TRP:HB3	2.48	0.44
3:2:115:LYS:HG2	3:2:146:PRO:HD3	1.99	0.44
2:W:9:ALA:HB1	2:W:121:MET:O	2.17	0.44
1:B:497:ASN:HD22	1:B:497:ASN:HA	1.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:83:GLU:H	3:N:83:GLU:CD	2.21	0.44
2:7:34:LEU:HD22	2:7:35:SER:N	2.31	0.44
2:S:100:GLU:N	2:S:111:TYR:HB2	2.14	0.44
2:M:34:LEU:N	2:M:99:VAL:HG13	2.32	0.44
2:5:55:ASP:OD2	2:5:57:GLN:HB2	2.17	0.44
1:E:19:ALA:CB	1:E:322:ASN:HD21	2.31	0.44
2:S:20:VAL:HG13	2:S:120:THR:HG21	2.00	0.44
1:J:191:GLN:NE2	1:J:217:ILE:HD11	2.24	0.44
2:O:167:TRP:HB3	2:O:172:LEU:HB3	2.00	0.44
2:3:179:PHE:CD1	3:4:140:LEU:HD22	2.52	0.44
2:U:60:TYR:CE1	2:U:70:MET:HG2	2.42	0.44
2:S:167:TRP:HB3	2:S:172:LEU:HB3	1.99	0.44
1:H:405:ARG:HH22	1:I:403:GLU:CD	2.21	0.44
3:T:6:GLN:NE2	3:T:105:GLY:H	2.15	0.44
2:7:155:VAL:HG11	2:7:211:VAL:HG11	1.99	0.44
1:D:380:LYS:HZ3	1:D:384:VAL:HG23	1.82	0.44
1:E:405:ARG:H	1:F:107:SER:CB	2.30	0.44
3:X:29:ILE:CD1	3:X:71:THR:HB	2.48	0.44
3:T:24:GLY:O	3:T:29:ILE:HD11	2.17	0.44
1:G:96:ASN:CA	1:G:224:ARG:HH11	2.31	0.44
3:6:37:TRP:HB2	3:6:50:ILE:HG13	1.99	0.44
3:T:37:TRP:CH2	3:T:90:CYS:HB3	2.53	0.44
3:8:37:TRP:HB2	3:8:50:ILE:HG13	1.99	0.44
2:Y:182:VAL:O	2:Y:189:TYR:HA	2.17	0.44
3:2:37:TRP:CH2	3:2:90:CYS:HB3	2.52	0.44
2:O:142:LYS:O	2:O:144:THR:HG23	2.17	0.44
2:7:142:LYS:O	2:7:144:THR:HG23	2.18	0.44
3:N:33:TYR:O	3:N:34:ALA:C	2.56	0.44
3:X:188:GLU:CD	3:X:188:GLU:H	2.21	0.44
3:6:188:GLU:H	3:6:188:GLU:CD	2.20	0.44
1:H:288:ILE:HG13	1:H:288:ILE:O	2.18	0.44
1:B:203:THR:HG23	1:B:212:THR:OG1	2.18	0.44
1:J:471:HIS:HB2	1:J:494:GLU:OE1	2.18	0.44
1:K:471:HIS:HB2	1:K:494:GLU:OE1	2.17	0.44
1:L:288:ILE:O	1:L:288:ILE:HG13	2.17	0.44
1:G:176:LYS:HD3	1:G:178:TYR:OH	2.18	0.44
3:X:113:GLN:HG3	3:X:175:ASN:HD22	1.77	0.44
2:7:34:LEU:N	2:7:99:VAL:HG13	2.33	0.44
2:W:55:ASP:OD2	2:W:57:GLN:HB2	2.18	0.44
2:Q:34:LEU:CD2	2:Q:35:SER:N	2.81	0.44
2:1:34:LEU:N	2:1:99:VAL:HG13	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:34:LEU:HD22	2:M:35:SER:H	1.82	0.44
2:S:148:THR:HA	2:S:199:SER:N	2.29	0.44
2:M:198:PRO:HG2	2:M:201:SER:OG	2.18	0.44
1:B:222:TRP:CH2	1:B:225:GLY:HA2	2.51	0.44
1:A:321:ARG:HG2	1:A:321:ARG:O	2.17	0.44
2:S:6:GLN:OE1	2:S:120:THR:HG23	2.18	0.44
2:9:61:VAL:O	2:9:65:GLN:HG3	2.18	0.44
2:1:2:VAL:HG21	2:1:115:VAL:HG21	1.99	0.44
2:7:167:TRP:CB	2:7:172:LEU:HB3	2.48	0.44
2:Q:195:VAL:HG12	2:Q:196:THR:N	2.33	0.44
2:O:167:TRP:CB	2:O:172:LEU:HB3	2.48	0.44
3:R:20:ILE:HG23	3:R:106:THR:HG21	1.98	0.44
1:B:346:MET:HE3	1:B:349:GLY:O	2.17	0.44
3:6:167:THR:CG2	3:6:180:SER:H	2.27	0.44
1:D:384:VAL:HG21	1:D:428:LEU:HD11	1.99	0.44
3:R:130:LEU:CD2	3:R:135:ALA:HB2	2.47	0.44
1:E:423:TYR:CE2	1:F:424:ASN:HB3	2.52	0.44
1:H:220:ARG:HB2	1:H:221:PRO:CD	2.47	0.44
1:G:229:ARG:HH11	1:G:229:ARG:HG2	1.83	0.44
2:5:98:ARG:NH1	2:5:98:ARG:HG2	2.33	0.44
1:A:220:ARG:HB2	1:A:221:PRO:CD	2.48	0.44
3:4:118:PRO:HB3	3:4:141:ILE:CG2	2.47	0.44
3:6:165:GLU:H	3:6:165:GLU:HG2	1.74	0.44
2:Q:142:LYS:O	2:Q:144:THR:HG23	2.17	0.44
1:I:352:GLY:CA	1:I:365:ALA:HA	2.48	0.44
3:T:118:PRO:HB2	3:T:207:VAL:HG11	2.00	0.44
3:V:146:PRO:HD2	3:V:203:GLU:OE1	2.17	0.44
1:K:203:THR:HG23	1:K:212:THR:OG1	2.18	0.44
1:H:141:ARG:HB2	1:H:141:ARG:NH1	2.33	0.44
3:6:91:GLN:HB2	3:6:102:PHE:HE2	1.82	0.44
1:A:176:LYS:HD3	1:A:178:TYR:OH	2.17	0.44
2:7:116:TRP:HZ2	3:8:38:TYR:CE1	2.36	0.44
2:3:198:PRO:HG2	2:3:201:SER:OG	2.18	0.44
2:3:19:THR:HG22	2:3:82:GLU:CG	2.46	0.44
1:E:17:HIS:HA	1:E:350:TRP:O	2.18	0.44
1:B:137:ASN:O	1:B:140:LYS:HG3	2.18	0.44
2:5:167:TRP:HB3	2:5:172:LEU:HB3	1.99	0.44
1:H:251:LEU:HD12	1:H:252:ILE:N	2.32	0.44
1:B:384:VAL:HG11	1:B:428:LEU:HD11	2.00	0.44
3:4:167:THR:CG2	3:4:180:SER:H	2.31	0.44
2:1:39:GLN:HE21	2:1:45:LEU:HD23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:346:MET:HE3	1:I:349:GLY:O	2.18	0.44
1:C:335:ILE:HG12	1:C:354:ARG:HB3	2.00	0.44
2:7:151:LEU:HB3	2:7:224:VAL:CG1	2.48	0.44
2:O:151:LEU:HB3	2:O:224:VAL:CG1	2.48	0.44
2:W:151:LEU:HB3	2:W:224:VAL:CG1	2.47	0.44
1:A:222:TRP:CH2	1:A:225:GLY:HA2	2.53	0.44
1:C:429:VAL:HG12	1:C:433:ASN:HD21	1.83	0.44
3:T:11:SER:HB3	3:T:111:LEU:HD11	2.00	0.44
3:V:51:SER:OG	3:V:55:ASN:HB3	2.18	0.44
3:8:24:GLY:O	3:8:29:ILE:HD11	2.18	0.44
1:B:421:TRP:HA	1:B:421:TRP:CE3	2.53	0.44
3:T:37:TRP:CZ3	3:T:90:CYS:HB3	2.53	0.44
1:K:433:ASN:O	1:K:437:ILE:HG13	2.18	0.44
1:L:134:GLY:CA	1:L:153:TRP:HB3	2.48	0.44
3:T:118:PRO:HB3	3:T:141:ILE:CG2	2.48	0.44
1:J:268:MET:CE	1:J:282:ILE:HG22	2.48	0.44
1:A:182:VAL:HG22	1:A:202:VAL:HG21	1.99	0.44
1:K:295:GLN:NE2	1:K:308:TYR:HB2	2.33	0.44
2:1:154:LEU:HD21	3:2:136:THR:HG21	1.98	0.44
3:Z:195:SER:HB3	3:Z:212:ALA:HB2	2.00	0.44
1:F:487:ASP:OD2	1:F:490:VAL:HG23	2.18	0.44
1:E:323:VAL:O	1:E:323:VAL:HG23	2.17	0.44
3:6:122:LEU:HD13	3:6:198:CYS:HB2	2.00	0.44
2:9:108:PHE:CB	2:9:111:TYR:HE2	2.30	0.43
3:6:174:ASN:HD21	3:6:176:LYS:HE3	1.83	0.43
3:6:172:GLN:N	3:6:176:LYS:O	2.48	0.43
2:Q:99:VAL:HA	2:Q:111:TYR:CD1	2.52	0.43
3:2:38:TYR:HE2	3:2:48:LEU:HD13	1.82	0.43
2:S:108:PHE:CB	2:S:111:TYR:HE2	2.30	0.43
2:S:55:ASP:OD2	2:S:57:GLN:HB2	2.18	0.43
2:Q:83:MET:HB3	2:Q:86:LEU:HD21	1.99	0.43
2:M:61:VAL:HG12	2:M:63:LYS:N	2.25	0.43
2:Q:4:LEU:HA	2:Q:23:GLN:O	2.18	0.43
1:B:220:ARG:HB2	1:B:221:PRO:CD	2.48	0.43
2:M:167:TRP:HB3	2:M:172:LEU:HB3	2.00	0.43
1:F:111:LEU:HD12	1:F:111:LEU:C	2.38	0.43
3:N:93:TYR:HD1	3:N:100:SER:HB3	1.80	0.43
1:B:433:ASN:O	1:B:437:ILE:HG13	2.17	0.43
1:K:339:ILE:HG22	1:K:340:GLU:N	2.33	0.43
2:W:109:HIS:HA	3:X:93:TYR:CD1	2.52	0.43
1:H:335:ILE:HG12	1:H:354:ARG:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:6:GLN:NE2	3:R:105:GLY:H	2.15	0.43
3:Z:139:CYS:CB	3:Z:153:TRP:HZ2	2.29	0.43
2:1:155:VAL:CG2	2:1:191:LEU:HG	2.48	0.43
2:O:210:ASN:N	2:O:210:ASN:HD22	2.16	0.43
1:G:114:SER:HA	1:G:265:SER:O	2.18	0.43
1:A:206:THR:CA	1:C:221:PRO:HG2	2.47	0.43
1:K:85:ASP:O	1:K:265:SER:HA	2.18	0.43
3:R:25:SER:O	3:R:29:ILE:HG13	2.18	0.43
1:L:109:ARG:NH2	1:L:267:ILE:HD13	2.32	0.43
1:G:470:TYR:CE2	1:G:499:ARG:HA	2.53	0.43
2:Y:32:TYR:CG	2:Y:98:ARG:HD3	2.53	0.43
2:3:98:ARG:HG2	2:3:98:ARG:NH1	2.32	0.43
1:G:15:LEU:HD22	1:G:448:PHE:HA	2.00	0.43
1:D:321:ARG:HG2	1:D:321:ARG:O	2.16	0.43
1:D:97:CYS:H	1:D:224:ARG:NH1	2.16	0.43
3:N:37:TRP:HB2	3:N:50:ILE:HG13	1.99	0.43
1:K:307:LYS:HE2	1:K:421:TRP:CZ2	2.52	0.43
1:C:471:HIS:HB2	1:C:494:GLU:OE1	2.17	0.43
1:K:176:LYS:HD3	1:K:178:TYR:OH	2.18	0.43
2:9:182:VAL:O	2:9:189:TYR:HA	2.17	0.43
1:E:298:ASN:OD1	1:E:300:ILE:N	2.42	0.43
3:X:174:ASN:HD21	3:X:176:LYS:HE3	1.83	0.43
3:R:174:ASN:HD21	3:R:176:LYS:HE3	1.83	0.43
2:Q:18:VAL:HG12	2:Q:19:THR:H	1.83	0.43
1:K:326:LYS:HD3	1:K:328:THR:H	1.83	0.43
1:J:326:LYS:NZ	1:J:341:ASN:HD22	2.16	0.43
1:D:203:THR:HG21	1:F:220:ARG:NH2	2.33	0.43
1:K:161:TYR:CZ	1:K:249:GLY:HA2	2.52	0.43
3:X:93:TYR:HD1	3:X:100:SER:HB3	1.80	0.43
1:K:220:ARG:HH21	1:L:203:THR:HG21	1.83	0.43
1:H:401:GLU:N	1:H:401:GLU:OE1	2.51	0.43
3:6:139:CYS:CB	3:6:153:TRP:HZ2	2.30	0.43
3:0:6:GLN:HG2	3:0:106:THR:HG23	1.98	0.43
1:E:103:PRO:HD2	1:E:232:ILE:O	2.17	0.43
3:R:24:GLY:O	3:R:29:ILE:HD11	2.18	0.43
1:C:470:TYR:CE2	1:C:499:ARG:HA	2.54	0.43
3:6:26:SER:HA	3:6:29:ILE:HD12	2.00	0.43
3:2:25:SER:O	3:2:29:ILE:HG13	2.17	0.43
1:L:376:GLN:HB2	1:L:439:LEU:HD11	2.00	0.43
1:L:97:CYS:H	1:L:224:ARG:NH1	2.16	0.43
1:D:372:ALA:O	1:D:376:GLN:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:ASN:CA	1:E:224:ARG:HH11	2.31	0.43
3:X:91:GLN:HB2	3:X:102:PHE:CE2	2.52	0.43
1:F:183:HIS:ND1	1:F:184:HIS:N	2.65	0.43
3:P:118:PRO:HB3	3:P:141:ILE:CG2	2.48	0.43
3:V:115:LYS:HG2	3:V:146:PRO:HD3	2.01	0.43
1:E:264:LYS:HB3	1:E:392:PHE:CG	2.54	0.43
3:2:195:SER:HB3	3:2:212:ALA:HB2	2.00	0.43
4:K:602:NAG:O7	2:7:55:ASP:OD1	2.36	0.43
2:M:18:VAL:HG12	2:M:19:THR:H	1.81	0.43
1:F:384:VAL:HG11	1:F:428:LEU:HD11	2.00	0.43
1:C:326:LYS:HZ3	1:C:341:ASN:ND2	2.14	0.43
1:E:350:TRP:HB2	1:E:370:THR:HG23	1.99	0.43
1:D:244:VAL:CB	1:F:221:PRO:HD3	2.45	0.43
2:Q:2:VAL:HG23	2:Q:115:VAL:CG1	2.46	0.43
1:K:251:LEU:HD12	1:K:252:ILE:N	2.33	0.43
1:F:272:ALA:N	2:W:105:VAL:HG23	2.33	0.43
2:U:4:LEU:HA	2:U:23:GLN:O	2.19	0.43
2:U:195:VAL:HG12	2:U:196:THR:N	2.34	0.43
2:Q:167:TRP:CB	2:Q:172:LEU:HB3	2.49	0.43
1:C:196:VAL:O	1:C:197:GLN:C	2.56	0.43
1:K:220:ARG:HG3	1:K:229:ARG:NH1	2.33	0.43
2:1:95:TYR:CE1	2:1:119:GLY:HA3	2.53	0.43
2:Y:181:ALA:HA	2:Y:190:SER:O	2.18	0.43
2:S:212:ASN:HB2	2:S:219:LYS:HD3	1.99	0.43
3:8:139:CYS:CB	3:8:153:TRP:HZ2	2.29	0.43
1:I:114:SER:HA	1:I:265:SER:O	2.18	0.43
2:7:136:PRO:O	3:8:126:SER:HB3	2.17	0.43
1:E:327:GLN:HG3	1:E:329:ARG:NE	2.31	0.43
2:Y:98:ARG:HG2	2:Y:98:ARG:NH1	2.31	0.43
1:C:423:TYR:CZ	1:C:427:LEU:HD22	2.53	0.43
1:B:96:ASN:CA	1:B:224:ARG:HH11	2.31	0.43
1:G:98:TYR:OH	1:G:228:SER:HB2	2.17	0.43
3:V:38:TYR:HD2	3:V:48:LEU:HA	1.84	0.43
1:K:414:GLU:O	1:K:418:ILE:HG13	2.18	0.43
1:C:288:ILE:HG13	1:C:288:ILE:O	2.18	0.43
1:K:288:ILE:HG13	1:K:288:ILE:O	2.18	0.43
1:D:280:GLU:HB2	1:D:290:ASN:ND2	2.33	0.43
3:X:33:TYR:O	3:X:34:ALA:C	2.56	0.43
1:I:49:GLY:O	1:I:273:PRO:HD2	2.18	0.43
1:B:414:GLU:O	1:B:418:ILE:HG13	2.18	0.43
3:V:81:GLN:O	3:V:110:VAL:HG11	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:174:ASN:ND2	3:P:176:LYS:HB3	2.34	0.43
2:U:179:PHE:CZ	3:V:140:LEU:HB3	2.53	0.43
2:M:2:VAL:CG2	2:M:115:VAL:HG21	2.48	0.43
2:9:38:ARG:HB3	2:9:94:TYR:HE1	1.83	0.43
1:F:271:ASP:C	2:W:105:VAL:HG23	2.39	0.43
2:7:195:VAL:HG12	2:7:196:THR:N	2.32	0.43
1:H:409:LEU:HD11	1:I:413:VAL:HG21	2.00	0.43
3:4:167:THR:HG22	3:4:180:SER:O	2.17	0.43
1:K:229:ARG:HH11	1:K:229:ARG:HG2	1.81	0.43
2:M:155:VAL:CG2	2:M:191:LEU:HG	2.48	0.43
1:B:29:ILE:H	1:B:434:GLN:HB2	1.83	0.43
1:L:103:PRO:HD2	1:L:232:ILE:O	2.18	0.43
3:T:6:GLN:HG2	3:T:106:THR:HG23	1.99	0.43
2:U:155:VAL:CG2	2:U:191:LEU:HG	2.49	0.43
1:F:470:TYR:CE2	1:F:499:ARG:HA	2.53	0.43
2:5:155:VAL:CG2	2:5:191:LEU:HG	2.49	0.43
2:5:155:VAL:HG11	2:5:211:VAL:HG11	1.99	0.43
3:N:6:GLN:NE2	3:N:105:GLY:H	2.17	0.43
1:A:405:ARG:H	1:B:107:SER:CB	2.31	0.43
1:H:17:HIS:HA	1:H:350:TRP:O	2.18	0.43
2:9:155:VAL:HG11	2:9:211:VAL:HG11	2.00	0.43
2:Q:155:VAL:CG2	2:Q:191:LEU:HG	2.48	0.43
1:H:85:ASP:O	1:H:265:SER:HA	2.17	0.43
1:K:470:TYR:CE2	1:K:499:ARG:HA	2.53	0.43
1:A:242:VAL:HG22	1:A:243:LEU:N	2.33	0.43
3:T:130:LEU:CD2	3:T:135:ALA:HB2	2.48	0.43
1:J:99:PRO:HB3	1:J:223:VAL:HG21	2.00	0.43
1:H:220:ARG:HD2	1:H:229:ARG:HG2	1.99	0.43
1:F:423:TYR:CZ	1:F:427:LEU:HD22	2.53	0.43
3:Z:118:PRO:HB3	3:Z:141:ILE:CG2	2.48	0.43
3:0:118:PRO:HB3	3:0:141:ILE:CG2	2.49	0.43
3:T:91:GLN:HB2	3:T:102:PHE:CE2	2.53	0.43
1:D:183:HIS:ND1	1:D:184:HIS:N	2.67	0.43
1:K:416:THR:HG22	1:K:420:LEU:CD1	2.48	0.43
1:H:176:LYS:HD3	1:H:178:TYR:OH	2.18	0.43
3:V:188:GLU:H	3:V:188:GLU:CD	2.21	0.43
3:N:167:THR:HG22	3:N:180:SER:O	2.18	0.43
3:N:167:THR:CG2	3:N:180:SER:H	2.31	0.43
2:Y:99:VAL:HB	2:Y:111:TYR:CE1	2.53	0.43
2:S:51:ILE:CD1	2:S:52:ASN:N	2.80	0.43
2:U:38:ARG:HB3	2:U:94:TYR:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:109:HIS:HA	3:6:93:TYR:CD1	2.54	0.43
1:K:384:VAL:HG11	1:K:428:LEU:HD11	2.01	0.43
2:O:195:VAL:HG12	2:O:196:THR:N	2.33	0.43
2:W:195:VAL:HG12	2:W:196:THR:N	2.32	0.43
2:M:155:VAL:HG11	2:M:211:VAL:HG11	1.99	0.43
3:P:7:PRO:HA	3:P:8:PRO:HD3	1.93	0.43
2:1:142:LYS:O	2:1:144:THR:HG23	2.18	0.43
2:3:158:TYR:CE2	2:3:163:VAL:HG12	2.53	0.43
3:8:20:ILE:HG23	3:8:106:THR:HG21	1.99	0.43
2:Y:151:LEU:HB3	2:Y:224:VAL:CG1	2.47	0.43
1:G:85:ASP:O	1:G:265:SER:HA	2.17	0.43
1:F:372:ALA:O	1:F:376:GLN:HG3	2.18	0.43
1:C:350:TRP:HB2	1:C:370:THR:HG23	2.01	0.43
3:0:5:THR:HB	3:0:23:THR:OG1	2.19	0.43
3:V:23:THR:HG22	3:V:72:SER:CB	2.47	0.43
3:6:51:SER:OG	3:6:55:ASN:HB3	2.18	0.43
1:F:84:TRP:HZ2	1:F:113:ALA:HA	1.83	0.43
1:F:15:LEU:HB3	1:F:444:MET:HE1	2.01	0.43
1:G:383:ARG:CZ	1:I:27:LYS:HD3	2.49	0.43
2:3:32:TYR:CG	2:3:98:ARG:HD3	2.54	0.43
1:G:220:ARG:HB2	1:G:221:PRO:CD	2.49	0.43
1:D:96:ASN:CA	1:D:224:ARG:HH11	2.31	0.43
1:E:421:TRP:HA	1:E:421:TRP:CE3	2.53	0.43
3:2:37:TRP:HB2	3:2:50:ILE:HG13	2.00	0.43
3:V:37:TRP:HB2	3:V:50:ILE:HG13	2.00	0.43
3:6:115:LYS:HG2	3:6:146:PRO:HD3	2.01	0.43
1:G:49:GLY:O	1:G:273:PRO:HD2	2.18	0.43
1:K:280:GLU:HB2	1:K:290:ASN:HD21	1.83	0.43
4:C:601:NAG:H61	4:C:602:NAG:O7	2.18	0.43
1:J:246:ASN:HD22	1:L:219:SER:HB3	1.83	0.43
3:Z:83:GLU:CD	3:Z:83:GLU:H	2.21	0.43
3:8:83:GLU:H	3:8:83:GLU:CD	2.21	0.43
2:9:2:VAL:HG12	2:9:25:SER:O	2.19	0.43
1:F:49:GLY:HA2	1:F:285:ASN:O	2.18	0.43
1:E:487:ASP:OD2	1:E:490:VAL:HG23	2.18	0.43
3:P:174:ASN:HD21	3:P:176:LYS:HE3	1.84	0.43
2:U:100:GLU:O	2:U:102:VAL:N	2.50	0.43
2:7:47:TRP:HZ2	2:7:50:TRP:HB2	1.83	0.43
2:U:154:LEU:HD23	3:V:129:GLU:OE2	2.18	0.43
2:3:51:ILE:CD1	2:3:52:ASN:N	2.80	0.43
3:2:38:TYR:HD2	3:2:48:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:34:LEU:HD22	2:5:35:SER:H	1.82	0.43
2:5:206:THR:CG2	2:5:223:LYS:HG2	2.49	0.43
2:Q:198:PRO:HG2	2:Q:201:SER:OG	2.18	0.43
2:U:198:PRO:HG2	2:U:201:SER:OG	2.19	0.43
1:G:326:LYS:HD3	1:G:328:THR:H	1.83	0.43
2:1:4:LEU:HA	2:1:23:GLN:O	2.19	0.43
1:K:185:PRO:O	1:K:217:ILE:HA	2.18	0.43
2:1:167:TRP:CB	2:1:172:LEU:HB3	2.48	0.43
2:5:167:TRP:CB	2:5:172:LEU:HB3	2.48	0.43
1:B:380:LYS:HE2	1:B:380:LYS:O	2.17	0.43
3:N:51:SER:O	3:N:53:ASN:N	2.51	0.43
1:D:196:VAL:O	1:D:197:GLN:C	2.55	0.43
3:6:6:GLN:NE2	3:6:105:GLY:H	2.16	0.43
2:3:155:VAL:CG2	2:3:191:LEU:HG	2.49	0.43
3:2:20:ILE:HG23	3:2:106:THR:HG21	2.00	0.43
2:S:155:VAL:CG2	2:S:191:LEU:HG	2.49	0.43
1:D:380:LYS:HE2	1:D:380:LYS:O	2.18	0.43
3:2:29:ILE:CD1	3:2:71:THR:HB	2.49	0.43
3:4:51:SER:OG	3:4:55:ASN:HB3	2.18	0.43
1:H:376:GLN:HB2	1:H:439:LEU:HD11	2.01	0.43
1:E:321:ARG:O	1:E:321:ARG:HG2	2.18	0.43
3:6:37:TRP:CZ3	3:6:90:CYS:HB3	2.53	0.43
1:G:134:GLY:CA	1:G:153:TRP:HB3	2.49	0.43
3:X:133:ASN:O	3:X:134:LYS:HG2	2.19	0.43
1:L:152:ASN:HB2	1:L:255:ARG:NH1	2.34	0.43
1:F:268:MET:SD	1:F:284:PRO:HG3	2.58	0.43
2:5:62:LYS:HE3	3:6:97:LEU:HD13	1.99	0.43
3:0:91:GLN:HB2	3:0:102:PHE:HE2	1.84	0.43
2:9:51:ILE:CD1	2:9:52:ASN:N	2.80	0.43
3:V:174:ASN:HD21	3:V:176:LYS:HE3	1.83	0.43
3:6:174:ASN:O	3:6:175:ASN:HB2	2.19	0.43
3:P:91:GLN:HB2	3:P:102:PHE:HE2	1.82	0.43
2:W:206:THR:CG2	2:W:223:LYS:HG2	2.48	0.43
1:C:187:THR:CB	1:C:189:GLN:HE21	2.17	0.43
6:C:609:NAG:C3	6:C:610:NAG:H82	2.40	0.43
1:B:326:LYS:HZ3	1:B:341:ASN:ND2	2.16	0.43
1:I:335:ILE:CG1	1:I:354:ARG:HB3	2.49	0.43
1:A:461:ASP:OD2	1:B:453:ARG:HG2	2.19	0.43
2:1:61:VAL:O	2:1:65:GLN:HG3	2.19	0.43
2:S:4:LEU:HA	2:S:23:GLN:O	2.19	0.43
1:H:185:PRO:HA	1:H:190:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:167:TRP:CB	2:M:172:LEU:HB3	2.48	0.43
1:C:183:HIS:O	1:C:185:PRO:HD3	2.19	0.43
1:G:339:ILE:HG22	1:G:340:GLU:N	2.34	0.43
3:6:7:PRO:HA	3:6:8:PRO:HD3	1.93	0.43
2:9:151:LEU:HB3	2:9:224:VAL:CG1	2.48	0.43
2:M:212:ASN:HB2	2:M:219:LYS:HD3	2.00	0.43
1:G:384:VAL:HG11	1:G:428:LEU:HD11	2.01	0.43
1:A:238:LYS:HE2	1:C:401:GLU:HG3	2.00	0.43
2:O:155:VAL:CG2	2:O:191:LEU:HG	2.48	0.43
1:K:29:ILE:H	1:K:434:GLN:HB2	1.84	0.43
2:S:210:ASN:HD22	2:S:210:ASN:N	2.17	0.43
2:Y:11:VAL:HG13	2:Y:123:THR:O	2.19	0.43
1:H:234:TRP:HE3	1:H:234:TRP:N	2.13	0.43
1:A:59:LEU:HD12	1:A:60:ASP:N	2.34	0.43
3:2:24:GLY:O	3:2:29:ILE:HD11	2.19	0.43
1:J:457:GLU:HG3	1:J:499:ARG:NH1	2.29	0.43
3:P:130:LEU:CD2	3:P:135:ALA:HB2	2.46	0.43
1:A:221:PRO:HD3	1:B:244:VAL:HB	2.01	0.43
1:G:244:VAL:HB	1:I:221:PRO:HD3	2.00	0.43
1:H:15:LEU:HD22	1:H:448:PHE:HA	2.01	0.43
1:D:421:TRP:HA	1:D:421:TRP:CE3	2.53	0.43
1:H:242:VAL:HG22	1:H:243:LEU:N	2.34	0.43
3:N:37:TRP:CZ3	3:N:90:CYS:HB3	2.54	0.43
3:0:117:ALA:HA	3:0:118:PRO:HD3	1.92	0.43
3:2:133:ASN:O	3:2:134:LYS:HG2	2.18	0.43
3:T:195:SER:HB3	3:T:212:ALA:HB2	2.01	0.43
1:K:143:PRO:HG2	1:K:144:GLY:H	1.84	0.43
2:5:9:ALA:HB1	2:5:121:MET:O	2.18	0.43
1:L:416:THR:HG22	1:L:420:LEU:CD1	2.49	0.43
3:P:67:SER:O	3:P:73:ALA:HB1	2.18	0.43
3:V:33:TYR:O	3:V:34:ALA:C	2.57	0.43
2:9:100:GLU:O	2:9:102:VAL:HG23	2.18	0.43
3:Z:174:ASN:O	3:Z:175:ASN:HB2	2.19	0.43
2:7:32:TYR:CG	2:7:98:ARG:HD3	2.54	0.43
2:M:108:PHE:CB	2:M:111:TYR:CE2	3.01	0.43
1:G:187:THR:CB	1:G:189:GLN:HE21	2.17	0.43
6:D:610:NAG:H62	1:F:222:TRP:CB	2.49	0.43
2:S:7:SER:O	2:S:120:THR:HG22	2.19	0.43
2:5:61:VAL:O	2:5:65:GLN:HG3	2.18	0.43
1:L:192:THR:HG22	1:L:198:ALA:HB2	2.01	0.43
1:B:161:TYR:CZ	1:B:249:GLY:HA2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:4:LEU:HA	2:3:23:GLN:O	2.19	0.43
2:S:91:THR:HB	2:S:124:VAL:HG23	2.01	0.43
1:J:147:PHE:CG	1:J:148:PHE:N	2.87	0.43
1:I:247:SER:HB3	1:I:251:LEU:HD22	2.01	0.43
1:J:108:LEU:O	1:J:112:VAL:HG23	2.18	0.43
1:G:29:ILE:H	1:G:434:GLN:HB2	1.84	0.43
1:A:382:ASN:O	1:A:385:ILE:O	2.36	0.43
1:E:208:ARG:HG3	1:E:241:ASP:OD2	2.17	0.43
2:3:210:ASN:HD22	2:3:210:ASN:N	2.17	0.43
1:C:234:TRP:HE3	1:C:234:TRP:N	2.14	0.43
3:Z:24:GLY:O	3:Z:29:ILE:HD11	2.19	0.43
2:S:105:VAL:HG12	2:S:107:GLY:O	2.19	0.43
1:I:311:GLN:HG2	1:I:426:GLU:OE1	2.19	0.43
1:A:183:HIS:ND1	1:A:184:HIS:N	2.67	0.43
1:H:84:TRP:HZ2	1:H:113:ALA:HA	1.84	0.43
1:K:15:LEU:HD22	1:K:448:PHE:HA	2.00	0.43
1:D:109:ARG:HG2	1:D:109:ARG:HH11	1.83	0.43
3:0:37:TRP:HB2	3:0:50:ILE:HG13	2.00	0.43
3:0:11:SER:HB3	3:0:111:LEU:HD12	2.01	0.43
1:D:414:GLU:O	1:D:418:ILE:HG13	2.18	0.43
1:F:200:GLY:HA3	1:F:250:ASN:OD1	2.18	0.43
1:I:471:HIS:HB2	1:I:494:GLU:OE1	2.19	0.43
3:0:122:LEU:HD13	3:0:198:CYS:HB2	2.01	0.43
1:J:264:LYS:HB3	1:J:392:PHE:CG	2.54	0.43
1:E:141:ARG:NH1	1:E:141:ARG:HB2	2.33	0.43
2:Q:170:GLY:O	2:Q:173:THR:HG23	2.19	0.43
3:8:33:TYR:O	3:8:34:ALA:C	2.57	0.43
2:U:108:PHE:H	2:U:108:PHE:HD2	1.60	0.43
2:U:33:GLY:C	2:U:99:VAL:HG13	2.39	0.43
2:7:108:PHE:CD2	2:7:108:PHE:N	2.75	0.43
4:H:602:NAG:H81	2:1:55:ASP:HA	2.01	0.43
2:S:99:VAL:HB	2:S:111:TYR:CG	2.54	0.43
2:W:88:SER:HA	2:W:124:VAL:HG12	2.01	0.43
1:F:222:TRP:CH2	1:F:225:GLY:HA2	2.53	0.43
1:A:326:LYS:CD	1:A:328:THR:H	2.31	0.43
3:Z:51:SER:OG	3:Z:55:ASN:HB3	2.19	0.43
1:F:220:ARG:HB2	1:F:221:PRO:CD	2.48	0.43
2:U:167:TRP:CB	2:U:172:LEU:HB3	2.49	0.43
1:G:409:LEU:HD21	1:H:409:LEU:HG	2.00	0.43
2:M:195:VAL:HG12	2:M:196:THR:N	2.33	0.43
1:D:137:ASN:O	1:D:140:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:167:TRP:CB	2:W:172:LEU:HB3	2.49	0.43
1:B:102:VAL:O	1:B:105:TYR:HB2	2.18	0.43
2:5:181:ALA:HA	2:5:190:SER:O	2.19	0.43
2:Y:158:TYR:CE2	2:Y:163:VAL:HG12	2.53	0.43
1:F:353:PHE:CE1	1:F:366:ASP:HB2	2.45	0.43
2:U:182:VAL:O	2:U:189:TYR:HA	2.19	0.43
3:R:38:TYR:HD2	3:R:48:LEU:HA	1.83	0.43
3:T:26:SER:HA	3:T:29:ILE:HD12	2.01	0.43
3:0:26:SER:HA	3:0:29:ILE:HD12	2.01	0.43
3:4:130:LEU:CD2	3:4:135:ALA:HB2	2.48	0.43
2:Q:88:SER:HA	2:Q:124:VAL:HG12	2.00	0.43
1:J:220:ARG:HB2	1:J:221:PRO:CD	2.49	0.43
1:L:15:LEU:HD22	1:L:448:PHE:HA	2.01	0.43
1:B:97:CYS:H	1:B:224:ARG:NH1	2.17	0.43
2:Q:32:TYR:CG	2:Q:98:ARG:HD3	2.54	0.43
3:4:37:TRP:HB2	3:4:50:ILE:CG1	2.48	0.43
1:G:433:ASN:O	1:G:437:ILE:HG13	2.19	0.43
2:W:32:TYR:CG	2:W:98:ARG:HD3	2.54	0.43
2:W:98:ARG:NH1	2:W:98:ARG:HG2	2.33	0.43
1:G:234:TRP:CE3	1:G:234:TRP:N	2.83	0.43
3:X:37:TRP:HB2	3:X:50:ILE:CG1	2.49	0.43
3:6:37:TRP:HB2	3:6:50:ILE:CG1	2.49	0.43
3:4:64:PHE:HD1	3:4:77:ILE:HG12	1.81	0.43
1:L:416:THR:HG22	1:L:420:LEU:HD11	1.99	0.43
1:L:200:GLY:HA3	1:L:250:ASN:OD1	2.19	0.43
1:B:355:HIS:NE2	1:B:362:GLY:HA3	2.34	0.43
1:H:268:MET:CE	1:H:282:ILE:HG22	2.49	0.43
3:R:133:ASN:O	3:R:134:LYS:HG2	2.19	0.43
3:4:83:GLU:CD	3:4:83:GLU:H	2.21	0.43
1:L:451:THR:HG22	1:L:455:LEU:HG	2.01	0.43
2:9:55:ASP:OD2	2:9:57:GLN:HB2	2.18	0.43
3:X:174:ASN:ND2	3:X:176:LYS:HB3	2.34	0.43
2:Q:33:GLY:C	2:Q:99:VAL:HG13	2.40	0.43
2:Y:33:GLY:C	2:Y:99:VAL:HG13	2.39	0.43
2:3:47:TRP:HZ2	2:3:50:TRP:HB2	1.84	0.43
2:1:198:PRO:HG2	2:1:201:SER:OG	2.19	0.43
2:U:206:THR:CG2	2:U:223:LYS:HG2	2.49	0.43
1:B:222:TRP:CD1	1:B:227:SER:HB2	2.54	0.43
1:C:326:LYS:HD3	1:C:328:THR:H	1.83	0.43
1:F:271:ASP:C	2:W:105:VAL:CG2	2.88	0.43
1:B:229:ARG:HH11	1:B:229:ARG:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:463:GLY:HA2	1:F:453:ARG:CG	2.48	0.43
2:3:167:TRP:HB3	2:3:172:LEU:HB3	2.01	0.43
2:M:36:TRP:NE1	2:M:70:MET:CE	2.82	0.43
1:L:242:VAL:HG22	1:L:243:LEU:N	2.34	0.43
2:1:91:THR:CB	2:1:124:VAL:H	2.32	0.43
1:A:383:ARG:HH12	1:C:426:GLU:CD	2.22	0.43
1:C:380:LYS:HZ3	1:C:384:VAL:HG23	1.84	0.43
1:J:85:ASP:O	1:J:265:SER:HA	2.19	0.43
2:S:158:TYR:CE2	2:S:163:VAL:HG12	2.54	0.43
3:V:6:GLN:NE2	3:V:105:GLY:H	2.17	0.43
1:L:222:TRP:CH2	1:L:225:GLY:HA2	2.53	0.43
2:3:39:GLN:HG2	2:3:45:LEU:CD2	2.49	0.43
3:V:51:SER:O	3:V:53:ASN:N	2.52	0.43
3:V:5:THR:HB	3:V:23:THR:OG1	2.19	0.43
3:2:5:THR:HB	3:2:23:THR:OG1	2.19	0.43
1:K:97:CYS:H	1:K:224:ARG:NH1	2.17	0.43
3:4:37:TRP:CZ3	3:4:90:CYS:HB3	2.54	0.43
1:C:155:THR:HB	1:D:143:PRO:HG3	2.01	0.43
3:2:118:PRO:HB3	3:2:141:ILE:CG2	2.49	0.43
3:R:118:PRO:HB3	3:R:141:ILE:CG2	2.48	0.43
1:I:416:THR:HG22	1:I:420:LEU:CD1	2.49	0.43
3:8:81:GLN:O	3:8:110:VAL:HG11	2.19	0.43
1:G:298:ASN:OD1	1:G:300:ILE:N	2.42	0.43
2:O:170:GLY:O	2:O:173:THR:HG23	2.19	0.43
1:C:451:THR:HG22	1:C:455:LEU:HG	2.01	0.43
1:G:487:ASP:OD2	1:G:490:VAL:HG23	2.18	0.43
1:C:454:GLN:NE2	1:C:484:GLY:HA2	2.34	0.43
1:E:180:TRP:CD2	1:E:204:VAL:HG21	2.54	0.43
1:K:9:SER:N	1:K:472:LYS:HZ3	2.17	0.43
3:N:143:ASP:HA	3:N:176:LYS:CD	2.49	0.42
3:Z:167:THR:CG2	3:Z:180:SER:H	2.29	0.42
3:8:174:ASN:HD21	3:8:176:LYS:HE3	1.83	0.42
2:7:112:PRO:O	2:7:113:MET:C	2.57	0.42
2:Q:51:ILE:CD1	2:Q:52:ASN:N	2.80	0.42
1:E:29:ILE:H	1:E:434:GLN:HB2	1.83	0.42
2:Q:95:TYR:CE1	2:Q:119:GLY:HA3	2.54	0.42
2:Q:61:VAL:O	2:Q:65:GLN:HG3	2.19	0.42
1:I:137:ASN:O	1:I:140:LYS:HG3	2.19	0.42
1:H:196:VAL:O	1:H:197:GLN:C	2.57	0.42
1:J:339:ILE:HG22	1:J:340:GLU:N	2.33	0.42
1:I:101:ASP:O	1:I:103:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:102:VAL:HG11	1:K:108:LEU:HD23	2.01	0.42
1:J:405:ARG:HH22	1:K:403:GLU:CD	2.21	0.42
1:I:196:VAL:O	1:I:197:GLN:C	2.58	0.42
2:Y:167:TRP:CB	2:Y:172:LEU:HB3	2.49	0.42
3:N:153:TRP:CE2	3:N:183:LEU:HD13	2.54	0.42
3:X:123:PHE:O	3:X:137:LEU:HD23	2.19	0.42
1:H:346:MET:HE3	1:H:349:GLY:O	2.19	0.42
2:5:158:TYR:CE2	2:5:163:VAL:HG12	2.54	0.42
2:1:158:TYR:CE2	2:1:163:VAL:HG12	2.54	0.42
1:D:220:ARG:HD2	1:D:229:ARG:HG2	2.01	0.42
1:H:429:VAL:HG12	1:H:433:ASN:HD21	1.84	0.42
1:E:85:ASP:O	1:E:265:SER:HA	2.18	0.42
1:L:316:LEU:HD12	1:L:433:ASN:OD1	2.19	0.42
1:C:220:ARG:HD2	1:C:229:ARG:HG2	2.00	0.42
1:G:222:TRP:CD1	1:G:227:SER:HB2	2.54	0.42
1:C:463:GLY:C	1:C:465:GLY:H	2.21	0.42
1:B:109:ARG:NH2	1:B:267:ILE:HD13	2.33	0.42
3:Z:155:ALA:N	3:Z:158:SER:O	2.48	0.42
1:D:437:ILE:O	1:D:441:ASP:HB2	2.19	0.42
1:C:134:GLY:CA	1:C:153:TRP:HB3	2.48	0.42
1:K:49:GLY:O	1:K:273:PRO:HD2	2.19	0.42
1:B:255:ARG:HH11	1:B:255:ARG:HG2	1.83	0.42
1:H:50:LYS:HD3	1:H:275:ASP:HB2	2.01	0.42
3:N:195:SER:HB3	3:N:212:ALA:HB2	2.01	0.42
1:J:49:GLY:O	1:J:273:PRO:HD2	2.19	0.42
1:K:200:GLY:HA3	1:K:250:ASN:OD1	2.19	0.42
3:8:67:SER:O	3:8:73:ALA:HB1	2.19	0.42
3:V:133:ASN:O	3:V:134:LYS:HG2	2.19	0.42
3:4:172:GLN:N	3:4:176:LYS:O	2.48	0.42
2:S:208:ILE:HA	2:S:222:LYS:O	2.19	0.42
3:8:51:SER:O	3:8:53:ASN:N	2.52	0.42
2:M:38:ARG:HB3	2:M:94:TYR:HE1	1.84	0.42
1:F:380:LYS:O	1:F:380:LYS:HE2	2.18	0.42
1:J:326:LYS:CD	1:J:328:THR:H	2.32	0.42
2:M:61:VAL:O	2:M:65:GLN:HG3	2.19	0.42
2:7:11:VAL:HG13	2:7:123:THR:HB	2.00	0.42
1:K:156:LYS:HD3	1:K:193:SER:O	2.20	0.42
2:U:167:TRP:HB3	2:U:172:LEU:HB3	2.01	0.42
2:Q:167:TRP:HB3	2:Q:172:LEU:HB3	2.01	0.42
2:M:36:TRP:HE1	2:M:70:MET:CE	2.33	0.42
2:W:167:TRP:HB3	2:W:172:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:161:TYR:HB2	1:J:196:VAL:HG21	2.01	0.42
1:B:409:LEU:HD11	1:C:413:VAL:HG21	2.01	0.42
1:K:220:ARG:HD2	1:K:229:ARG:HG2	2.00	0.42
1:H:103:PRO:HG2	1:H:233:TYR:CE1	2.54	0.42
3:8:153:TRP:CB	3:8:183:LEU:HD22	2.50	0.42
3:V:153:TRP:CD2	3:V:183:LEU:HD13	2.54	0.42
1:K:350:TRP:HB2	1:K:370:THR:HG23	2.00	0.42
1:K:114:SER:O	1:K:265:SER:HB2	2.20	0.42
3:R:29:ILE:CD1	3:R:71:THR:HB	2.49	0.42
1:B:84:TRP:HZ2	1:B:113:ALA:HA	1.83	0.42
3:V:29:ILE:CD1	3:V:71:THR:HB	2.49	0.42
1:B:234:TRP:N	1:B:234:TRP:HE3	2.15	0.42
1:B:388:THR:HG23	1:B:389:ASN:N	2.32	0.42
2:S:32:TYR:CG	2:S:98:ARG:HD3	2.54	0.42
2:5:32:TYR:CG	2:5:98:ARG:HD3	2.53	0.42
1:D:97:CYS:N	1:D:224:ARG:NH1	2.67	0.42
1:D:423:TYR:CZ	1:D:427:LEU:HD22	2.54	0.42
1:D:295:GLN:HE22	1:D:308:TYR:HB2	1.84	0.42
3:0:37:TRP:HB2	3:0:50:ILE:CG1	2.50	0.42
1:F:471:HIS:HB2	1:F:494:GLU:OE1	2.19	0.42
1:H:200:GLY:HA3	1:H:250:ASN:OD1	2.19	0.42
2:S:9:ALA:HB1	2:S:121:MET:O	2.19	0.42
1:D:288:ILE:O	1:D:288:ILE:HG13	2.19	0.42
3:2:83:GLU:CD	3:2:83:GLU:H	2.22	0.42
1:F:395:ILE:HG13	1:F:395:ILE:O	2.19	0.42
1:I:268:MET:CE	1:I:282:ILE:HG22	2.49	0.42
3:X:195:SER:HB3	3:X:212:ALA:HB2	2.00	0.42
2:5:208:ILE:HA	2:5:222:LYS:O	2.20	0.42
3:T:174:ASN:O	3:T:175:ASN:HB2	2.20	0.42
3:N:174:ASN:O	3:N:175:ASN:HB2	2.19	0.42
3:4:113:GLN:HG3	3:4:175:ASN:ND2	2.34	0.42
2:O:98:ARG:NH1	2:O:98:ARG:HG2	2.32	0.42
2:Q:108:PHE:H	2:Q:108:PHE:HD2	1.59	0.42
2:Y:34:LEU:HD22	2:Y:35:SER:H	1.85	0.42
2:7:206:THR:HG21	2:7:223:LYS:CE	2.33	0.42
2:M:148:THR:HA	2:M:199:SER:N	2.29	0.42
3:X:12:GLY:CA	3:X:111:LEU:HD13	2.49	0.42
2:5:129:THR:HG22	2:5:160:PRO:CD	2.44	0.42
2:O:129:THR:HG22	2:O:160:PRO:CD	2.45	0.42
2:Q:208:ILE:HA	2:Q:222:LYS:O	2.20	0.42
2:U:61:VAL:O	2:U:65:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:61:VAL:O	2:S:65:GLN:HG3	2.20	0.42
1:F:161:TYR:HB2	1:F:196:VAL:HG21	2.01	0.42
2:W:36:TRP:NE1	2:W:70:MET:CE	2.82	0.42
1:I:67:ILE:HG13	1:I:105:TYR:CE2	2.53	0.42
1:J:196:VAL:O	1:J:197:GLN:C	2.57	0.42
1:B:101:ASP:O	1:B:103:PRO:HD3	2.18	0.42
2:9:105:VAL:HG12	2:9:107:GLY:O	2.20	0.42
2:5:212:ASN:HB2	2:5:219:LYS:HD3	2.00	0.42
3:N:7:PRO:HA	3:N:8:PRO:HD3	1.93	0.42
3:4:6:GLN:NE2	3:4:105:GLY:H	2.17	0.42
2:Y:155:VAL:CG2	2:Y:191:LEU:HG	2.49	0.42
1:E:357:ASN:HB2	1:E:473:CYS:O	2.19	0.42
3:4:29:ILE:CD1	3:4:71:THR:HB	2.49	0.42
2:W:44:GLY:HA2	3:X:89:TYR:OH	2.19	0.42
3:V:24:GLY:O	3:V:29:ILE:HD11	2.19	0.42
1:L:97:CYS:N	1:L:224:ARG:NH1	2.66	0.42
3:2:130:LEU:CD2	3:2:135:ALA:HB2	2.49	0.42
2:7:44:GLY:HA2	3:8:89:TYR:CZ	2.55	0.42
1:K:234:TRP:CE3	1:K:234:TRP:N	2.82	0.42
3:4:5:THR:HB	3:4:23:THR:OG1	2.19	0.42
1:A:220:ARG:HD2	1:A:229:ARG:HG2	2.01	0.42
3:X:37:TRP:CH2	3:X:90:CYS:HB3	2.54	0.42
1:H:421:TRP:HA	1:H:421:TRP:CE3	2.53	0.42
1:K:463:GLY:C	1:K:465:GLY:H	2.22	0.42
3:0:51:SER:OG	3:0:55:ASN:HB3	2.18	0.42
3:N:115:LYS:HG2	3:N:146:PRO:HD3	2.01	0.42
1:G:280:GLU:HB2	1:G:290:ASN:HD21	1.85	0.42
1:A:50:LYS:HD3	1:A:275:ASP:HB2	2.01	0.42
3:N:45:ALA:HA	3:N:46:PRO:HD3	1.92	0.42
3:6:33:TYR:O	3:6:34:ALA:C	2.57	0.42
1:F:152:ASN:HB2	1:F:255:ARG:NH1	2.34	0.42
3:6:133:ASN:O	3:6:134:LYS:HG2	2.19	0.42
3:2:174:ASN:HD21	3:2:176:LYS:HE3	1.83	0.42
3:T:172:GLN:N	3:T:176:LYS:O	2.49	0.42
3:0:174:ASN:O	3:0:175:ASN:HB2	2.20	0.42
3:N:172:GLN:HE21	3:N:176:LYS:NZ	2.18	0.42
3:Z:174:ASN:HD21	3:Z:176:LYS:HE3	1.84	0.42
2:U:47:TRP:HZ2	2:U:50:TRP:HB2	1.84	0.42
2:Y:108:PHE:HD2	2:Y:108:PHE:H	1.61	0.42
2:5:34:LEU:N	2:5:99:VAL:HG13	2.34	0.42
2:W:122:VAL:HG23	2:W:123:THR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:129:THR:HG22	2:M:160:PRO:CD	2.46	0.42
1:F:311:GLN:HG2	1:F:426:GLU:OE1	2.19	0.42
2:Q:109:HIS:O	3:R:93:TYR:CE2	2.73	0.42
2:O:4:LEU:HA	2:O:23:GLN:O	2.19	0.42
2:1:167:TRP:HB3	2:1:172:LEU:HB3	2.01	0.42
1:I:251:LEU:HD12	1:I:252:ILE:N	2.32	0.42
1:K:102:VAL:HG22	1:K:232:ILE:CB	2.45	0.42
1:C:190:GLU:O	1:C:194:LEU:HD13	2.19	0.42
1:A:111:LEU:C	1:A:111:LEU:HD12	2.39	0.42
3:T:123:PHE:O	3:T:137:LEU:HD23	2.20	0.42
2:W:158:TYR:CE2	2:W:163:VAL:HG12	2.54	0.42
2:9:167:TRP:HB3	2:9:172:LEU:HB3	2.01	0.42
2:U:158:TYR:CE2	2:U:163:VAL:HG12	2.54	0.42
1:C:29:ILE:H	1:C:434:GLN:HB2	1.84	0.42
2:9:158:TYR:CE2	2:9:163:VAL:HG12	2.55	0.42
3:V:7:PRO:HA	3:V:8:PRO:HD3	1.93	0.42
3:P:26:SER:HA	3:P:29:ILE:HD12	2.02	0.42
3:N:26:SER:HA	3:N:29:ILE:HD12	2.00	0.42
2:9:208:ILE:HA	2:9:222:LYS:O	2.19	0.42
2:Y:39:GLN:HE21	2:Y:45:LEU:HD23	1.84	0.42
2:Q:105:VAL:HG12	2:Q:107:GLY:O	2.20	0.42
1:L:83:THR:O	1:L:84:TRP:HB3	2.20	0.42
2:S:44:GLY:HA2	3:T:89:TYR:CZ	2.54	0.42
1:D:376:GLN:HB2	1:D:439:LEU:HD11	2.01	0.42
1:G:388:THR:HG23	1:G:389:ASN:N	2.33	0.42
1:F:15:LEU:HD22	1:F:448:PHE:HA	2.01	0.42
3:T:158:SER:HA	3:T:159:PRO:HD3	1.86	0.42
1:C:109:ARG:HH11	1:C:109:ARG:HG2	1.85	0.42
1:A:423:TYR:CE2	1:B:424:ASN:HB3	2.55	0.42
3:V:118:PRO:HB3	3:V:141:ILE:CG2	2.49	0.42
3:4:115:LYS:HG2	3:4:146:PRO:HD3	2.02	0.42
3:V:91:GLN:HB2	3:V:102:PHE:CE2	2.55	0.42
1:G:421:TRP:HA	1:G:421:TRP:CE3	2.53	0.42
1:C:49:GLY:HA2	1:C:285:ASN:O	2.19	0.42
3:6:80:LEU:HD11	3:6:108:LEU:HD21	2.00	0.42
1:B:50:LYS:HD3	1:B:275:ASP:HB2	2.00	0.42
3:V:83:GLU:H	3:V:83:GLU:CD	2.22	0.42
1:D:401:GLU:N	1:D:401:GLU:OE1	2.51	0.42
1:C:110:SER:OG	1:C:393:HIS:NE2	2.48	0.42
1:L:50:LYS:HD3	1:L:275:ASP:HB2	2.01	0.42
1:C:131:THR:HG22	1:C:132:GLN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:174:ASN:O	3:V:175:ASN:HB2	2.20	0.42
2:O:33:GLY:C	2:O:99:VAL:HG13	2.39	0.42
2:S:108:PHE:H	2:S:108:PHE:HD2	1.60	0.42
2:M:108:PHE:HB2	2:M:111:TYR:HE2	1.80	0.42
2:O:206:THR:CG2	2:O:223:LYS:HG2	2.50	0.42
1:H:326:LYS:CD	1:H:328:THR:H	2.32	0.42
2:S:118:GLN:HG3	2:S:118:GLN:H	1.55	0.42
1:D:311:GLN:HG2	1:D:426:GLU:OE1	2.19	0.42
1:K:161:TYR:HB2	1:K:196:VAL:HG21	2.02	0.42
1:F:137:ASN:O	1:F:140:LYS:HG3	2.20	0.42
2:3:167:TRP:CB	2:3:172:LEU:HB3	2.48	0.42
1:C:185:PRO:O	1:C:217:ILE:HA	2.18	0.42
1:A:156:LYS:HD2	1:A:196:VAL:CG2	2.45	0.42
1:J:382:ASN:O	1:J:385:ILE:O	2.37	0.42
3:R:51:SER:O	3:R:53:ASN:N	2.53	0.42
1:G:384:VAL:HG21	1:G:428:LEU:HD11	2.02	0.42
2:9:155:VAL:CG2	2:9:191:LEU:HG	2.49	0.42
3:8:123:PHE:O	3:8:137:LEU:HD23	2.19	0.42
1:A:470:TYR:CE2	1:A:499:ARG:HA	2.54	0.42
1:E:203:THR:HG23	1:E:212:THR:OG1	2.20	0.42
2:M:208:ILE:HA	2:M:222:LYS:O	2.20	0.42
3:6:155:ALA:N	3:6:158:SER:O	2.48	0.42
1:J:421:TRP:HA	1:J:421:TRP:CE3	2.53	0.42
1:G:427:LEU:O	1:G:431:LEU:HD12	2.19	0.42
2:U:32:TYR:CG	2:U:98:ARG:HD3	2.54	0.42
3:6:37:TRP:CH2	3:6:90:CYS:HB3	2.54	0.42
3:8:37:TRP:CH2	3:8:90:CYS:HB3	2.55	0.42
3:N:118:PRO:HB3	3:N:141:ILE:CG2	2.50	0.42
3:4:122:LEU:HD13	3:4:198:CYS:HB2	2.00	0.42
1:J:414:GLU:O	1:J:418:ILE:HG13	2.20	0.42
3:Z:33:TYR:O	3:Z:34:ALA:C	2.57	0.42
1:K:152:ASN:HB2	1:K:255:ARG:NH1	2.34	0.42
2:7:182:VAL:O	2:7:189:TYR:HA	2.19	0.42
2:3:14:PRO:HD2	2:3:126:SER:HA	2.01	0.42
3:N:133:ASN:O	3:N:134:LYS:HG2	2.19	0.42
3:6:81:GLN:O	3:6:110:VAL:HG11	2.19	0.42
2:M:182:VAL:O	2:M:189:TYR:HA	2.20	0.42
3:0:113:GLN:HG3	3:0:175:ASN:HD21	1.84	0.42
3:0:143:ASP:HA	3:0:176:LYS:CD	2.49	0.42
3:V:172:GLN:HE21	3:V:176:LYS:NZ	2.18	0.42
3:R:174:ASN:O	3:R:175:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:38:ARG:HB3	2:5:94:TYR:HE1	1.84	0.42
1:J:326:LYS:HD3	1:J:328:THR:H	1.84	0.42
2:W:61:VAL:O	2:W:65:GLN:HG3	2.19	0.42
2:U:2:VAL:HG12	2:U:25:SER:O	2.19	0.42
1:C:183:HIS:ND1	1:C:184:HIS:N	2.68	0.42
2:1:36:TRP:NE1	2:1:70:MET:CE	2.83	0.42
1:D:103:PRO:HG2	1:D:233:TYR:CE1	2.54	0.42
3:P:123:PHE:O	3:P:137:LEU:HD23	2.20	0.42
3:N:123:PHE:O	3:N:137:LEU:HD23	2.19	0.42
2:W:155:VAL:HG23	2:W:155:VAL:O	2.20	0.42
2:5:179:PHE:HA	2:5:180:PRO:HD3	1.95	0.42
1:H:470:TYR:CE2	1:H:499:ARG:HA	2.54	0.42
2:7:155:VAL:HG23	2:7:155:VAL:O	2.20	0.42
2:7:181:ALA:HA	2:7:190:SER:O	2.19	0.42
1:C:85:ASP:O	1:C:265:SER:HA	2.20	0.42
1:C:143:PRO:HG3	1:D:155:THR:HB	1.99	0.42
1:L:437:ILE:O	1:L:441:ASP:HB2	2.20	0.42
2:O:181:ALA:HA	2:O:190:SER:O	2.20	0.42
2:W:210:ASN:N	2:W:210:ASN:HD22	2.17	0.42
1:A:222:TRP:CD1	1:A:227:SER:HB2	2.53	0.42
1:I:439:LEU:HD23	1:I:440:THR:N	2.34	0.42
1:A:376:GLN:HB2	1:A:439:LEU:HD11	2.01	0.42
3:8:5:THR:HB	3:8:23:THR:OG1	2.18	0.42
1:G:83:THR:O	1:G:84:TRP:HB3	2.20	0.42
3:R:37:TRP:CZ3	3:R:90:CYS:HB3	2.54	0.42
1:E:307:LYS:HE2	1:E:421:TRP:CZ2	2.54	0.42
2:Y:182:VAL:CG1	3:Z:182:TYR:HD2	2.32	0.42
3:V:37:TRP:HB2	3:V:50:ILE:CG1	2.50	0.42
3:N:37:TRP:CH2	3:N:90:CYS:HB3	2.54	0.42
1:A:134:GLY:CA	1:A:153:TRP:HB3	2.50	0.42
1:C:421:TRP:HA	1:C:421:TRP:CE3	2.54	0.42
1:J:143:PRO:HG2	1:J:144:GLY:H	1.84	0.42
3:R:81:GLN:O	3:R:110:VAL:HG11	2.19	0.42
1:C:141:ARG:NH1	1:C:141:ARG:HB2	2.34	0.42
3:V:195:SER:HB3	3:V:212:ALA:HB2	2.02	0.42
1:E:451:THR:HG22	1:E:455:LEU:HG	2.01	0.42
1:L:49:GLY:O	1:L:273:PRO:HD2	2.19	0.42
3:4:33:TYR:O	3:4:34:ALA:C	2.57	0.42
3:X:174:ASN:O	3:X:175:ASN:HB2	2.19	0.42
2:S:99:VAL:HA	2:S:111:TYR:CD1	2.55	0.42
2:1:206:THR:CG2	2:1:223:LYS:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:24:VAL:HG23	2:W:77:ASN:O	2.20	0.42
2:Q:206:THR:CG2	2:Q:223:LYS:HG2	2.49	0.42
1:C:326:LYS:CD	1:C:328:THR:H	2.33	0.42
1:E:322:ASN:O	1:E:324:PRO:HD3	2.20	0.42
1:G:326:LYS:CD	1:G:328:THR:H	2.33	0.42
1:F:326:LYS:HD3	1:F:327:GLN:H	1.85	0.42
2:7:91:THR:HB	2:7:124:VAL:N	2.35	0.42
1:C:251:LEU:HD12	1:C:252:ILE:N	2.32	0.42
2:3:36:TRP:NE1	2:3:70:MET:CE	2.83	0.42
1:H:147:PHE:CG	1:H:148:PHE:N	2.88	0.42
1:A:103:PRO:HD2	1:A:232:ILE:O	2.19	0.42
1:D:339:ILE:HG22	1:D:340:GLU:N	2.34	0.42
1:L:111:LEU:C	1:L:111:LEU:HD12	2.40	0.42
2:7:158:TYR:CE2	2:7:163:VAL:HG12	2.54	0.42
1:C:220:ARG:HB2	1:C:221:PRO:CD	2.49	0.42
1:A:114:SER:HA	1:A:265:SER:O	2.19	0.42
1:B:114:SER:O	1:B:265:SER:HB2	2.20	0.42
1:I:222:TRP:CH2	1:I:225:GLY:HA2	2.54	0.42
3:0:24:GLY:O	3:0:29:ILE:HD11	2.20	0.42
3:4:51:SER:O	3:4:53:ASN:N	2.52	0.42
3:0:23:THR:HG22	3:0:72:SER:CB	2.49	0.42
2:S:39:GLN:HE21	2:S:45:LEU:HD23	1.85	0.42
3:N:5:THR:HB	3:N:23:THR:OG1	2.20	0.42
2:Q:98:ARG:HG2	2:Q:98:ARG:NH1	2.33	0.42
3:8:37:TRP:HB2	3:8:50:ILE:CG1	2.50	0.42
1:H:97:CYS:H	1:H:224:ARG:NH1	2.18	0.42
1:J:268:MET:SD	1:J:284:PRO:HG3	2.59	0.42
1:L:49:GLY:HA2	1:L:285:ASN:O	2.19	0.42
1:J:131:THR:HG22	1:J:132:GLN:N	2.35	0.42
3:4:195:SER:HB3	3:4:212:ALA:HB2	2.01	0.42
3:2:122:LEU:HD13	3:2:198:CYS:HB2	2.00	0.42
3:2:110:VAL:HG23	3:2:110:VAL:O	2.19	0.42
1:K:301:THR:HB	1:K:305:CYS:SG	2.60	0.42
2:7:170:GLY:O	2:7:173:THR:HG23	2.19	0.42
2:W:161:GLU:HA	2:W:162:PRO:HA	1.77	0.42
3:6:83:GLU:CD	3:6:83:GLU:H	2.23	0.42
3:2:33:TYR:O	3:2:34:ALA:C	2.58	0.42
3:8:122:LEU:HD13	3:8:198:CYS:HB2	2.00	0.42
3:P:80:LEU:HD11	3:P:108:LEU:HD21	2.02	0.42
1:H:414:GLU:O	1:H:418:ILE:HG13	2.19	0.42
1:H:416:THR:HG22	1:H:420:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:143:ASP:HA	3:P:176:LYS:CD	2.50	0.42
3:4:174:ASN:O	3:4:175:ASN:HB2	2.20	0.42
3:R:174:ASN:ND2	3:R:176:LYS:HB3	2.34	0.42
2:7:108:PHE:H	2:7:108:PHE:HD2	1.61	0.42
3:8:47:LYS:HG2	3:8:48:LEU:N	2.35	0.42
1:A:273:PRO:HB3	2:M:110:TYR:CD1	2.54	0.42
2:7:198:PRO:HG2	2:7:201:SER:OG	2.20	0.42
2:O:118:GLN:HG3	2:O:118:GLN:H	1.56	0.42
1:H:222:TRP:CD1	1:H:227:SER:HB2	2.55	0.42
2:O:61:VAL:O	2:O:65:GLN:HG3	2.19	0.42
1:G:183:HIS:ND1	1:G:184:HIS:N	2.67	0.42
1:C:243:LEU:HD12	1:C:244:VAL:N	2.33	0.42
1:E:196:VAL:O	1:E:197:GLN:C	2.58	0.42
2:M:36:TRP:HE1	2:M:70:MET:HE2	1.85	0.42
1:C:191:GLN:NE2	1:C:198:ALA:O	2.53	0.42
2:1:36:TRP:HE1	2:1:70:MET:CE	2.32	0.42
2:5:194:VAL:HG21	3:6:140:LEU:CD1	2.49	0.42
1:D:229:ARG:HG2	1:D:229:ARG:HH11	1.84	0.42
2:7:155:VAL:CG2	2:7:191:LEU:HG	2.49	0.42
1:A:203:THR:HG23	1:A:212:THR:OG1	2.20	0.42
1:J:327:GLN:HG3	1:J:329:ARG:NE	2.28	0.42
1:L:433:ASN:O	1:L:437:ILE:HG13	2.20	0.42
2:7:40:ALA:HA	2:7:92:ALA:CB	2.50	0.42
1:H:29:ILE:HA	1:I:380:LYS:HZ1	1.84	0.42
2:O:39:GLN:HE21	2:O:45:LEU:HD23	1.85	0.42
2:O:44:GLY:HA2	3:P:89:TYR:CZ	2.55	0.42
3:8:29:ILE:CD1	3:8:71:THR:HB	2.49	0.42
1:J:15:LEU:HD22	1:J:448:PHE:HA	2.01	0.42
3:X:37:TRP:CZ3	3:X:90:CYS:HB3	2.54	0.42
3:2:37:TRP:HB2	3:2:50:ILE:CG1	2.50	0.42
3:V:37:TRP:CH2	3:V:90:CYS:HB3	2.54	0.42
3:N:118:PRO:HB2	3:N:207:VAL:HG11	2.02	0.42
3:4:91:GLN:HB2	3:4:102:PHE:CE2	2.54	0.42
2:O:161:GLU:HA	2:O:162:PRO:HA	1.77	0.42
3:4:81:GLN:O	3:4:110:VAL:HG11	2.20	0.42
1:E:416:THR:HG22	1:E:420:LEU:CD1	2.50	0.42
3:N:80:LEU:HD11	3:N:108:LEU:HD21	2.02	0.42
1:I:474:ASP:O	1:I:477:CYS:HB3	2.20	0.42
1:H:264:LYS:HB3	1:H:392:PHE:CG	2.55	0.42
2:9:99:VAL:HB	2:9:111:TYR:CZ	2.54	0.42
3:8:174:ASN:ND2	3:8:176:LYS:HB3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:55:ASP:OD2	2:7:57:GLN:HB2	2.19	0.42
2:M:47:TRP:HZ2	2:M:50:TRP:HB2	1.84	0.42
2:M:33:GLY:C	2:M:99:VAL:HG13	2.40	0.42
2:7:148:THR:CG2	2:7:198:PRO:HA	2.50	0.42
2:7:206:THR:CG2	2:7:223:LYS:HG2	2.50	0.42
2:1:2:VAL:HG12	2:1:25:SER:O	2.20	0.42
2:S:36:TRP:NE1	2:S:70:MET:HE1	2.35	0.42
2:3:172:LEU:CD2	2:3:195:VAL:HG11	2.46	0.42
1:B:251:LEU:HD12	1:B:252:ILE:N	2.32	0.42
1:I:147:PHE:CG	1:I:148:PHE:N	2.88	0.42
1:C:346:MET:HE3	1:C:349:GLY:O	2.18	0.42
1:A:246:ASN:HD22	1:C:219:SER:HB3	1.85	0.42
1:E:241:ASP:OD1	1:E:242:VAL:N	2.53	0.42
2:Q:158:TYR:CE2	2:Q:163:VAL:HG12	2.54	0.42
1:E:470:TYR:CE2	1:E:499:ARG:HA	2.54	0.42
3:8:153:TRP:CD2	3:8:183:LEU:HD13	2.55	0.42
1:C:229:ARG:HG2	1:C:229:ARG:HH11	1.85	0.42
2:W:208:ILE:HA	2:W:222:LYS:O	2.20	0.42
1:J:372:ALA:O	1:J:376:GLN:HG3	2.20	0.42
1:J:439:LEU:HD12	1:L:30:THR:HG22	2.02	0.42
1:C:97:CYS:H	1:C:224:ARG:NH1	2.18	0.42
2:9:32:TYR:CG	2:9:98:ARG:HD3	2.55	0.42
3:R:115:LYS:HG2	3:R:146:PRO:HD3	2.00	0.42
1:G:50:LYS:HD3	1:G:275:ASP:HB2	2.01	0.42
1:F:49:GLY:O	1:F:273:PRO:HD2	2.20	0.42
1:H:416:THR:HG22	1:H:420:LEU:CD1	2.49	0.42
1:A:451:THR:HG22	1:A:455:LEU:HG	2.01	0.42
1:J:451:THR:HG22	1:J:455:LEU:HG	2.01	0.42
2:O:182:VAL:O	2:O:189:TYR:HA	2.19	0.42
3:P:195:SER:HB3	3:P:212:ALA:HB2	2.01	0.42
2:Y:170:GLY:O	2:Y:173:THR:HG23	2.20	0.42
2:S:170:GLY:O	2:S:173:THR:HG23	2.19	0.42
3:N:174:ASN:HD21	3:N:176:LYS:HE3	1.84	0.42
3:Z:174:ASN:ND2	3:Z:176:LYS:HB3	2.34	0.42
3:6:174:ASN:ND2	3:6:176:LYS:HB3	2.35	0.42
3:P:47:LYS:HG2	3:P:48:LEU:N	2.35	0.42
3:R:172:GLN:N	3:R:176:LYS:O	2.49	0.42
1:A:49:GLY:O	1:A:273:PRO:HD2	2.20	0.42
2:3:24:VAL:HG23	2:3:77:ASN:O	2.20	0.42
2:M:24:VAL:HG23	2:M:77:ASN:O	2.20	0.42
2:W:148:THR:CG2	2:W:198:PRO:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:198:PRO:HG2	2:Y:201:SER:OG	2.20	0.42
2:M:206:THR:CG2	2:M:223:LYS:HG2	2.50	0.42
1:D:326:LYS:HD3	1:D:328:THR:H	1.84	0.42
2:U:61:VAL:HG12	2:U:63:LYS:N	2.25	0.42
2:7:61:VAL:O	2:7:65:GLN:HG3	2.20	0.42
2:1:208:ILE:HA	2:1:222:LYS:O	2.19	0.42
2:Q:2:VAL:HG12	2:Q:25:SER:O	2.19	0.42
2:U:118:GLN:HG3	2:U:118:GLN:H	1.61	0.42
2:W:36:TRP:HE1	2:W:70:MET:CE	2.33	0.42
2:5:60:TYR:CE1	2:5:70:MET:HG2	2.43	0.42
1:E:220:ARG:HB2	1:E:221:PRO:CD	2.50	0.42
1:E:223:VAL:CG1	1:F:207:ARG:HG3	2.50	0.42
1:B:111:LEU:C	1:B:111:LEU:HD12	2.40	0.42
1:B:339:ILE:HG22	1:B:340:GLU:N	2.35	0.42
2:Y:167:TRP:HB3	2:Y:172:LEU:HB3	2.01	0.42
3:6:123:PHE:O	3:6:137:LEU:HD23	2.20	0.42
3:4:153:TRP:CD2	3:4:183:LEU:HD13	2.55	0.42
1:H:111:LEU:HD12	1:H:111:LEU:C	2.41	0.42
2:3:155:VAL:HG23	2:3:155:VAL:O	2.20	0.42
3:0:153:TRP:CD2	3:0:183:LEU:HD13	2.55	0.42
1:C:143:PRO:HG2	1:D:155:THR:HG21	2.02	0.42
2:Q:179:PHE:CZ	3:R:140:LEU:HB3	2.55	0.42
3:8:167:THR:CG2	3:8:180:SER:H	2.29	0.42
3:V:153:TRP:CB	3:V:183:LEU:HD22	2.50	0.42
1:L:293:PRO:C	1:L:306:PRO:HB3	2.40	0.42
1:C:320:MET:HG2	1:C:321:ARG:N	2.35	0.42
3:R:47:LYS:HG2	3:R:48:LEU:N	2.35	0.42
3:R:26:SER:HA	3:R:29:ILE:HD12	2.02	0.42
1:D:470:TYR:CE2	1:D:499:ARG:HA	2.55	0.42
3:T:29:ILE:CD1	3:T:71:THR:HB	2.50	0.42
2:Y:105:VAL:HG12	2:Y:107:GLY:O	2.20	0.42
2:W:39:GLN:HE21	2:W:45:LEU:HD23	1.85	0.42
1:L:220:ARG:HB2	1:L:221:PRO:CD	2.50	0.42
2:1:105:VAL:HG12	2:1:107:GLY:O	2.20	0.42
1:C:15:LEU:HD22	1:C:448:PHE:HA	2.01	0.42
2:U:98:ARG:HG2	2:U:98:ARG:NH1	2.35	0.42
3:T:37:TRP:HB2	3:T:50:ILE:CG1	2.50	0.42
3:Z:118:PRO:HB2	3:Z:207:VAL:HG11	2.02	0.42
3:8:115:LYS:HG2	3:8:146:PRO:HD3	2.02	0.42
1:J:44:GLN:HG2	1:J:288:ILE:HD12	2.01	0.42
1:F:474:ASP:O	1:F:477:CYS:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:141:ARG:NH1	1:J:141:ARG:HB2	2.35	0.42
1:J:203:THR:HG23	1:J:212:THR:OG1	2.20	0.42
3:2:174:ASN:ND2	3:2:176:LYS:HB3	2.35	0.41
3:0:174:ASN:ND2	3:0:176:LYS:HB3	2.34	0.41
3:4:174:ASN:ND2	3:4:176:LYS:HB3	2.35	0.41
3:X:172:GLN:HE21	3:X:176:LYS:NZ	2.18	0.41
2:U:208:ILE:HA	2:U:222:LYS:O	2.20	0.41
2:Q:34:LEU:HD22	2:Q:35:SER:H	1.82	0.41
2:9:206:THR:CG2	2:9:223:LYS:HG2	2.50	0.41
1:F:292:LYS:HB3	1:F:293:PRO:HD2	2.02	0.41
1:E:401:GLU:OE1	1:E:401:GLU:N	2.53	0.41
1:L:196:VAL:O	1:L:197:GLN:C	2.57	0.41
1:E:161:TYR:HB2	1:E:196:VAL:HG21	2.01	0.41
1:G:192:THR:HG22	1:G:198:ALA:HB2	2.02	0.41
2:3:105:VAL:HG12	2:3:107:GLY:O	2.20	0.41
1:I:272:ALA:N	2:3:105:VAL:HG23	2.35	0.41
1:F:437:ILE:O	1:F:441:ASP:HB2	2.19	0.41
1:A:101:ASP:O	1:A:103:PRO:HD3	2.19	0.41
2:U:36:TRP:HE1	2:U:70:MET:CE	2.33	0.41
1:A:27:LYS:HZ3	1:B:383:ARG:HD3	1.85	0.41
1:L:335:ILE:CG1	1:L:354:ARG:HB3	2.50	0.41
2:M:158:TYR:CE2	2:M:163:VAL:HG12	2.55	0.41
3:T:153:TRP:CD2	3:T:183:LEU:HD13	2.55	0.41
2:5:155:VAL:HG23	2:5:155:VAL:O	2.20	0.41
1:D:429:VAL:HG12	1:D:433:ASN:HD21	1.85	0.41
3:R:167:THR:CG2	3:R:180:SER:H	2.28	0.41
1:E:495:ALA:O	1:E:499:ARG:HG3	2.19	0.41
2:5:210:ASN:N	2:5:210:ASN:HD22	2.17	0.41
1:K:114:SER:HA	1:K:265:SER:O	2.20	0.41
3:4:26:SER:HA	3:4:29:ILE:HD12	2.02	0.41
3:Z:26:SER:HA	3:Z:29:ILE:HD12	2.02	0.41
1:B:376:GLN:HB2	1:B:439:LEU:HD11	2.02	0.41
3:6:51:SER:O	3:6:53:ASN:N	2.52	0.41
3:8:23:THR:HG22	3:8:72:SER:CB	2.48	0.41
1:I:15:LEU:HD22	1:I:448:PHE:HA	2.01	0.41
1:I:229:ARG:HH11	1:I:229:ARG:HG2	1.85	0.41
1:G:84:TRP:HZ2	1:G:113:ALA:HA	1.85	0.41
1:H:229:ARG:HH11	1:H:229:ARG:HG2	1.84	0.41
2:Q:62:LYS:NZ	3:R:97:LEU:HD13	2.35	0.41
3:R:118:PRO:HB2	3:R:207:VAL:HG11	2.02	0.41
2:9:112:PRO:HB3	3:0:36:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ILE:O	1:B:288:ILE:HG13	2.20	0.41
1:J:280:GLU:HB2	1:J:290:ASN:HD21	1.85	0.41
1:G:255:ARG:HG2	1:G:255:ARG:HH11	1.85	0.41
1:B:152:ASN:HB2	1:B:255:ARG:NH1	2.35	0.41
1:J:98:TYR:OH	1:J:228:SER:HB2	2.20	0.41
1:H:49:GLY:HA2	1:H:285:ASN:O	2.19	0.41
1:B:451:THR:HG22	1:B:455:LEU:HG	2.02	0.41
2:1:170:GLY:O	2:1:173:THR:HG23	2.19	0.41
1:B:474:ASP:O	1:B:477:CYS:HB3	2.20	0.41
1:L:141:ARG:NH1	1:L:141:ARG:HB2	2.35	0.41
3:T:83:GLU:CD	3:T:83:GLU:H	2.23	0.41
3:R:83:GLU:CD	3:R:83:GLU:H	2.22	0.41
1:E:176:LYS:HD3	1:E:178:TYR:OH	2.20	0.41
2:Y:161:GLU:HA	2:Y:162:PRO:HA	1.76	0.41
2:9:34:LEU:HD22	2:9:35:SER:N	2.34	0.41
2:Y:179:PHE:CE2	3:Z:140:LEU:HB3	2.55	0.41
2:Y:180:PRO:O	3:Z:167:THR:HG21	2.19	0.41
2:Q:99:VAL:HB	2:Q:111:TYR:CE1	2.55	0.41
2:3:99:VAL:HB	2:3:111:TYR:CZ	2.56	0.41
3:2:47:LYS:HG2	3:2:48:LEU:N	2.35	0.41
2:9:198:PRO:HG2	2:9:201:SER:OG	2.20	0.41
2:5:24:VAL:HG23	2:5:77:ASN:O	2.19	0.41
2:Q:206:THR:HG21	2:Q:223:LYS:CE	2.34	0.41
1:A:322:ASN:O	1:A:324:PRO:HD3	2.20	0.41
1:J:326:LYS:NZ	1:J:341:ASN:ND2	2.68	0.41
3:Z:51:SER:O	3:Z:53:ASN:N	2.53	0.41
1:A:137:ASN:O	1:A:140:LYS:HG3	2.20	0.41
1:G:102:VAL:HG22	1:G:232:ILE:CB	2.47	0.41
3:N:153:TRP:CB	3:N:183:LEU:HD22	2.50	0.41
1:G:335:ILE:CG1	1:G:354:ARG:HB3	2.50	0.41
3:Z:153:TRP:CB	3:Z:183:LEU:HD22	2.50	0.41
3:0:123:PHE:O	3:0:137:LEU:HD23	2.20	0.41
2:U:210:ASN:N	2:U:210:ASN:HD22	2.19	0.41
2:9:210:ASN:HD22	2:9:210:ASN:N	2.17	0.41
2:O:105:VAL:HG12	2:O:107:GLY:O	2.19	0.41
2:1:98:ARG:NH1	2:1:98:ARG:HG2	2.34	0.41
1:G:203:THR:HG23	1:G:212:THR:OG1	2.19	0.41
3:2:165:GLU:HG2	3:2:165:GLU:H	1.75	0.41
3:0:12:GLY:CA	3:0:111:LEU:HD13	2.50	0.41
3:8:118:PRO:HB3	3:8:141:ILE:CG2	2.49	0.41
1:F:463:GLY:C	1:F:465:GLY:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:288:ILE:O	1:J:288:ILE:HG13	2.20	0.41
1:G:50:LYS:HG2	1:G:273:PRO:HG2	2.01	0.41
1:L:418:ILE:HG13	1:L:418:ILE:H	1.70	0.41
3:X:133:ASN:HA	3:X:187:PRO:HG2	2.03	0.41
1:E:451:THR:HB	1:E:467:PHE:CE2	2.55	0.41
1:C:152:ASN:HB2	1:C:255:ARG:NH1	2.34	0.41
3:O:83:GLU:H	3:O:83:GLU:CD	2.22	0.41
1:J:395:ILE:O	1:J:395:ILE:HG13	2.19	0.41
2:M:116:TRP:CD1	2:M:116:TRP:N	2.88	0.41
2:W:182:VAL:O	2:W:189:TYR:HA	2.20	0.41
1:J:487:ASP:OD2	1:J:490:VAL:HG23	2.19	0.41
1:H:143:PRO:HG2	1:H:144:GLY:H	1.85	0.41
3:R:33:TYR:O	3:R:34:ALA:C	2.58	0.41
3:R:195:SER:HB3	3:R:212:ALA:HB2	2.02	0.41
3:2:172:GLN:HE21	3:2:176:LYS:NZ	2.18	0.41
2:S:179:PHE:HA	2:S:180:PRO:HD3	1.95	0.41
2:9:34:LEU:HD22	2:9:35:SER:H	1.85	0.41
3:P:174:ASN:O	3:P:175:ASN:HB2	2.20	0.41
3:X:47:LYS:HG2	3:X:48:LEU:N	2.34	0.41
2:M:2:VAL:HG12	2:M:25:SER:O	2.20	0.41
2:7:148:THR:O	2:7:199:SER:HB2	2.20	0.41
2:Y:206:THR:CG2	2:Y:223:LYS:HG2	2.50	0.41
2:M:105:VAL:HG12	2:M:107:GLY:O	2.20	0.41
2:S:2:VAL:HG12	2:S:25:SER:O	2.21	0.41
2:1:2:VAL:HG23	2:1:115:VAL:HG11	2.02	0.41
1:B:221:PRO:HD3	1:C:244:VAL:CB	2.45	0.41
2:5:105:VAL:HG12	2:5:107:GLY:O	2.20	0.41
1:F:196:VAL:O	1:F:197:GLN:C	2.57	0.41
2:O:208:ILE:HA	2:O:222:LYS:O	2.20	0.41
1:C:61:GLY:O	1:C:62:ILE:C	2.58	0.41
1:K:111:LEU:HD12	1:K:111:LEU:C	2.41	0.41
1:L:326:LYS:HD3	1:L:328:THR:H	1.85	0.41
3:Z:123:PHE:O	3:Z:137:LEU:HD23	2.20	0.41
2:Q:155:VAL:O	2:Q:155:VAL:HG23	2.20	0.41
1:D:212:THR:HG21	1:F:216:ASN:CG	2.40	0.41
2:O:40:ALA:HA	2:O:92:ALA:CB	2.50	0.41
3:N:29:ILE:CD1	3:N:71:THR:HB	2.50	0.41
2:7:210:ASN:N	2:7:210:ASN:HD22	2.18	0.41
1:I:436:THR:O	1:I:440:THR:HG23	2.20	0.41
1:J:222:TRP:CH2	1:J:225:GLY:HA2	2.55	0.41
3:R:5:THR:HB	3:R:23:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:155:ALA:HA	3:6:196:TYR:CE1	2.55	0.41
2:M:30:THR:HB	2:M:54:TYR:CD2	2.56	0.41
1:D:15:LEU:HD22	1:D:448:PHE:HA	2.02	0.41
1:A:96:ASN:CA	1:A:224:ARG:HH11	2.32	0.41
2:9:98:ARG:NH1	2:9:98:ARG:HG2	2.34	0.41
3:T:38:TYR:CD2	3:T:48:LEU:HA	2.56	0.41
3:P:118:PRO:HB2	3:P:207:VAL:HG11	2.02	0.41
1:I:356:GLN:OE1	1:I:361:THR:HG22	2.20	0.41
1:F:131:THR:HG22	1:F:132:GLN:N	2.35	0.41
1:H:255:ARG:HG2	1:H:255:ARG:HH11	1.85	0.41
3:Z:122:LEU:HD13	3:Z:198:CYS:HB2	2.02	0.41
3:T:122:LEU:HD13	3:T:198:CYS:HB2	2.01	0.41
1:D:176:LYS:HD3	1:D:178:TYR:OH	2.21	0.41
1:C:487:ASP:OD2	1:C:490:VAL:HG23	2.20	0.41
1:B:416:THR:HG22	1:B:420:LEU:HD11	2.02	0.41
3:0:172:GLN:HE21	3:0:176:LYS:NZ	2.18	0.41
2:M:177:HIS:CD2	3:N:172:GLN:NE2	2.89	0.41
3:8:172:GLN:HE21	3:8:176:LYS:NZ	2.19	0.41
2:U:99:VAL:HB	2:U:111:TYR:CG	2.54	0.41
2:W:33:GLY:C	2:W:99:VAL:HG13	2.41	0.41
2:W:99:VAL:HB	2:W:111:TYR:CZ	2.55	0.41
2:M:99:VAL:HB	2:M:111:TYR:CE1	2.55	0.41
2:U:118:GLN:OE1	2:U:119:GLY:N	2.53	0.41
1:K:380:LYS:O	1:K:380:LYS:HE2	2.20	0.41
2:9:36:TRP:NE1	2:9:70:MET:CE	2.83	0.41
1:L:147:PHE:CG	1:L:148:PHE:N	2.89	0.41
1:C:161:TYR:HB2	1:C:196:VAL:HG21	2.02	0.41
2:5:36:TRP:NE1	2:5:70:MET:CE	2.83	0.41
1:K:220:ARG:HB2	1:K:221:PRO:CD	2.49	0.41
1:A:357:ASN:HB2	1:A:473:CYS:O	2.19	0.41
1:G:182:VAL:HG21	1:G:213:ILE:HB	2.02	0.41
2:M:155:VAL:O	2:M:155:VAL:HG23	2.20	0.41
2:W:181:ALA:HA	2:W:190:SER:O	2.20	0.41
2:U:155:VAL:HG23	2:U:155:VAL:O	2.21	0.41
2:U:181:ALA:HA	2:U:190:SER:O	2.19	0.41
1:E:61:GLY:O	1:E:62:ILE:C	2.59	0.41
1:H:320:MET:HG2	1:H:321:ARG:N	2.36	0.41
1:D:131:THR:HB	1:D:155:THR:OG1	2.19	0.41
2:O:155:VAL:O	2:O:155:VAL:HG23	2.20	0.41
1:C:67:ILE:HG13	1:C:105:TYR:CE2	2.56	0.41
1:F:29:ILE:HG12	1:F:434:GLN:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:SER:HB3	1:C:227:SER:O	2.20	0.41
1:D:222:TRP:CH2	1:D:225:GLY:HA2	2.55	0.41
1:L:463:GLY:C	1:L:465:GLY:H	2.24	0.41
2:M:39:GLN:HE21	2:M:45:LEU:HD23	1.84	0.41
3:2:23:THR:HG22	3:2:72:SER:CB	2.49	0.41
1:L:423:TYR:OH	1:L:427:LEU:HD22	2.20	0.41
2:S:112:PRO:HB3	3:T:36:HIS:CE1	2.54	0.41
3:0:75:LEU:HD12	3:0:76:ALA:N	2.35	0.41
3:0:37:TRP:CZ3	3:0:90:CYS:HB3	2.55	0.41
3:V:118:PRO:HB2	3:V:207:VAL:HG11	2.03	0.41
3:2:51:SER:O	3:2:53:ASN:N	2.54	0.41
3:Z:91:GLN:HB2	3:Z:102:PHE:CE2	2.55	0.41
1:K:49:GLY:HA2	1:K:285:ASN:O	2.20	0.41
1:L:44:GLN:HG2	1:L:288:ILE:HD12	2.02	0.41
2:9:2:VAL:HG21	2:9:115:VAL:HG21	2.02	0.41
1:C:50:LYS:HD3	1:C:275:ASP:HB2	2.01	0.41
3:Z:133:ASN:O	3:Z:134:LYS:HG2	2.20	0.41
3:N:81:GLN:O	3:N:110:VAL:HG11	2.20	0.41
3:V:80:LEU:HD11	3:V:108:LEU:HD21	2.02	0.41
3:0:174:ASN:HD21	3:0:176:LYS:HE3	1.85	0.41
2:7:179:PHE:HA	2:7:180:PRO:HD3	1.95	0.41
2:U:99:VAL:HB	2:U:111:TYR:CD1	2.55	0.41
2:U:55:ASP:OD2	2:U:57:GLN:HB2	2.20	0.41
4:K:602:NAG:C8	2:7:55:ASP:OD1	2.67	0.41
2:1:100:GLU:HB2	2:1:111:TYR:HB2	2.03	0.41
2:Q:29:LEU:N	2:Q:29:LEU:CD2	2.83	0.41
1:D:326:LYS:CD	1:D:328:THR:H	2.33	0.41
3:P:51:SER:O	3:P:53:ASN:N	2.53	0.41
1:I:185:PRO:O	1:I:217:ILE:HA	2.21	0.41
1:G:147:PHE:CG	1:G:148:PHE:N	2.88	0.41
2:9:36:TRP:HE1	2:9:70:MET:CE	2.33	0.41
2:M:36:TRP:NE1	2:M:70:MET:HE1	2.36	0.41
1:H:357:ASN:HB2	1:H:473:CYS:O	2.20	0.41
1:D:357:ASN:HB2	1:D:473:CYS:O	2.20	0.41
2:1:155:VAL:O	2:1:155:VAL:HG23	2.20	0.41
1:E:242:VAL:HG22	1:E:243:LEU:N	2.36	0.41
1:J:335:ILE:CG1	1:J:354:ARG:HB3	2.51	0.41
2:U:182:VAL:HG21	3:V:165:GLU:C	2.40	0.41
3:P:29:ILE:CD1	3:P:71:THR:HB	2.51	0.41
2:7:208:ILE:HA	2:7:222:LYS:O	2.20	0.41
2:Q:40:ALA:HA	2:Q:92:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:ARG:CZ	1:H:267:ILE:HD13	2.50	0.41
1:H:327:GLN:HG3	1:H:329:ARG:NE	2.32	0.41
3:X:155:ALA:N	3:X:158:SER:O	2.48	0.41
1:E:427:LEU:O	1:E:431:LEU:HD12	2.20	0.41
3:4:37:TRP:CH2	3:4:90:CYS:HB3	2.55	0.41
1:G:97:CYS:H	1:G:224:ARG:NH1	2.18	0.41
1:J:152:ASN:HB2	1:J:255:ARG:NH1	2.35	0.41
1:L:131:THR:HG22	1:L:132:GLN:N	2.35	0.41
3:0:195:SER:HB3	3:0:212:ALA:HB2	2.01	0.41
1:D:44:GLN:OE1	1:D:289:PRO:HG2	2.19	0.41
2:Y:154:LEU:HD21	3:Z:136:THR:HG21	2.01	0.41
1:L:176:LYS:HD3	1:L:178:TYR:OH	2.20	0.41
3:2:174:ASN:O	3:2:175:ASN:HB2	2.21	0.41
2:M:179:PHE:CZ	3:N:142:SER:HB3	2.55	0.41
3:N:174:ASN:ND2	3:N:176:LYS:HB3	2.35	0.41
3:P:172:GLN:HE21	3:P:176:LYS:NZ	2.19	0.41
3:8:143:ASP:HA	3:8:176:LYS:CD	2.50	0.41
3:6:47:LYS:HG2	3:6:48:LEU:N	2.36	0.41
2:1:148:THR:O	2:1:199:SER:HB2	2.21	0.41
2:W:48:VAL:HG13	2:W:64:PHE:CE2	2.56	0.41
1:L:185:PRO:HA	1:L:190:GLU:OE2	2.20	0.41
1:I:161:TYR:HB2	1:I:196:VAL:HG21	2.03	0.41
1:C:339:ILE:HG22	1:C:340:GLU:N	2.36	0.41
1:E:343:TRP:C	1:E:345:GLY:N	2.74	0.41
2:U:184:GLN:CG	3:V:165:GLU:OE1	2.69	0.41
3:V:153:TRP:CE2	3:V:183:LEU:HD13	2.55	0.41
2:Q:210:ASN:HD22	2:Q:210:ASN:N	2.17	0.41
2:O:130:LYS:NZ	2:W:130:LYS:CD	2.83	0.41
1:I:222:TRP:CD1	1:I:227:SER:HB2	2.55	0.41
3:2:123:PHE:O	3:2:137:LEU:HD23	2.21	0.41
2:S:216:SER:HG	2:S:218:THR:CB	2.34	0.41
3:4:133:ASN:HA	3:4:187:PRO:HG2	2.02	0.41
1:C:52:CYS:HB3	1:C:277:CYS:O	2.21	0.41
1:J:220:ARG:HD2	1:J:229:ARG:HG2	2.01	0.41
2:U:30:THR:HB	2:U:54:TYR:CD2	2.55	0.41
1:K:427:LEU:O	1:K:431:LEU:HD12	2.20	0.41
3:Z:47:LYS:HG2	3:Z:48:LEU:N	2.35	0.41
3:N:117:ALA:HA	3:N:118:PRO:HD3	1.92	0.41
3:N:37:TRP:HB2	3:N:50:ILE:CG1	2.50	0.41
1:H:134:GLY:CA	1:H:153:TRP:HB3	2.50	0.41
1:K:50:LYS:HD3	1:K:275:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:91:GLN:HB2	3:6:102:PHE:CE2	2.56	0.41
3:4:110:VAL:HG23	3:4:110:VAL:O	2.21	0.41
1:H:49:GLY:O	1:H:273:PRO:HD2	2.20	0.41
1:A:268:MET:CE	1:A:282:ILE:HG22	2.50	0.41
1:A:497:ASN:HA	1:A:497:ASN:HD22	1.53	0.41
3:0:80:LEU:HD11	3:0:108:LEU:HD21	2.02	0.41
2:9:161:GLU:HA	2:9:162:PRO:HA	1.77	0.41
3:N:122:LEU:HD13	3:N:198:CYS:HB2	2.01	0.41
1:I:110:SER:OG	1:I:393:HIS:NE2	2.47	0.41
1:K:44:GLN:OE1	1:K:289:PRO:HG2	2.21	0.41
2:3:182:VAL:O	2:3:189:TYR:HA	2.20	0.41
2:M:170:GLY:O	2:M:173:THR:HG23	2.21	0.41
1:F:143:PRO:HG2	1:F:144:GLY:H	1.85	0.41
2:3:9:ALA:HB1	2:3:121:MET:O	2.20	0.41
3:T:174:ASN:ND2	3:T:176:LYS:HB3	2.35	0.41
3:P:116:ALA:HB1	3:P:143:ASP:O	2.21	0.41
2:U:34:LEU:CD2	2:U:35:SER:N	2.83	0.41
2:7:34:LEU:HD22	2:7:35:SER:H	1.86	0.41
2:W:108:PHE:CZ	3:X:99:GLY:HA2	2.55	0.41
2:9:83:MET:HB3	2:9:86:LEU:HD21	2.02	0.41
1:E:222:TRP:CD1	1:E:227:SER:HB2	2.56	0.41
2:Q:222:LYS:NZ	3:R:128:GLU:OE1	2.52	0.41
1:D:147:PHE:CG	1:D:148:PHE:N	2.87	0.41
1:B:220:ARG:HH21	1:C:203:THR:HG21	1.85	0.41
2:U:20:VAL:HG13	2:U:120:THR:HG21	2.03	0.41
1:L:161:TYR:CZ	1:L:249:GLY:HA2	2.56	0.41
1:J:51:ILE:HD11	1:J:272:ALA:HB3	2.01	0.41
2:7:167:TRP:HB3	2:7:172:LEU:HB3	2.02	0.41
1:I:102:VAL:HG22	1:I:232:ILE:CB	2.45	0.41
3:N:51:SER:OG	3:N:55:ASN:HB3	2.20	0.41
3:P:153:TRP:CB	3:P:183:LEU:HD22	2.50	0.41
2:Y:155:VAL:O	2:Y:155:VAL:HG23	2.20	0.41
2:1:181:ALA:HA	2:1:190:SER:O	2.20	0.41
1:D:220:ARG:HB2	1:D:221:PRO:CD	2.51	0.41
2:U:184:GLN:CB	3:V:165:GLU:OE1	2.69	0.41
1:G:463:GLY:C	1:G:465:GLY:H	2.23	0.41
1:L:222:TRP:CD1	1:L:227:SER:HB2	2.55	0.41
1:C:222:TRP:CD1	1:C:227:SER:HB2	2.56	0.41
1:I:320:MET:HG2	1:I:321:ARG:N	2.36	0.41
1:I:321:ARG:HD2	1:I:437:ILE:CG2	2.50	0.41
2:U:105:VAL:HG12	2:U:107:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:372:ALA:O	1:G:376:GLN:HG3	2.20	0.41
2:Q:62:LYS:HE3	3:R:97:LEU:HD13	2.02	0.41
1:C:84:TRP:HZ2	1:C:113:ALA:HA	1.86	0.41
1:B:423:TYR:OH	1:B:427:LEU:HD22	2.21	0.41
3:O:47:LYS:HG2	3:O:48:LEU:N	2.36	0.41
3:4:38:TYR:CD2	3:4:48:LEU:HA	2.55	0.41
3:N:91:GLN:HB2	3:N:102:PHE:CE2	2.56	0.41
3:2:34:ALA:HB1	3:2:36:HIS:CE1	2.56	0.41
1:L:56:HIS:O	1:L:58:ILE:HG12	2.20	0.41
1:E:98:TYR:OH	1:E:228:SER:HB2	2.20	0.41
3:O:33:TYR:O	3:O:34:ALA:C	2.58	0.41
1:F:98:TYR:OH	1:F:228:SER:HB2	2.20	0.41
7:G:615:NAG:H82	7:G:615:NAG:H3	2.02	0.41
3:T:133:ASN:O	3:T:134:LYS:HG2	2.20	0.41
1:G:416:THR:HG22	1:G:420:LEU:CD1	2.51	0.41
2:7:33:GLY:C	2:7:99:VAL:HG13	2.41	0.41
2:1:33:GLY:C	2:1:99:VAL:HG13	2.41	0.41
2:Q:148:THR:O	2:Q:199:SER:HB2	2.21	0.41
2:Y:29:LEU:CD2	2:Y:29:LEU:N	2.84	0.41
1:K:222:TRP:CD1	1:K:227:SER:HB2	2.56	0.41
2:S:159:PHE:HB2	2:S:188:LEU:CD2	2.51	0.41
1:G:183:HIS:O	1:G:185:PRO:HD3	2.21	0.41
2:S:36:TRP:HE1	2:S:70:MET:CE	2.34	0.41
2:O:36:TRP:NE1	2:O:70:MET:CE	2.84	0.41
2:W:4:LEU:HA	2:W:23:GLN:O	2.20	0.41
1:B:293:PRO:C	1:B:306:PRO:HB3	2.42	0.41
1:B:380:LYS:HZ2	1:B:384:VAL:HG23	1.85	0.41
1:E:229:ARG:HH11	1:E:229:ARG:HG2	1.85	0.41
1:B:102:VAL:HG22	1:B:232:ILE:CB	2.45	0.41
1:G:103:PRO:HG2	1:G:233:TYR:CE1	2.56	0.41
3:R:153:TRP:CD2	3:R:183:LEU:HD13	2.55	0.41
3:4:123:PHE:O	3:4:137:LEU:HD23	2.20	0.41
1:F:357:ASN:HB2	1:F:473:CYS:O	2.21	0.41
1:A:335:ILE:CG1	1:A:354:ARG:HB3	2.51	0.41
2:S:181:ALA:HA	2:S:190:SER:O	2.20	0.41
1:K:63:ASP:CA	1:K:93:ALA:HA	2.49	0.41
2:Q:194:VAL:HG21	3:R:140:LEU:HD13	2.02	0.41
2:1:210:ASN:HD22	2:1:210:ASN:N	2.17	0.41
1:A:206:THR:C	1:C:221:PRO:HG2	2.41	0.41
3:6:12:GLY:O	3:6:111:LEU:HB2	2.21	0.41
1:E:97:CYS:H	1:E:224:ARG:NH1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:155:ALA:N	3:0:158:SER:O	2.47	0.41
3:P:155:ALA:HA	3:P:196:TYR:CE1	2.56	0.41
1:I:242:VAL:HG22	1:I:243:LEU:N	2.36	0.41
2:M:154:LEU:HD22	3:N:138:VAL:CG2	2.51	0.41
3:4:117:ALA:HA	3:4:118:PRO:HD3	1.92	0.41
2:Q:184:GLN:HA	3:R:165:GLU:OE1	2.20	0.41
1:J:242:VAL:HG22	1:J:243:LEU:N	2.35	0.41
3:2:118:PRO:HB2	3:2:207:VAL:HG11	2.03	0.41
1:D:453:ARG:HD3	1:F:463:GLY:CA	2.50	0.41
2:O:194:VAL:HG21	3:P:140:LEU:HD13	2.03	0.41
1:L:298:ASN:OD1	1:L:300:ILE:N	2.42	0.41
3:P:33:TYR:O	3:P:34:ALA:C	2.58	0.41
1:K:131:THR:HG22	1:K:132:GLN:N	2.36	0.41
3:Z:80:LEU:HD11	3:Z:108:LEU:HD21	2.03	0.41
2:U:59:LYS:HE3	2:U:59:LYS:HB2	1.93	0.41
1:B:200:GLY:HA3	1:B:250:ASN:OD1	2.21	0.41
1:I:203:THR:HG23	1:I:212:THR:OG1	2.21	0.41
3:0:133:ASN:O	3:0:134:LYS:HG2	2.21	0.41
3:V:174:ASN:ND2	3:V:176:LYS:HB3	2.35	0.41
2:O:34:LEU:CD2	2:O:35:SER:N	2.84	0.41
2:O:51:ILE:CD1	2:O:52:ASN:N	2.81	0.41
3:X:116:ALA:HB1	3:X:143:ASP:O	2.21	0.41
2:W:99:VAL:HB	2:W:111:TYR:CG	2.56	0.41
2:U:11:VAL:HG13	2:U:123:THR:O	2.21	0.41
2:5:111:TYR:CD1	2:5:111:TYR:O	2.74	0.41
2:5:34:LEU:CD2	2:5:35:SER:N	2.84	0.41
3:6:38:TYR:CD2	3:6:48:LEU:HA	2.55	0.41
2:S:198:PRO:HG2	2:S:201:SER:OG	2.20	0.41
2:5:198:PRO:HG2	2:5:201:SER:OG	2.20	0.41
2:7:29:LEU:CD2	2:7:29:LEU:N	2.84	0.41
2:3:88:SER:HA	2:3:124:VAL:HG12	2.03	0.41
2:3:208:ILE:HA	2:3:222:LYS:O	2.20	0.41
1:F:222:TRP:CD1	1:F:227:SER:HB2	2.56	0.41
2:5:159:PHE:HB2	2:5:188:LEU:CD2	2.50	0.41
1:I:326:LYS:NZ	1:I:343:TRP:CD1	2.83	0.41
2:5:4:LEU:HA	2:5:23:GLN:O	2.21	0.41
1:A:185:PRO:O	1:A:217:ILE:HA	2.21	0.41
1:E:156:LYS:HD3	1:E:193:SER:O	2.21	0.41
1:H:161:TYR:HB2	1:H:196:VAL:HG21	2.02	0.41
1:B:161:TYR:HB2	1:B:196:VAL:HG21	2.02	0.41
2:5:36:TRP:HE1	2:5:70:MET:CE	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:THR:N	1:A:434:GLN:OE1	2.50	0.41
1:B:380:LYS:C	1:B:380:LYS:HD3	2.41	0.41
2:3:179:PHE:HA	2:3:180:PRO:HD3	1.95	0.41
1:H:339:ILE:HG22	1:H:340:GLU:N	2.36	0.41
2:Y:208:ILE:HA	2:Y:222:LYS:O	2.20	0.41
1:G:111:LEU:HD12	1:G:111:LEU:C	2.41	0.41
3:R:123:PHE:O	3:R:137:LEU:HD23	2.20	0.41
3:T:153:TRP:CB	3:T:183:LEU:HD22	2.50	0.41
1:C:293:PRO:C	1:C:306:PRO:HB3	2.41	0.41
1:G:293:PRO:C	1:G:306:PRO:HB3	2.41	0.41
1:L:108:LEU:O	1:L:112:VAL:HG23	2.20	0.41
1:A:147:PHE:CG	1:A:148:PHE:N	2.89	0.41
1:A:384:VAL:HG11	1:A:428:LEU:HD11	2.01	0.41
3:2:7:PRO:O	3:2:105:GLY:O	2.39	0.41
2:S:155:VAL:O	2:S:155:VAL:HG23	2.21	0.41
1:L:208:ARG:HG3	1:L:241:ASP:OD2	2.20	0.41
1:A:241:ASP:OD1	1:A:242:VAL:N	2.54	0.41
2:S:109:HIS:HA	3:T:93:TYR:CD1	2.55	0.41
2:7:105:VAL:HG12	2:7:107:GLY:O	2.20	0.41
1:G:238:LYS:HE2	1:I:401:GLU:HG3	2.03	0.41
2:M:210:ASN:HD22	2:M:210:ASN:N	2.17	0.41
1:L:229:ARG:HG2	1:L:229:ARG:HH11	1.86	0.41
2:M:216:SER:HG	2:M:218:THR:CB	2.34	0.41
1:E:234:TRP:HE3	1:E:234:TRP:N	2.17	0.41
3:Z:29:ILE:CD1	3:Z:71:THR:HB	2.51	0.41
3:X:23:THR:HG22	3:X:72:SER:CB	2.49	0.41
1:J:222:TRP:CD1	1:J:227:SER:HB2	2.56	0.41
3:8:26:SER:HA	3:8:29:ILE:HD12	2.03	0.41
1:L:234:TRP:CE3	1:L:234:TRP:N	2.80	0.41
1:L:388:THR:HG23	1:L:389:ASN:H	1.86	0.41
3:4:133:ASN:O	3:4:134:LYS:HG2	2.21	0.41
3:8:155:ALA:HA	3:8:196:TYR:CE1	2.56	0.41
3:P:50:ILE:CD1	3:P:75:LEU:HD13	2.51	0.41
1:B:109:ARG:CZ	1:B:267:ILE:HD13	2.51	0.41
3:N:158:SER:HA	3:N:159:PRO:HD3	1.86	0.41
1:J:229:ARG:HG2	1:J:229:ARG:HH11	1.85	0.41
1:C:109:ARG:NH1	1:C:109:ARG:HG2	2.36	0.41
1:J:96:ASN:CA	1:J:224:ARG:HH11	2.32	0.41
1:J:234:TRP:CE3	1:J:234:TRP:N	2.82	0.41
3:R:37:TRP:CH2	3:R:90:CYS:HB3	2.56	0.41
1:G:437:ILE:O	1:G:441:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:32:TYR:CG	2:1:98:ARG:HD3	2.55	0.41
1:D:109:ARG:HG2	1:D:109:ARG:NH1	2.36	0.41
1:J:170:ASN:OD1	1:J:176:LYS:HE3	2.21	0.41
3:0:51:SER:O	3:0:53:ASN:N	2.53	0.41
1:I:239:PRO:HB3	2:1:75:GLY:HA2	2.02	0.41
3:V:47:LYS:HG2	3:V:48:LEU:N	2.35	0.41
1:K:421:TRP:CE3	1:K:421:TRP:HA	2.56	0.41
1:G:307:LYS:HE2	1:G:421:TRP:CZ2	2.56	0.41
3:2:81:GLN:O	3:2:110:VAL:HG11	2.19	0.41
1:B:176:LYS:HD3	1:B:178:TYR:OH	2.21	0.41
1:E:131:THR:HG22	1:E:132:GLN:N	2.36	0.41
1:L:401:GLU:N	1:L:401:GLU:OE1	2.54	0.41
1:C:474:ASP:O	1:C:477:CYS:HB3	2.20	0.41
1:F:356:GLN:OE1	1:F:361:THR:HG22	2.21	0.41
1:B:143:PRO:HG2	1:B:144:GLY:H	1.85	0.41
3:X:122:LEU:HD13	3:X:198:CYS:HB2	2.02	0.41
3:X:80:LEU:HD11	3:X:108:LEU:HD21	2.02	0.41
2:U:161:GLU:HA	2:U:162:PRO:HA	1.77	0.41
3:T:33:TYR:O	3:T:34:ALA:C	2.58	0.41
2:U:9:ALA:HB1	2:U:121:MET:O	2.20	0.41
1:G:497:ASN:HA	1:G:497:ASN:HD22	1.54	0.41
1:I:56:HIS:O	1:I:58:ILE:HG12	2.20	0.41
2:Q:182:VAL:O	2:Q:189:TYR:HA	2.21	0.41
1:K:455:LEU:O	1:K:456:ARG:HB2	2.21	0.41
1:I:180:TRP:CD2	1:I:204:VAL:HG21	2.55	0.41
2:W:114:ASP:CG	2:W:115:VAL:HG23	2.41	0.41
2:W:51:ILE:CD1	2:W:52:ASN:N	2.81	0.41
2:3:148:THR:O	2:3:199:SER:HB2	2.21	0.41
2:W:19:THR:HG22	2:W:82:GLU:CG	2.47	0.41
1:E:187:THR:CB	1:E:189:GLN:HE21	2.16	0.41
2:Y:24:VAL:HG23	2:Y:77:ASN:O	2.21	0.41
2:1:83:MET:HB3	2:1:86:LEU:HD21	2.02	0.41
2:U:159:PHE:HB2	2:U:188:LEU:CD2	2.51	0.41
1:I:326:LYS:CD	1:I:328:THR:H	2.35	0.41
1:A:320:MET:HG2	1:A:321:ARG:N	2.36	0.41
1:A:437:ILE:O	1:A:441:ASP:HB2	2.21	0.41
1:D:383:ARG:CD	1:F:27:LYS:HZ2	2.29	0.41
1:L:183:HIS:O	1:L:185:PRO:HD3	2.20	0.41
2:7:2:VAL:HG12	2:7:25:SER:O	2.20	0.41
1:J:251:LEU:HD12	1:J:252:ILE:N	2.34	0.41
2:7:36:TRP:NE1	2:7:70:MET:HE1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:SER:C	1:C:93:ALA:N	2.73	0.41
2:U:36:TRP:NE1	2:U:70:MET:CE	2.84	0.41
1:C:311:GLN:HG2	1:C:426:GLU:OE1	2.20	0.41
1:C:292:LYS:HB3	1:C:293:PRO:HD2	2.03	0.41
3:4:153:TRP:CB	3:4:183:LEU:HD22	2.51	0.41
1:A:251:LEU:HD12	1:A:252:ILE:N	2.35	0.41
1:C:401:GLU:N	1:C:401:GLU:OE1	2.54	0.41
1:I:292:LYS:HB3	1:I:293:PRO:HD2	2.02	0.41
2:Y:210:ASN:N	2:Y:210:ASN:HD22	2.17	0.41
1:D:19:ALA:CB	1:D:322:ASN:HD21	2.34	0.41
1:B:234:TRP:CE3	1:B:234:TRP:N	2.80	0.41
3:4:130:LEU:HD23	3:4:187:PRO:HG3	2.03	0.41
2:W:87:ARG:HB3	2:W:87:ARG:HE	1.74	0.41
3:P:75:LEU:HD12	3:P:76:ALA:N	2.36	0.41
1:J:15:LEU:HB3	1:J:444:MET:HE1	2.03	0.41
1:I:98:TYR:OH	1:I:228:SER:HB2	2.21	0.41
1:I:49:GLY:HA2	1:I:285:ASN:O	2.21	0.41
1:F:255:ARG:HH11	1:F:255:ARG:HG2	1.86	0.41
2:5:182:VAL:O	2:5:189:TYR:HA	2.21	0.41
1:B:301:THR:HB	1:B:305:CYS:SG	2.61	0.41
3:V:122:LEU:HD13	3:V:198:CYS:HB2	2.01	0.41
3:8:174:ASN:O	3:8:175:ASN:HB2	2.21	0.40
4:E:601:NAG:H61	4:E:602:NAG:O7	2.20	0.40
2:7:99:VAL:HB	2:7:111:TYR:CD1	2.56	0.40
2:W:84:LYS:HZ3	2:9:142:LYS:HE3	1.86	0.40
2:M:159:PHE:HB2	2:M:188:LEU:CD2	2.51	0.40
2:5:48:VAL:HG13	2:5:64:PHE:CE2	2.55	0.40
1:F:433:ASN:O	1:F:437:ILE:HG13	2.20	0.40
2:7:36:TRP:NE1	2:7:70:MET:CE	2.84	0.40
1:A:29:ILE:HG12	1:A:434:GLN:CB	2.51	0.40
3:6:153:TRP:CD2	3:6:183:LEU:HD13	2.56	0.40
3:X:153:TRP:CB	3:X:183:LEU:HD22	2.51	0.40
3:0:153:TRP:CB	3:0:183:LEU:HD22	2.50	0.40
3:2:6:GLN:NE2	3:2:105:GLY:H	2.19	0.40
1:E:292:LYS:HB3	1:E:293:PRO:HD2	2.03	0.40
1:E:111:LEU:HD12	1:E:111:LEU:C	2.41	0.40
1:K:19:ALA:CB	1:K:322:ASN:HD21	2.34	0.40
1:L:384:VAL:HG21	1:L:428:LEU:HD11	2.04	0.40
1:I:380:LYS:O	1:I:380:LYS:HE2	2.20	0.40
1:D:222:TRP:CD1	1:D:227:SER:HB2	2.56	0.40
1:C:437:ILE:O	1:C:441:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:26:SER:HA	3:X:29:ILE:HD12	2.03	0.40
1:H:59:LEU:HD12	1:H:60:ASP:N	2.36	0.40
1:G:311:GLN:HG2	1:G:426:GLU:OE1	2.21	0.40
3:8:130:LEU:CD2	3:8:135:ALA:HB2	2.49	0.40
3:X:155:ALA:HA	3:X:196:TYR:CE1	2.56	0.40
1:H:423:TYR:OH	1:H:427:LEU:HD22	2.21	0.40
1:E:437:ILE:O	1:E:441:ASP:HB2	2.21	0.40
1:K:437:ILE:O	1:K:441:ASP:HB2	2.22	0.40
1:D:268:MET:SD	1:D:284:PRO:HG3	2.61	0.40
1:B:49:GLY:O	1:B:273:PRO:HD2	2.21	0.40
3:8:133:ASN:O	3:8:134:LYS:HG2	2.20	0.40
2:S:14:PRO:HD3	2:S:125:SER:C	2.42	0.40
1:H:131:THR:HG22	1:H:132:GLN:N	2.35	0.40
1:G:246:ASN:ND2	1:I:219:SER:H	2.19	0.40
1:I:143:PRO:HG2	1:I:144:GLY:H	1.85	0.40
2:Q:55:ASP:OD2	2:Q:57:GLN:HB2	2.21	0.40
2:Y:100:GLU:HB2	2:Y:111:TYR:HB2	2.03	0.40
2:S:34:LEU:HD22	2:S:35:SER:H	1.86	0.40
3:N:111:LEU:N	3:N:111:LEU:HD12	2.36	0.40
2:Y:206:THR:HG21	2:Y:223:LYS:CE	2.34	0.40
2:S:140:SER:CB	3:T:211:VAL:HG13	2.51	0.40
1:C:203:THR:HG23	1:C:212:THR:OG1	2.22	0.40
2:U:4:LEU:HB2	2:U:117:GLY:HA2	2.04	0.40
2:Y:4:LEU:HA	2:Y:23:GLN:O	2.21	0.40
2:3:36:TRP:HE1	2:3:70:MET:CE	2.33	0.40
2:5:172:LEU:CD2	2:5:195:VAL:HG11	2.48	0.40
2:1:118:GLN:H	2:1:118:GLN:HG3	1.43	0.40
1:A:383:ARG:HD3	1:C:27:LYS:HZ2	1.85	0.40
1:C:241:ASP:OD1	1:C:242:VAL:N	2.54	0.40
3:4:153:TRP:CE2	3:4:183:LEU:HD13	2.57	0.40
1:D:316:LEU:HD12	1:D:433:ASN:OD1	2.21	0.40
1:H:433:ASN:O	1:H:437:ILE:HG13	2.21	0.40
1:D:131:THR:HG22	1:D:132:GLN:N	2.35	0.40
1:K:51:ILE:HD11	1:K:272:ALA:HB3	2.03	0.40
1:I:433:ASN:O	1:I:437:ILE:HG13	2.20	0.40
1:J:93:ALA:O	1:J:94:PHE:HB3	2.22	0.40
1:K:109:ARG:NH2	1:K:267:ILE:HD13	2.37	0.40
1:D:83:THR:O	1:D:84:TRP:HB3	2.20	0.40
1:I:84:TRP:HZ2	1:I:113:ALA:HA	1.86	0.40
3:4:75:LEU:HD12	3:4:76:ALA:N	2.36	0.40
1:G:98:TYR:CD1	1:G:99:PRO:HD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:GLN:HE22	1:E:308:TYR:HB2	1.86	0.40
3:6:133:ASN:HA	3:6:187:PRO:HG2	2.03	0.40
1:C:49:GLY:O	1:C:273:PRO:HD2	2.21	0.40
2:U:170:GLY:O	2:U:173:THR:HG23	2.21	0.40
1:G:56:HIS:O	1:G:58:ILE:HG12	2.21	0.40
1:E:355:HIS:NE2	1:E:362:GLY:HA3	2.36	0.40
1:I:131:THR:HG22	1:I:132:GLN:N	2.37	0.40
1:C:416:THR:HG22	1:C:420:LEU:CD1	2.51	0.40
1:G:331:LEU:N	1:G:331:LEU:CD2	2.70	0.40
3:P:91:GLN:HB2	3:P:102:PHE:CE2	2.57	0.40
4:G:602:NAG:H81	2:Y:55:ASP:OD1	2.21	0.40
2:Y:2:VAL:HG12	2:Y:25:SER:O	2.21	0.40
2:M:55:ASP:OD2	2:M:57:GLN:HB2	2.21	0.40
2:W:148:THR:O	2:W:199:SER:HB2	2.22	0.40
2:W:198:PRO:HG2	2:W:201:SER:OG	2.21	0.40
2:S:40:ALA:HA	2:S:92:ALA:CB	2.52	0.40
2:U:94:TYR:CE2	2:U:122:VAL:HG21	2.54	0.40
1:F:229:ARG:HG2	1:F:229:ARG:HH11	1.86	0.40
2:W:105:VAL:HG12	2:W:107:GLY:O	2.20	0.40
2:7:91:THR:HB	2:7:124:VAL:H	1.87	0.40
2:5:91:THR:HB	2:5:124:VAL:HG23	2.04	0.40
2:Q:36:TRP:HE1	2:Q:70:MET:CE	2.34	0.40
1:K:220:ARG:NH2	1:L:203:THR:HG21	2.37	0.40
1:D:61:GLY:O	1:D:62:ILE:C	2.60	0.40
1:D:292:LYS:HB3	1:D:293:PRO:HD2	2.04	0.40
1:F:29:ILE:HD13	1:F:430:ALA:HB1	2.03	0.40
1:E:372:ALA:O	1:E:376:GLN:HG3	2.21	0.40
1:L:220:ARG:HD2	1:L:229:ARG:HG2	2.04	0.40
3:P:158:SER:HA	3:P:159:PRO:HD3	1.87	0.40
3:6:5:THR:HB	3:6:23:THR:OG1	2.22	0.40
1:L:15:LEU:HD13	1:L:448:PHE:CD2	2.57	0.40
1:B:242:VAL:HG22	1:B:243:LEU:N	2.36	0.40
3:X:75:LEU:HD12	3:X:76:ALA:N	2.36	0.40
1:D:268:MET:CE	1:D:282:ILE:HG22	2.51	0.40
1:J:451:THR:HB	1:J:467:PHE:CE2	2.57	0.40
1:I:451:THR:HG22	1:I:455:LEU:HG	2.04	0.40
1:A:19:ALA:HB3	1:A:344:GLU:HG2	2.03	0.40
3:P:122:LEU:HD13	3:P:198:CYS:HB2	2.03	0.40
2:5:170:GLY:O	2:5:173:THR:HG23	2.20	0.40
3:2:116:ALA:HB1	3:2:143:ASP:O	2.22	0.40
2:9:34:LEU:N	2:9:99:VAL:HG13	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:143:ASP:HA	3:Z:176:LYS:CD	2.51	0.40
3:V:172:GLN:N	3:V:176:LYS:O	2.49	0.40
1:F:331:LEU:N	1:F:331:LEU:CD1	2.75	0.40
2:W:34:LEU:CD2	2:W:35:SER:N	2.84	0.40
2:O:19:THR:HG22	2:O:82:GLU:CG	2.47	0.40
2:W:159:PHE:HB2	2:W:188:LEU:CD2	2.52	0.40
1:B:222:TRP:CG	6:C:610:NAG:H5	2.56	0.40
1:F:380:LYS:C	1:F:380:LYS:HD3	2.42	0.40
1:E:221:PRO:HG3	1:F:244:VAL:HG23	2.02	0.40
1:L:203:THR:HG23	1:L:212:THR:OG1	2.21	0.40
3:R:137:LEU:HD13	3:R:153:TRP:HZ3	1.87	0.40
1:C:380:LYS:O	1:C:380:LYS:HE2	2.21	0.40
3:T:153:TRP:CE2	3:T:183:LEU:HD13	2.57	0.40
2:1:141:SER:O	2:1:142:LYS:C	2.60	0.40
3:4:7:PRO:O	3:4:105:GLY:O	2.40	0.40
1:L:380:LYS:O	1:L:380:LYS:HE2	2.22	0.40
1:I:293:PRO:C	1:I:306:PRO:HB3	2.42	0.40
3:6:29:ILE:CD1	3:6:71:THR:HB	2.51	0.40
2:Q:216:SER:HG	2:Q:218:THR:CB	2.34	0.40
3:T:5:THR:HB	3:T:23:THR:OG1	2.21	0.40
1:C:388:THR:HG23	1:C:389:ASN:H	1.87	0.40
2:M:32:TYR:CG	2:M:98:ARG:HD3	2.56	0.40
1:F:448:PHE:HZ	1:F:461:ASP:OD1	2.05	0.40
2:S:30:THR:HB	2:S:54:TYR:CD2	2.57	0.40
1:D:234:TRP:CE3	1:D:234:TRP:N	2.83	0.40
3:0:37:TRP:CH2	3:0:90:CYS:HB3	2.57	0.40
1:H:96:ASN:CA	1:H:224:ARG:HH11	2.33	0.40
1:B:280:GLU:HB2	1:B:290:ASN:HD21	1.85	0.40
2:O:2:VAL:HG12	2:O:25:SER:O	2.21	0.40
3:N:38:TYR:CD2	3:N:48:LEU:HA	2.57	0.40
2:3:13:LYS:HB3	2:3:14:PRO:HD2	2.04	0.40
1:D:98:TYR:OH	1:D:228:SER:HB2	2.21	0.40
1:C:176:LYS:HD3	1:C:178:TYR:OH	2.22	0.40
1:I:288:ILE:HG13	1:I:288:ILE:O	2.21	0.40
3:X:83:GLU:CD	3:X:83:GLU:H	2.24	0.40
1:B:471:HIS:HB2	1:B:494:GLU:OE1	2.21	0.40
1:E:268:MET:CE	1:E:282:ILE:HG22	2.51	0.40
1:G:355:HIS:NE2	1:G:362:GLY:HA3	2.36	0.40
2:9:37:VAL:HG11	3:0:102:PHE:HE1	1.85	0.40
2:9:33:GLY:C	2:9:99:VAL:HG13	2.42	0.40
2:W:177:HIS:NE2	3:X:172:GLN:OE1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:24:VAL:HG23	2:U:77:ASN:O	2.21	0.40
1:B:326:LYS:CD	1:B:328:THR:H	2.34	0.40
1:D:242:VAL:HG22	1:D:243:LEU:N	2.37	0.40
1:K:292:LYS:HB3	1:K:293:PRO:HD2	2.03	0.40
2:U:172:LEU:CD2	2:U:195:VAL:HG11	2.47	0.40
1:J:410:GLU:HG3	1:L:409:LEU:HD22	2.03	0.40
1:B:292:LYS:HB3	1:B:293:PRO:HD2	2.03	0.40
1:F:242:VAL:HG22	1:F:243:LEU:N	2.37	0.40
1:B:316:LEU:HD12	1:B:433:ASN:OD1	2.21	0.40
1:D:161:TYR:CZ	1:D:249:GLY:HA2	2.57	0.40
1:B:27:LYS:HZ2	1:C:383:ARG:HD3	1.87	0.40
3:X:153:TRP:CD2	3:X:183:LEU:HD13	2.56	0.40
3:Z:153:TRP:CD2	3:Z:183:LEU:HD13	2.56	0.40
1:G:346:MET:HE3	1:G:349:GLY:O	2.21	0.40
2:9:155:VAL:O	2:9:155:VAL:HG23	2.20	0.40
2:Q:181:ALA:HA	2:Q:190:SER:O	2.22	0.40
2:U:184:GLN:CA	3:V:165:GLU:OE1	2.65	0.40
1:A:210:GLN:HE21	1:C:220:ARG:CZ	2.34	0.40
1:E:147:PHE:CG	1:E:148:PHE:N	2.89	0.40
1:F:93:ALA:O	1:F:94:PHE:HB3	2.22	0.40
3:2:26:SER:HA	3:2:29:ILE:HD12	2.03	0.40
3:2:137:LEU:HD21	3:2:190:TRP:CZ3	2.57	0.40
3:N:23:THR:HG22	3:N:72:SER:CB	2.49	0.40
2:9:168:ASN:CB	2:9:171:ALA:HB3	2.50	0.40
2:7:30:THR:HB	2:7:54:TYR:CD2	2.57	0.40
1:D:109:ARG:NH2	1:D:267:ILE:HD13	2.37	0.40
1:J:437:ILE:O	1:J:441:ASP:HB2	2.21	0.40
2:3:30:THR:HB	2:3:54:TYR:CD2	2.57	0.40
3:6:118:PRO:HB2	3:6:207:VAL:HG11	2.02	0.40
3:0:38:TYR:CD2	3:0:48:LEU:HA	2.57	0.40
2:9:194:VAL:HG21	3:0:140:LEU:CD1	2.51	0.40
1:I:98:TYR:CE2	1:I:226:LEU:HD13	2.56	0.40
3:V:133:ASN:HA	3:V:187:PRO:HG2	2.04	0.40
3:N:110:VAL:HG23	3:N:110:VAL:O	2.21	0.40
1:H:451:THR:HG22	1:H:455:LEU:HG	2.03	0.40
3:Z:4:LEU:HG	3:Z:101:VAL:CG1	2.51	0.40
1:C:364:ALA:HB3	1:C:482:ARG:NH1	2.35	0.40
1:D:451:THR:HB	1:D:467:PHE:CE2	2.57	0.40
1:F:91:SER:O	2:W:31:SER:HB2	2.21	0.40
1:D:471:HIS:HB2	1:D:494:GLU:OE1	2.21	0.40
1:D:474:ASP:O	1:D:477:CYS:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:451:THR:HG22	1:G:455:LEU:HG	2.02	0.40
1:B:264:LYS:HB3	1:B:392:PHE:CG	2.56	0.40

All (2) 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)
2:3:171:ALA:CB	2:3:171:ALA:CB[2_556]	1.73	0.47
2:3:206:THR:OG1	2:3:206:THR:OG1[2_556]	1.74	0.46

## 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	491/493 (100%)	431 (88%)	54 (11%)	6 (1%)	16	62
1	B	491/493 (100%)	425 (87%)	60 (12%)	6 (1%)	16	62
1	C	491/493 (100%)	427 (87%)	57 (12%)	7 (1%)	14	59
1	D	491/493 (100%)	429 (87%)	55 (11%)	7 (1%)	14	59
1	E	491/493 (100%)	426 (87%)	58 (12%)	7 (1%)	14	59
1	F	491/493 (100%)	430 (88%)	54 (11%)	7 (1%)	14	59
1	G	491/493 (100%)	431 (88%)	54 (11%)	6 (1%)	16	62
1	H	491/493 (100%)	426 (87%)	58 (12%)	7 (1%)	14	59
1	I	491/493 (100%)	431 (88%)	54 (11%)	6 (1%)	16	62
1	J	491/493 (100%)	430 (88%)	54 (11%)	7 (1%)	14	59
1	K	491/493 (100%)	424 (86%)	60 (12%)	7 (1%)	14	59
1	L	491/493 (100%)	429 (87%)	56 (11%)	6 (1%)	16	62
2	1	224/226 (99%)	200 (89%)	18 (8%)	6 (3%)	6	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3	224/226 (99%)	203 (91%)	16 (7%)	5 (2%)	8	52
2	5	224/226 (99%)	202 (90%)	17 (8%)	5 (2%)	8	52
2	7	224/226 (99%)	198 (88%)	20 (9%)	6 (3%)	6	47
2	9	224/226 (99%)	201 (90%)	18 (8%)	5 (2%)	8	52
2	M	224/226 (99%)	197 (88%)	22 (10%)	5 (2%)	8	52
2	O	224/226 (99%)	197 (88%)	22 (10%)	5 (2%)	8	52
2	Q	224/226 (99%)	203 (91%)	16 (7%)	5 (2%)	8	52
2	S	224/226 (99%)	200 (89%)	19 (8%)	5 (2%)	8	52
2	U	224/226 (99%)	199 (89%)	20 (9%)	5 (2%)	8	52
2	W	224/226 (99%)	200 (89%)	19 (8%)	5 (2%)	8	52
2	Y	224/226 (99%)	197 (88%)	22 (10%)	5 (2%)	8	52
3	0	210/220 (96%)	190 (90%)	15 (7%)	5 (2%)	7	50
3	2	210/220 (96%)	191 (91%)	16 (8%)	3 (1%)	14	59
3	4	210/220 (96%)	190 (90%)	16 (8%)	4 (2%)	10	54
3	6	210/220 (96%)	192 (91%)	15 (7%)	3 (1%)	14	59
3	8	210/220 (96%)	190 (90%)	16 (8%)	4 (2%)	10	54
3	N	210/220 (96%)	189 (90%)	16 (8%)	5 (2%)	7	50
3	P	210/220 (96%)	191 (91%)	15 (7%)	4 (2%)	10	54
3	R	210/220 (96%)	190 (90%)	17 (8%)	3 (1%)	14	59
3	T	210/220 (96%)	192 (91%)	14 (7%)	4 (2%)	10	54
3	V	210/220 (96%)	190 (90%)	16 (8%)	4 (2%)	10	54
3	X	210/220 (96%)	191 (91%)	15 (7%)	4 (2%)	10	54
3	Z	210/220 (96%)	190 (90%)	15 (7%)	5 (2%)	7	50
All	All	11100/11268 (98%)	9822 (88%)	1089 (10%)	189 (2%)	11	56

All (189) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	330	GLY
2	5	115	VAL
3	N	175	ASN
3	P	175	ASN
3	R	175	ASN
3	T	175	ASN

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Mol	Chain	Res	Type
3	V	175	ASN
3	X	175	ASN
3	Z	175	ASN
3	2	175	ASN
3	4	175	ASN
3	6	175	ASN
3	8	175	ASN
3	0	175	ASN
1	A	330	GLY
1	A	339	ILE
1	B	330	GLY
1	B	339	ILE
1	C	62	ILE
1	C	330	GLY
1	C	339	ILE
1	D	62	ILE
1	D	330	GLY
1	D	339	ILE
1	E	62	ILE
1	E	330	GLY
1	E	339	ILE
1	F	339	ILE
1	G	330	GLY
1	G	339	ILE
1	H	62	ILE
1	H	330	GLY
1	H	339	ILE
1	I	330	GLY
1	I	339	ILE
1	J	330	GLY
1	J	339	ILE
1	K	62	ILE
1	K	330	GLY
1	K	339	ILE
1	L	330	GLY
1	L	339	ILE
2	M	101	GLY
2	M	109	HIS
2	M	115	VAL
2	O	101	GLY
2	O	109	HIS
2	Q	101	GLY

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Mol	Chain	Res	Type
2	Q	109	HIS
2	S	101	GLY
2	S	109	HIS
2	S	115	VAL
2	U	101	GLY
2	U	109	HIS
2	W	101	GLY
2	W	109	HIS
2	Y	101	GLY
2	Y	109	HIS
2	Y	115	VAL
2	1	101	GLY
2	1	109	HIS
2	3	101	GLY
2	3	109	HIS
2	5	101	GLY
2	5	109	HIS
2	7	101	GLY
2	7	109	HIS
2	7	113	MET
2	7	115	VAL
2	9	101	GLY
2	9	109	HIS
3	N	52	GLY
3	P	52	GLY
3	R	52	GLY
3	T	52	GLY
3	V	52	GLY
3	X	52	GLY
3	Z	52	GLY
3	2	52	GLY
3	4	52	GLY
3	6	52	GLY
3	8	52	GLY
3	0	52	GLY
1	A	62	ILE
1	B	62	ILE
1	B	336	ALA
1	F	62	ILE
1	F	336	ALA
1	G	62	ILE
1	I	62	ILE

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Mol	Chain	Res	Type
1	I	336	ALA
1	J	62	ILE
1	J	336	ALA
1	L	62	ILE
2	O	115	VAL
2	Q	115	VAL
2	U	115	VAL
2	1	115	VAL
3	Z	114	PRO
3	8	114	PRO
3	0	111	LEU
1	A	196	VAL
1	A	336	ALA
1	B	196	VAL
1	C	196	VAL
1	C	336	ALA
1	D	196	VAL
1	D	336	ALA
1	D	458	ASN
1	E	196	VAL
1	E	336	ALA
1	E	458	ASN
1	F	196	VAL
1	G	196	VAL
1	G	336	ALA
1	H	196	VAL
1	H	336	ALA
1	I	196	VAL
1	J	196	VAL
1	K	196	VAL
1	K	336	ALA
1	L	196	VAL
1	L	336	ALA
2	M	112	PRO
2	O	112	PRO
2	S	112	PRO
2	Y	112	PRO
2	3	115	VAL
2	5	112	PRO
2	7	112	PRO
3	X	84	ASP
3	4	84	ASP

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Mol	Chain	Res	Type
3	0	84	ASP
1	C	458	ASN
1	I	335	ILE
1	J	93	ALA
1	K	458	ASN
2	W	112	PRO
2	W	115	VAL
2	3	112	PRO
2	9	112	PRO
2	9	115	VAL
3	N	84	ASP
3	P	84	ASP
3	V	114	PRO
1	A	335	ILE
1	B	335	ILE
1	C	335	ILE
1	D	335	ILE
1	E	335	ILE
1	F	93	ALA
1	F	335	ILE
1	G	335	ILE
1	H	335	ILE
1	H	458	ASN
1	J	335	ILE
1	K	335	ILE
1	L	335	ILE
2	1	112	PRO
3	N	112	GLY
3	P	29	ILE
3	T	84	ASP
3	Z	84	ASP
3	2	29	ILE
3	6	29	ILE
3	8	29	ILE
2	U	112	PRO
3	N	29	ILE
3	R	29	ILE
3	T	29	ILE
3	V	29	ILE
3	X	29	ILE
3	Z	29	ILE
3	4	29	ILE

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Mol	Chain	Res	Type
3	0	29	ILE
2	Q	112	PRO
2	1	117	GLY
2	M	162	PRO
2	O	162	PRO
2	Q	162	PRO
2	S	162	PRO
2	U	162	PRO
2	W	162	PRO
2	1	162	PRO
2	3	162	PRO
2	5	162	PRO
2	7	162	PRO
2	9	162	PRO
2	Y	162	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	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	B	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	C	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	D	430/430 (100%)	405 (94%)	25 (6%)	25	64
1	E	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	F	430/430 (100%)	405 (94%)	25 (6%)	25	64
1	G	430/430 (100%)	405 (94%)	25 (6%)	25	64
1	H	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	I	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	J	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	K	430/430 (100%)	405 (94%)	25 (6%)	25	64
1	L	430/430 (100%)	406 (94%)	24 (6%)	26	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	191/191 (100%)	166 (87%)	25 (13%)	5	30
2	3	191/191 (100%)	166 (87%)	25 (13%)	5	30
2	5	191/191 (100%)	168 (88%)	23 (12%)	6	33
2	7	191/191 (100%)	163 (85%)	28 (15%)	4	26
2	9	191/191 (100%)	165 (86%)	26 (14%)	5	30
2	M	191/191 (100%)	167 (87%)	24 (13%)	5	31
2	O	191/191 (100%)	164 (86%)	27 (14%)	4	28
2	Q	191/191 (100%)	166 (87%)	25 (13%)	5	30
2	S	191/191 (100%)	166 (87%)	25 (13%)	5	30
2	U	191/191 (100%)	165 (86%)	26 (14%)	5	30
2	W	191/191 (100%)	166 (87%)	25 (13%)	5	30
2	Y	191/191 (100%)	167 (87%)	24 (13%)	5	31
3	0	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	2	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	4	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	6	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	8	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	N	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	P	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	R	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	T	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	V	174/181 (96%)	161 (92%)	13 (8%)	17	56
3	X	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	Z	174/181 (96%)	161 (92%)	13 (8%)	17	56
All	All	9540/9624 (99%)	8802 (92%)	738 (8%)	16	55

All (738) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	63	ASP
1	A	85	ASP
1	A	189	GLN
1	A	222	TRP

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Mol	Chain	Res	Type
1	A	274	ILE
1	A	277	CYS
1	A	283	THR
1	A	294	PHE
1	A	296	ASN
1	A	321	ARG
1	A	325	GLU
1	A	327	GLN
1	A	331	LEU
1	A	340	GLU
1	A	347	ILE
1	A	348	ASP
1	A	380	LYS
1	A	384	VAL
1	A	387	LYS
1	A	421	TRP
1	A	457	GLU
1	A	483	ASN
1	A	497	ASN
1	B	18	HIS
1	B	63	ASP
1	B	85	ASP
1	B	189	GLN
1	B	222	TRP
1	B	274	ILE
1	B	277	CYS
1	B	283	THR
1	B	294	PHE
1	B	296	ASN
1	B	321	ARG
1	B	325	GLU
1	B	327	GLN
1	B	331	LEU
1	B	340	GLU
1	B	347	ILE
1	B	348	ASP
1	B	380	LYS
1	B	384	VAL
1	B	387	LYS
1	B	421	TRP
1	B	457	GLU
1	B	483	ASN

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Mol	Chain	Res	Type
1	B	497	ASN
1	C	18	HIS
1	C	85	ASP
1	C	189	GLN
1	C	222	TRP
1	C	274	ILE
1	C	277	CYS
1	C	283	THR
1	C	294	PHE
1	C	296	ASN
1	C	321	ARG
1	C	325	GLU
1	C	327	GLN
1	C	331	LEU
1	C	340	GLU
1	C	347	ILE
1	C	348	ASP
1	C	380	LYS
1	C	384	VAL
1	C	387	LYS
1	C	421	TRP
1	C	457	GLU
1	C	483	ASN
1	C	497	ASN
1	D	18	HIS
1	D	63	ASP
1	D	85	ASP
1	D	189	GLN
1	D	222	TRP
1	D	274	ILE
1	D	277	CYS
1	D	283	THR
1	D	294	PHE
1	D	296	ASN
1	D	321	ARG
1	D	325	GLU
1	D	327	GLN
1	D	331	LEU
1	D	340	GLU
1	D	347	ILE
1	D	348	ASP
1	D	380	LYS

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Mol	Chain	Res	Type
1	D	384	VAL
1	D	387	LYS
1	D	400	SER
1	D	421	TRP
1	D	457	GLU
1	D	483	ASN
1	D	497	ASN
1	E	18	HIS
1	E	85	ASP
1	E	189	GLN
1	E	222	TRP
1	E	274	ILE
1	E	277	CYS
1	E	283	THR
1	E	294	PHE
1	E	296	ASN
1	E	321	ARG
1	E	325	GLU
1	E	327	GLN
1	E	331	LEU
1	E	340	GLU
1	E	347	ILE
1	E	348	ASP
1	E	380	LYS
1	E	384	VAL
1	E	387	LYS
1	E	421	TRP
1	E	457	GLU
1	E	483	ASN
1	E	497	ASN
1	F	18	HIS
1	F	63	ASP
1	F	85	ASP
1	F	189	GLN
1	F	222	TRP
1	F	274	ILE
1	F	277	CYS
1	F	283	THR
1	F	294	PHE
1	F	296	ASN
1	F	321	ARG
1	F	325	GLU

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Mol	Chain	Res	Type
1	F	327	GLN
1	F	331	LEU
1	F	340	GLU
1	F	347	ILE
1	F	348	ASP
1	F	380	LYS
1	F	384	VAL
1	F	387	LYS
1	F	400	SER
1	F	421	TRP
1	F	457	GLU
1	F	483	ASN
1	F	497	ASN
1	G	18	HIS
1	G	63	ASP
1	G	85	ASP
1	G	189	GLN
1	G	222	TRP
1	G	274	ILE
1	G	277	CYS
1	G	283	THR
1	G	294	PHE
1	G	296	ASN
1	G	321	ARG
1	G	325	GLU
1	G	327	GLN
1	G	331	LEU
1	G	340	GLU
1	G	347	ILE
1	G	348	ASP
1	G	380	LYS
1	G	384	VAL
1	G	387	LYS
1	G	400	SER
1	G	421	TRP
1	G	457	GLU
1	G	483	ASN
1	G	497	ASN
1	H	18	HIS
1	H	85	ASP
1	H	189	GLN
1	H	222	TRP

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Mol	Chain	Res	Type
1	H	274	ILE
1	H	277	CYS
1	H	283	THR
1	H	294	PHE
1	H	296	ASN
1	H	321	ARG
1	H	325	GLU
1	H	327	GLN
1	H	331	LEU
1	H	340	GLU
1	H	347	ILE
1	H	348	ASP
1	H	380	LYS
1	H	384	VAL
1	H	387	LYS
1	H	421	TRP
1	H	457	GLU
1	H	483	ASN
1	H	497	ASN
1	I	18	HIS
1	I	63	ASP
1	I	85	ASP
1	I	189	GLN
1	I	222	TRP
1	I	274	ILE
1	I	277	CYS
1	I	283	THR
1	I	294	PHE
1	I	296	ASN
1	I	321	ARG
1	I	325	GLU
1	I	327	GLN
1	I	331	LEU
1	I	340	GLU
1	I	347	ILE
1	I	348	ASP
1	I	380	LYS
1	I	384	VAL
1	I	387	LYS
1	I	421	TRP
1	I	457	GLU
1	I	483	ASN

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Mol	Chain	Res	Type
1	I	497	ASN
1	J	18	HIS
1	J	85	ASP
1	J	189	GLN
1	J	222	TRP
1	J	274	ILE
1	J	277	CYS
1	J	283	THR
1	J	294	PHE
1	J	296	ASN
1	J	321	ARG
1	J	325	GLU
1	J	327	GLN
1	J	331	LEU
1	J	340	GLU
1	J	347	ILE
1	J	348	ASP
1	J	380	LYS
1	J	384	VAL
1	J	387	LYS
1	J	400	SER
1	J	421	TRP
1	J	457	GLU
1	J	483	ASN
1	J	497	ASN
1	K	18	HIS
1	K	63	ASP
1	K	85	ASP
1	K	189	GLN
1	K	222	TRP
1	K	274	ILE
1	K	277	CYS
1	K	283	THR
1	K	294	PHE
1	K	296	ASN
1	K	321	ARG
1	K	325	GLU
1	K	327	GLN
1	K	331	LEU
1	K	340	GLU
1	K	347	ILE
1	K	348	ASP

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Mol	Chain	Res	Type
1	K	380	LYS
1	K	384	VAL
1	K	387	LYS
1	K	400	SER
1	K	421	TRP
1	K	457	GLU
1	K	483	ASN
1	K	497	ASN
1	L	18	HIS
1	L	85	ASP
1	L	189	GLN
1	L	222	TRP
1	L	274	ILE
1	L	277	CYS
1	L	283	THR
1	L	294	PHE
1	L	296	ASN
1	L	321	ARG
1	L	325	GLU
1	L	327	GLN
1	L	331	LEU
1	L	340	GLU
1	L	347	ILE
1	L	348	ASP
1	L	380	LYS
1	L	384	VAL
1	L	387	LYS
1	L	400	SER
1	L	421	TRP
1	L	457	GLU
1	L	483	ASN
1	L	497	ASN
2	M	24	VAL
2	M	34	LEU
2	M	39	GLN
2	M	43	GLN
2	M	45	LEU
2	M	51	ILE
2	M	54	TYR
2	M	64	PHE
2	M	69	THR
2	M	73	HIS

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Mol	Chain	Res	Type
2	M	74	THR
2	M	82	GLU
2	M	83	MET
2	M	91	THR
2	M	99	VAL
2	M	100	GLU
2	M	108	PHE
2	M	110	TYR
2	M	111	TYR
2	M	118	GLN
2	M	123	THR
2	M	143	SER
2	M	163	VAL
2	M	219	LYS
2	O	24	VAL
2	O	34	LEU
2	O	39	GLN
2	O	43	GLN
2	O	45	LEU
2	O	51	ILE
2	O	54	TYR
2	O	64	PHE
2	O	69	THR
2	O	73	HIS
2	O	74	THR
2	O	82	GLU
2	O	83	MET
2	O	91	THR
2	O	99	VAL
2	O	100	GLU
2	O	108	PHE
2	O	110	TYR
2	O	111	TYR
2	O	113	MET
2	O	118	GLN
2	O	121	MET
2	O	123	THR
2	O	125	SER
2	O	143	SER
2	O	163	VAL
2	O	219	LYS
2	Q	24	VAL

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Mol	Chain	Res	Type
2	Q	34	LEU
2	Q	39	GLN
2	Q	43	GLN
2	Q	45	LEU
2	Q	51	ILE
2	Q	54	TYR
2	Q	64	PHE
2	Q	69	THR
2	Q	73	HIS
2	Q	74	THR
2	Q	82	GLU
2	Q	83	MET
2	Q	91	THR
2	Q	99	VAL
2	Q	100	GLU
2	Q	108	PHE
2	Q	110	TYR
2	Q	111	TYR
2	Q	118	GLN
2	Q	121	MET
2	Q	123	THR
2	Q	143	SER
2	Q	163	VAL
2	Q	219	LYS
2	S	24	VAL
2	S	34	LEU
2	S	39	GLN
2	S	43	GLN
2	S	45	LEU
2	S	51	ILE
2	S	54	TYR
2	S	64	PHE
2	S	69	THR
2	S	73	HIS
2	S	74	THR
2	S	82	GLU
2	S	83	MET
2	S	91	THR
2	S	99	VAL
2	S	100	GLU
2	S	108	PHE
2	S	110	TYR

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Mol	Chain	Res	Type
2	S	111	TYR
2	S	118	GLN
2	S	121	MET
2	S	123	THR
2	S	143	SER
2	S	163	VAL
2	S	219	LYS
2	U	24	VAL
2	U	34	LEU
2	U	39	GLN
2	U	43	GLN
2	U	45	LEU
2	U	51	ILE
2	U	54	TYR
2	U	64	PHE
2	U	69	THR
2	U	73	HIS
2	U	74	THR
2	U	82	GLU
2	U	83	MET
2	U	91	THR
2	U	99	VAL
2	U	100	GLU
2	U	108	PHE
2	U	110	TYR
2	U	111	TYR
2	U	118	GLN
2	U	121	MET
2	U	123	THR
2	U	125	SER
2	U	143	SER
2	U	163	VAL
2	U	219	LYS
2	W	24	VAL
2	W	34	LEU
2	W	39	GLN
2	W	43	GLN
2	W	45	LEU
2	W	51	ILE
2	W	54	TYR
2	W	64	PHE
2	W	69	THR

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Mol	Chain	Res	Type
2	W	73	HIS
2	W	74	THR
2	W	82	GLU
2	W	83	MET
2	W	91	THR
2	W	99	VAL
2	W	100	GLU
2	W	108	PHE
2	W	110	TYR
2	W	111	TYR
2	W	118	GLN
2	W	121	MET
2	W	122	VAL
2	W	143	SER
2	W	163	VAL
2	W	219	LYS
2	Y	24	VAL
2	Y	34	LEU
2	Y	39	GLN
2	Y	43	GLN
2	Y	45	LEU
2	Y	51	ILE
2	Y	54	TYR
2	Y	64	PHE
2	Y	69	THR
2	Y	73	HIS
2	Y	74	THR
2	Y	82	GLU
2	Y	83	MET
2	Y	91	THR
2	Y	99	VAL
2	Y	100	GLU
2	Y	108	PHE
2	Y	110	TYR
2	Y	111	TYR
2	Y	118	GLN
2	Y	123	THR
2	Y	143	SER
2	Y	163	VAL
2	Y	219	LYS
2	1	24	VAL
2	1	34	LEU

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Mol	Chain	Res	Type
2	1	39	GLN
2	1	43	GLN
2	1	45	LEU
2	1	51	ILE
2	1	54	TYR
2	1	64	PHE
2	1	69	THR
2	1	73	HIS
2	1	74	THR
2	1	82	GLU
2	1	83	MET
2	1	91	THR
2	1	99	VAL
2	1	100	GLU
2	1	108	PHE
2	1	110	TYR
2	1	111	TYR
2	1	118	GLN
2	1	123	THR
2	1	125	SER
2	1	143	SER
2	1	163	VAL
2	1	219	LYS
2	3	24	VAL
2	3	34	LEU
2	3	39	GLN
2	3	43	GLN
2	3	45	LEU
2	3	51	ILE
2	3	54	TYR
2	3	64	PHE
2	3	69	THR
2	3	73	HIS
2	3	74	THR
2	3	82	GLU
2	3	83	MET
2	3	91	THR
2	3	99	VAL
2	3	100	GLU
2	3	108	PHE
2	3	110	TYR
2	3	111	TYR

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Mol	Chain	Res	Type
2	3	118	GLN
2	3	121	MET
2	3	125	SER
2	3	143	SER
2	3	163	VAL
2	3	219	LYS
2	5	24	VAL
2	5	34	LEU
2	5	39	GLN
2	5	43	GLN
2	5	51	ILE
2	5	54	TYR
2	5	64	PHE
2	5	69	THR
2	5	73	HIS
2	5	74	THR
2	5	82	GLU
2	5	83	MET
2	5	91	THR
2	5	99	VAL
2	5	100	GLU
2	5	108	PHE
2	5	110	TYR
2	5	111	TYR
2	5	118	GLN
2	5	123	THR
2	5	143	SER
2	5	163	VAL
2	5	219	LYS
2	7	24	VAL
2	7	34	LEU
2	7	39	GLN
2	7	43	GLN
2	7	45	LEU
2	7	51	ILE
2	7	54	TYR
2	7	64	PHE
2	7	69	THR
2	7	73	HIS
2	7	74	THR
2	7	82	GLU
2	7	83	MET

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Mol	Chain	Res	Type
2	7	91	THR
2	7	99	VAL
2	7	100	GLU
2	7	108	PHE
2	7	110	TYR
2	7	111	TYR
2	7	113	MET
2	7	118	GLN
2	7	121	MET
2	7	123	THR
2	7	125	SER
2	7	126	SER
2	7	143	SER
2	7	163	VAL
2	7	219	LYS
2	9	24	VAL
2	9	34	LEU
2	9	39	GLN
2	9	43	GLN
2	9	45	LEU
2	9	51	ILE
2	9	54	TYR
2	9	64	PHE
2	9	69	THR
2	9	73	HIS
2	9	74	THR
2	9	82	GLU
2	9	83	MET
2	9	91	THR
2	9	99	VAL
2	9	100	GLU
2	9	108	PHE
2	9	110	TYR
2	9	111	TYR
2	9	118	GLN
2	9	121	MET
2	9	123	THR
2	9	125	SER
2	9	143	SER
2	9	163	VAL
2	9	219	LYS
3	N	18	VAL

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Mol	Chain	Res	Type
3	N	97	LEU
3	N	102	PHE
3	N	109	THR
3	N	134	LYS
3	N	154	LYS
3	N	165	GLU
3	N	167	THR
3	N	172	GLN
3	N	174	ASN
3	N	176	LYS
3	N	180	SER
3	P	18	VAL
3	P	97	LEU
3	P	102	PHE
3	P	109	THR
3	P	134	LYS
3	P	154	LYS
3	P	165	GLU
3	P	167	THR
3	P	172	GLN
3	P	174	ASN
3	P	176	LYS
3	P	180	SER
3	R	18	VAL
3	R	97	LEU
3	R	102	PHE
3	R	109	THR
3	R	134	LYS
3	R	154	LYS
3	R	165	GLU
3	R	167	THR
3	R	172	GLN
3	R	174	ASN
3	R	176	LYS
3	R	180	SER
3	T	18	VAL
3	T	97	LEU
3	T	102	PHE
3	T	109	THR
3	T	134	LYS
3	T	154	LYS
3	T	165	GLU

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Mol	Chain	Res	Type
3	T	167	THR
3	T	172	GLN
3	T	174	ASN
3	T	176	LYS
3	T	180	SER
3	V	18	VAL
3	V	51	SER
3	V	97	LEU
3	V	102	PHE
3	V	109	THR
3	V	134	LYS
3	V	154	LYS
3	V	165	GLU
3	V	167	THR
3	V	172	GLN
3	V	174	ASN
3	V	176	LYS
3	V	180	SER
3	X	18	VAL
3	X	97	LEU
3	X	102	PHE
3	X	109	THR
3	X	134	LYS
3	X	154	LYS
3	X	165	GLU
3	X	167	THR
3	X	172	GLN
3	X	174	ASN
3	X	176	LYS
3	X	180	SER
3	Z	18	VAL
3	Z	51	SER
3	Z	97	LEU
3	Z	102	PHE
3	Z	109	THR
3	Z	134	LYS
3	Z	154	LYS
3	Z	165	GLU
3	Z	167	THR
3	Z	172	GLN
3	Z	174	ASN
3	Z	176	LYS

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Mol	Chain	Res	Type
3	Z	180	SER
3	2	18	VAL
3	2	97	LEU
3	2	102	PHE
3	2	109	THR
3	2	134	LYS
3	2	154	LYS
3	2	165	GLU
3	2	167	THR
3	2	172	GLN
3	2	174	ASN
3	2	176	LYS
3	2	180	SER
3	4	18	VAL
3	4	97	LEU
3	4	102	PHE
3	4	109	THR
3	4	134	LYS
3	4	154	LYS
3	4	165	GLU
3	4	167	THR
3	4	172	GLN
3	4	174	ASN
3	4	176	LYS
3	4	180	SER
3	6	18	VAL
3	6	97	LEU
3	6	102	PHE
3	6	109	THR
3	6	134	LYS
3	6	154	LYS
3	6	165	GLU
3	6	167	THR
3	6	172	GLN
3	6	174	ASN
3	6	176	LYS
3	6	180	SER
3	8	18	VAL
3	8	97	LEU
3	8	102	PHE
3	8	109	THR
3	8	134	LYS

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Mol	Chain	Res	Type
3	8	154	LYS
3	8	165	GLU
3	8	167	THR
3	8	172	GLN
3	8	174	ASN
3	8	176	LYS
3	8	180	SER
3	0	18	VAL
3	0	97	LEU
3	0	102	PHE
3	0	109	THR
3	0	134	LYS
3	0	154	LYS
3	0	165	GLU
3	0	167	THR
3	0	172	GLN
3	0	174	ASN
3	0	176	LYS
3	0	180	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (369) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	53	ASN
1	A	54	ASN
1	A	80	GLN
1	A	96	ASN
1	A	137	ASN
1	A	171	ASN
1	A	189	GLN
1	A	210	GLN
1	A	211	GLN
1	A	246	ASN
1	A	290	ASN
1	A	322	ASN
1	A	341	ASN
1	A	371	GLN
1	A	407	GLN
1	A	424	ASN
1	A	458	ASN
1	A	497	ASN

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Mol	Chain	Res	Type
1	A	501	GLN
1	B	18	HIS
1	B	53	ASN
1	B	54	ASN
1	B	80	GLN
1	B	96	ASN
1	B	137	ASN
1	B	171	ASN
1	B	189	GLN
1	B	211	GLN
1	B	216	ASN
1	B	290	ASN
1	B	322	ASN
1	B	341	ASN
1	B	371	GLN
1	B	407	GLN
1	B	424	ASN
1	B	458	ASN
1	B	497	ASN
1	B	501	GLN
1	C	18	HIS
1	C	53	ASN
1	C	54	ASN
1	C	80	GLN
1	C	96	ASN
1	C	137	ASN
1	C	171	ASN
1	C	189	GLN
1	C	211	GLN
1	C	216	ASN
1	C	246	ASN
1	C	290	ASN
1	C	322	ASN
1	C	341	ASN
1	C	407	GLN
1	C	424	ASN
1	C	458	ASN
1	C	497	ASN
1	C	501	GLN
1	D	18	HIS
1	D	53	ASN
1	D	54	ASN

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Mol	Chain	Res	Type
1	D	80	GLN
1	D	96	ASN
1	D	137	ASN
1	D	171	ASN
1	D	189	GLN
1	D	211	GLN
1	D	216	ASN
1	D	246	ASN
1	D	290	ASN
1	D	322	ASN
1	D	341	ASN
1	D	371	GLN
1	D	407	GLN
1	D	424	ASN
1	D	458	ASN
1	D	497	ASN
1	D	501	GLN
1	E	18	HIS
1	E	53	ASN
1	E	54	ASN
1	E	80	GLN
1	E	96	ASN
1	E	137	ASN
1	E	171	ASN
1	E	189	GLN
1	E	210	GLN
1	E	211	GLN
1	E	246	ASN
1	E	290	ASN
1	E	322	ASN
1	E	341	ASN
1	E	371	GLN
1	E	382	ASN
1	E	407	GLN
1	E	424	ASN
1	E	458	ASN
1	E	497	ASN
1	E	501	GLN
1	F	18	HIS
1	F	53	ASN
1	F	54	ASN
1	F	80	GLN

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Mol	Chain	Res	Type
1	F	96	ASN
1	F	137	ASN
1	F	171	ASN
1	F	189	GLN
1	F	211	GLN
1	F	246	ASN
1	F	290	ASN
1	F	322	ASN
1	F	341	ASN
1	F	407	GLN
1	F	424	ASN
1	F	458	ASN
1	F	497	ASN
1	F	501	GLN
1	G	18	HIS
1	G	53	ASN
1	G	54	ASN
1	G	80	GLN
1	G	96	ASN
1	G	137	ASN
1	G	171	ASN
1	G	189	GLN
1	G	210	GLN
1	G	211	GLN
1	G	216	ASN
1	G	246	ASN
1	G	290	ASN
1	G	322	ASN
1	G	341	ASN
1	G	407	GLN
1	G	424	ASN
1	G	458	ASN
1	G	497	ASN
1	G	501	GLN
1	H	17	HIS
1	H	18	HIS
1	H	53	ASN
1	H	54	ASN
1	H	80	GLN
1	H	96	ASN
1	H	137	ASN
1	H	171	ASN

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Mol	Chain	Res	Type
1	H	189	GLN
1	H	210	GLN
1	H	211	GLN
1	H	216	ASN
1	H	290	ASN
1	H	322	ASN
1	H	341	ASN
1	H	407	GLN
1	H	424	ASN
1	H	458	ASN
1	H	497	ASN
1	H	501	GLN
1	I	18	HIS
1	I	53	ASN
1	I	54	ASN
1	I	80	GLN
1	I	96	ASN
1	I	137	ASN
1	I	171	ASN
1	I	189	GLN
1	I	210	GLN
1	I	211	GLN
1	I	216	ASN
1	I	246	ASN
1	I	290	ASN
1	I	322	ASN
1	I	341	ASN
1	I	371	GLN
1	I	407	GLN
1	I	424	ASN
1	I	458	ASN
1	I	497	ASN
1	I	501	GLN
1	J	17	HIS
1	J	18	HIS
1	J	53	ASN
1	J	54	ASN
1	J	80	GLN
1	J	96	ASN
1	J	137	ASN
1	J	171	ASN
1	J	189	GLN

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Mol	Chain	Res	Type
1	J	210	GLN
1	J	211	GLN
1	J	216	ASN
1	J	246	ASN
1	J	290	ASN
1	J	322	ASN
1	J	341	ASN
1	J	371	GLN
1	J	407	GLN
1	J	424	ASN
1	J	458	ASN
1	J	497	ASN
1	J	501	GLN
1	K	18	HIS
1	K	53	ASN
1	K	54	ASN
1	K	80	GLN
1	K	96	ASN
1	K	137	ASN
1	K	171	ASN
1	K	189	GLN
1	K	210	GLN
1	K	211	GLN
1	K	290	ASN
1	K	322	ASN
1	K	341	ASN
1	K	371	GLN
1	K	407	GLN
1	K	424	ASN
1	K	458	ASN
1	K	497	ASN
1	K	501	GLN
1	L	18	HIS
1	L	53	ASN
1	L	54	ASN
1	L	80	GLN
1	L	96	ASN
1	L	137	ASN
1	L	171	ASN
1	L	189	GLN
1	L	211	GLN
1	L	216	ASN

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Mol	Chain	Res	Type
1	L	246	ASN
1	L	290	ASN
1	L	322	ASN
1	L	341	ASN
1	L	407	GLN
1	L	424	ASN
1	L	458	ASN
1	L	497	ASN
1	L	501	GLN
2	M	1	GLN
2	M	6	GLN
2	M	39	GLN
2	M	57	GLN
2	M	210	ASN
2	O	1	GLN
2	O	6	GLN
2	O	39	GLN
2	O	57	GLN
2	O	210	ASN
2	Q	1	GLN
2	Q	6	GLN
2	Q	39	GLN
2	Q	210	ASN
2	S	1	GLN
2	S	6	GLN
2	S	39	GLN
2	S	57	GLN
2	S	210	ASN
2	U	1	GLN
2	U	6	GLN
2	U	39	GLN
2	U	210	ASN
2	W	1	GLN
2	W	6	GLN
2	W	39	GLN
2	W	210	ASN
2	Y	1	GLN
2	Y	6	GLN
2	Y	39	GLN
2	Y	210	ASN
2	1	1	GLN
2	1	6	GLN

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Mol	Chain	Res	Type
2	1	39	GLN
2	1	210	ASN
2	3	1	GLN
2	3	6	GLN
2	3	39	GLN
2	3	210	ASN
2	5	1	GLN
2	5	6	GLN
2	5	39	GLN
2	5	57	GLN
2	5	210	ASN
2	7	1	GLN
2	7	6	GLN
2	7	39	GLN
2	7	57	GLN
2	7	210	ASN
2	9	1	GLN
2	9	6	GLN
2	9	39	GLN
2	9	57	GLN
2	9	210	ASN
3	N	6	GLN
3	N	81	GLN
3	N	133	ASN
3	N	172	GLN
3	N	199	GLN
3	P	6	GLN
3	P	36	HIS
3	P	40	GLN
3	P	81	GLN
3	P	133	ASN
3	P	172	GLN
3	P	174	ASN
3	P	199	GLN
3	R	6	GLN
3	R	36	HIS
3	R	81	GLN
3	R	133	ASN
3	R	172	GLN
3	R	199	GLN
3	T	6	GLN
3	T	36	HIS

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Mol	Chain	Res	Type
3	T	40	GLN
3	T	81	GLN
3	T	133	ASN
3	T	172	GLN
3	T	174	ASN
3	T	199	GLN
3	V	6	GLN
3	V	36	HIS
3	V	81	GLN
3	V	133	ASN
3	V	172	GLN
3	V	199	GLN
3	X	6	GLN
3	X	36	HIS
3	X	81	GLN
3	X	133	ASN
3	X	172	GLN
3	X	174	ASN
3	X	199	GLN
3	Z	6	GLN
3	Z	36	HIS
3	Z	81	GLN
3	Z	133	ASN
3	Z	172	GLN
3	Z	174	ASN
3	Z	199	GLN
3	2	6	GLN
3	2	81	GLN
3	2	133	ASN
3	2	172	GLN
3	2	199	GLN
3	4	6	GLN
3	4	81	GLN
3	4	133	ASN
3	4	172	GLN
3	4	174	ASN
3	4	199	GLN
3	6	6	GLN
3	6	36	HIS
3	6	81	GLN
3	6	133	ASN
3	6	172	GLN

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Mol	Chain	Res	Type
3	6	199	GLN
3	8	6	GLN
3	8	36	HIS
3	8	40	GLN
3	8	81	GLN
3	8	133	ASN
3	8	172	GLN
3	8	199	GLN
3	0	6	GLN
3	0	40	GLN
3	0	81	GLN
3	0	133	ASN
3	0	172	GLN
3	0	199	GLN

### 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 ⓘ

192 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	A	601	1,4	14,14,15	0.55	0	15,19,21	0.79	1 (6%)
4	NAG	A	602	4	14,14,15	0.54	0	15,19,21	0.75	1 (6%)
4	BMA	A	603	4	11,11,12	0.92	1 (9%)	14,15,17	0.51	0
4	MAN	A	604	4	11,11,12	0.76	0	14,15,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	A	605	4	11,11,12	1.07	2 (18%)	14,15,17	1.34	1 (7%)
4	MAN	A	606	4	11,11,12	0.72	0	14,15,17	0.96	2 (14%)
4	MAN	A	607	4	11,11,12	0.63	0	14,15,17	0.74	0
6	NAG	A	609	1,6	14,14,15	0.77	0	15,19,21	1.14	2 (13%)
6	NAG	A	610	6	14,14,15	0.83	1 (7%)	15,19,21	1.29	2 (13%)
6	BMA	A	611	6	11,11,12	0.93	1 (9%)	14,15,17	0.82	1 (7%)
6	MAN	A	612	6	11,11,12	0.92	1 (9%)	14,15,17	1.28	1 (7%)
6	MAN	A	613	6	11,11,12	0.66	0	14,15,17	0.92	2 (14%)
6	MAN	A	614	6	11,11,12	0.65	0	14,15,17	0.84	1 (7%)
7	NAG	A	615	1,7	14,14,15	0.76	0	15,19,21	1.25	2 (13%)
7	NAG	A	616	7	14,14,15	0.75	1 (7%)	15,19,21	0.71	1 (6%)
7	BMA	A	617	7	11,11,12	0.74	0	14,15,17	0.33	0
4	NAG	B	601	1,4	14,14,15	0.60	0	15,19,21	0.74	1 (6%)
4	NAG	B	602	4	14,14,15	0.47	0	15,19,21	0.83	1 (6%)
4	BMA	B	603	4	11,11,12	0.91	1 (9%)	14,15,17	0.55	0
4	MAN	B	604	4	11,11,12	0.75	0	14,15,17	0.62	0
4	MAN	B	605	4	11,11,12	1.05	1 (9%)	14,15,17	1.34	1 (7%)
4	MAN	B	606	4	11,11,12	0.80	0	14,15,17	1.01	2 (14%)
4	MAN	B	607	4	11,11,12	0.62	0	14,15,17	0.74	0
6	NAG	B	609	1,6	14,14,15	0.89	0	15,19,21	1.17	2 (13%)
6	NAG	B	610	6	14,14,15	0.93	1 (7%)	15,19,21	1.23	2 (13%)
6	BMA	B	611	6	11,11,12	0.77	0	14,15,17	0.83	1 (7%)
6	MAN	B	612	6	11,11,12	0.93	1 (9%)	14,15,17	1.34	1 (7%)
6	MAN	B	613	6	11,11,12	0.69	0	14,15,17	0.88	2 (14%)
6	MAN	B	614	6	11,11,12	0.71	0	14,15,17	0.82	1 (7%)
7	NAG	B	615	1,7	14,14,15	0.79	0	15,19,21	1.27	2 (13%)
7	NAG	B	616	7	14,14,15	0.73	0	15,19,21	0.72	1 (6%)
7	BMA	B	617	7	11,11,12	0.75	0	14,15,17	0.30	0
4	NAG	C	601	1,4	14,14,15	0.52	0	15,19,21	0.75	1 (6%)
4	NAG	C	602	4	14,14,15	0.49	0	15,19,21	0.77	1 (6%)
4	BMA	C	603	4	11,11,12	0.91	1 (9%)	14,15,17	0.53	0
4	MAN	C	604	4	11,11,12	0.76	0	14,15,17	0.66	0
4	MAN	C	605	4	11,11,12	1.08	2 (18%)	14,15,17	1.34	1 (7%)
4	MAN	C	606	4	11,11,12	0.73	0	14,15,17	0.96	2 (14%)
4	MAN	C	607	4	11,11,12	0.63	0	14,15,17	0.75	0
6	NAG	C	609	1,6	14,14,15	0.78	0	15,19,21	1.22	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	C	610	6	14,14,15	0.84	1 (7%)	15,19,21	1.35	2 (13%)
6	BMA	C	611	6	11,11,12	0.74	0	14,15,17	0.92	1 (7%)
6	MAN	C	612	6	11,11,12	0.84	0	14,15,17	1.35	1 (7%)
6	MAN	C	613	6	11,11,12	0.63	0	14,15,17	0.88	1 (7%)
6	MAN	C	614	6	11,11,12	0.69	0	14,15,17	0.86	1 (7%)
7	NAG	C	615	1,7	14,14,15	0.85	1 (7%)	15,19,21	1.20	2 (13%)
7	NAG	C	616	7	14,14,15	0.83	1 (7%)	15,19,21	0.73	1 (6%)
7	BMA	C	617	7	11,11,12	0.75	0	14,15,17	0.33	0
4	NAG	D	601	1,4	14,14,15	0.60	0	15,19,21	0.73	1 (6%)
4	NAG	D	602	4	14,14,15	0.59	0	15,19,21	0.78	1 (6%)
4	BMA	D	603	4	11,11,12	0.84	1 (9%)	14,15,17	0.49	0
4	MAN	D	604	4	11,11,12	0.68	0	14,15,17	0.63	0
4	MAN	D	605	4	11,11,12	1.08	1 (9%)	14,15,17	1.36	1 (7%)
4	MAN	D	606	4	11,11,12	0.75	0	14,15,17	1.00	2 (14%)
4	MAN	D	607	4	11,11,12	0.62	0	14,15,17	0.73	0
6	NAG	D	609	1,6	14,14,15	0.83	0	15,19,21	1.22	2 (13%)
6	NAG	D	610	6	14,14,15	0.86	1 (7%)	15,19,21	1.29	2 (13%)
6	BMA	D	611	6	11,11,12	0.87	1 (9%)	14,15,17	0.85	1 (7%)
6	MAN	D	612	6	11,11,12	0.93	1 (9%)	14,15,17	1.33	1 (7%)
6	MAN	D	613	6	11,11,12	0.67	0	14,15,17	0.89	2 (14%)
6	MAN	D	614	6	11,11,12	0.72	0	14,15,17	0.82	1 (7%)
7	NAG	D	615	1,7	14,14,15	0.83	1 (7%)	15,19,21	1.19	2 (13%)
7	NAG	D	616	7	14,14,15	0.76	1 (7%)	15,19,21	0.69	1 (6%)
7	BMA	D	617	7	11,11,12	0.72	0	14,15,17	0.30	0
4	NAG	E	601	1,4	14,14,15	0.50	0	15,19,21	0.76	1 (6%)
4	NAG	E	602	4	14,14,15	0.40	0	15,19,21	0.79	1 (6%)
4	BMA	E	603	4	11,11,12	0.99	1 (9%)	14,15,17	0.54	0
4	MAN	E	604	4	11,11,12	0.79	0	14,15,17	0.69	0
4	MAN	E	605	4	11,11,12	1.12	1 (9%)	14,15,17	1.34	1 (7%)
4	MAN	E	606	4	11,11,12	0.72	0	14,15,17	0.95	2 (14%)
4	MAN	E	607	4	11,11,12	0.58	0	14,15,17	0.74	0
6	NAG	E	609	1,6	14,14,15	0.81	0	15,19,21	1.17	2 (13%)
6	NAG	E	610	6	14,14,15	0.84	1 (7%)	15,19,21	1.31	2 (13%)
6	BMA	E	611	6	11,11,12	0.85	0	14,15,17	0.84	1 (7%)
6	MAN	E	612	6	11,11,12	0.90	1 (9%)	14,15,17	1.32	1 (7%)
6	MAN	E	613	6	11,11,12	0.71	0	14,15,17	0.91	2 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	E	614	6	11,11,12	0.65	0	14,15,17	0.84	1 (7%)
7	NAG	E	615	1,7	14,14,15	0.82	0	15,19,21	1.26	2 (13%)
7	NAG	E	616	7	14,14,15	0.70	0	15,19,21	0.74	1 (6%)
7	BMA	E	617	7	11,11,12	0.71	0	14,15,17	0.32	0
4	NAG	F	601	1,4	14,14,15	0.66	0	15,19,21	0.81	1 (6%)
4	NAG	F	602	4	14,14,15	0.44	0	15,19,21	0.84	1 (6%)
4	BMA	F	603	4	11,11,12	0.99	1 (9%)	14,15,17	0.54	0
4	MAN	F	604	4	11,11,12	0.73	0	14,15,17	0.67	0
4	MAN	F	605	4	11,11,12	1.08	2 (18%)	14,15,17	1.37	1 (7%)
4	MAN	F	606	4	11,11,12	0.73	0	14,15,17	1.01	2 (14%)
4	MAN	F	607	4	11,11,12	0.57	0	14,15,17	0.73	0
6	NAG	F	609	1,6	14,14,15	0.84	0	15,19,21	1.12	2 (13%)
6	NAG	F	610	6	14,14,15	0.92	1 (7%)	15,19,21	1.24	2 (13%)
6	BMA	F	611	6	11,11,12	0.86	1 (9%)	14,15,17	0.94	1 (7%)
6	MAN	F	612	6	11,11,12	0.88	1 (9%)	14,15,17	1.34	1 (7%)
6	MAN	F	613	6	11,11,12	0.69	0	14,15,17	0.91	2 (14%)
6	MAN	F	614	6	11,11,12	0.66	0	14,15,17	0.83	1 (7%)
7	NAG	F	615	1,7	14,14,15	0.78	0	15,19,21	1.26	2 (13%)
7	NAG	F	616	7	14,14,15	0.67	0	15,19,21	0.74	1 (6%)
7	BMA	F	617	7	11,11,12	0.71	0	14,15,17	0.32	0
4	NAG	G	601	1,4	14,14,15	0.61	0	15,19,21	0.76	1 (6%)
4	NAG	G	602	4	14,14,15	0.53	0	15,19,21	0.82	1 (6%)
4	BMA	G	603	4	11,11,12	0.92	1 (9%)	14,15,17	0.58	0
4	MAN	G	604	4	11,11,12	0.70	0	14,15,17	0.68	0
4	MAN	G	605	4	11,11,12	1.03	1 (9%)	14,15,17	1.33	1 (7%)
4	MAN	G	606	4	11,11,12	0.69	0	14,15,17	0.96	2 (14%)
4	MAN	G	607	4	11,11,12	0.59	0	14,15,17	0.75	0
6	NAG	G	609	1,6	14,14,15	0.92	0	15,19,21	1.16	2 (13%)
6	NAG	G	610	6	14,14,15	0.89	1 (7%)	15,19,21	1.27	2 (13%)
6	BMA	G	611	6	11,11,12	0.85	1 (9%)	14,15,17	0.80	1 (7%)
6	MAN	G	612	6	11,11,12	0.78	0	14,15,17	1.38	1 (7%)
6	MAN	G	613	6	11,11,12	0.67	0	14,15,17	0.87	2 (14%)
6	MAN	G	614	6	11,11,12	0.70	0	14,15,17	0.82	1 (7%)
7	NAG	G	615	1,7	14,14,15	0.86	1 (7%)	15,19,21	1.26	2 (13%)
7	NAG	G	616	7	14,14,15	0.80	1 (7%)	15,19,21	0.70	1 (6%)
7	BMA	G	617	7	11,11,12	0.77	0	14,15,17	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	H	601	1,4	14,14,15	0.63	0	15,19,21	0.74	1 (6%)
4	NAG	H	602	4	14,14,15	0.67	0	15,19,21	0.75	1 (6%)
4	BMA	H	603	4	11,11,12	0.89	1 (9%)	14,15,17	0.46	0
4	MAN	H	604	4	11,11,12	0.73	0	14,15,17	0.63	0
4	MAN	H	605	4	11,11,12	1.11	2 (18%)	14,15,17	1.35	1 (7%)
4	MAN	H	606	4	11,11,12	0.72	0	14,15,17	1.01	2 (14%)
4	MAN	H	607	4	11,11,12	0.64	0	14,15,17	0.76	0
6	NAG	H	609	1,6	14,14,15	0.88	0	15,19,21	1.16	2 (13%)
6	NAG	H	610	6	14,14,15	0.86	1 (7%)	15,19,21	1.27	2 (13%)
6	BMA	H	611	6	11,11,12	0.86	0	14,15,17	0.83	1 (7%)
6	MAN	H	612	6	11,11,12	0.90	1 (9%)	14,15,17	1.34	1 (7%)
6	MAN	H	613	6	11,11,12	0.68	0	14,15,17	0.86	2 (14%)
6	MAN	H	614	6	11,11,12	0.64	0	14,15,17	0.81	1 (7%)
7	NAG	H	615	1,7	14,14,15	1.02	1 (7%)	15,19,21	1.14	3 (20%)
7	NAG	H	616	7	14,14,15	0.74	0	15,19,21	0.67	0
7	BMA	H	617	7	11,11,12	0.73	0	14,15,17	0.33	0
4	NAG	I	601	1,4	14,14,15	0.59	0	15,19,21	0.77	1 (6%)
4	NAG	I	602	4	14,14,15	0.43	0	15,19,21	0.80	1 (6%)
4	BMA	I	603	4	11,11,12	1.07	1 (9%)	14,15,17	0.54	0
4	MAN	I	604	4	11,11,12	0.83	0	14,15,17	0.70	0
4	MAN	I	605	4	11,11,12	1.12	2 (18%)	14,15,17	1.39	1 (7%)
4	MAN	I	606	4	11,11,12	0.73	0	14,15,17	1.02	2 (14%)
4	MAN	I	607	4	11,11,12	0.64	0	14,15,17	0.74	0
6	NAG	I	609	1,6	14,14,15	0.88	0	15,19,21	1.18	2 (13%)
6	NAG	I	610	6	14,14,15	0.91	1 (7%)	15,19,21	1.25	2 (13%)
6	BMA	I	611	6	11,11,12	0.74	0	14,15,17	0.85	1 (7%)
6	MAN	I	612	6	11,11,12	0.85	1 (9%)	14,15,17	1.35	1 (7%)
6	MAN	I	613	6	11,11,12	0.68	0	14,15,17	0.86	1 (7%)
6	MAN	I	614	6	11,11,12	0.70	0	14,15,17	0.84	1 (7%)
7	NAG	I	615	1,7	14,14,15	0.86	1 (7%)	15,19,21	1.20	2 (13%)
7	NAG	I	616	7	14,14,15	0.73	0	15,19,21	0.70	0
7	BMA	I	617	7	11,11,12	0.74	0	14,15,17	0.30	0
4	NAG	J	601	1,4	14,14,15	0.61	0	15,19,21	0.76	1 (6%)
4	NAG	J	602	4	14,14,15	0.49	0	15,19,21	0.77	1 (6%)
4	BMA	J	603	4	11,11,12	0.81	0	14,15,17	0.55	0
4	MAN	J	604	4	11,11,12	0.72	0	14,15,17	0.66	0
4	MAN	J	605	4	11,11,12	1.04	1 (9%)	14,15,17	1.36	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	J	606	4	11,11,12	0.76	0	14,15,17	1.01	2 (14%)
4	MAN	J	607	4	11,11,12	0.58	0	14,15,17	0.74	0
6	NAG	J	609	1,6	14,14,15	0.88	0	15,19,21	1.20	2 (13%)
6	NAG	J	610	6	14,14,15	0.87	1 (7%)	15,19,21	1.32	2 (13%)
6	BMA	J	611	6	11,11,12	0.80	0	14,15,17	0.83	1 (7%)
6	MAN	J	612	6	11,11,12	0.84	0	14,15,17	1.36	1 (7%)
6	MAN	J	613	6	11,11,12	0.67	0	14,15,17	0.88	1 (7%)
6	MAN	J	614	6	11,11,12	0.75	0	14,15,17	0.84	1 (7%)
7	NAG	J	615	1,7	14,14,15	0.83	1 (7%)	15,19,21	1.20	2 (13%)
7	NAG	J	616	7	14,14,15	0.72	0	15,19,21	0.73	1 (6%)
7	BMA	J	617	7	11,11,12	0.77	0	14,15,17	0.32	0
4	NAG	K	601	1,4	14,14,15	0.53	0	15,19,21	0.75	1 (6%)
4	NAG	K	602	4	14,14,15	0.57	0	15,19,21	0.76	1 (6%)
4	BMA	K	603	4	11,11,12	0.90	1 (9%)	14,15,17	0.53	0
4	MAN	K	604	4	11,11,12	0.65	0	14,15,17	0.69	0
4	MAN	K	605	4	11,11,12	1.09	1 (9%)	14,15,17	1.33	1 (7%)
4	MAN	K	606	4	11,11,12	0.68	0	14,15,17	0.96	2 (14%)
4	MAN	K	607	4	11,11,12	0.62	0	14,15,17	0.77	0
6	NAG	K	609	1,6	14,14,15	0.89	0	15,19,21	1.16	2 (13%)
6	NAG	K	610	6	14,14,15	0.86	1 (7%)	15,19,21	1.25	2 (13%)
6	BMA	K	611	6	11,11,12	0.87	1 (9%)	14,15,17	0.82	1 (7%)
6	MAN	K	612	6	11,11,12	0.87	1 (9%)	14,15,17	1.35	1 (7%)
6	MAN	K	613	6	11,11,12	0.68	0	14,15,17	0.86	1 (7%)
6	MAN	K	614	6	11,11,12	0.72	0	14,15,17	0.79	1 (7%)
7	NAG	K	615	1,7	14,14,15	0.93	1 (7%)	15,19,21	1.21	2 (13%)
7	NAG	K	616	7	14,14,15	0.75	0	15,19,21	0.69	1 (6%)
7	BMA	K	617	7	11,11,12	0.72	0	14,15,17	0.30	0
4	NAG	L	601	1,4	14,14,15	0.71	0	15,19,21	0.76	1 (6%)
4	NAG	L	602	4	14,14,15	0.54	0	15,19,21	0.77	1 (6%)
4	BMA	L	603	4	11,11,12	0.84	0	14,15,17	0.52	0
4	MAN	L	604	4	11,11,12	0.75	0	14,15,17	0.68	0
4	MAN	L	605	4	11,11,12	1.15	2 (18%)	14,15,17	1.39	1 (7%)
4	MAN	L	606	4	11,11,12	0.76	0	14,15,17	1.01	2 (14%)
4	MAN	L	607	4	11,11,12	0.66	0	14,15,17	0.73	0
6	NAG	L	609	1,6	14,14,15	0.87	0	15,19,21	1.15	2 (13%)
6	NAG	L	610	6	14,14,15	0.88	1 (7%)	15,19,21	1.29	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BMA	L	611	6	11,11,12	0.81	0	14,15,17	0.85	1 (7%)
6	MAN	L	612	6	11,11,12	0.87	1 (9%)	14,15,17	1.35	1 (7%)
6	MAN	L	613	6	11,11,12	0.68	0	14,15,17	0.89	2 (14%)
6	MAN	L	614	6	11,11,12	0.69	0	14,15,17	0.82	1 (7%)
7	NAG	L	615	1,7	14,14,15	0.90	1 (7%)	15,19,21	1.20	2 (13%)
7	NAG	L	616	7	14,14,15	0.71	0	15,19,21	0.73	1 (6%)
7	BMA	L	617	7	11,11,12	0.75	0	14,15,17	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	602	4	-	0/6/23/26	0/1/1/1
4	BMA	A	603	4	-	0/2/19/22	0/1/1/1
4	MAN	A	604	4	-	0/2/19/22	0/1/1/1
4	MAN	A	605	4	-	0/2/19/22	0/1/1/1
4	MAN	A	606	4	-	0/2/19/22	0/1/1/1
4	MAN	A	607	4	-	0/2/19/22	0/1/1/1
6	NAG	A	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	610	6	-	0/6/23/26	0/1/1/1
6	BMA	A	611	6	-	0/2/19/22	0/1/1/1
6	MAN	A	612	6	-	0/2/19/22	0/1/1/1
6	MAN	A	613	6	-	0/2/19/22	0/1/1/1
6	MAN	A	614	6	-	0/2/19/22	0/1/1/1
7	NAG	A	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	616	7	-	1/6/23/26	0/1/1/1
7	BMA	A	617	7	-	0/2/19/22	0/1/1/1
4	NAG	B	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	602	4	-	0/6/23/26	0/1/1/1
4	BMA	B	603	4	-	0/2/19/22	0/1/1/1
4	MAN	B	604	4	-	0/2/19/22	0/1/1/1
4	MAN	B	605	4	-	0/2/19/22	0/1/1/1
4	MAN	B	606	4	-	0/2/19/22	0/1/1/1
4	MAN	B	607	4	-	0/2/19/22	0/1/1/1
6	NAG	B	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	610	6	-	0/6/23/26	0/1/1/1
6	BMA	B	611	6	-	0/2/19/22	0/1/1/1
6	MAN	B	612	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	B	613	6	-	0/2/19/22	0/1/1/1
6	MAN	B	614	6	-	0/2/19/22	0/1/1/1
7	NAG	B	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	616	7	-	1/6/23/26	0/1/1/1
7	BMA	B	617	7	-	0/2/19/22	0/1/1/1
4	NAG	C	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	602	4	-	0/6/23/26	0/1/1/1
4	BMA	C	603	4	-	0/2/19/22	0/1/1/1
4	MAN	C	604	4	-	0/2/19/22	0/1/1/1
4	MAN	C	605	4	-	0/2/19/22	0/1/1/1
4	MAN	C	606	4	-	0/2/19/22	0/1/1/1
4	MAN	C	607	4	-	0/2/19/22	0/1/1/1
6	NAG	C	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	610	6	-	0/6/23/26	0/1/1/1
6	BMA	C	611	6	-	0/2/19/22	0/1/1/1
6	MAN	C	612	6	-	0/2/19/22	0/1/1/1
6	MAN	C	613	6	-	0/2/19/22	0/1/1/1
6	MAN	C	614	6	-	0/2/19/22	0/1/1/1
7	NAG	C	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	616	7	-	1/6/23/26	0/1/1/1
7	BMA	C	617	7	-	0/2/19/22	0/1/1/1
4	NAG	D	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	602	4	-	0/6/23/26	0/1/1/1
4	BMA	D	603	4	-	0/2/19/22	0/1/1/1
4	MAN	D	604	4	-	0/2/19/22	0/1/1/1
4	MAN	D	605	4	-	0/2/19/22	0/1/1/1
4	MAN	D	606	4	-	0/2/19/22	0/1/1/1
4	MAN	D	607	4	-	0/2/19/22	0/1/1/1
6	NAG	D	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	610	6	-	0/6/23/26	0/1/1/1
6	BMA	D	611	6	-	0/2/19/22	0/1/1/1
6	MAN	D	612	6	-	0/2/19/22	0/1/1/1
6	MAN	D	613	6	-	0/2/19/22	0/1/1/1
6	MAN	D	614	6	-	0/2/19/22	0/1/1/1
7	NAG	D	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	616	7	-	1/6/23/26	0/1/1/1
7	BMA	D	617	7	-	0/2/19/22	0/1/1/1
4	NAG	E	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	602	4	-	0/6/23/26	0/1/1/1
4	BMA	E	603	4	-	0/2/19/22	0/1/1/1
4	MAN	E	604	4	-	0/2/19/22	0/1/1/1
4	MAN	E	605	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	E	606	4	-	0/2/19/22	0/1/1/1
4	MAN	E	607	4	-	0/2/19/22	0/1/1/1
6	NAG	E	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	610	6	-	0/6/23/26	0/1/1/1
6	BMA	E	611	6	-	0/2/19/22	0/1/1/1
6	MAN	E	612	6	-	0/2/19/22	0/1/1/1
6	MAN	E	613	6	-	0/2/19/22	0/1/1/1
6	MAN	E	614	6	-	0/2/19/22	0/1/1/1
7	NAG	E	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	616	7	-	1/6/23/26	0/1/1/1
7	BMA	E	617	7	-	0/2/19/22	0/1/1/1
4	NAG	F	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	602	4	-	0/6/23/26	0/1/1/1
4	BMA	F	603	4	-	0/2/19/22	0/1/1/1
4	MAN	F	604	4	-	0/2/19/22	0/1/1/1
4	MAN	F	605	4	-	0/2/19/22	0/1/1/1
4	MAN	F	606	4	-	0/2/19/22	0/1/1/1
4	MAN	F	607	4	-	0/2/19/22	0/1/1/1
6	NAG	F	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	F	610	6	-	0/6/23/26	0/1/1/1
6	BMA	F	611	6	-	0/2/19/22	0/1/1/1
6	MAN	F	612	6	-	0/2/19/22	0/1/1/1
6	MAN	F	613	6	-	0/2/19/22	0/1/1/1
6	MAN	F	614	6	-	0/2/19/22	0/1/1/1
7	NAG	F	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	F	616	7	-	1/6/23/26	0/1/1/1
7	BMA	F	617	7	-	0/2/19/22	0/1/1/1
4	NAG	G	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	602	4	-	0/6/23/26	0/1/1/1
4	BMA	G	603	4	-	0/2/19/22	0/1/1/1
4	MAN	G	604	4	-	0/2/19/22	0/1/1/1
4	MAN	G	605	4	-	0/2/19/22	0/1/1/1
4	MAN	G	606	4	-	0/2/19/22	0/1/1/1
4	MAN	G	607	4	-	0/2/19/22	0/1/1/1
6	NAG	G	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	610	6	-	0/6/23/26	0/1/1/1
6	BMA	G	611	6	-	0/2/19/22	0/1/1/1
6	MAN	G	612	6	-	0/2/19/22	0/1/1/1
6	MAN	G	613	6	-	0/2/19/22	0/1/1/1
6	MAN	G	614	6	-	0/2/19/22	0/1/1/1
7	NAG	G	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	616	7	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	G	617	7	-	0/2/19/22	0/1/1/1
4	NAG	H	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	602	4	-	0/6/23/26	0/1/1/1
4	BMA	H	603	4	-	0/2/19/22	0/1/1/1
4	MAN	H	604	4	-	0/2/19/22	0/1/1/1
4	MAN	H	605	4	-	0/2/19/22	0/1/1/1
4	MAN	H	606	4	-	0/2/19/22	0/1/1/1
4	MAN	H	607	4	-	0/2/19/22	0/1/1/1
6	NAG	H	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	H	610	6	-	0/6/23/26	0/1/1/1
6	BMA	H	611	6	-	0/2/19/22	0/1/1/1
6	MAN	H	612	6	-	0/2/19/22	0/1/1/1
6	MAN	H	613	6	-	0/2/19/22	0/1/1/1
6	MAN	H	614	6	-	0/2/19/22	0/1/1/1
7	NAG	H	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	H	616	7	-	1/6/23/26	0/1/1/1
7	BMA	H	617	7	-	0/2/19/22	0/1/1/1
4	NAG	I	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	602	4	-	0/6/23/26	0/1/1/1
4	BMA	I	603	4	-	0/2/19/22	0/1/1/1
4	MAN	I	604	4	-	0/2/19/22	0/1/1/1
4	MAN	I	605	4	-	0/2/19/22	0/1/1/1
4	MAN	I	606	4	-	0/2/19/22	0/1/1/1
4	MAN	I	607	4	-	0/2/19/22	0/1/1/1
6	NAG	I	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	610	6	-	0/6/23/26	0/1/1/1
6	BMA	I	611	6	-	0/2/19/22	0/1/1/1
6	MAN	I	612	6	-	0/2/19/22	0/1/1/1
6	MAN	I	613	6	-	0/2/19/22	0/1/1/1
6	MAN	I	614	6	-	0/2/19/22	0/1/1/1
7	NAG	I	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	I	616	7	-	1/6/23/26	0/1/1/1
7	BMA	I	617	7	-	0/2/19/22	0/1/1/1
4	NAG	J	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	602	4	-	0/6/23/26	0/1/1/1
4	BMA	J	603	4	-	0/2/19/22	0/1/1/1
4	MAN	J	604	4	-	0/2/19/22	0/1/1/1
4	MAN	J	605	4	-	0/2/19/22	0/1/1/1
4	MAN	J	606	4	-	0/2/19/22	0/1/1/1
4	MAN	J	607	4	-	0/2/19/22	0/1/1/1
6	NAG	J	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	610	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	J	611	6	-	0/2/19/22	0/1/1/1
6	MAN	J	612	6	-	0/2/19/22	0/1/1/1
6	MAN	J	613	6	-	0/2/19/22	0/1/1/1
6	MAN	J	614	6	-	0/2/19/22	0/1/1/1
7	NAG	J	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	J	616	7	-	1/6/23/26	0/1/1/1
7	BMA	J	617	7	-	0/2/19/22	0/1/1/1
4	NAG	K	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	602	4	-	0/6/23/26	0/1/1/1
4	BMA	K	603	4	-	0/2/19/22	0/1/1/1
4	MAN	K	604	4	-	0/2/19/22	0/1/1/1
4	MAN	K	605	4	-	0/2/19/22	0/1/1/1
4	MAN	K	606	4	-	0/2/19/22	0/1/1/1
4	MAN	K	607	4	-	0/2/19/22	0/1/1/1
6	NAG	K	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	610	6	-	0/6/23/26	0/1/1/1
6	BMA	K	611	6	-	0/2/19/22	0/1/1/1
6	MAN	K	612	6	-	0/2/19/22	0/1/1/1
6	MAN	K	613	6	-	0/2/19/22	0/1/1/1
6	MAN	K	614	6	-	0/2/19/22	0/1/1/1
7	NAG	K	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	K	616	7	-	1/6/23/26	0/1/1/1
7	BMA	K	617	7	-	0/2/19/22	0/1/1/1
4	NAG	L	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	602	4	-	0/6/23/26	0/1/1/1
4	BMA	L	603	4	-	0/2/19/22	0/1/1/1
4	MAN	L	604	4	-	0/2/19/22	0/1/1/1
4	MAN	L	605	4	-	0/2/19/22	0/1/1/1
4	MAN	L	606	4	-	0/2/19/22	0/1/1/1
4	MAN	L	607	4	-	0/2/19/22	0/1/1/1
6	NAG	L	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	L	610	6	-	0/6/23/26	0/1/1/1
6	BMA	L	611	6	-	0/2/19/22	0/1/1/1
6	MAN	L	612	6	-	0/2/19/22	0/1/1/1
6	MAN	L	613	6	-	0/2/19/22	0/1/1/1
6	MAN	L	614	6	-	0/2/19/22	0/1/1/1
7	NAG	L	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	L	616	7	-	1/6/23/26	0/1/1/1
7	BMA	L	617	7	-	0/2/19/22	0/1/1/1

All (66) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	611	BMA	C4-C3	2.01	1.57	1.52
4	G	605	MAN	C2-C3	2.02	1.55	1.52
7	J	615	NAG	C4-C3	2.02	1.57	1.52
4	A	605	MAN	C2-C3	2.03	1.55	1.52
4	H	605	MAN	C2-C3	2.03	1.55	1.52
4	L	605	MAN	C2-C3	2.04	1.55	1.52
6	A	612	MAN	C2-C3	2.04	1.55	1.52
6	I	612	MAN	C2-C3	2.05	1.55	1.52
7	D	615	NAG	C4-C3	2.06	1.57	1.52
6	E	612	MAN	C2-C3	2.07	1.55	1.52
6	L	612	MAN	C2-C3	2.08	1.55	1.52
7	A	616	NAG	C4-C3	2.08	1.57	1.52
7	D	616	NAG	C4-C3	2.09	1.57	1.52
4	F	605	MAN	C2-C3	2.09	1.55	1.52
4	D	603	BMA	C4-C3	2.09	1.57	1.52
4	G	603	BMA	C4-C3	2.10	1.57	1.52
6	F	611	BMA	C4-C3	2.10	1.57	1.52
4	C	605	MAN	C2-C3	2.11	1.55	1.52
6	D	611	BMA	C4-C3	2.11	1.57	1.52
6	K	612	MAN	C2-C3	2.11	1.55	1.52
4	J	605	MAN	C2-C3	2.12	1.55	1.52
6	K	611	BMA	C4-C3	2.12	1.58	1.52
7	G	615	NAG	C4-C3	2.12	1.58	1.52
6	F	612	MAN	C2-C3	2.13	1.55	1.52
6	H	612	MAN	C2-C3	2.14	1.55	1.52
4	I	605	MAN	C2-C3	2.14	1.55	1.52
7	C	615	NAG	C4-C3	2.15	1.58	1.52
4	A	605	MAN	C4-C3	2.15	1.58	1.52
4	F	605	MAN	C4-C3	2.18	1.58	1.52
4	C	605	MAN	C4-C3	2.19	1.58	1.52
4	K	603	BMA	C4-C3	2.20	1.58	1.52
6	B	612	MAN	C2-C3	2.20	1.55	1.52
7	I	615	NAG	C4-C3	2.21	1.58	1.52
7	G	616	NAG	C4-C3	2.21	1.58	1.52
6	A	611	BMA	C4-C3	2.22	1.58	1.52
6	D	612	MAN	C2-C3	2.23	1.55	1.52
4	H	603	BMA	C4-C3	2.24	1.58	1.52
4	K	605	MAN	C4-C3	2.24	1.58	1.52
6	C	610	NAG	C1-C2	2.24	1.55	1.52
6	K	610	NAG	C1-C2	2.25	1.55	1.52
4	B	603	BMA	C4-C3	2.26	1.58	1.52
6	H	610	NAG	C1-C2	2.27	1.55	1.52
6	A	610	NAG	C1-C2	2.27	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	BMA	C4-C3	2.28	1.58	1.52
6	E	610	NAG	C1-C2	2.28	1.55	1.52
4	B	605	MAN	C4-C3	2.29	1.58	1.52
6	J	610	NAG	C1-C2	2.30	1.55	1.52
4	I	605	MAN	C4-C3	2.31	1.58	1.52
6	D	610	NAG	C1-C2	2.31	1.55	1.52
4	D	605	MAN	C4-C3	2.32	1.58	1.52
7	L	615	NAG	C4-C3	2.32	1.58	1.52
6	L	610	NAG	C1-C2	2.33	1.55	1.52
6	I	610	NAG	C1-C2	2.34	1.55	1.52
4	H	605	MAN	C4-C3	2.36	1.58	1.52
4	C	603	BMA	C4-C3	2.37	1.58	1.52
7	C	616	NAG	C4-C3	2.37	1.58	1.52
6	B	610	NAG	C1-C2	2.38	1.55	1.52
6	G	610	NAG	C1-C2	2.40	1.55	1.52
6	F	610	NAG	C1-C2	2.41	1.55	1.52
7	K	615	NAG	C4-C3	2.47	1.58	1.52
4	E	605	MAN	C4-C3	2.48	1.58	1.52
4	L	605	MAN	C4-C3	2.49	1.58	1.52
4	F	603	BMA	C4-C3	2.59	1.59	1.52
4	E	603	BMA	C4-C3	2.64	1.59	1.52
7	H	615	NAG	C4-C3	2.86	1.59	1.52
4	I	603	BMA	C4-C3	2.93	1.60	1.52

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	610	NAG	C2-N2-C7	-3.24	118.88	123.04
6	J	610	NAG	C2-N2-C7	-3.23	118.89	123.04
6	K	610	NAG	C2-N2-C7	-3.23	118.89	123.04
6	L	610	NAG	C2-N2-C7	-3.22	118.91	123.04
6	D	610	NAG	C2-N2-C7	-3.20	118.93	123.04
6	G	610	NAG	C2-N2-C7	-3.19	118.94	123.04
6	C	610	NAG	C2-N2-C7	-3.19	118.94	123.04
6	I	610	NAG	C2-N2-C7	-3.18	118.95	123.04
6	B	610	NAG	C2-N2-C7	-3.17	118.96	123.04
6	E	610	NAG	C2-N2-C7	-3.17	118.97	123.04
6	A	610	NAG	C2-N2-C7	-3.15	119.00	123.04
6	F	610	NAG	C2-N2-C7	-3.14	119.00	123.04
4	K	602	NAG	C2-N2-C7	-2.40	119.95	123.04
4	B	602	NAG	C2-N2-C7	-2.40	119.96	123.04
4	H	601	NAG	C2-N2-C7	-2.39	119.97	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	602	NAG	C2-N2-C7	-2.39	119.97	123.04
4	L	601	NAG	C2-N2-C7	-2.39	119.97	123.04
4	F	602	NAG	C2-N2-C7	-2.39	119.97	123.04
4	E	601	NAG	C2-N2-C7	-2.39	119.97	123.04
4	D	601	NAG	C2-N2-C7	-2.38	119.98	123.04
4	D	602	NAG	C2-N2-C7	-2.37	120.00	123.04
4	J	601	NAG	C2-N2-C7	-2.36	120.01	123.04
4	A	601	NAG	C2-N2-C7	-2.34	120.03	123.04
4	B	601	NAG	C2-N2-C7	-2.34	120.03	123.04
4	A	602	NAG	C2-N2-C7	-2.34	120.04	123.04
4	K	601	NAG	C2-N2-C7	-2.33	120.04	123.04
4	C	601	NAG	C2-N2-C7	-2.33	120.04	123.04
4	E	602	NAG	C2-N2-C7	-2.33	120.04	123.04
4	C	602	NAG	C2-N2-C7	-2.32	120.06	123.04
4	G	601	NAG	C2-N2-C7	-2.32	120.06	123.04
4	J	602	NAG	C2-N2-C7	-2.31	120.07	123.04
4	L	602	NAG	C2-N2-C7	-2.31	120.07	123.04
4	I	601	NAG	C2-N2-C7	-2.31	120.08	123.04
4	I	602	NAG	C2-N2-C7	-2.31	120.08	123.04
4	F	601	NAG	C2-N2-C7	-2.30	120.08	123.04
4	H	602	NAG	C2-N2-C7	-2.30	120.08	123.04
6	L	609	NAG	C2-N2-C7	-2.28	120.12	123.04
6	H	609	NAG	C2-N2-C7	-2.27	120.12	123.04
6	F	609	NAG	C2-N2-C7	-2.26	120.14	123.04
6	I	609	NAG	C2-N2-C7	-2.26	120.14	123.04
6	B	609	NAG	C2-N2-C7	-2.25	120.14	123.04
6	G	609	NAG	C2-N2-C7	-2.25	120.14	123.04
6	E	609	NAG	C2-N2-C7	-2.25	120.15	123.04
6	J	609	NAG	C2-N2-C7	-2.25	120.15	123.04
6	A	609	NAG	C2-N2-C7	-2.24	120.16	123.04
6	K	609	NAG	C2-N2-C7	-2.23	120.17	123.04
6	C	609	NAG	C2-N2-C7	-2.23	120.18	123.04
6	D	609	NAG	C2-N2-C7	-2.21	120.19	123.04
7	C	616	NAG	C2-N2-C7	-2.08	120.37	123.04
7	B	616	NAG	C2-N2-C7	-2.08	120.37	123.04
7	E	616	NAG	C2-N2-C7	-2.08	120.37	123.04
7	J	616	NAG	C2-N2-C7	-2.07	120.38	123.04
7	F	616	NAG	C2-N2-C7	-2.06	120.40	123.04
7	K	616	NAG	C2-N2-C7	-2.05	120.41	123.04
7	L	616	NAG	C2-N2-C7	-2.05	120.41	123.04
7	A	616	NAG	C2-N2-C7	-2.04	120.42	123.04
7	G	616	NAG	C2-N2-C7	-2.04	120.42	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	615	NAG	C2-N2-C7	-2.02	120.44	123.04
7	D	616	NAG	C2-N2-C7	-2.02	120.45	123.04
6	G	613	MAN	C1-O5-C5	2.01	114.81	112.25
6	L	613	MAN	C1-O5-C5	2.02	114.81	112.25
6	H	613	MAN	C1-O5-C5	2.02	114.81	112.25
6	D	613	MAN	C1-O5-C5	2.02	114.81	112.25
6	B	613	MAN	C1-O5-C5	2.03	114.83	112.25
6	A	613	MAN	C1-O5-C5	2.05	114.85	112.25
6	F	613	MAN	C1-O5-C5	2.05	114.86	112.25
6	E	613	MAN	C1-O5-C5	2.06	114.86	112.25
4	L	606	MAN	C1-C2-C3	2.09	112.01	109.54
4	B	606	MAN	C1-C2-C3	2.09	112.02	109.54
4	J	606	MAN	C1-C2-C3	2.10	112.03	109.54
4	A	606	MAN	C1-C2-C3	2.14	112.08	109.54
4	F	606	MAN	C1-C2-C3	2.15	112.09	109.54
4	C	606	MAN	C1-C2-C3	2.16	112.10	109.54
4	D	606	MAN	C1-C2-C3	2.16	112.10	109.54
4	H	606	MAN	C1-C2-C3	2.16	112.10	109.54
6	H	613	MAN	C1-C2-C3	2.18	112.12	109.54
4	K	606	MAN	C1-C2-C3	2.18	112.12	109.54
4	E	606	MAN	C1-C2-C3	2.19	112.14	109.54
6	J	614	MAN	C1-C2-C3	2.20	112.14	109.54
6	E	613	MAN	C1-C2-C3	2.20	112.14	109.54
4	G	606	MAN	C1-C2-C3	2.20	112.14	109.54
6	B	613	MAN	C1-C2-C3	2.20	112.14	109.54
4	I	606	MAN	C1-C2-C3	2.21	112.15	109.54
6	K	614	MAN	C1-C2-C3	2.22	112.17	109.54
6	I	613	MAN	C1-C2-C3	2.23	112.18	109.54
6	D	613	MAN	C1-C2-C3	2.25	112.20	109.54
6	G	613	MAN	C1-C2-C3	2.25	112.20	109.54
6	J	613	MAN	C1-C2-C3	2.26	112.21	109.54
6	L	613	MAN	C1-C2-C3	2.26	112.22	109.54
6	G	614	MAN	C1-C2-C3	2.26	112.22	109.54
6	F	613	MAN	C1-C2-C3	2.27	112.22	109.54
6	K	613	MAN	C1-C2-C3	2.27	112.23	109.54
6	B	614	MAN	C1-C2-C3	2.28	112.23	109.54
6	C	614	MAN	C1-C2-C3	2.28	112.23	109.54
7	H	615	NAG	C3-C4-C5	2.28	114.17	110.20
6	D	614	MAN	C1-C2-C3	2.28	112.24	109.54
6	I	614	MAN	C1-C2-C3	2.28	112.24	109.54
6	C	613	MAN	C1-C2-C3	2.30	112.26	109.54
6	G	611	BMA	C1-C2-C3	2.30	112.27	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	614	MAN	C1-C2-C3	2.31	112.28	109.54
6	J	611	BMA	C1-C2-C3	2.32	112.28	109.54
6	F	610	NAG	C4-C3-C2	2.32	114.83	111.23
6	E	614	MAN	C1-C2-C3	2.32	112.28	109.54
6	A	613	MAN	C1-C2-C3	2.33	112.29	109.54
6	A	611	BMA	C1-C2-C3	2.34	112.31	109.54
6	E	611	BMA	C1-C2-C3	2.36	112.33	109.54
6	A	614	MAN	C1-C2-C3	2.37	112.34	109.54
6	H	614	MAN	C1-C2-C3	2.37	112.34	109.54
7	G	615	NAG	C3-C4-C5	2.37	114.34	110.20
6	H	611	BMA	C1-C2-C3	2.38	112.35	109.54
4	C	606	MAN	C1-O5-C5	2.38	115.27	112.25
6	K	611	BMA	C1-C2-C3	2.38	112.36	109.54
4	K	606	MAN	C1-O5-C5	2.39	115.28	112.25
7	L	615	NAG	C3-C4-C5	2.40	114.38	110.20
6	B	610	NAG	C4-C3-C2	2.40	114.96	111.23
7	B	615	NAG	C3-C4-C5	2.40	114.38	110.20
6	F	614	MAN	C1-C2-C3	2.40	112.38	109.54
4	A	606	MAN	C1-O5-C5	2.40	115.30	112.25
4	F	606	MAN	C1-O5-C5	2.42	115.32	112.25
4	E	606	MAN	C1-O5-C5	2.42	115.33	112.25
7	I	615	NAG	C3-C4-C5	2.43	114.42	110.20
4	G	606	MAN	C1-O5-C5	2.43	115.33	112.25
6	K	610	NAG	C4-C3-C2	2.43	115.01	111.23
4	I	606	MAN	C1-O5-C5	2.45	115.36	112.25
4	D	606	MAN	C1-O5-C5	2.45	115.36	112.25
6	B	611	BMA	C1-C2-C3	2.46	112.45	109.54
7	K	615	NAG	C3-C4-C5	2.46	114.48	110.20
7	D	615	NAG	C3-C4-C5	2.47	114.50	110.20
4	B	606	MAN	C1-O5-C5	2.47	115.38	112.25
7	J	615	NAG	C3-C4-C5	2.47	114.50	110.20
4	H	606	MAN	C1-O5-C5	2.47	115.39	112.25
6	I	610	NAG	C4-C3-C2	2.47	115.07	111.23
7	C	615	NAG	C3-C4-C5	2.48	114.51	110.20
6	I	611	BMA	C1-C2-C3	2.48	112.47	109.54
7	F	615	NAG	C3-C4-C5	2.49	114.53	110.20
4	L	606	MAN	C1-O5-C5	2.49	115.41	112.25
4	J	606	MAN	C1-O5-C5	2.50	115.42	112.25
6	H	610	NAG	C4-C3-C2	2.52	115.15	111.23
6	D	611	BMA	C1-C2-C3	2.52	112.53	109.54
6	G	610	NAG	C4-C3-C2	2.53	115.16	111.23
6	C	611	BMA	C1-C2-C3	2.54	112.54	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	611	BMA	C1-C2-C3	2.54	112.55	109.54
6	L	610	NAG	C4-C3-C2	2.58	115.23	111.23
7	E	615	NAG	C3-C4-C5	2.59	114.71	110.20
6	A	610	NAG	C4-C3-C2	2.60	115.27	111.23
6	F	609	NAG	O4-C4-C3	2.60	116.20	110.34
7	H	615	NAG	C4-C3-C2	2.61	115.28	111.23
7	A	615	NAG	C3-C4-C5	2.68	114.88	110.20
6	A	609	NAG	O4-C4-C3	2.68	116.38	110.34
6	D	610	NAG	C4-C3-C2	2.70	115.42	111.23
6	E	610	NAG	C4-C3-C2	2.74	115.49	111.23
6	J	610	NAG	C4-C3-C2	2.78	115.55	111.23
7	K	615	NAG	C4-C3-C2	2.78	115.56	111.23
6	K	609	NAG	O4-C4-C3	2.80	116.65	110.34
7	C	615	NAG	C4-C3-C2	2.82	115.61	111.23
6	L	609	NAG	O4-C4-C3	2.82	116.69	110.34
6	B	609	NAG	O4-C4-C3	2.83	116.70	110.34
7	L	615	NAG	C4-C3-C2	2.83	115.63	111.23
7	D	615	NAG	C4-C3-C2	2.84	115.64	111.23
6	H	609	NAG	O4-C4-C3	2.86	116.77	110.34
7	J	615	NAG	C4-C3-C2	2.87	115.68	111.23
7	I	615	NAG	C4-C3-C2	2.88	115.70	111.23
6	F	611	BMA	C1-C2-C3	2.88	112.95	109.54
7	A	615	NAG	C4-C3-C2	2.91	115.75	111.23
6	E	609	NAG	O4-C4-C3	2.91	116.89	110.34
6	G	609	NAG	O4-C4-C3	2.94	116.95	110.34
6	C	610	NAG	C4-C3-C2	2.96	115.83	111.23
7	E	615	NAG	C4-C3-C2	3.00	115.89	111.23
6	C	609	NAG	O4-C4-C3	3.02	117.14	110.34
6	J	609	NAG	O4-C4-C3	3.02	117.14	110.34
6	D	609	NAG	O4-C4-C3	3.06	117.23	110.34
6	I	609	NAG	O4-C4-C3	3.07	117.26	110.34
7	F	615	NAG	C4-C3-C2	3.16	116.15	111.23
7	G	615	NAG	C4-C3-C2	3.17	116.15	111.23
7	B	615	NAG	C4-C3-C2	3.29	116.34	111.23
6	A	612	MAN	C1-C2-C3	3.99	114.26	109.54
6	E	612	MAN	C1-C2-C3	4.02	114.29	109.54
6	B	612	MAN	C1-C2-C3	4.06	114.34	109.54
6	D	612	MAN	C1-C2-C3	4.08	114.37	109.54
6	H	612	MAN	C1-C2-C3	4.12	114.42	109.54
6	C	612	MAN	C1-C2-C3	4.18	114.49	109.54
6	I	612	MAN	C1-C2-C3	4.19	114.50	109.54
6	F	612	MAN	C1-C2-C3	4.19	114.50	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	612	MAN	C1-C2-C3	4.21	114.52	109.54
6	K	612	MAN	C1-C2-C3	4.25	114.57	109.54
6	J	612	MAN	C1-C2-C3	4.25	114.57	109.54
4	F	605	MAN	C1-C2-C3	4.25	114.57	109.54
4	L	605	MAN	C1-C2-C3	4.30	114.62	109.54
4	I	605	MAN	C1-C2-C3	4.31	114.64	109.54
4	A	605	MAN	C1-C2-C3	4.31	114.64	109.54
4	K	605	MAN	C1-C2-C3	4.31	114.64	109.54
4	E	605	MAN	C1-C2-C3	4.32	114.65	109.54
4	H	605	MAN	C1-C2-C3	4.34	114.68	109.54
4	D	605	MAN	C1-C2-C3	4.35	114.69	109.54
4	C	605	MAN	C1-C2-C3	4.36	114.70	109.54
6	G	612	MAN	C1-C2-C3	4.36	114.70	109.54
4	G	605	MAN	C1-C2-C3	4.37	114.71	109.54
4	J	605	MAN	C1-C2-C3	4.39	114.73	109.54
4	B	605	MAN	C1-C2-C3	4.42	114.77	109.54

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	616	NAG	O7-C7-N2-C2
7	E	616	NAG	O7-C7-N2-C2
7	D	616	NAG	O7-C7-N2-C2
7	K	616	NAG	O7-C7-N2-C2
7	A	616	NAG	O7-C7-N2-C2
7	C	616	NAG	O7-C7-N2-C2
7	B	616	NAG	O7-C7-N2-C2
7	J	616	NAG	O7-C7-N2-C2
7	F	616	NAG	O7-C7-N2-C2
7	H	616	NAG	O7-C7-N2-C2
7	G	616	NAG	O7-C7-N2-C2
7	L	616	NAG	O7-C7-N2-C2

There are no ring outliers.

74 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	NAG	1	0
4	A	602	NAG	4	0
6	A	609	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	610	NAG	2	0
7	A	616	NAG	1	0
7	A	617	BMA	1	0
4	B	601	NAG	1	0
4	B	602	NAG	5	0
6	B	609	NAG	3	0
6	B	610	NAG	2	0
7	B	616	NAG	1	0
7	B	617	BMA	1	0
4	C	601	NAG	1	0
4	C	602	NAG	1	0
6	C	609	NAG	4	0
6	C	610	NAG	8	0
7	C	616	NAG	1	0
7	C	617	BMA	1	0
4	D	601	NAG	1	0
4	D	602	NAG	4	0
6	D	609	NAG	3	0
6	D	610	NAG	6	0
7	D	616	NAG	1	0
7	D	617	BMA	1	0
4	E	601	NAG	1	0
4	E	602	NAG	2	0
6	E	609	NAG	3	0
6	E	610	NAG	2	0
7	E	616	NAG	1	0
7	E	617	BMA	1	0
4	F	601	NAG	1	0
4	F	602	NAG	2	0
6	F	609	NAG	3	0
6	F	610	NAG	8	0
6	F	611	BMA	2	0
7	F	616	NAG	1	0
7	F	617	BMA	1	0
4	G	601	NAG	1	0
4	G	602	NAG	2	0
6	G	609	NAG	3	0
6	G	610	NAG	2	0
7	G	615	NAG	1	0
7	G	616	NAG	1	0
7	G	617	BMA	1	0
4	H	601	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	602	NAG	2	0
6	H	609	NAG	3	0
6	H	610	NAG	2	0
7	H	616	NAG	1	0
7	H	617	BMA	1	0
4	I	601	NAG	1	0
4	I	602	NAG	1	0
6	I	609	NAG	3	0
6	I	610	NAG	3	0
7	I	616	NAG	1	0
7	I	617	BMA	1	0
4	J	601	NAG	1	0
4	J	602	NAG	4	0
6	J	609	NAG	3	0
6	J	610	NAG	2	0
7	J	616	NAG	1	0
7	J	617	BMA	1	0
4	K	601	NAG	1	0
4	K	602	NAG	7	0
6	K	609	NAG	3	0
6	K	610	NAG	2	0
7	K	616	NAG	1	0
7	K	617	BMA	1	0
4	L	601	NAG	1	0
4	L	602	NAG	5	0
6	L	609	NAG	3	0
6	L	610	NAG	3	0
7	L	616	NAG	1	0
7	L	617	BMA	1	0

## 5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	608	1	14,14,15	0.61	0	15,19,21	0.73	1 (6%)
5	NAG	A	618	1	14,14,15	0.71	0	15,19,21	0.70	0
5	NAG	B	608	1	14,14,15	0.75	1 (7%)	15,19,21	0.73	1 (6%)
5	NAG	B	618	1	14,14,15	0.77	1 (7%)	15,19,21	0.69	0
5	NAG	C	608	1	14,14,15	0.68	0	15,19,21	0.73	1 (6%)
5	NAG	C	618	1	14,14,15	0.71	0	15,19,21	0.70	0
5	NAG	D	608	1	14,14,15	0.77	1 (7%)	15,19,21	0.72	1 (6%)
5	NAG	D	618	1	14,14,15	0.74	0	15,19,21	0.70	0
5	NAG	E	608	1	14,14,15	0.67	0	15,19,21	0.73	1 (6%)
5	NAG	E	618	1	14,14,15	0.71	0	15,19,21	0.69	0
5	NAG	F	608	1	14,14,15	0.65	0	15,19,21	0.72	1 (6%)
5	NAG	F	618	1	14,14,15	0.74	0	15,19,21	0.68	0
5	NAG	G	608	1	14,14,15	0.66	0	15,19,21	0.74	1 (6%)
5	NAG	G	618	1	14,14,15	0.70	0	15,19,21	0.69	0
5	NAG	H	608	1	14,14,15	0.76	1 (7%)	15,19,21	0.74	1 (6%)
5	NAG	H	618	1	14,14,15	1.08	1 (7%)	15,19,21	1.35	4 (26%)
5	NAG	I	608	1	14,14,15	0.68	0	15,19,21	0.73	1 (6%)
5	NAG	I	618	1	14,14,15	0.72	0	15,19,21	0.70	0
5	NAG	J	608	1	14,14,15	0.64	0	15,19,21	0.72	1 (6%)
5	NAG	J	618	1	14,14,15	0.72	0	15,19,21	0.66	0
5	NAG	K	608	1	14,14,15	0.69	0	15,19,21	0.74	1 (6%)
5	NAG	K	618	1	14,14,15	0.73	0	15,19,21	0.68	0
5	NAG	L	608	1	14,14,15	0.65	0	15,19,21	0.74	1 (6%)
5	NAG	L	618	1	14,14,15	0.70	0	15,19,21	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	608	1	-	0/6/23/26	0/1/1/1
5	NAG	A	618	1	-	0/6/23/26	0/1/1/1
5	NAG	B	608	1	-	0/6/23/26	0/1/1/1
5	NAG	B	618	1	-	0/6/23/26	0/1/1/1
5	NAG	C	608	1	-	0/6/23/26	0/1/1/1
5	NAG	C	618	1	-	0/6/23/26	0/1/1/1
5	NAG	D	608	1	-	0/6/23/26	0/1/1/1
5	NAG	D	618	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	608	1	-	0/6/23/26	0/1/1/1
5	NAG	E	618	1	-	0/6/23/26	0/1/1/1
5	NAG	F	608	1	-	0/6/23/26	0/1/1/1
5	NAG	F	618	1	-	0/6/23/26	0/1/1/1
5	NAG	G	608	1	-	0/6/23/26	0/1/1/1
5	NAG	G	618	1	-	0/6/23/26	0/1/1/1
5	NAG	H	608	1	-	0/6/23/26	0/1/1/1
5	NAG	H	618	1	-	0/6/23/26	0/1/1/1
5	NAG	I	608	1	-	0/6/23/26	0/1/1/1
5	NAG	I	618	1	-	0/6/23/26	0/1/1/1
5	NAG	J	608	1	-	0/6/23/26	0/1/1/1
5	NAG	J	618	1	-	0/6/23/26	0/1/1/1
5	NAG	K	608	1	-	0/6/23/26	0/1/1/1
5	NAG	K	618	1	-	0/6/23/26	0/1/1/1
5	NAG	L	608	1	-	0/6/23/26	0/1/1/1
5	NAG	L	618	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	618	NAG	C4-C3	2.01	1.57	1.52
5	B	608	NAG	C4-C3	2.10	1.57	1.52
5	H	608	NAG	C4-C3	2.17	1.58	1.52
5	D	608	NAG	C4-C3	2.19	1.58	1.52
5	H	618	NAG	O5-C5	2.26	1.48	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	608	NAG	C2-N2-C7	-2.33	120.04	123.04
5	H	608	NAG	C2-N2-C7	-2.33	120.04	123.04
5	G	608	NAG	C2-N2-C7	-2.32	120.06	123.04
5	B	608	NAG	C2-N2-C7	-2.32	120.06	123.04
5	D	608	NAG	C2-N2-C7	-2.30	120.08	123.04
5	I	608	NAG	C2-N2-C7	-2.29	120.10	123.04
5	A	608	NAG	C2-N2-C7	-2.29	120.10	123.04
5	E	608	NAG	C2-N2-C7	-2.29	120.10	123.04
5	C	608	NAG	C2-N2-C7	-2.29	120.10	123.04
5	K	608	NAG	C2-N2-C7	-2.27	120.13	123.04
5	F	608	NAG	C2-N2-C7	-2.25	120.14	123.04
5	J	608	NAG	C2-N2-C7	-2.25	120.15	123.04
5	H	618	NAG	C2-N2-C7	-2.09	120.36	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	618	NAG	C1-O5-C5	2.11	114.93	112.25
5	H	618	NAG	C3-C4-C5	2.67	114.85	110.20
5	H	618	NAG	O4-C4-C3	2.70	116.42	110.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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	493/493 (100%)	-0.28	4 (0%) 87 82	113, 184, 248, 333	0
1	B	493/493 (100%)	-0.32	3 (0%) 90 86	113, 184, 249, 332	0
1	C	493/493 (100%)	-0.21	6 (1%) 81 72	112, 184, 249, 333	0
1	D	493/493 (100%)	-0.16	10 (2%) 68 57	114, 184, 249, 333	0
1	E	493/493 (100%)	-0.14	10 (2%) 68 57	113, 184, 249, 333	0
1	F	493/493 (100%)	-0.21	3 (0%) 90 86	114, 184, 248, 333	0
1	G	493/493 (100%)	-0.25	7 (1%) 78 68	114, 184, 249, 333	0
1	H	493/493 (100%)	-0.20	4 (0%) 87 82	113, 184, 248, 333	0
1	I	493/493 (100%)	-0.29	3 (0%) 90 86	114, 184, 249, 333	0
1	J	493/493 (100%)	-0.27	9 (1%) 71 61	113, 184, 248, 333	0
1	K	493/493 (100%)	-0.24	5 (1%) 84 77	113, 184, 249, 333	0
1	L	493/493 (100%)	-0.16	14 (2%) 56 44	114, 184, 249, 333	0
2	1	226/226 (100%)	0.18	14 (6%) 24 16	125, 213, 300, 359	0
2	3	226/226 (100%)	0.34	17 (7%) 17 12	114, 213, 300, 359	0
2	5	226/226 (100%)	0.28	20 (8%) 12 9	134, 215, 300, 359	0
2	7	226/226 (100%)	0.05	9 (3%) 42 31	137, 212, 300, 359	0
2	9	226/226 (100%)	0.00	6 (2%) 58 46	131, 213, 300, 359	0
2	M	226/226 (100%)	0.19	13 (5%) 26 18	133, 213, 304, 359	0
2	O	226/226 (100%)	0.05	8 (3%) 48 37	136, 212, 306, 359	0
2	Q	226/226 (100%)	0.25	18 (7%) 15 11	140, 214, 306, 359	0
2	S	226/226 (100%)	0.42	25 (11%) 7 6	146, 214, 306, 359	0
2	U	226/226 (100%)	0.46	23 (10%) 9 7	145, 214, 306, 359	0
2	W	226/226 (100%)	0.42	26 (11%) 6 6	121, 213, 306, 359	0
2	Y	226/226 (100%)	0.24	19 (8%) 14 10	145, 214, 306, 359	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	0	212/220 (96%)	-0.12	0 100 100	146, 221, 284, 324	0
3	2	212/220 (96%)	-0.08	4 (1%) 70 59	146, 222, 284, 325	0
3	4	212/220 (96%)	0.08	4 (1%) 70 59	146, 221, 284, 325	0
3	6	212/220 (96%)	0.26	16 (7%) 17 12	146, 223, 284, 325	0
3	8	212/220 (96%)	0.03	3 (1%) 78 68	146, 223, 284, 324	0
3	N	212/220 (96%)	0.13	6 (2%) 56 44	146, 222, 284, 324	0
3	P	212/220 (96%)	0.06	4 (1%) 70 59	146, 222, 284, 324	0
3	R	212/220 (96%)	0.28	11 (5%) 31 23	146, 224, 284, 324	0
3	T	212/220 (96%)	0.36	15 (7%) 19 13	146, 224, 284, 324	0
3	V	212/220 (96%)	0.60	30 (14%) 4 4	146, 223, 284, 325	0
3	X	212/220 (96%)	0.36	18 (8%) 13 10	146, 222, 284, 325	0
3	Z	212/220 (96%)	0.24	11 (5%) 31 23	146, 223, 284, 325	0
All	All	11172/11268 (99%)	-0.02	398 (3%) 46 36	112, 200, 279, 359	0

All (398) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	3	139	PRO	8.9
2	U	174	SER	8.7
2	U	139	PRO	8.0
2	5	226	PRO	7.8
2	5	138	ALA	7.8
2	U	224	VAL	7.6
2	U	226	PRO	7.1
2	U	138	ALA	6.9
3	R	212	ALA	6.9
3	V	118	PRO	6.4
3	X	152	ALA	6.4
2	Q	146	GLY	6.3
1	L	331	LEU	6.3
1	H	352	GLY	6.2
2	5	198	PRO	6.1
2	3	138	ALA	5.9
2	S	207	TYR	5.9
2	3	134	VAL	5.7
2	U	173	THR	5.7
1	E	333	GLY	5.6
3	V	160	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
2	U	225	GLU	5.4
3	V	159	PRO	5.4
3	T	179	ALA	5.3
2	1	151	LEU	5.2
2	W	151	LEU	5.0
2	7	144	THR	5.0
1	D	135	GLY	4.9
2	5	199	SER	4.9
2	Q	197	VAL	4.9
2	W	193	SER	4.8
2	1	146	GLY	4.7
2	U	136	PRO	4.6
2	U	172	LEU	4.6
2	3	141	SER	4.6
1	L	330	GLY	4.6
2	5	139	PRO	4.5
2	5	207	TYR	4.5
2	Y	150	ALA	4.4
2	5	149	ALA	4.4
2	Y	139	PRO	4.4
1	J	329	ARG	4.4
3	V	187	PRO	4.3
3	T	151	VAL	4.3
3	R	198	CYS	4.2
2	W	200	SER	4.2
3	6	194	ARG	4.2
2	U	140	SER	4.2
2	W	206	THR	4.1
2	Q	145	SER	4.1
2	3	150	ALA	4.1
3	6	121	THR	4.1
3	N	161	LYS	4.0
3	R	197	SER	4.0
1	E	12	THR	4.0
1	J	333	GLY	4.0
1	E	329	ARG	4.0
2	U	151	LEU	4.0
3	X	160	VAL	4.0
1	I	331	LEU	4.0
2	S	226	PRO	3.9
1	H	331	LEU	3.9
2	Y	151	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	M	146	GLY	3.9
3	R	196	TYR	3.9
2	S	195	VAL	3.9
3	V	153	TRP	3.8
3	V	139	CYS	3.8
3	V	199	GLN	3.8
3	T	152	ALA	3.7
2	W	155	VAL	3.7
3	V	133	ASN	3.7
2	S	139	PRO	3.7
2	W	164	THR	3.7
3	T	178	ALA	3.6
3	2	119	SER	3.6
3	V	193	HIS	3.6
2	1	207	TYR	3.6
1	F	331	LEU	3.6
2	W	195	VAL	3.6
2	S	138	ALA	3.5
1	K	325	GLU	3.5
1	C	356	GLN	3.5
2	5	220	VAL	3.5
3	V	146	PRO	3.5
3	X	158	SER	3.5
2	5	202	LEU	3.5
3	V	120	VAL	3.5
1	G	470	TYR	3.5
2	7	151	LEU	3.5
3	4	135	ALA	3.5
3	N	196	TYR	3.5
3	R	158	SER	3.5
2	W	134	VAL	3.5
1	L	143	PRO	3.5
2	5	132	PRO	3.5
2	Q	198	PRO	3.4
1	D	134	GLY	3.4
1	L	365	ALA	3.4
1	J	12	THR	3.4
3	V	209	LYS	3.4
2	7	226	PRO	3.4
3	6	152	ALA	3.4
1	L	458	ASN	3.4
3	Z	199	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
3	V	201	THR	3.4
2	W	138	ALA	3.4
2	W	226	PRO	3.4
1	E	332	PHE	3.4
2	Y	140	SER	3.3
2	5	200	SER	3.3
3	R	213	PRO	3.3
3	T	199	GLN	3.3
2	5	197	VAL	3.3
3	T	180	SER	3.3
3	X	207	VAL	3.3
2	Y	138	ALA	3.3
3	4	120	VAL	3.3
2	Q	143	SER	3.3
1	I	330	GLY	3.3
3	T	141	ILE	3.2
2	S	151	LEU	3.2
2	3	155	VAL	3.2
3	T	198	CYS	3.2
1	G	325	GLU	3.2
1	C	333	GLY	3.2
2	Y	207	TYR	3.2
3	R	155	ALA	3.2
3	V	124	PRO	3.1
2	M	140	SER	3.1
1	K	334	ALA	3.1
2	5	201	SER	3.1
1	E	334	ALA	3.1
2	S	225	GLU	3.1
2	3	219	LYS	3.1
2	5	148	THR	3.1
3	V	202	HIS	3.1
3	6	201	THR	3.1
2	Y	133	SER	3.1
2	S	196	THR	3.1
2	U	193	SER	3.0
3	X	159	PRO	3.0
2	Y	225	GLU	3.0
2	1	172	LEU	3.0
2	Q	152	GLY	3.0
2	3	135	PHE	3.0
2	U	134	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
3	6	199	GLN	2.9
1	G	324	PRO	2.9
3	X	206	THR	2.9
2	Y	146	GLY	2.9
3	V	198	CYS	2.9
2	Q	139	PRO	2.9
2	1	211	VAL	2.9
3	X	197	SER	2.9
2	U	207	TYR	2.9
3	6	123	PHE	2.9
1	J	328	THR	2.9
2	9	146	GLY	2.9
1	E	327	GLN	2.9
2	1	125	SER	2.9
2	1	219	LYS	2.9
2	S	142	LYS	2.8
1	D	325	GLU	2.8
3	V	152	ALA	2.8
2	3	140	SER	2.8
2	W	212	ASN	2.8
2	W	170	GLY	2.8
3	T	175	ASN	2.8
2	M	202	LEU	2.8
2	Q	147	GLY	2.8
2	W	225	GLU	2.8
2	1	212	ASN	2.8
1	A	458	ASN	2.8
2	M	163	VAL	2.8
2	Y	149	ALA	2.8
3	X	39	GLN	2.8
1	E	336	ALA	2.8
2	Q	134	VAL	2.8
3	X	151	VAL	2.8
1	G	334	ALA	2.8
3	R	211	VAL	2.8
2	S	144	THR	2.8
2	Q	138	ALA	2.8
3	N	115	LYS	2.7
3	8	208	GLU	2.7
3	T	139	CYS	2.7
2	W	135	PHE	2.7
3	N	147	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	Y	214	LYS	2.7
2	S	134	VAL	2.7
1	L	145	SER	2.7
2	1	144	THR	2.7
2	O	226	PRO	2.7
2	1	195	VAL	2.7
2	O	136	PRO	2.7
3	T	181	SER	2.7
2	Q	132	PRO	2.7
2	U	195	VAL	2.7
2	5	211	VAL	2.7
2	M	125	SER	2.7
2	5	219	LYS	2.7
2	S	224	VAL	2.7
2	S	146	GLY	2.7
2	5	195	VAL	2.7
3	T	186	THR	2.7
2	3	136	PRO	2.6
1	H	329	ARG	2.6
2	3	3	GLN	2.6
2	7	143	SER	2.6
1	J	11	ALA	2.6
1	E	331	LEU	2.6
3	P	159	PRO	2.6
3	X	125	PRO	2.6
1	D	332	PHE	2.6
1	J	334	ALA	2.6
2	W	125	SER	2.6
3	Z	110	VAL	2.6
2	W	207	TYR	2.6
3	N	146	PRO	2.6
3	6	186	THR	2.6
2	O	197	VAL	2.6
1	G	498	ASN	2.6
3	V	119	SER	2.6
2	5	140	SER	2.5
2	S	141	SER	2.5
3	X	127	SER	2.5
3	P	118	PRO	2.5
2	3	220	VAL	2.5
3	4	160	VAL	2.5
3	Z	205	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	5	196	THR	2.5
2	5	225	GLU	2.5
3	V	117	ALA	2.5
2	O	224	VAL	2.5
2	W	196	THR	2.5
3	Z	207	VAL	2.5
3	Z	175	ASN	2.5
1	L	328	THR	2.5
2	3	125	SER	2.5
2	S	193	SER	2.5
1	A	351	TYR	2.5
2	S	197	VAL	2.5
1	C	145	SER	2.5
1	K	12	THR	2.5
2	7	136	PRO	2.4
2	S	205	GLN	2.4
3	V	186	THR	2.4
3	N	159	PRO	2.4
3	Z	159	PRO	2.4
2	W	201	SER	2.4
2	Y	126	SER	2.4
1	B	458	ASN	2.4
2	Y	206	THR	2.4
2	Y	195	VAL	2.4
3	4	196	TYR	2.4
2	Q	149	ALA	2.4
3	V	121	THR	2.4
2	M	152	GLY	2.4
2	Y	152	GLY	2.4
2	S	220	VAL	2.4
2	Y	143	SER	2.4
3	6	187	PRO	2.4
3	V	113	GLN	2.4
2	9	149	ALA	2.4
3	X	153	TRP	2.4
3	R	154	LYS	2.4
1	A	365	ALA	2.4
2	9	132	PRO	2.4
1	D	133	ASN	2.4
2	Y	197	VAL	2.4
3	6	120	VAL	2.4
2	U	198	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	6	118	PRO	2.4
2	Q	133	SER	2.3
3	V	192	SER	2.3
1	G	365	ALA	2.3
2	1	218	THR	2.3
2	7	207	TYR	2.3
3	Z	109	THR	2.3
1	C	458	ASN	2.3
2	S	198	PRO	2.3
3	8	121	THR	2.3
2	7	224	VAL	2.3
3	P	139	CYS	2.3
1	D	324	PRO	2.3
1	I	387	LYS	2.3
1	F	132	GLN	2.3
2	U	220	VAL	2.3
2	S	206	THR	2.3
1	J	352	GLY	2.3
2	M	220	VAL	2.3
2	U	141	SER	2.3
3	6	151	VAL	2.3
1	B	331	LEU	2.3
3	6	185	LEU	2.3
1	C	332	PHE	2.3
2	S	211	VAL	2.3
1	B	325	GLU	2.3
1	L	349	GLY	2.3
1	E	330	GLY	2.3
2	O	207	TYR	2.3
3	6	207	VAL	2.3
1	L	335	ILE	2.3
1	L	329	ARG	2.3
2	Q	199	SER	2.3
2	9	193	SER	2.3
3	X	205	SER	2.3
2	M	97	ALA	2.3
2	Y	200	SER	2.2
3	2	139	CYS	2.2
2	O	144	THR	2.2
2	M	203	GLY	2.2
2	M	226	PRO	2.2
3	V	158	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	U	131	GLY	2.2
3	V	156	ASP	2.2
2	9	153	CYS	2.2
3	2	208	GLU	2.2
3	8	139	CYS	2.2
3	R	159	PRO	2.2
2	W	142	LYS	2.2
2	Q	225	GLU	2.2
2	O	145	SER	2.2
3	R	195	SER	2.2
1	J	327	GLN	2.2
2	7	202	LEU	2.2
3	V	189	GLN	2.2
1	D	356	GLN	2.2
2	U	205	GLN	2.2
3	V	134	LYS	2.2
3	X	165	GLU	2.2
2	3	151	LEU	2.2
1	L	333	GLY	2.2
2	Q	226	PRO	2.2
2	W	150	ALA	2.2
3	T	149	VAL	2.2
1	K	329	ARG	2.2
3	P	113	GLN	2.2
2	9	107	GLY	2.2
2	S	222	LYS	2.2
3	T	196	TYR	2.2
3	Z	191	LYS	2.2
1	A	387	LYS	2.2
2	W	139	PRO	2.1
3	X	155	ALA	2.1
2	W	137	LEU	2.1
3	X	201	THR	2.1
1	D	330	GLY	2.1
2	Y	147	GLY	2.1
3	6	124	PRO	2.1
2	S	140	SER	2.1
1	K	349	GLY	2.1
2	M	149	ALA	2.1
3	V	125	PRO	2.1
3	V	196	TYR	2.1
2	W	163	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	335	ILE	2.1
2	W	140	SER	2.1
3	V	188	GLU	2.1
2	M	144	THR	2.1
2	1	145	SER	2.1
2	Q	200	SER	2.1
2	W	133	SER	2.1
1	L	344	GLU	2.1
2	3	146	GLY	2.1
3	2	190	TRP	2.1
2	1	140	SER	2.1
3	6	115	LYS	2.1
1	L	501	GLN	2.1
1	L	351	TYR	2.1
3	Z	158	SER	2.1
2	S	201	SER	2.1
2	7	145	SER	2.1
3	X	124	PRO	2.0
2	3	152	GLY	2.0
3	X	181	SER	2.0
1	D	461	ASP	2.0
1	E	135	GLY	2.0
2	U	101	GLY	2.0
3	Z	161	LYS	2.0
2	Q	202	LEU	2.0
2	1	224	VAL	2.0
1	C	472	LYS	2.0
1	F	248	ASN	2.0
2	U	137	LEU	2.0
2	W	205	GLN	2.0
2	S	143	SER	2.0
2	3	200	SER	2.0
1	G	497	ASN	2.0
2	M	35	SER	2.0
3	Z	196	TYR	2.0
3	T	188	GLU	2.0
2	U	143	SER	2.0
1	H	135	GLY	2.0
2	O	146	GLY	2.0
1	D	458	ASN	2.0
3	6	208	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	G	601	14/15	0.86	0.27	0.27	168,168,168,168	0
4	NAG	E	601	14/15	0.94	0.32	0.07	169,169,169,169	0
6	NAG	D	609	14/15	0.88	0.23	-0.09	181,181,181,181	0
4	NAG	K	602	14/15	0.76	0.31	-0.16	199,199,199,199	0
4	NAG	A	601	14/15	0.90	0.23	-0.19	168,168,168,168	0
4	NAG	K	601	14/15	0.87	0.24	-0.25	168,168,168,168	0
4	NAG	H	601	14/15	0.90	0.24	-0.30	168,168,168,168	0
4	NAG	L	601	14/15	0.77	0.26	-0.33	169,169,169,169	0
4	NAG	I	601	14/15	0.93	0.22	-0.41	168,168,168,168	0
4	NAG	F	601	14/15	0.94	0.23	-0.54	169,169,169,169	0
4	NAG	B	601	14/15	0.86	0.23	-0.58	168,168,168,168	0
4	NAG	B	602	14/15	0.81	0.24	-0.72	198,198,198,198	0
4	NAG	J	602	14/15	0.86	0.26	-0.72	198,198,198,198	0
4	NAG	J	601	14/15	0.90	0.19	-0.73	169,169,169,169	0
6	NAG	F	609	14/15	0.89	0.16	-1.49	181,181,181,181	0
4	NAG	D	601	14/15	0.93	0.17	-1.84	168,168,168,168	0
4	MAN	B	604	11/12	0.96	0.10	-	235,235,235,235	0
6	NAG	B	609	14/15	0.87	0.24	-	181,181,181,181	0
4	MAN	C	607	11/12	0.80	0.45	-	244,244,244,244	0
6	BMA	G	611	11/12	0.94	0.23	-	224,224,224,224	0
6	BMA	L	611	11/12	0.85	0.11	-	223,223,223,223	0
4	MAN	L	605	11/12	0.83	0.36	-	235,235,235,235	0
4	BMA	G	603	11/12	0.84	0.22	-	212,212,212,212	0
4	MAN	A	607	11/12	0.84	0.36	-	244,244,244,244	0
7	NAG	K	615	14/15	0.77	0.33	-	251,251,251,251	0
4	NAG	C	602	14/15	0.81	0.35	-	199,199,199,199	0
6	MAN	E	614	11/12	0.78	0.13	-	253,253,253,253	0
4	BMA	J	603	11/12	0.88	0.25	-	212,212,212,212	0
4	MAN	K	606	11/12	0.86	0.28	-	222,222,222,222	0
6	MAN	L	614	11/12	0.84	0.17	-	254,254,254,254	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	L	607	11/12	0.84	0.55	-	245,245,245,245	0
6	NAG	I	609	14/15	0.88	0.22	-	181,181,181,181	0
4	MAN	G	607	11/12	0.88	0.35	-	244,244,244,244	0
6	MAN	F	614	11/12	0.85	0.14	-	253,253,253,253	0
6	BMA	H	611	11/12	0.83	0.17	-	223,223,223,223	0
4	MAN	K	604	11/12	0.85	0.17	-	236,236,236,236	0
4	MAN	E	606	11/12	0.66	0.33	-	222,222,222,222	0
7	NAG	J	615	14/15	0.89	0.23	-	251,251,251,251	0
6	MAN	K	613	11/12	0.75	0.46	-	294,294,294,294	0
4	BMA	F	603	11/12	0.84	0.36	-	212,212,212,212	0
4	MAN	G	605	11/12	0.83	0.29	-	235,235,235,235	0
7	BMA	A	617	11/12	0.46	0.54	-	301,301,301,301	0
4	MAN	J	606	11/12	0.64	0.36	-	222,222,222,222	0
4	NAG	I	602	14/15	0.89	0.23	-	199,199,199,199	0
6	BMA	F	611	11/12	0.73	0.19	-	224,224,224,224	0
4	MAN	H	607	11/12	0.79	0.37	-	245,245,245,245	0
6	BMA	C	611	11/12	0.87	0.10	-	223,223,223,223	0
4	NAG	G	602	14/15	0.93	0.30	-	198,198,198,198	0
6	MAN	B	614	11/12	0.79	0.18	-	254,254,254,254	0
4	MAN	K	607	11/12	0.77	0.35	-	244,244,244,244	0
7	NAG	I	616	14/15	0.78	0.33	-	270,270,270,270	0
4	MAN	J	605	11/12	0.69	0.29	-	235,235,235,235	0
7	BMA	B	617	11/12	0.11	0.46	-	301,301,301,301	0
6	MAN	I	614	11/12	0.79	0.19	-	254,254,254,254	0
4	MAN	B	607	11/12	0.57	0.54	-	245,245,245,245	0
6	NAG	G	609	14/15	0.84	0.23	-	181,181,181,181	0
6	NAG	A	610	14/15	0.91	0.27	-	201,201,201,201	0
6	NAG	J	610	14/15	0.86	0.21	-	202,202,202,202	0
7	BMA	I	617	11/12	0.44	0.41	-	301,301,301,301	0
6	MAN	G	614	11/12	0.79	0.24	-	254,254,254,254	0
4	MAN	B	605	11/12	0.80	0.35	-	235,235,235,235	0
4	MAN	F	606	11/12	0.71	0.30	-	222,222,222,222	0
6	MAN	B	612	11/12	0.72	0.20	-	271,271,271,271	0
4	MAN	C	606	11/12	0.45	0.50	-	223,223,223,223	0
6	NAG	I	610	14/15	0.85	0.30	-	202,202,202,202	0
4	BMA	A	603	11/12	0.94	0.23	-	212,212,212,212	0
4	MAN	F	607	11/12	0.87	0.19	-	244,244,244,244	0
4	MAN	D	607	11/12	0.69	0.35	-	244,244,244,244	0
6	BMA	D	611	11/12	0.61	0.21	-	224,224,224,224	0
6	MAN	H	614	11/12	0.79	0.23	-	253,253,253,253	0
6	MAN	L	613	11/12	0.47	0.40	-	294,294,294,294	0
4	MAN	A	604	11/12	0.79	0.20	-	236,236,236,236	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	I	605	11/12	0.85	0.12	-	235,235,235,235	0
6	NAG	H	609	14/15	0.94	0.14	-	181,181,181,181	0
6	BMA	I	611	11/12	0.85	0.21	-	224,224,224,224	0
6	MAN	D	612	11/12	0.59	0.31	-	271,271,271,271	0
6	MAN	F	612	11/12	0.75	0.32	-	271,271,271,271	0
7	NAG	G	616	14/15	0.82	0.36	-	270,270,270,270	0
4	MAN	E	604	11/12	0.90	0.12	-	236,236,236,236	0
6	NAG	L	610	14/15	0.80	0.25	-	202,202,202,202	0
4	MAN	K	605	11/12	0.73	0.24	-	235,235,235,235	0
6	BMA	J	611	11/12	0.86	0.20	-	223,223,223,223	0
4	BMA	L	603	11/12	0.85	0.21	-	212,212,212,212	0
6	BMA	K	611	11/12	0.85	0.15	-	224,224,224,224	0
6	NAG	C	609	14/15	0.92	0.20	-	180,180,180,180	0
6	NAG	B	610	14/15	0.90	0.21	-	202,202,202,202	0
6	NAG	A	609	14/15	0.87	0.24	-	180,180,180,180	0
7	BMA	F	617	11/12	0.68	0.42	-	301,301,301,301	0
7	NAG	L	615	14/15	0.74	0.29	-	251,251,251,251	0
6	BMA	B	611	11/12	0.89	0.21	-	223,223,223,223	0
6	MAN	H	613	11/12	0.61	0.54	-	294,294,294,294	0
6	BMA	E	611	11/12	0.87	0.12	-	223,223,223,223	0
6	MAN	C	612	11/12	0.84	0.14	-	271,271,271,271	0
7	BMA	L	617	11/12	0.69	0.38	-	301,301,301,301	0
4	MAN	H	604	11/12	0.92	0.11	-	235,235,235,235	0
4	MAN	J	604	11/12	0.87	0.22	-	236,236,236,236	0
6	MAN	J	614	11/12	0.35	0.33	-	254,254,254,254	0
4	BMA	E	603	11/12	0.94	0.22	-	212,212,212,212	0
7	BMA	K	617	11/12	0.37	0.44	-	301,301,301,301	0
4	BMA	C	603	11/12	0.66	0.28	-	212,212,212,212	0
4	NAG	D	602	14/15	0.84	0.36	-	199,199,199,199	0
6	BMA	A	611	11/12	0.70	0.29	-	223,223,223,223	0
4	MAN	J	607	11/12	0.81	0.38	-	244,244,244,244	0
4	MAN	L	604	11/12	0.83	0.15	-	236,236,236,236	0
4	MAN	I	604	11/12	0.72	0.26	-	235,235,235,235	0
7	NAG	L	616	14/15	0.89	0.37	-	270,270,270,270	0
4	MAN	I	607	11/12	0.86	0.27	-	245,245,245,245	0
6	MAN	K	614	11/12	0.79	0.27	-	254,254,254,254	0
4	MAN	L	606	11/12	0.63	0.52	-	222,222,222,222	0
4	MAN	I	606	11/12	0.74	0.35	-	222,222,222,222	0
4	MAN	D	604	11/12	0.90	0.39	-	236,236,236,236	0
4	MAN	D	606	11/12	0.63	0.39	-	223,223,223,223	0
6	MAN	K	612	11/12	0.87	0.20	-	271,271,271,271	0
6	MAN	I	612	11/12	0.72	0.22	-	271,271,271,271	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	C	610	14/15	0.91	0.17	-	201,201,201,201	0
6	MAN	E	612	11/12	0.71	0.17	-	271,271,271,271	0
4	BMA	D	603	11/12	0.87	0.28	-	212,212,212,212	0
6	NAG	J	609	14/15	0.88	0.16	-	181,181,181,181	0
4	MAN	A	606	11/12	0.72	0.41	-	222,222,222,222	0
6	MAN	J	612	11/12	0.71	0.21	-	271,271,271,271	0
7	NAG	J	616	14/15	0.91	0.39	-	270,270,270,270	0
7	BMA	H	617	11/12	0.48	0.47	-	301,301,301,301	0
4	MAN	C	605	11/12	0.78	0.38	-	235,235,235,235	0
6	MAN	E	613	11/12	0.74	0.24	-	293,293,293,293	0
4	BMA	H	603	11/12	0.88	0.15	-	212,212,212,212	0
4	MAN	F	605	11/12	0.77	0.21	-	235,235,235,235	0
6	NAG	G	610	14/15	0.84	0.26	-	202,202,202,202	0
4	NAG	A	602	14/15	0.90	0.20	-	198,198,198,198	0
6	NAG	L	609	14/15	0.92	0.18	-	181,181,181,181	0
6	MAN	A	613	11/12	0.68	0.44	-	293,293,293,293	0
4	MAN	H	605	11/12	0.90	0.20	-	235,235,235,235	0
4	MAN	B	606	11/12	0.38	0.47	-	222,222,222,222	0
6	NAG	F	610	14/15	0.87	0.21	-	202,202,202,202	0
7	NAG	H	615	14/15	0.62	0.35	-	251,251,251,251	0
6	NAG	D	610	14/15	0.84	0.27	-	202,202,202,202	0
7	NAG	H	616	14/15	0.85	0.45	-	270,270,270,270	0
6	MAN	A	614	11/12	0.59	0.33	-	253,253,253,253	0
6	NAG	E	609	14/15	0.87	0.25	-	180,180,180,180	0
4	MAN	G	606	11/12	0.75	0.30	-	222,222,222,222	0
4	NAG	C	601	14/15	0.84	0.34	-	168,168,168,168	0
6	MAN	G	612	11/12	0.55	0.25	-	271,271,271,271	0
4	NAG	L	602	14/15	0.77	0.42	-	199,199,199,199	0
7	BMA	E	617	11/12	0.60	0.31	-	301,301,301,301	0
7	NAG	B	616	14/15	0.88	0.27	-	270,270,270,270	0
7	NAG	E	616	14/15	0.84	0.28	-	270,270,270,270	0
4	MAN	G	604	11/12	0.90	0.18	-	236,236,236,236	0
7	NAG	E	615	14/15	0.86	0.22	-	251,251,251,251	0
7	NAG	D	615	14/15	0.91	0.15	-	250,250,250,250	0
6	MAN	D	613	11/12	0.44	0.35	-	294,294,294,294	0
6	MAN	B	613	11/12	0.56	0.34	-	294,294,294,294	0
4	BMA	I	603	11/12	0.76	0.24	-	212,212,212,212	0
6	MAN	C	613	11/12	0.59	0.25	-	294,294,294,294	0
6	MAN	I	613	11/12	0.51	0.59	-	294,294,294,294	0
6	NAG	K	610	14/15	0.94	0.14	-	202,202,202,202	0
7	NAG	C	616	14/15	0.84	0.30	-	270,270,270,270	0
7	NAG	A	616	14/15	0.81	0.32	-	271,271,271,271	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	C	615	14/15	0.90	0.19	-	251,251,251,251	0
4	NAG	F	602	14/15	0.86	0.40	-	198,198,198,198	0
4	MAN	F	604	11/12	0.83	0.20	-	236,236,236,236	0
4	MAN	C	604	11/12	0.73	0.24	-	236,236,236,236	0
6	MAN	L	612	11/12	0.39	0.29	-	271,271,271,271	0
6	NAG	E	610	14/15	0.92	0.18	-	201,201,201,201	0
7	BMA	J	617	11/12	0.33	0.40	-	301,301,301,301	0
4	NAG	E	602	14/15	0.95	0.32	-	198,198,198,198	0
4	NAG	H	602	14/15	0.83	0.25	-	199,199,199,199	0
6	MAN	H	612	11/12	0.72	0.26	-	271,271,271,271	0
6	MAN	J	613	11/12	0.68	0.44	-	294,294,294,294	0
4	BMA	B	603	11/12	0.92	0.17	-	212,212,212,212	0
6	NAG	K	609	14/15	0.91	0.20	-	181,181,181,181	0
6	MAN	D	614	11/12	0.53	0.32	-	254,254,254,254	0
6	NAG	H	610	14/15	0.93	0.15	-	202,202,202,202	0
6	MAN	F	613	11/12	0.39	0.43	-	293,293,293,293	0
4	BMA	K	603	11/12	0.84	0.28	-	212,212,212,212	0
7	NAG	F	616	14/15	0.87	0.23	-	270,270,270,270	0
7	NAG	A	615	14/15	0.89	0.16	-	250,250,250,250	0
4	MAN	D	605	11/12	0.79	0.35	-	235,235,235,235	0
4	MAN	E	605	11/12	0.86	0.32	-	235,235,235,235	0
6	MAN	G	613	11/12	0.58	0.39	-	294,294,294,294	0
7	NAG	I	615	14/15	0.82	0.25	-	250,250,250,250	0
7	NAG	G	615	14/15	0.87	0.27	-	251,251,251,251	0
4	MAN	A	605	11/12	0.78	0.32	-	235,235,235,235	0
7	NAG	B	615	14/15	0.88	0.19	-	251,251,251,251	0
4	MAN	E	607	11/12	0.88	0.33	-	244,244,244,244	0
7	NAG	D	616	14/15	0.90	0.26	-	270,270,270,270	0
7	BMA	D	617	11/12	0.53	0.29	-	301,301,301,301	0
7	BMA	G	617	11/12	0.48	0.41	-	301,301,301,301	0
6	MAN	A	612	11/12	0.72	0.41	-	271,271,271,271	0
7	BMA	C	617	11/12	0.34	0.40	-	301,301,301,301	0
7	NAG	F	615	14/15	0.87	0.25	-	250,250,250,250	0
7	NAG	K	616	14/15	0.82	0.45	-	270,270,270,270	0
4	MAN	H	606	11/12	0.68	0.39	-	222,222,222,222	0
6	MAN	C	614	11/12	0.91	0.23	-	253,253,253,253	0

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	H	608	14/15	0.19	0.80	8.60	238,238,238,238	0
5	NAG	H	618	14/15	0.71	0.45	1.16	291,291,291,291	0
5	NAG	C	618	14/15	0.75	0.32	-	290,290,290,290	0
5	NAG	A	608	14/15	0.73	0.27	-	238,238,238,238	0
5	NAG	J	618	14/15	0.72	0.48	-	291,291,291,291	0
5	NAG	C	608	14/15	0.76	0.40	-	238,238,238,238	0
5	NAG	D	618	14/15	0.61	0.49	-	291,291,291,291	0
5	NAG	E	608	14/15	0.61	0.33	-	238,238,238,238	0
5	NAG	F	608	14/15	0.80	0.27	-	238,238,238,238	0
5	NAG	F	618	14/15	0.62	0.37	-	291,291,291,291	0
5	NAG	L	608	14/15	0.68	0.33	-	238,238,238,238	0
5	NAG	I	618	14/15	0.70	0.25	-	290,290,290,290	0
5	NAG	A	618	14/15	0.63	0.29	-	291,291,291,291	0
5	NAG	G	618	14/15	0.73	0.49	-	291,291,291,291	0
5	NAG	D	608	14/15	0.67	0.30	-	238,238,238,238	0
5	NAG	G	608	14/15	0.77	0.20	-	238,238,238,238	0
5	NAG	J	608	14/15	0.79	0.19	-	238,238,238,238	0
5	NAG	K	608	14/15	0.72	0.29	-	238,238,238,238	0
5	NAG	I	608	14/15	0.74	0.23	-	238,238,238,238	0
5	NAG	B	608	14/15	0.73	0.33	-	238,238,238,238	0
5	NAG	L	618	14/15	0.67	0.52	-	291,291,291,291	0
5	NAG	B	618	14/15	0.60	0.54	-	291,291,291,291	0
5	NAG	K	618	14/15	0.64	0.55	-	291,291,291,291	0
5	NAG	E	618	14/15	0.81	0.41	-	291,291,291,291	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.