



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:41 PM UTC

PDB ID : 4YD9 / pdb_00004yd9
Title : Crystal structure of squid hemocyanin
Authors : Matsuno, A.; Gai, Z.; Kato, K.; Tanaka, Y.; Yao, M.
Deposited on : 2015-02-21
Resolution : 3.00 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

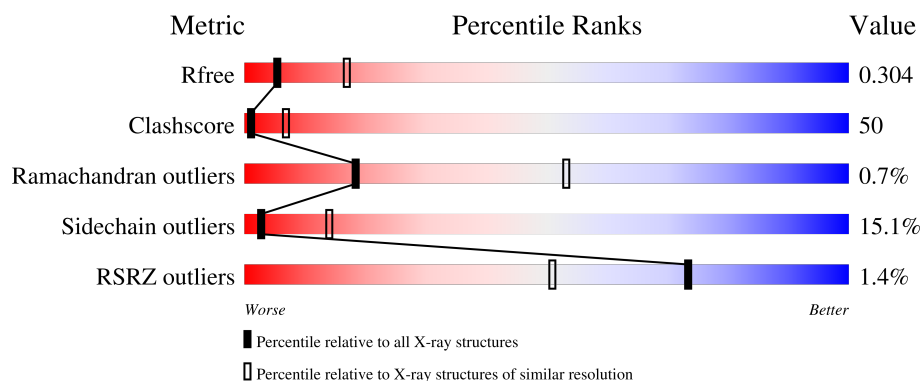
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2000	49% 28% 5% 17%
1	D	2000	48% 30% 5% 17%
1	G	2000	47% 30% 6% 17%
1	J	2000	47% 31% 5% 17%
1	M	2000	50% 27% 5% 17%

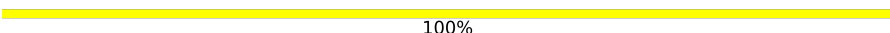
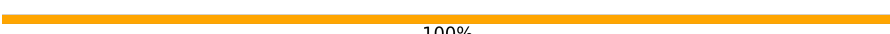
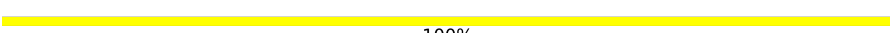
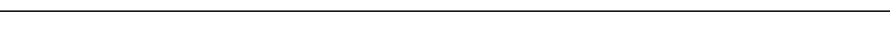
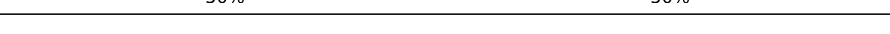
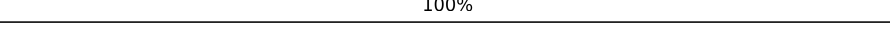
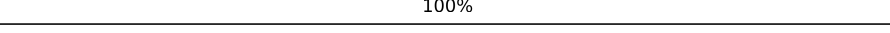
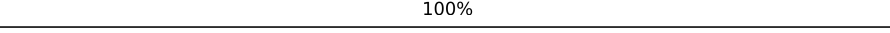
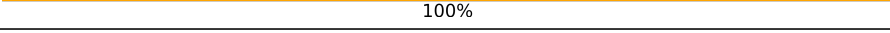
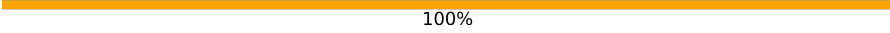
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Mol	Chain	Length	Quality of chain
1	P	2000	
1	S	2000	
1	V	2000	
1	Y	2000	
1	b	2000	
2	B	920	
2	E	920	
2	H	920	
2	K	920	
2	N	920	
2	Q	920	
2	T	920	
2	W	920	
2	Z	920	
2	c	920	
3	C	394	
3	F	394	
3	I	394	
3	L	394	
3	O	394	
3	R	394	
3	U	394	
3	X	394	
3	a	394	
3	d	394	

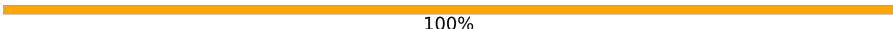
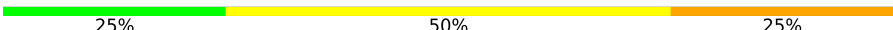
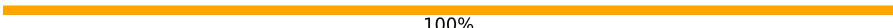
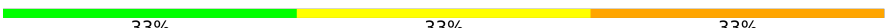
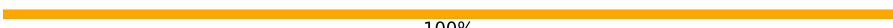
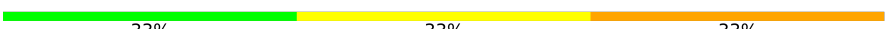
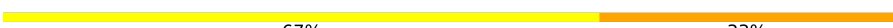
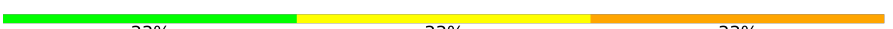
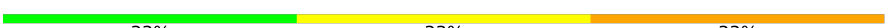
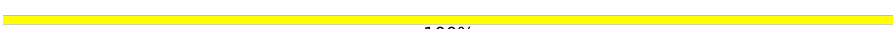
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Mol	Chain	Length	Quality of chain
4	1	2	 50% 50%
4	2	2	 50% 50%
4	4	2	 100%
4	6	2	 50% 50%
4	7	2	 100%
4	8	2	 100%
4	9	2	 100%
4	BA	2	 100%
4	HA	2	 50% 50%
4	IA	2	 100%
4	JA	2	 50% 50%
4	MA	2	 100%
4	OA	2	 100%
4	QA	2	 50% 50%
4	RA	2	 50% 50%
4	e	2	 50% 50%
4	f	2	 50% 50%
4	i	2	 100%
4	j	2	 100%
4	m	2	 100%
4	n	2	 100%
4	o	2	 50% 50%
4	p	2	 50% 50%
4	q	2	 100%
4	s	2	 50% 50%

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Mol	Chain	Length	Quality of chain
4	t	2	 50% 50%
4	u	2	 50% 50%
4	v	2	 100%
4	x	2	 50% 50%
5	AA	4	 25% 50% 25%
5	FA	4	 100%
5	KA	4	 75% 25%
5	PA	4	 25% 25% 50%
5	g	4	 50% 50%
5	l	4	 50% 50%
6	3	3	 33% 33% 33%
6	5	3	 100%
6	CA	3	 33% 67%
6	DA	3	 33% 67%
6	EA	3	 33% 33% 33%
6	GA	3	 33% 67%
6	LA	3	 33% 67%
6	NA	3	 67% 33%
6	h	3	 67% 33%
6	k	3	 33% 67%
6	r	3	 33% 33% 33%
6	w	3	 33% 33% 33%
6	y	3	 100%
7	z	5	 20% 40% 40%
8	0	4	 25% 75%

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	MA	1	-	-	X	-
4	NAG	m	1	-	-	X	-
4	NAG	q	2	-	-	X	-
6	NAG	GA	1	-	-	X	-
6	NAG	GA	2	-	-	X	-
6	NAG	r	1	-	-	X	-
8	NAG	0	2	-	-	X	-
9	CUO	A	5001	-	-	X	-
9	CUO	C	3401[A]	-	-	X	-
9	CUO	C	3401[B]	-	-	X	-
9	CUO	F	3401[A]	-	-	X	-
9	CUO	F	3401[B]	-	-	X	-
9	CUO	I	3401[A]	-	-	X	-
9	CUO	L	3401[A]	-	-	X	-
9	CUO	L	3401[B]	-	-	X	-
9	CUO	M	2105	-	-	X	-
9	CUO	O	3401[A]	-	-	X	-
9	CUO	O	3401[B]	-	-	X	-
9	CUO	R	3401[A]	-	-	X	-
9	CUO	S	2104	-	-	X	-
9	CUO	U	3401[A]	-	-	X	-
9	CUO	U	3401[B]	-	-	X	-
9	CUO	X	3401[A]	-	-	X	-
9	CUO	X	3401[B]	-	-	X	-
9	CUO	a	3401[A]	-	-	X	-
9	CUO	a	3401[B]	-	-	X	-
9	CUO	d	3401[A]	-	-	X	-
9	CUO	d	3401[B]	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 261470 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 hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	D	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	G	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	J	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	M	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	P	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	S	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	V	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	Y	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	b	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			

- Molecule 2 is a protein called hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	E	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	H	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	K	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	Q	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	T	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	W	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	Z	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	c	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			

- Molecule 3 is a protein called hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	F	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	I	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	L	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	O	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	R	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	U	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	X	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	a	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	d	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	e	2	Total 28	C 16	N 2	O 10	0	0	0
4	f	2	Total 28	C 16	N 2	O 10	0	0	0
4	i	2	Total 28	C 16	N 2	O 10	0	0	0
4	j	2	Total 28	C 16	N 2	O 10	0	0	0
4	m	2	Total 28	C 16	N 2	O 10	0	0	0
4	n	2	Total 28	C 16	N 2	O 10	0	0	0
4	o	2	Total 28	C 16	N 2	O 10	0	0	0
4	p	2	Total 28	C 16	N 2	O 10	0	0	0
4	q	2	Total 28	C 16	N 2	O 10	0	0	0
4	s	2	Total 28	C 16	N 2	O 10	0	0	0
4	t	2	Total 28	C 16	N 2	O 10	0	0	0
4	u	2	Total 28	C 16	N 2	O 10	0	0	0
4	v	2	Total 28	C 16	N 2	O 10	0	0	0
4	x	2	Total 28	C 16	N 2	O 10	0	0	0
4	1	2	Total 28	C 16	N 2	O 10	0	0	0
4	2	2	Total 28	C 16	N 2	O 10	0	0	0
4	4	2	Total 28	C 16	N 2	O 10	0	0	0
4	6	2	Total 28	C 16	N 2	O 10	0	0	0
4	7	2	Total 28	C 16	N 2	O 10	0	0	0
4	8	2	Total 28	C 16	N 2	O 10	0	0	0
4	9	2	Total 28	C 16	N 2	O 10	0	0	0
4	BA	2	Total 28	C 16	N 2	O 10	0	0	0

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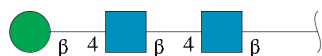
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	HA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	IA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	JA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	MA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	OA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	QA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	RA	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



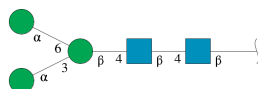
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	g	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	l	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	AA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	FA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	KA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	PA	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



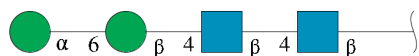
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	h	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	k	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	r	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	w	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	y	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	3	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	5	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	CA	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	DA	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	EA	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	GA	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	LA	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	NA	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



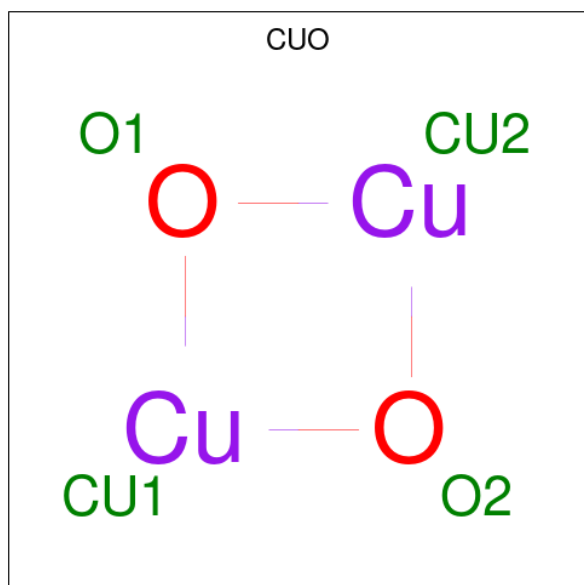
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	z	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	0	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 9 is CU2-O2 CLUSTER (CCD ID: CUO) (formula: Cu_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	Cu	O	0	0
			4	2	2		
9	A	1	Total	Cu	O	0	0
			4	2	2		
9	A	1	Total	Cu	O	0	0
			4	2	2		
9	A	1	Total	Cu	O	0	0
			4	2	2		
9	A	1	Total	Cu	O	0	1
			8	4	4		
9	B	1	Total	Cu	O	0	0
			4	2	2		
9	B	1	Total	Cu	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	Cu	O	0	1
			8	4	4		
9	D	1	Total	Cu	O	0	0
			4	2	2		
9	D	1	Total	Cu	O	0	0
			4	2	2		
9	D	1	Total	Cu	O	0	0
			4	2	2		
9	D	1	Total	Cu	O	0	0
			4	2	2		
9	D	1	Total	Cu	O	0	1
			8	4	4		
9	E	1	Total	Cu	O	0	0
			4	2	2		
9	E	1	Total	Cu	O	0	0
			4	2	2		
9	F	1	Total	Cu	O	0	1
			8	4	4		
9	G	1	Total	Cu	O	0	1
			8	4	4		
9	G	1	Total	Cu	O	0	0
			4	2	2		
9	G	1	Total	Cu	O	0	0
			4	2	2		
9	G	1	Total	Cu	O	0	0
			4	2	2		
9	G	1	Total	Cu	O	0	0
			4	2	2		
9	H	1	Total	Cu	O	0	0
			4	2	2		
9	H	1	Total	Cu	O	0	0
			4	2	2		
9	I	1	Total	Cu	O	0	1
			8	4	4		
9	J	1	Total	Cu	O	0	0
			4	2	2		
9	J	1	Total	Cu	O	0	0
			4	2	2		
9	J	1	Total	Cu	O	0	0
			4	2	2		
9	J	1	Total	Cu	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	J	1	Total 8	Cu 4	O 4	0	1
9	K	1	Total 4	Cu 2	O 2	0	0
9	K	1	Total 4	Cu 2	O 2	0	0
9	L	1	Total 8	Cu 4	O 4	0	1
9	M	1	Total 8	Cu 4	O 4	0	1
9	M	1	Total 4	Cu 2	O 2	0	0
9	M	1	Total 4	Cu 2	O 2	0	0
9	M	1	Total 4	Cu 2	O 2	0	0
9	M	1	Total 4	Cu 2	O 2	0	0
9	M	1	Total 4	Cu 2	O 2	0	0
9	N	1	Total 4	Cu 2	O 2	0	0
9	N	1	Total 4	Cu 2	O 2	0	0
9	O	1	Total 8	Cu 4	O 4	0	1
9	P	1	Total 4	Cu 2	O 2	0	0
9	P	1	Total 4	Cu 2	O 2	0	0
9	P	1	Total 4	Cu 2	O 2	0	0
9	P	1	Total 4	Cu 2	O 2	0	0
9	P	1	Total 8	Cu 4	O 4	0	1
9	Q	1	Total 4	Cu 2	O 2	0	0
9	Q	1	Total 4	Cu 2	O 2	0	0
9	R	1	Total 8	Cu 4	O 4	0	1
9	S	1	Total 8	Cu 4	O 4	0	1

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	S	1	Total 4	Cu 2	O 2	0	0
9	S	1	Total 4	Cu 2	O 2	0	0
9	S	1	Total 4	Cu 2	O 2	0	0
9	S	1	Total 4	Cu 2	O 2	0	0
9	T	1	Total 4	Cu 2	O 2	0	0
9	T	1	Total 4	Cu 2	O 2	0	0
9	U	1	Total 8	Cu 4	O 4	0	1
9	V	1	Total 4	Cu 2	O 2	0	0
9	V	1	Total 4	Cu 2	O 2	0	0
9	V	1	Total 4	Cu 2	O 2	0	0
9	V	1	Total 4	Cu 2	O 2	0	0
9	V	1	Total 8	Cu 4	O 4	0	1
9	W	1	Total 4	Cu 2	O 2	0	0
9	W	1	Total 4	Cu 2	O 2	0	0
9	X	1	Total 8	Cu 4	O 4	0	1
9	Y	1	Total 8	Cu 4	O 4	0	1
9	Y	1	Total 4	Cu 2	O 2	0	0
9	Y	1	Total 4	Cu 2	O 2	0	0
9	Y	1	Total 4	Cu 2	O 2	0	0
9	Y	1	Total 4	Cu 2	O 2	0	0
9	Z	1	Total 4	Cu 2	O 2	0	0

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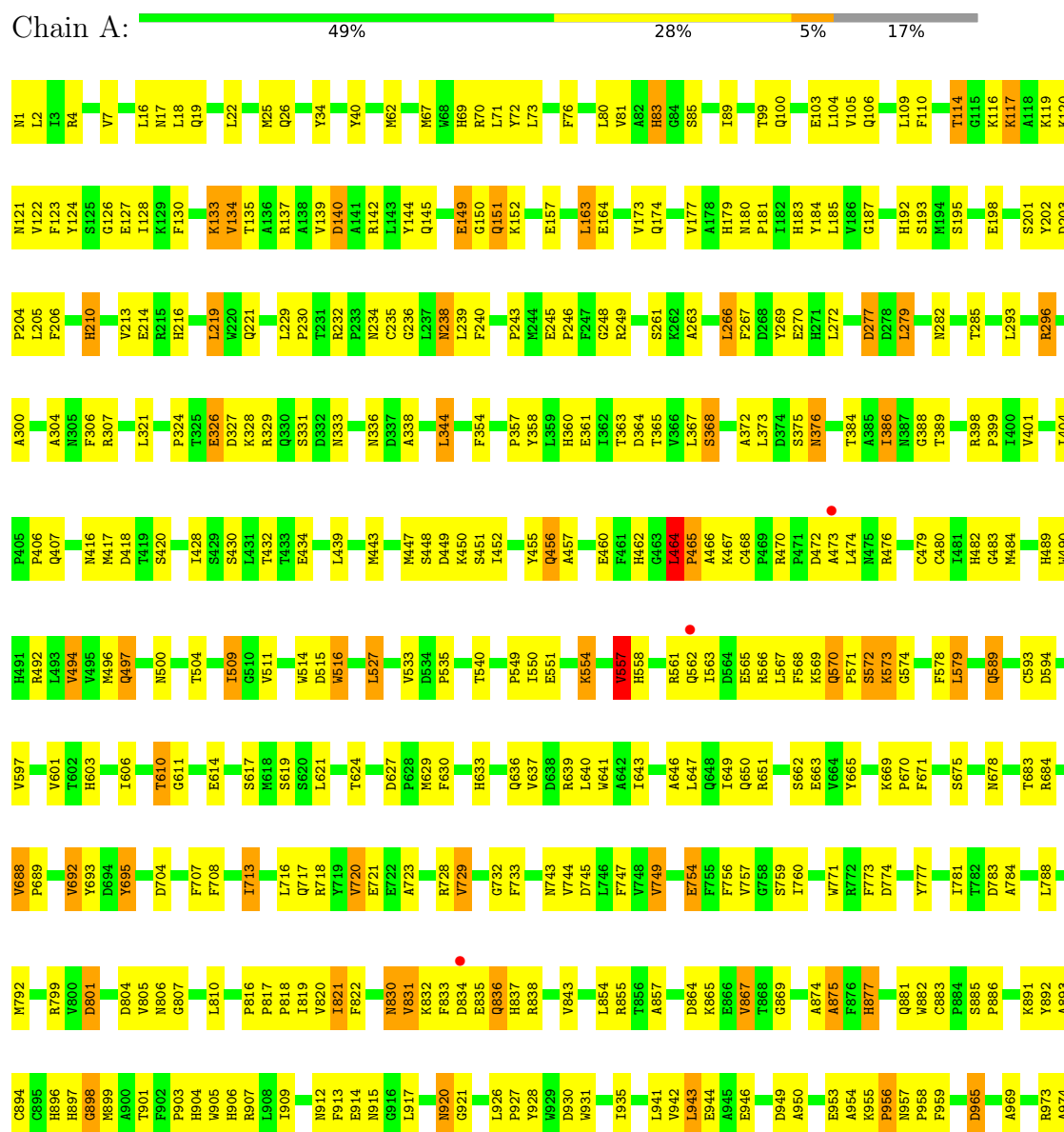
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	Z	1	Total 4	Cu 2	O 2	0	0
9	a	1	Total 8	Cu 4	O 4	0	1
9	b	1	Total 8	Cu 4	O 4	0	1
9	b	1	Total 4	Cu 2	O 2	0	0
9	b	1	Total 4	Cu 2	O 2	0	0
9	b	1	Total 4	Cu 2	O 2	0	0
9	b	1	Total 4	Cu 2	O 2	0	0
9	c	1	Total 4	Cu 2	O 2	0	0
9	c	1	Total 4	Cu 2	O 2	0	0
9	d	1	Total 8	Cu 4	O 4	0	1

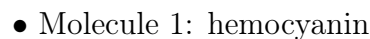
3 Residue-property plots

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

- Molecule 1: hemocyanin



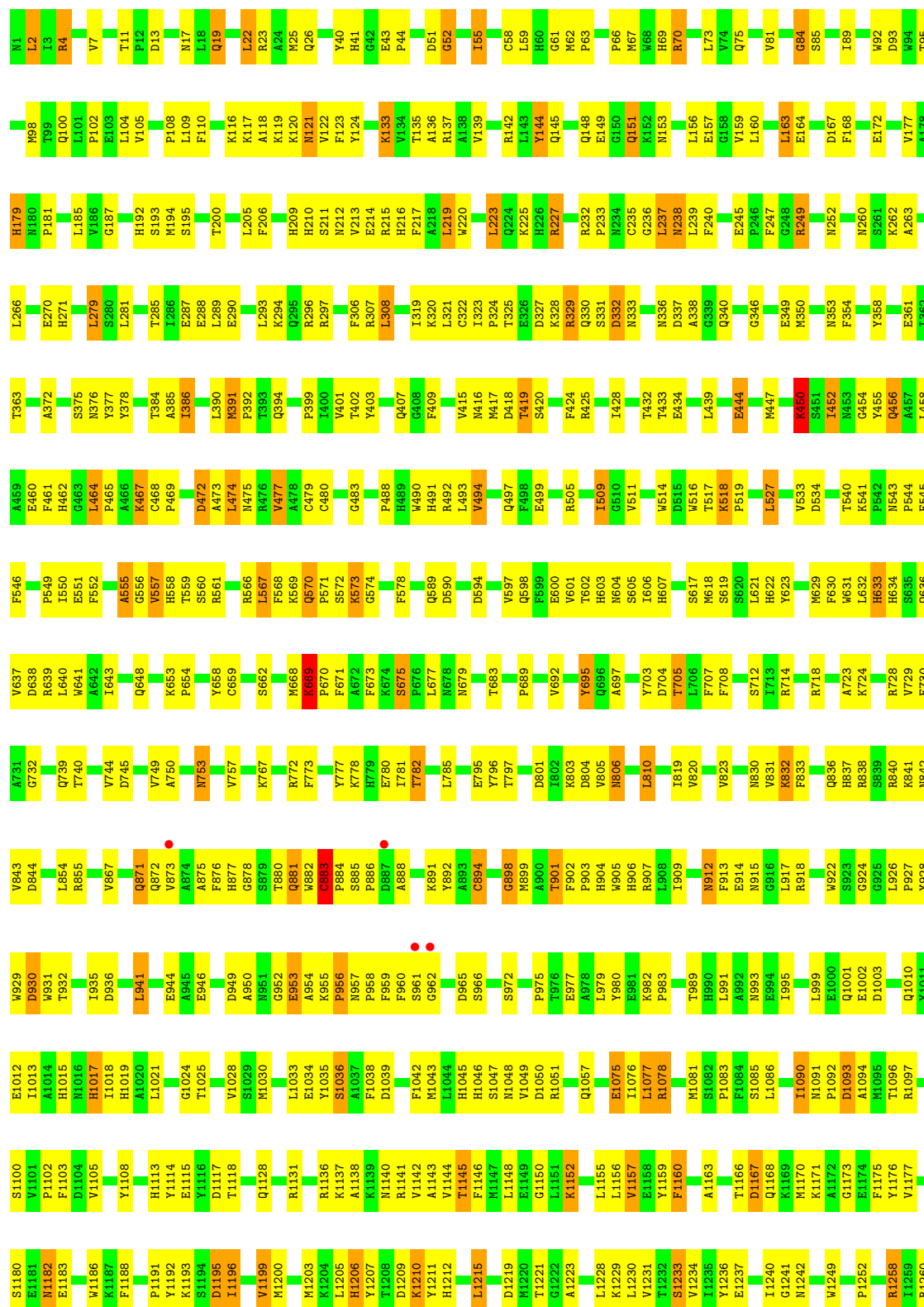




WORLDWIDE
PDB
PROTEIN DATA BANK

● Molecule 1: hemocyanin

Chain J:  47% 31% 5% 17%







LEU	ASN	LEU	LEU	ASP	ASP	PRO	MET	ARG	PRO	PHE	GLY	PHE	ASN	ASN	LYS	THR	THR	ASN	GLN	ALA	ASP	HIS	LEU	THR	THR	ASP	VAL	ASP	PRO	CYS	VAL	PRO	P44	VAL	PHE	VAL	GLU	TYR	GLN	ASN	SER	SER	LEU	ASN	TYR	LYS	PHE	ASP	SER	LEU	SER	PHE	GLY	LEU	SER	ILE	ARG	LEU	ASP	ASP	LEU	GLU
SER	ARG	GLN	SER	HIS	ASP	ARG	VAL	PHE	ALA	GLY	PHE	TRP	LEU	SER	THR	ILE	GLY	VAL	ASP	ASN	ASN	THR	ALA	LEU	THR	THR	ASP	VAL	PRO	VAL	PRO	ASP	ILE	GLY	VAL	GLU	GLU	GLN	ASN	ASP	SER	LEU	ASN	TYR	LYS	PHE	ASP	SER	LEU	SER	PHE	GLY	LEU	SER	ILE	ARG	LEU	ASP	ASP	LEU	GLU	

● Molecule 1: hemocyanin

Chain P: 49% 28% 6% 17%

H1046	H1047	N1048	D1049	R1051	T1055	K1065	A1066	Y1067	N1068	A1073	I1074	E1075	I1076	R1078	K1079	P1080	M1081	S1082	P1083	F1084	S1085	L1086	D1089	I1090	N1091	P1092	D1093	S1100	V1101	P1102	V1105	K1109	H1113	D1117	T1118	E1119	I1120	L1121	N1122	S1125	I1126	A1127	K1128	S1130	L1131			
T971	S972	A974	P975	T976	E977	L979	G980	E981	K982	P983	D984	K987	H990	L991	I995	S997	A996	L999	Q1001	E1002	D1003	F1007	Y1011	I1012	I1013	A1014	H1015	N1016	H1017	I1018	G1024	T1025	E1026	A1027	V1028	L1033	E1034	Y1035	S1036	A1037	F1038	D1039	P1040	T1041	F1042	M1043	L1044	
S885	K891	A893	C894	C895	H896	H897	G898	E981	K982	P983	D984	H904	W905	H906	R907	L908	I909	E914	N915	G916	L917	L926	P927	Y928	W929	D930	W931	I935	P939	A940	L941	E944	A945	Y947	T948	D949	A950	E953	A954	K955	P956	N957	P958	S961	G962	I964	R965	
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
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L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
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L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
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L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
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L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802	K803	D804	W805	L810	P816	P817	L734	L735	M736	Q739	W744	D745	L746	V749	E754	N841	N842	W843	T847	R855	E865	E866	W867	T868	G869	Y870	Q871	K872	W873	N957	P958	S961	T980	Q981	W982	C983
L788	G789	V790	D791	W792	A794	E795	T796	L798	W799	W800	D801	L802</																																				

T1133	K1210	V1308	T1407	R1494	L1615	GLU	ARG	ASP	SER	HIS
N1134	Y1211	H1309	F1411	S1497	K1616	ASN	LYS	PRO	ARG	ILE
R1135	H1212	T1310	N1498	N1498	K1617	LEU	PRO	ILE	PRO	CYS
K1137	V1213	C1311	T1414	S1499	L1618	LEU	ASP	PHE	ASN	VAL
	D1219	C1312	T1500	T1500	Q1622	ALA	GLN	LEU	VAL	ILE
N1140	M1220	L1313	C1417	T1507	R1627	ARG	LEU	HIS	PHE	GLY
R1141	T1221	H1314	E1420	T1507	Y1628	GLY	PHE	HIS	ASP	VAL
V1142	G1222	G1315	V1421	S1511	E1629	SER	ASN	SER	TYR	GLU
A1143	A1223	M1316	H1422	S1511	M1630	ASP	ASN	THR	ASN	HIS
V1144	E1224	P1317	Y1423	V1516	E1631	VAL	ARG	VAL	ASN	GLU
T1145	V1225	V1318	E1424	V1516	E1631	ALA	TYR	ASP	SER	CYS
	T1226	F1319	V1425	Y1519	M1636	VAL	LEU	ARG	LEU	ASP
E1149	L1230	P1320	H1426	Y1519	G1637	PRO	TYR	LEU	ASN	ASN
	K1152	H1321	H1427	H1524	G1637	GLY	GLY	TRP	TYR	TYR
K1153	S1233	W1322	H1427	Y1525	S1638	TRP	HIS	ALA	LYS	LYS
L1156	Y1236	R1324	I1430	D1528	I1640	TRP	LEU	ALA	PHE	ASP
V1157		L1325	W1433	T1529	T1641	ILE	PHE	GLN	SER	LEU
	G1241	L1329		T1530	Q1642	GLU	ALA	ASP	LEU	ASP
F1160	N1242	V1330	G1436	E1541	K1643	PRO	PHE	ALA	PHE	PHE
T1161	F1243	E1331	R1437	E1541	F1645	ALA	GLU	GLN	GLU	GLN
A1162	R1247	D1332	D1438	I1542	P1646	ASP	HIS	ARG	HIS	ASP
A1163	R1248	E1333	V1439	I1543	P1647	LEU	THR	GLY	THR	GLY
			H1440	L1544	P1648	PRO	ASP	LYS	PHE	LEU
T1166	R1337	R1337	S1441	D1551	T1649	GLY	CYS	LEU	CYS	ILE
D1167	W1249	G1338	M1442	D1559	F1652	LEU	PHE	TYR	ASP	ARG
Q1168	I1250	S1339	D1446	L1559		ILE	ASP	ASN	LEU	LEU
K1169	P1252	G1340		H1560	D1656	ASP	VAL	VAL	ASP	ASP
M1170	S1255		Y1450	G1561	VAL	GLU	HIS	ALA	LEU	LEU
K1171				I1562	GLU	THR	PHE	ASN	LEU	LEU
A1172	R1258	G1173	F1454	K1563	PHE	TYR	GLU	CYS	GLY	GLY
E1174	I1259	D1347	F1455	K1563	GLU	LYS	VAL	VAL	VAL	GLY
F1175	R1260	W1348	L1456	V1568	GLU	HIS	LEU	LEU	LEU	ARG
Y1176			H1457	R1569	ASP	PRO	HIS	ASN	ASN	GLN
V1177	F1266	L1355	H1458	C1573	THR	LYS	ASN	LEU	LEU	SER
L1178		P1356		V1574	TRP	THR	SER	LEU	LEU	THR
G1179	M1271	R1357	V1461	V1574	ARG	ASN	ILE	ASN	ASN	HIS
S1180	E1272	L1358	D1462	P1575	ASP	THR	ILE	ASP	ASP	ASP
E1181	S1273		W1465	T1576	VAL	ASP	TRP	PRO	PRO	ARG
N1182	L1274	I1372		G1577	VAL	ILE	ILE	ARG	ARG	PHE
E1183			E1470	I1578	THR	HIS	ILE	PRO	ALA	ALA
	K1279	P1376	L1471	G1579	SER	GLY	GLY	PRO	PHE	GLY
W1186	Q1280		Q1472	E1580	ALA	PRO	GLY	PHE	ASN	GLY
K1187	R1286	G1380	R1473	E1581	ASN	THR	ASN	PRO	ASN	PHE
			Y1474	N1582	ARG	HIS	THR	ASN	ASN	THR
Y1192	F1293	T1369	R1475	C1583	ILE	GLY	PHE	PRO	ILE	ILE
K1193			K1476	G1584	ARG	LYS	HIS	HIS	SER	GLY
S1194	V1296	Q1394	L1477	A1587	ASN	TRP	ILE	ALA	MET	ILE
D1195	Q1299	P1395	Y1479	W1601	LYS	ARG	SER	ALA	SER	LYS
I1196		E1396		F1603	ASP	HIS	LEU	ASP	LEU	ASP
V1199	G1300	N1400	C1483	F1603	LEU	TYR	ALA	ASP	LEU	ALA
M1200	P1301	R1401	A1485	D1604	SER	LEU	PHE	THR	PHE	THR
M1203	S1302	Y1402		R1605	LYS	VAL	ALA	ALA	ALA	THR
	D1304	L1403	P1492		GLU	THR	ALA	ALA	ALA	ILE
D1209	G1305		M1493	E1614	ASP	VAL	TYR	TYR	TYR	

• Molecule 1: hemocyanin

Chain S: 50% 27% 6% 17%

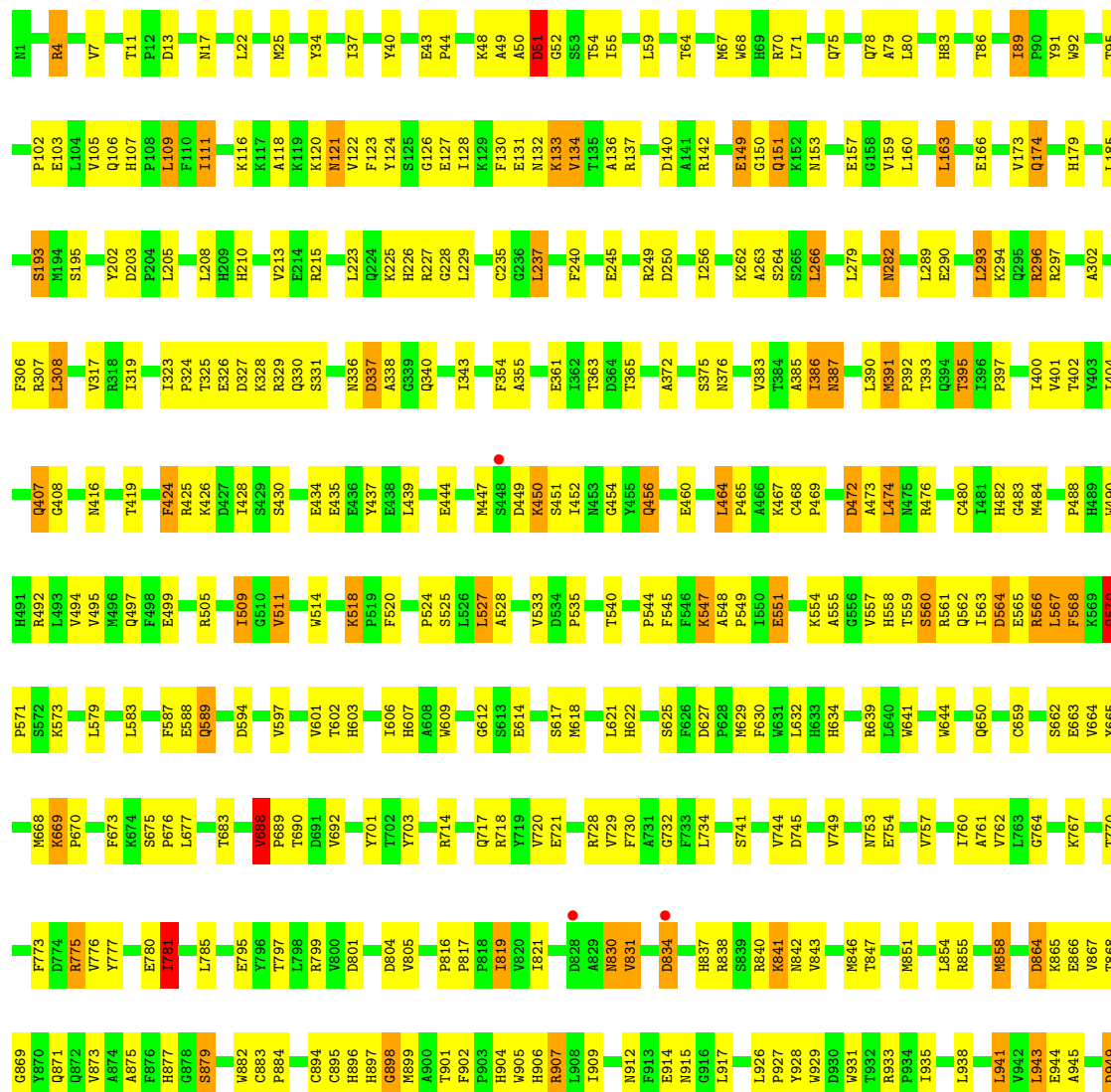
H1	V105	T200	H116	V105	H1
L2	L109	S201	K117	L109	L2
I3	F110	L205	K118	F110	I3
R4	I111	L205	K119	I111	R4
V7		L205	K120		V7
		L205	K121		
T11	K116	L208	K122	K116	T11
P12	K117	H209	V122	K117	P12
D13	A118	G209	Y124	A118	D13
E14	K119	S211	Y124	K119	E14
	K120	N212	E214	K120	
N17	N121	V213	E214	N121	N17
L16	V122	R215		V122	L16
Q19	Y124	Q221		Y124	Q19
V20	F123	H226		F123	V20
S21	Y124	R227		Y124	S21
L22					L22
W25	F130			F130	W25
	T135	G236		T135	
Y34	A136	N238		A136	Y34
I37	R137	L239		R137	I37
H41	R142	F240		R142	H41
G42	Q145	H241		Q145	G42
E43	Q148	E245		Q148	E43
P44	E149	P246		E149	P44
A49	G150	F247		G150	A49
A50	Q151	G248		Q151	A50
D51	K152	D250		K152	D51
I55	N153	K258		N153	I55
G61	E157	A263		E157	G61
M62	M161	L266		M161	M62
M67	E164	F267		E164	M67
W68	Q165	D277		Q165	W68
H69	E166	D278		E166	H69
R70					R70
L71	Q174	L281		Q174	L71
Y72	L175	M284		L175	Y72
L73	E176	T285		E176	L73
V74	H179	L286		H179	V74
Q75	L185	E287		L185	Q75
F76	V186	E288		V186	F76
E77	G187	L289		G187	E77
	G188	L292		G188	
V81	T191	R296		T191	V81
A82	H192	R297		H192	A82
H83	S193	R301		S193	H83
S85	M194			M194	S85
I89	P190			P190	I89
	S195			S195	

L1618	G1619	N1620	N1621	Q1622	R1627	N1498	S1499	T1500	L1632	T1633	A1634	V1635	N1636	G1637	S1638	K1639	T1640	T1641	K1642	I1643	I1644	I1651	D1656	VAL	GLU	PHE	GLU	GLU	ASP	THR	TRP	ARG	ASP	VAL	VAL	THR	SER	ALA	ASN	ARG	ILE	ARG	ARG	ASN	LEU	LYS	ASP	LEU	SER	LYS	GLU	ASP	MET	PHE	SER	LEU
W1490	Q1491	M1492	M1493	R1494	M1498	S1499	T1500	L1511	S1512	P1513	V1516	V1517	L1523	L1524	F1532	I1537	E1541	G1549	F1557	L1558	L1559	S1565	N1566	D1567	V1568	P1574	P1575	I1578	G1579	E1580	E1581	N1582	C1583	S1591	G1594	G1595	E1596	T1597	W1601	D1604	R1605	R1608	L1616	K1617												
T1407	L1408	T1414	F1415	F1416	V1421	H1422	H1423	H1424	H1425	H1426	H1427	H1428	H1429	H1430	H1431	S1432	H1433	G1436	H1437	H1438	H1439	H1440	M1442	D1446	Y1447	Y1450	F1454	F1455	F1456	N1460	V1461	ALA	D1462	W1465	A1466	W1467	Q1469	E1470	R1473	L1477	C1484	L1485	L1486	L1487	L1488	M1489										
W1322	H1323	R1324	L1325	S1328	E1331	D1332	E1333	L1334	L1335	A1336	R1337	G1338	S1339	G1340	V1341	W1346	D1347	W1348	F1352	D1353	E1354	R1357	L1358	I1359	A1362	S1367	R1368	T1369	L1370	F1378	K1379	G1380	K1381	I1382	S1383	F1384	E1385	D1390	R1391	D1392	Q1393	P1395	E1396	L1397	F1398	G1399	L1403									
I1217	D1218	T1219	A1223	E1224	V1225	L1228	K1229	L1230	V1231	T1232	S1233	V1234	I1235	V1236	G1239	R1248	W1249	I1250	S1251	R1258	I1259	R1260	L1263	M1271	R1275	E1284	G1285	R1286	V1296	Q1299	I1300	P1301	D1304	G1305	T1306	V1307	V1308	C1312	L1313	H1314	G1315	F1319														
W1025	E1026	A1027	V1028	M1030	E1034	Y1035	S1036	H1046	S1047	N1048	V1049	Q1052	R1051	T1055	W1056	Q1057	A1058	K1059	Q1060	K1061	F1062	A1063	G1064	K1065	P1066	A1067	I1074	H1075	I1076	L1077	R1078	M1081	S1082	P1083	S1084	S1085	L1086	A1087	D1088	I1089	N1090	N1091	Y1011	E1012	H1015	N1016	H1017	I1018	H1019	A1020	E1021					
E1120	N1121	N1122	I1126	R1131	E1132	T1133	K1137	M1140	T1145	K1152	K1153	S1154	L1155	V1157	F1160	L1161	A1162	A1163	D1164	G1165	T1166	D1167	Q1168	K1169	M1170	K1171	A1172	G1173	E1174	Y1176	G1179	S1180	E1181	M1182	E1183	W1186	R1190	D1195	T1196	C1312	L1313	H1314	G1315	F1319												
R865	E866	V867	T868	G869	Y870	Q871	G872	F876	H877	S879	T880	Q881	A888	A889	Q890	K891	C895	H896	H897	G898	N899	F902	P903	P904	H905	H906	R907	H908	L909	F913	E914	N915	G916	L917	N920	L926	P927	Y928	K929	D930	K931	T932	L935	L941	V942	L943	E944	N958	A945							
F773	D774	Y777	E780	T781	T782	L785	L788	W792	E795	T796	T797	L798	R799	W800	D801	L802	K803	D804	W805	N806	G807	T808	A809	L810	T813	P816	P817	P818	T819	V820	D828	V831	K832	F833	D834	E835	H837	B838	K841	N842	W843	L854	R855	V942	L943	E944	N958	A945								
H686	S687	P688	P689	D691	E696	Y701	T705	F708	S712	T713	R714	E715	L716	Q717	R718	Y719	W720	E721	E722	K724	R728	P903	P904	L810	T813	P816	P817	P818	T819	V820	D828	V831	K832	F833	D834	E835	H837	B838	K841	N842	W843	L854	R855	V942	L943	E944	N958	A945								
V601	T602	H603	T606	W609	S613	E614	P615	M618	L621	H622	F623	T624	D627	P628	M629	F630	H633	Q636	V637	K724	R728	P903	P904	L810	T813	P816	P817	P818	T819	V820	D828	V831	K832	F833	D834	E835	H837	B838	K841	N842	W843	L854	R855	V942	L943	E944	N958	A945								
H516	T517	K518	L523	P524	S525	L526	L527	V533	T540	N543	S544	L545	Q546	E548	P549	T550	E551	K554	V557	H558	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598										
S420	R423	F424	I428	T432	E435	F446	K450	S451	L452	Y455	Q456	E460	F461	H462	G463	L464	P465	P471	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598											
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E361	L362	T363	A372	D472	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T572	S573	G574	D575	H576	L579	L585	E588	Q589	F590	C593	D594	V597	Q598												
N305	F306	R307	L308	R318	T319	K320	Q329	S331	D332	N336	N353	F354	A355	E3																																										

PRO	ASP	PHE	ASP	LEU	ARG
ILE	VAL	LEU	GLN	LEU	ALA
GLY	PHE	HIS	LEU	PHE	ARG
VAL	HIS	HIS	PHE	GLY	ALA
GLU	TYR	SER	ASN	SER	PHE
HIS	GLN	THR	ASN	ASP	LYS
ASN	ASN	VAL	ARG	VAL	ARG
ASP	SER	ASN	TYR	ALA	THR
ASP	LEU	ARG	TYR	VAL	ASP
ASN	ASN	LEU	TYR	PRO	ASP
	TYR	TRP	GLU	TYR	GLY
	LYS	ALA	HIS	TRP	ARG
	PHE	ILE	ALA	ASP	TYR
	SER	TRP	LEU	TRP	GLU
	ASP	GLN	PHE	ILE	GLU
	LEU	ASP	ALA	GLU	ILE
	PHE	LEU	PHE	PRO	ALA
	SER	GLN	GLU	PHE	ALA
	SER	ARG	HIS	ASP	PHE
	GLY	TYR	THR	SER	PHE
	LEU	LYS	ASP	LEU	GLY
	ILE	LEU	PHE	PRO	LEU
	PRO	ASP	CYS	GLY	PRO
	ARG	TYR	ASP	LEU	ALA
	LEU	ASN	GLU	ILE	GLN
	ASP	ALA	HIS	GLU	CYS
	LEU	VAL	VAL	ASP	PRO
	ASN	ASN	HIS	GLU	ASN
	LEU	ASN	PHE	THR	ALA
	GLU	CYS	GLU	TYR	ASP
	GLU	ALA	VAL	LYS	GLY
	GLN	ASN	HIS	PRO	ASN
	SER	LEU	SER	THR	HIS
	HIS	ASN	ILE	ASN	THR
	ASP	ASP	HIS	CYS	THR
	ARG	PRO	SER	ASP	CYS
	VAL	MET	TRP	ILE	GLY
	PHE	ARG	ILE	GLU	HIS
	ALA	PRO	GLY	ASN	GLY
	GLY	PHE	GLY	PRO	MET
	PHE	ASN	PRO	PHE	THR
	TRP	ASN	ASN	HIS	THR
	LEU	LYS	PRO	HIS	PHE
	GLY	THR	HIS	GLY	PRO
	ILE	ASN	MET	LYS	HIS
	LYS	GLN	SER	ILE	THR
	ALA	ASP	SER	SER	HIS
	SER	HIS	LEU	PHE	ARG
	ASP	THR	ASP	ASP	TYR
	VAL	PHE	ALA	VAL	LEU
	THR	THR	ALA	THR	SER
	ASN	THR	ALA	THR	VAL
	ILE	ASN	TYR	VAL	VAL
	HIS	SER	ASP	ARG	GLU
	ILE	ARG	PRO	LYS	ASN
	CYS	ASN	ILE	VAL	GLU
	VAL	PRO	PHE	ARG	LEU

- Molecule 1: hemocyanin

Chain V: 48% 29% 5% 17%



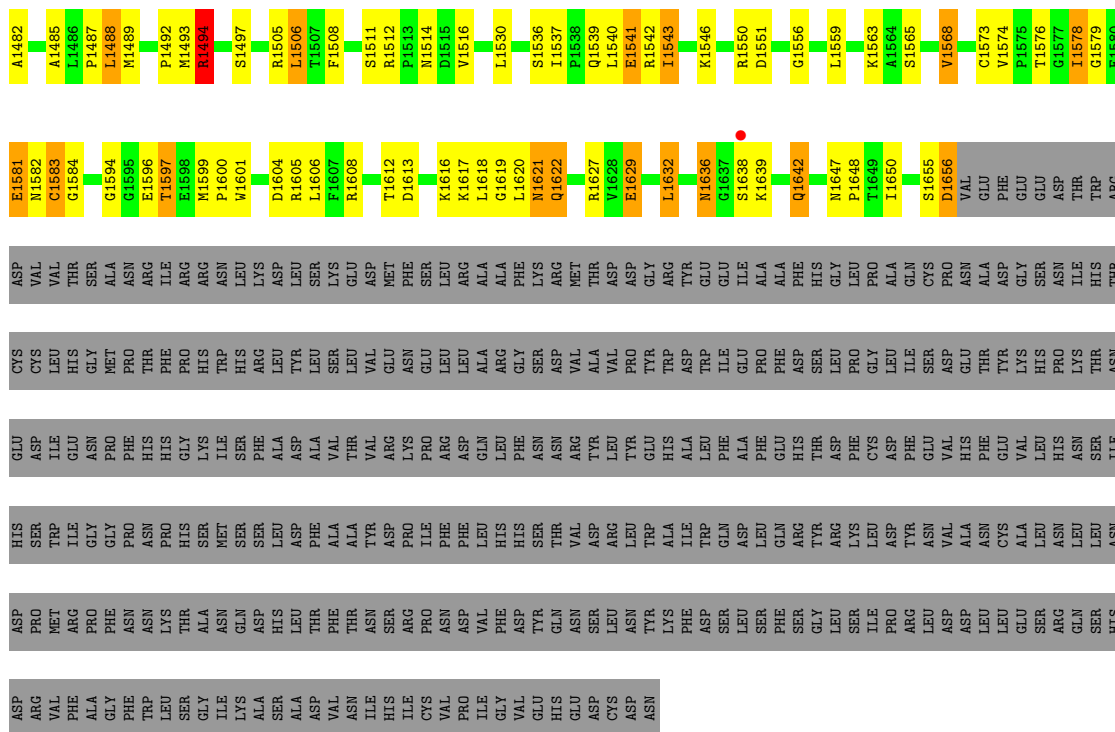
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N951	G1024	P1102	K1187	E1396	P1492	V1577	GLU	LYS	VAL	ALA	GLU
G952				L1397	M1493	G1577	GLU	HIS	LEU	ASN	SER
E953	V1028	V1105	G1295	N1400	P1494	T1578	ASP	PRO	HIS	ASN	ARG
P956	M1030	F1107	P1191	H1406	P1496	E1580	THR	LYS	ASN	LEU	GLN
N957	A1031	N1107	Y1192	T1407	S1497	E1581	THR	ASN	ILE	ASN	HIS
P958	S1032	Y1108	D1195	T1407	N1498	N1582	ASP	GLU	HIS	ASP	ASP
F959	S1033	Y1116	T1196	L1408	C1499	C1583	VAL	ASP	ASP	PRO	ARG
F960	E1034	D1117	Y1199	F1409	T1500	G1584	VAL	ILE	TRP	MET	VAL
S961	Y1035	T1118	V1199	F1410	N1505	N1585	THR	GLU	ILE	ARG	PHE
G962	S1036	L1119	M1200	F1411	R1505	Y1586	SER	ASN	GLY	PRO	ALA
A963	A1037	L1122	M1203	T1414	T1509	A1587	ALA	PRO	GLY	PHE	ALA
D964	F1038	N1122	M1203	D1415	M1510	F1590	ASN	PHE	PRO	ASN	PHE
D965	D1039	G1123	K1204	D1415	N1510	F1590	THR	HIS	ASN	ASN	THR
	P1040	L1124	L1205	L1421	R1512	S1591	ILE	HIS	PRO	LYS	THR
S972	I1041	S1125	H1206	H1421	R1512	G1594	ARG	GLY	HIS	ALA	THR
R973	F1042	Y1126	Y1207	H1422	P1513		ARG	LYS	ILE	ASN	GLN
A974	M1043	L1129	T1208	Y1423	V1516		ASN	ILE	ILE	ASN	GLN
P975	L1044	L1129	D1209					SER	SER	ASN	GLN
	H1045		K1210	L1426			LEU	LYS	PHE	ASN	ALA
L979	H1046	R1136	E1214	H1427	Y1519	P1600	LYS	ALA	ALA	HIS	ALA
Y980	S1047	K1137	L1215	H1427	W1601	W1601	ASP	ALA	ASP	LEU	ALA
E981	N1048	P1137	L1215	I1430	D1604	D1605	LEU	VAL	PHE	ASP	THR
X982	V1049	N1140	T1221	W1433	L1523	L1605	LYS	THR	ALA	THR	THR
P983		R1141		L1434	H1524		GLU	THR	ALA	THR	ASN
D984	T1055	Y1142		G1435	Y1525	E1614	ASP	VAL	VAL	VAL	ILE
F985	W1056	L1143		G1436	A1526	L1615	MET	GLU	ARG	ASP	HIS
G986		V1144		G1437	Y1527	L1616	PHE	ASN	LYS	PRO	ILE
X987	L1059	T1145	K1229	R1437	D1528	K1617	GLU	PRO	PRO	ILE	ILE
Y988		F1146	L1230	T1438	T1529		LEU	ARG	ARG	PHE	PHE
	F1062	M1147	V1231	V1439	L1530	L1620	ARG	ASP	ASP	ASP	PRO
L991	R1063	L1148	T1232	H1440	N1531	N1621	ALA	GLN	LEU	VAL	ILE
A992	E1149	G1150	S1233	S1441	F1532	Q1622	ALA	LEU	PHE	PHE	GLY
N993	K1065	G1150	T1234	M1442			PHE	GLY	GLY	ASP	VAL
E994			I1235	L1333	I1537	R1627	LYS	ASN	ASN	LYS	TYR
Y995	M1071	K1153	Y1236	L1334	P1538	V1628	ASP	ASN	THR	ALA	ILE
					Q1539	E1629	ARG	VAL	ARG	ASP	TRP
L999	I1074	L1156	I1240	V1343	Y1539	E1629	MET	VAL	TYR	LEU	TRP
E1000	E1075	V1157			L1540	P1630	THR	ALA	ILE	PHE	GLN
Q1001	I1076	F1160	F1243	E1350	E1541	E1631	THR	LEU	ALA	LEU	ASP
E1002	L1077	I1161	G1244	P1351	R1542	L1632	GLY	TYR	PRO	TYR	LEU
	R1078	A1162	E1245		K1546		GLY	TRP	TRP	ALA	TRP
C1005		A1162	G1246	P1356		N1636	ARG	ALA	HIS	ALA	ILE
	M1081	A1163	R1247	R1357	G1549	K1639	TYR	ASP	ALA	ASP	TRP
E1008	S1082		R1248	L1358		T1640	GLU	TRP	GLN	SER	GLN
V1009	P1083	T1166	W1249	I1359	L1559	T1641	ILE	ILE	ALA	LEU	ASP
Q1010		D1167	I1250			Q1642	ALA	PHE	GLU	LEU	PHE
Y1011	L1086	M1170	R1258	S1367	I1562	T1644	ALA	GLU	GLU	GLN	ARG
E1012	A1087	K1171	Y1259	R1368	K1563	F1645	PHE	HIS	THR	THR	ARG
I1013	S1088	A1172	R1260	T1372	A1564		GLY	HIS	ASP	ASP	GLY
A1014	D1089	G1173	R1260		S1565		GLY	ASP	ASP	ASP	LEU
H1015	I1090	O1174	E1267	K1381	A1566	T1649	LEU	PHE	PRO	LYS	LEU
N1016	N1091	E1174			D1567		PRO	CYS	CYS	ILE	ILE
H1017	P1092	F1175	E1267		D1567	F1652	ALA	ASP	ASP	ASP	PRO
H1018	D1093	V1176	M1271	D1390	R1569		GLN	ASP	ASP	ASP	ARG
H1019		V1177		R1591	V1570	S1655	CYS	PHE	PHE	GLU	LEU
A1020	T1096		L1274	D1392	Y1571	D1656	PRO	GLU	VAL	VAL	ASP
L1021	S1180		Q1280	T1393	I1572	VAL	ASN	HIS	ASN	ALA	ASP
V1022	E1181			Q1394	C1573	GLU	ALA	PHE	PHE	ASN	LEU

• Molecule 1: hemocyanin

Chain Y:  48% 29% 5% 17%

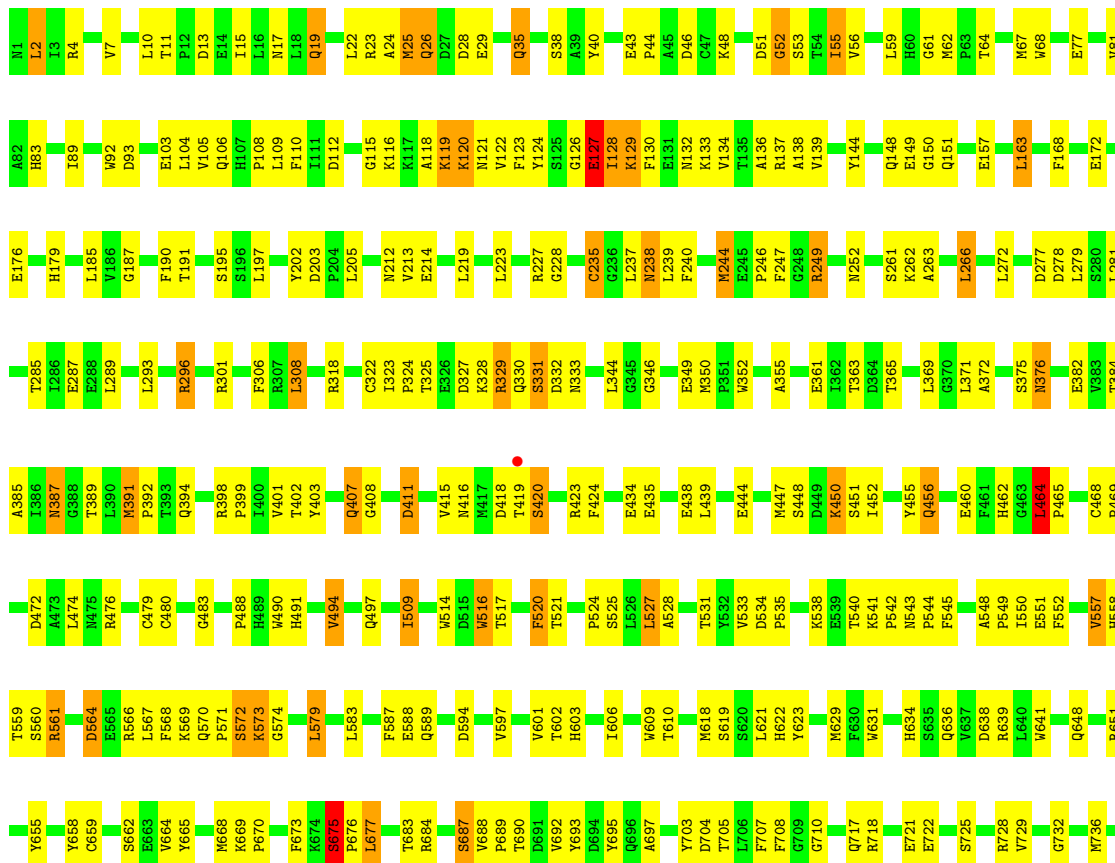
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E1396	C1311	R1190	F1103	E1012	L926	V848	V757	M688	E565	A473	T365	D250	Q145	G84
L1397	C1312	P1191	D1104	I1013	P927	V848	V757	K669	R566	L474	T371	D258	E166	S85
N1400	L1313	Y1192	V1105	H1015	Y928	N852	G758	P670	L567	R476	A372	K259	D167	L87
R1401	H1314	D1195	Y1108	N1016	Q929	A853	I760	A672	F568	G483	S375	N260	H170	Y91
L1403	M1315	I1196	H1113	H1017	D930	L854	K767	F673	K576	T486	K376	K262	F171	W92
Y1404	P1317	T1197	Y1114	I1018	W931	R855	K767	K674	Q570	G483	Y377	Z263	E172	D93
	V1318			H1019	T932			S675	D575	T486		S264	V173	W94
T1407	F1319	M1200	T1118	A1020	I935	A859	W771	P676	F578	H489	A385	S265	Q174	
F1411	P1320		L1021	V1022	I935	A860	R772	L677	L579	W490	I386	L266	V177	M98
T1414	H1321	M1203	L1119	G1023	L941	A862	F773	N678	L579	H491	N387	H271	A178	T99
D1415	L1121	V1213	L1121	G1024	E946	A863	D774	M679		R492	M391		H179	Q100
F1416	H1122		N1122	T1025	E947	S684	W776	T683	E588	L493	P392	D277	M180	E103
C1417	I1133	T1221	I1133	A1026	T948	R865	Y777	A694	C593	V494	P392	D278	P181	I104
	N1134		N1134	E1027	D948	E866	I781	S687	D594	Q497	Q394	L279	I182	V105
	R1135	D1227	R1135	S1028	A950	V867	I781	P689		F498	R398	S280	H184	
	K1137	K1229	K1137	M1030	N951	Y870	A784	T690	V597	E499	P399	L281	L185	L109
	N1140	K1229	N1140	L1033	K955	Q871	L785	D691	T602	I509	I400	N282	V186	T114
	R1141	K1229	R1141	I1041	N957	Q872	L788	V692	H603	G510	V401	T285	G187	G115
	V1142	P958	V1142	H1045	P958	T880	E795	Q696	M604	V511	T402	L289	F190	K117
	T1145	F959	T1145	H1046	F960	Q881	Y796		S605	W514	Q407	R296	S193	A118
	E1149	P960	E1149	H1047	S961	C883	T797	Y703		D515	G408	R297	M194	K119
	S1154	I964	S1154	N1048	I964	P884	L798	D704	W609	W516	D411	N305	S195	V122
	L1155	D065	L1155	V1049	D065	S885	R799	T705	T610	T517	V412	F306	S201	F123
	L1156	S966	L1156	D1060	S966	P886	W800	L706	G611	L527	N413	K307	Y202	Y124
	V1157	I967	V1157	R1051	I967	A888	I802	F707	G612		M414	L308	G126	S125
	Y1157	S972	Y1157	H1055	S972	K891	K803	G709	S619	T531	V415		L205	G127
	F1158	R973	F1158	W1056	R973	Y892	D804	G710	H622	Y532	N416	N316	F207	K133
	I1160	A974	I1160	L1059	A974	A893	G807	S712	V533	D534	M417	L321	L208	V134
	A1161	P975	A1161	C895	P975	C894	L810	R714	T624	T540	L422	I323	H209	T135
	A1162	T976	A1162	H896	T976	H897	L810	E715	M629	K541	R493	I324	H210	A136
	A1163	E977	A1163	H897	E977	G898	P817	L716	F630	P542	F424	P394	S211	R137
	G1064	A978	G1064	H898	A978	C899	P818	Q717	W631		R493	E326	N212	A138
	G1065	L979	G1065	M899	L979	A900	P819	R718	L632	F545	L439	D327	E214	V139
	A1070	Y980	A1070	A900	Y980	T901	I819	Y719	H633	K547	E444	K328	E214	D140
	I1074	E981	I1074	T901	E981		V823	W720		A548		R329	R215	A141
	E1075	K987	E1075	H904	K987	H904	V823	E721	V637	A548		R329	H216	R142
	I1076	Y988	I1076	W905	Y988	W905	I826	E722	D638	P649	S448	Q330	F217	L143
	L1077	T989	L1077	H906	T989	H906	I827		R639	I550	D449	Q331	W220	Y144
	R1078	H990	R1078	R907	H990	R907	D828	V729	L640	E551	K450	D332	Q221	Q145
	P1083	L991	P1083	L998	L991	L998	A829	W736	F552	L553	Q456	N336	A222	A146
	L1086	I995	L1086	I909	I995	I909	N830	M736	A642	K554		Q340	L223	S147
	I1090	L999	I1090	N912	L999	N912	V831	G737	I643	A555	H462	Q340	H226	Q148
	N1091	E1000	N1091	F913	E1000	F913	R832	I738	P654	G556	G463		H226	E149
	P1092	Q1001	P1092	E914	Q1001	E914	F833	Q739	V557	L464	L464	M350	C235	G150
	D1093	F1007	D1093	N915	F1007	N915	D834	W744	P658	H558	P465	P357	C236	Q151
	R1097	E1008	R1097	N916	E1008	N916	E836	L746	C659	T559	A466		Q236	N153
	K1187	Y1011	K1187	Q916	Y1011	Q916	R841	D745	S662	S560	K467	E361	N238	E157
				L917		L917	R842	L746	V664	R561	C468	I362	L239	
				R918		R918	W748	F747	I563	G562	P469	T363		L163
				N920		N920	V749	V749		D564	D472	D364		E164



- Molecule 1: hemocyanin

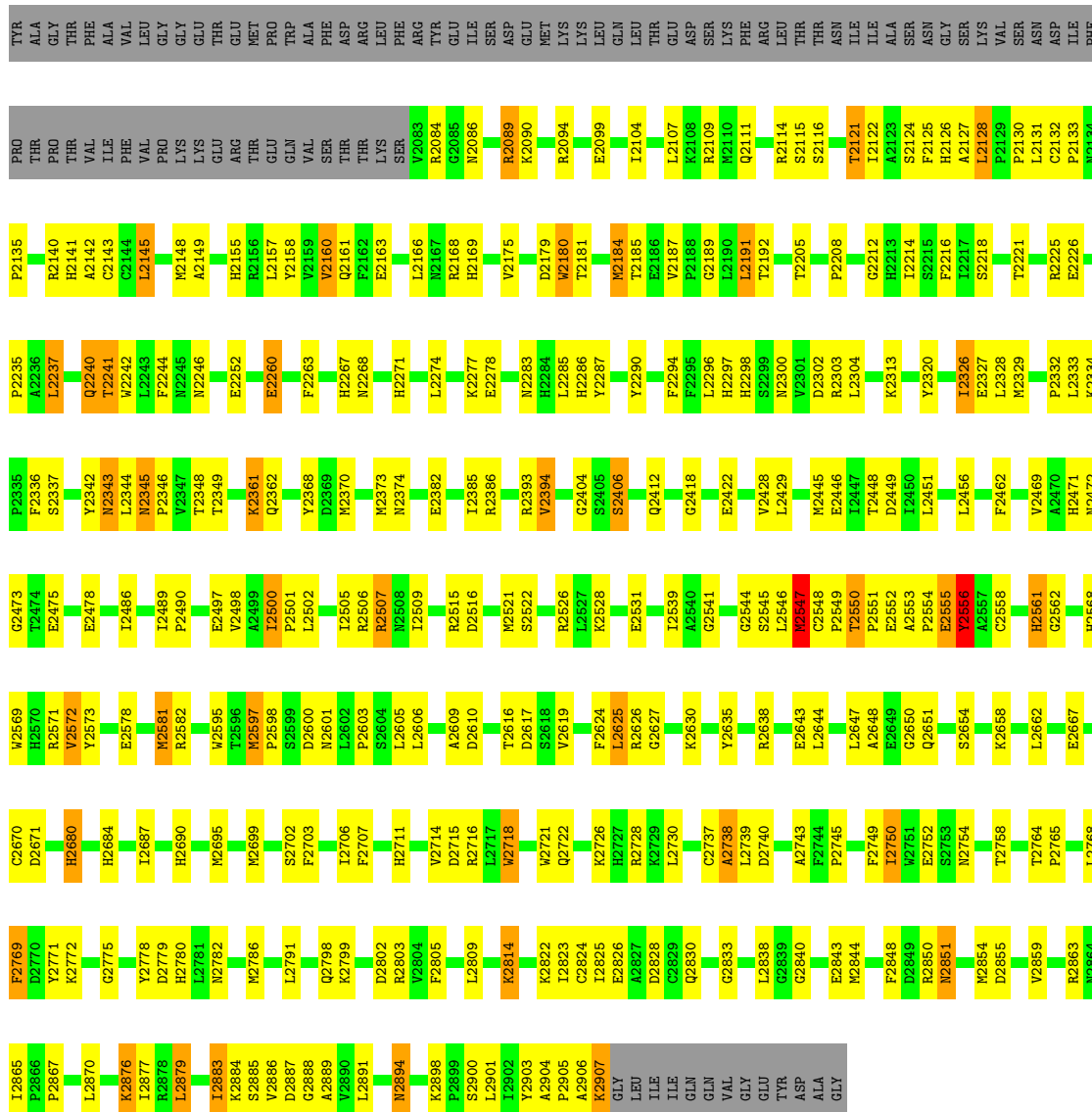
Chain b:





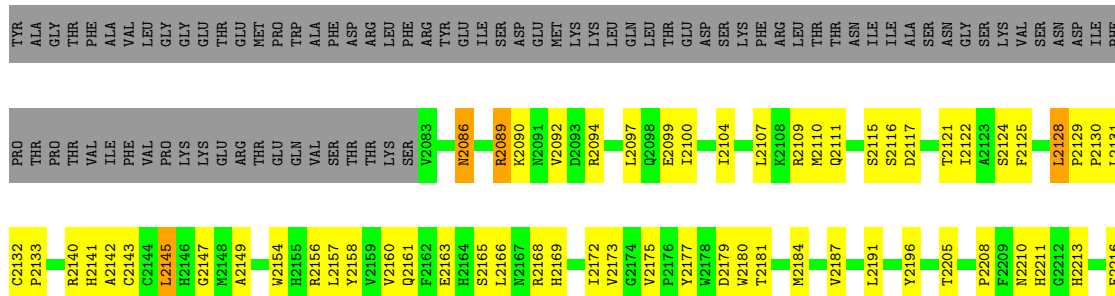
- Molecule 2: hemocyanin

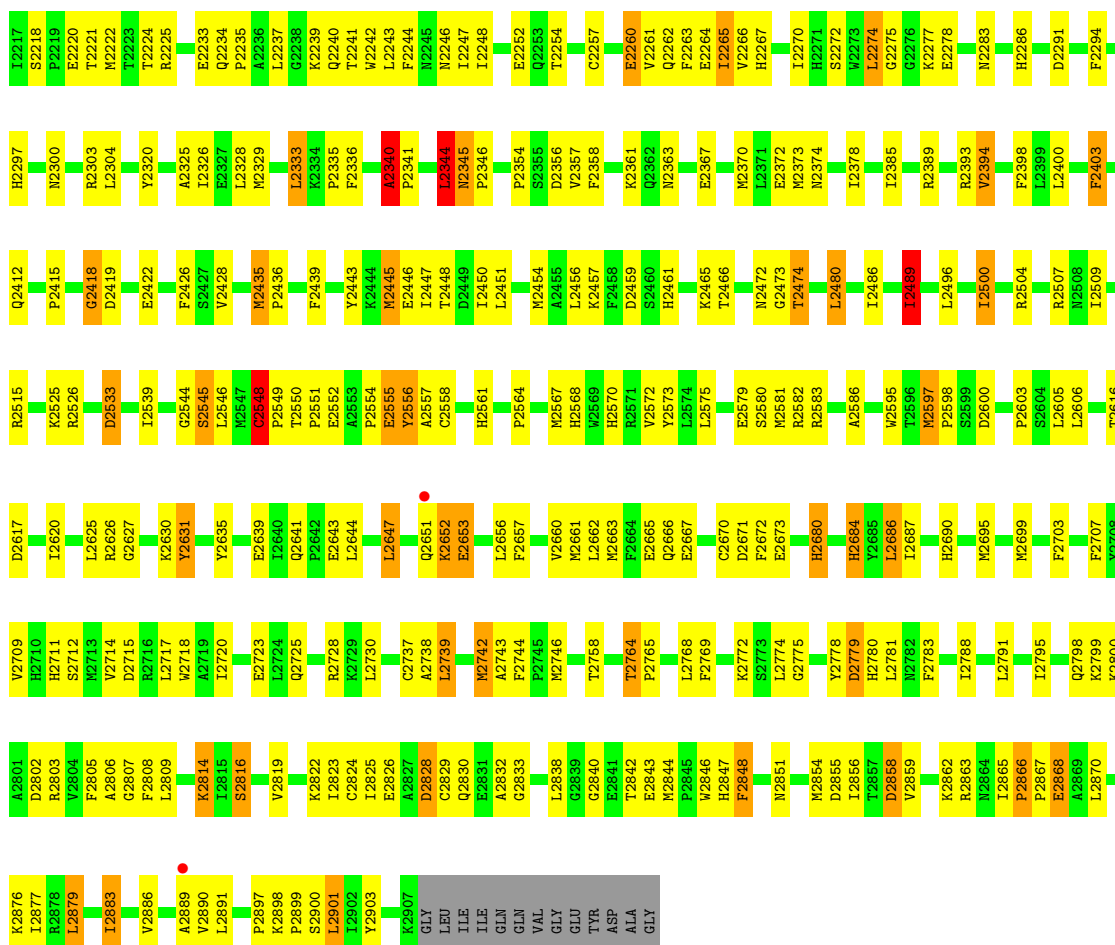
Chain B:  56% 29% 1% 10%



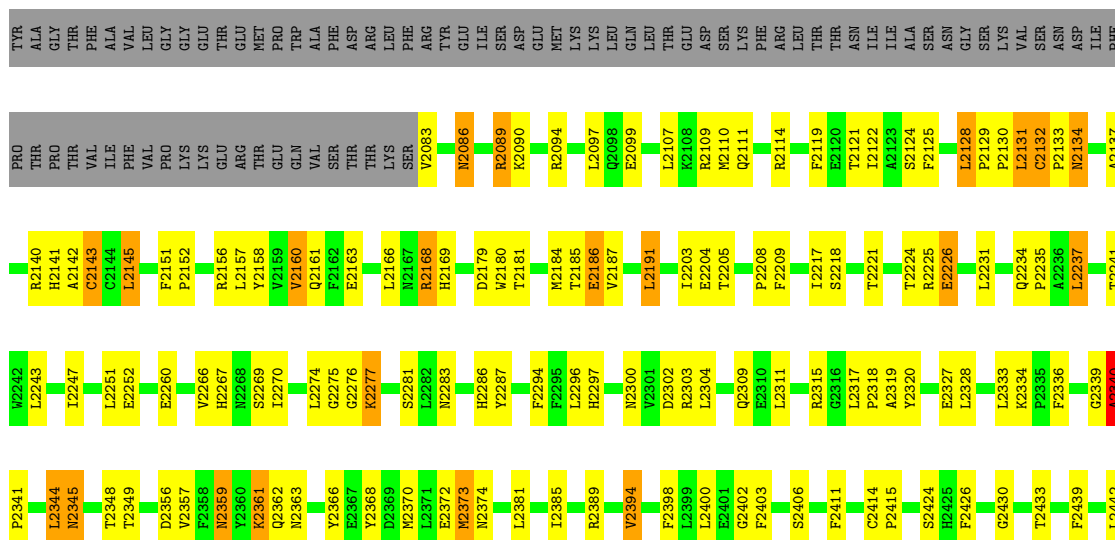
- Molecule 2: hemocyanin

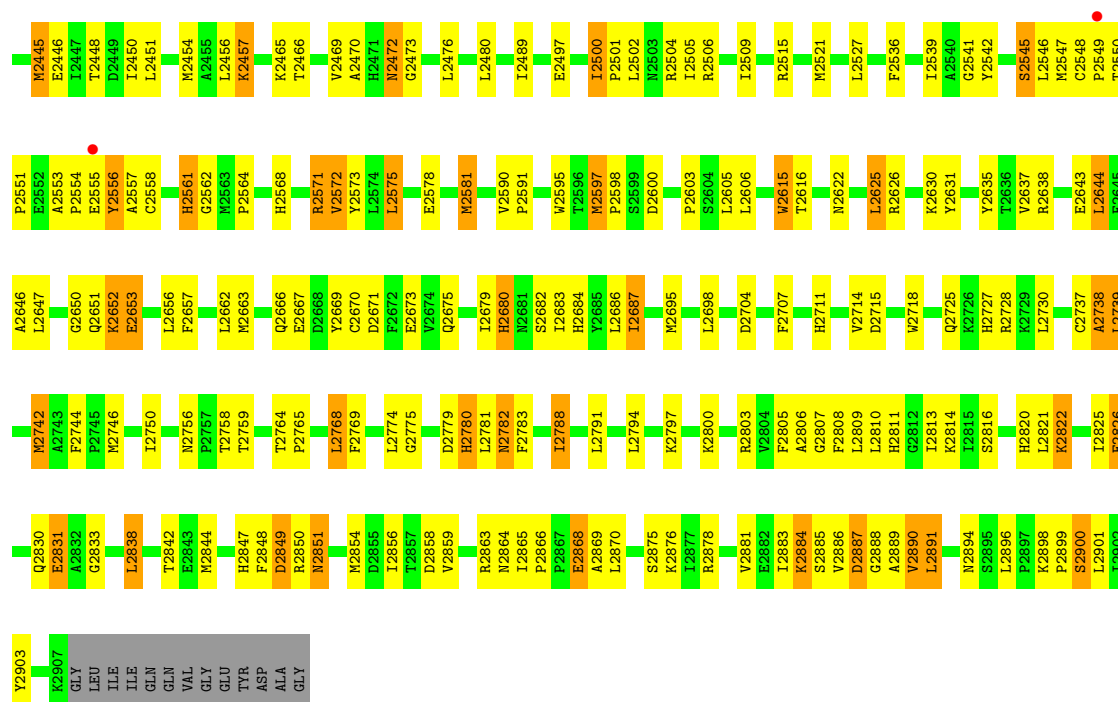
Chain E: 52% 32% 5% 10%





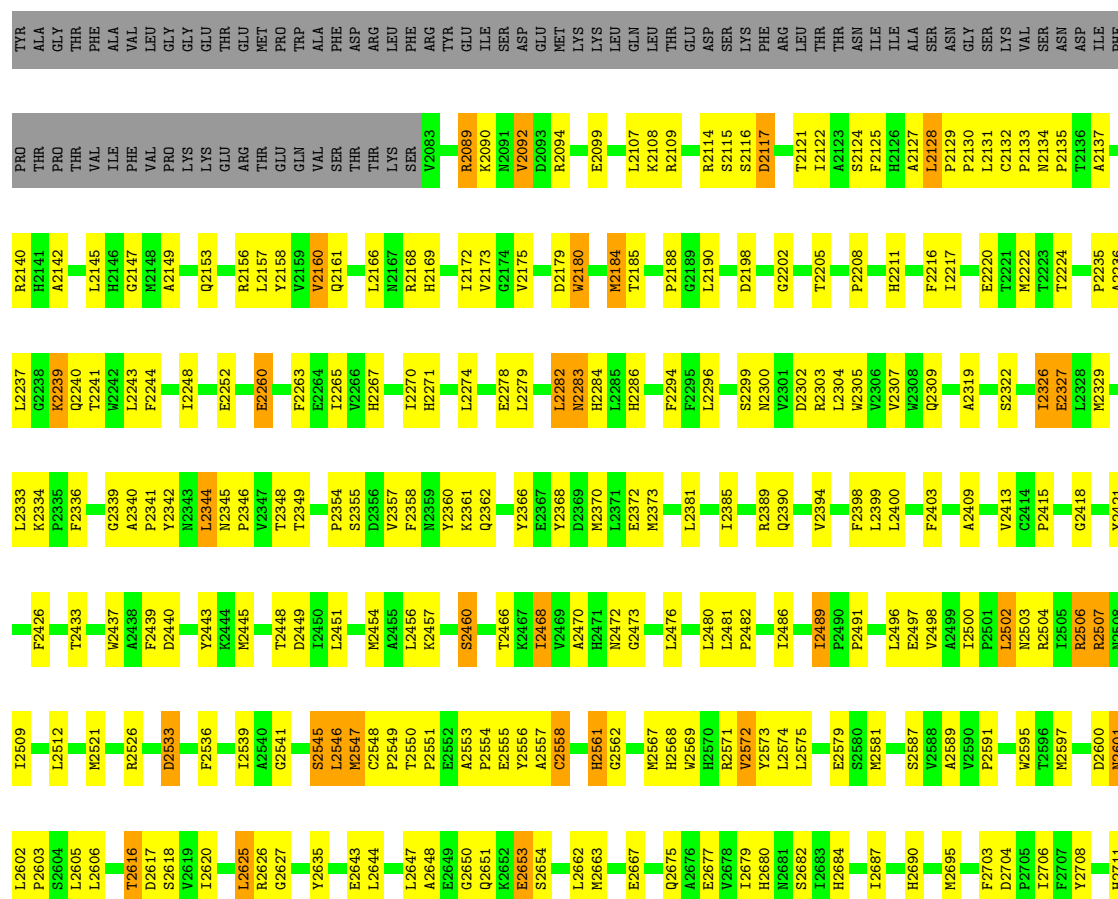
- Molecule 2: hemocyanin

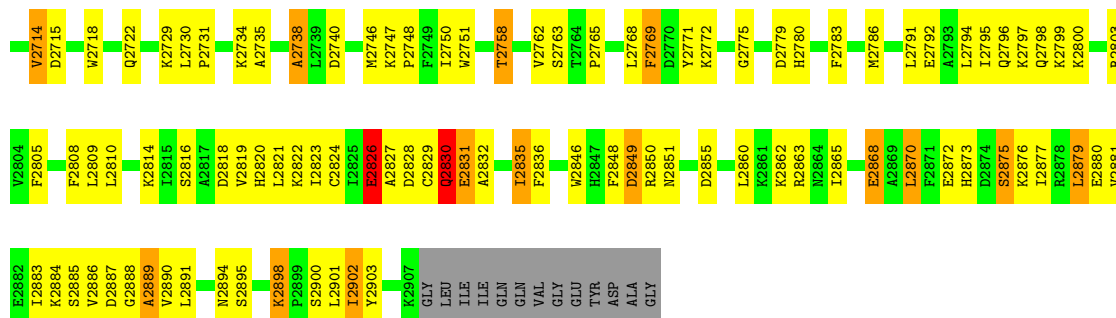




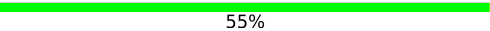
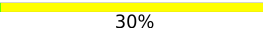
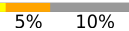
• Molecule 2: hemocyanin

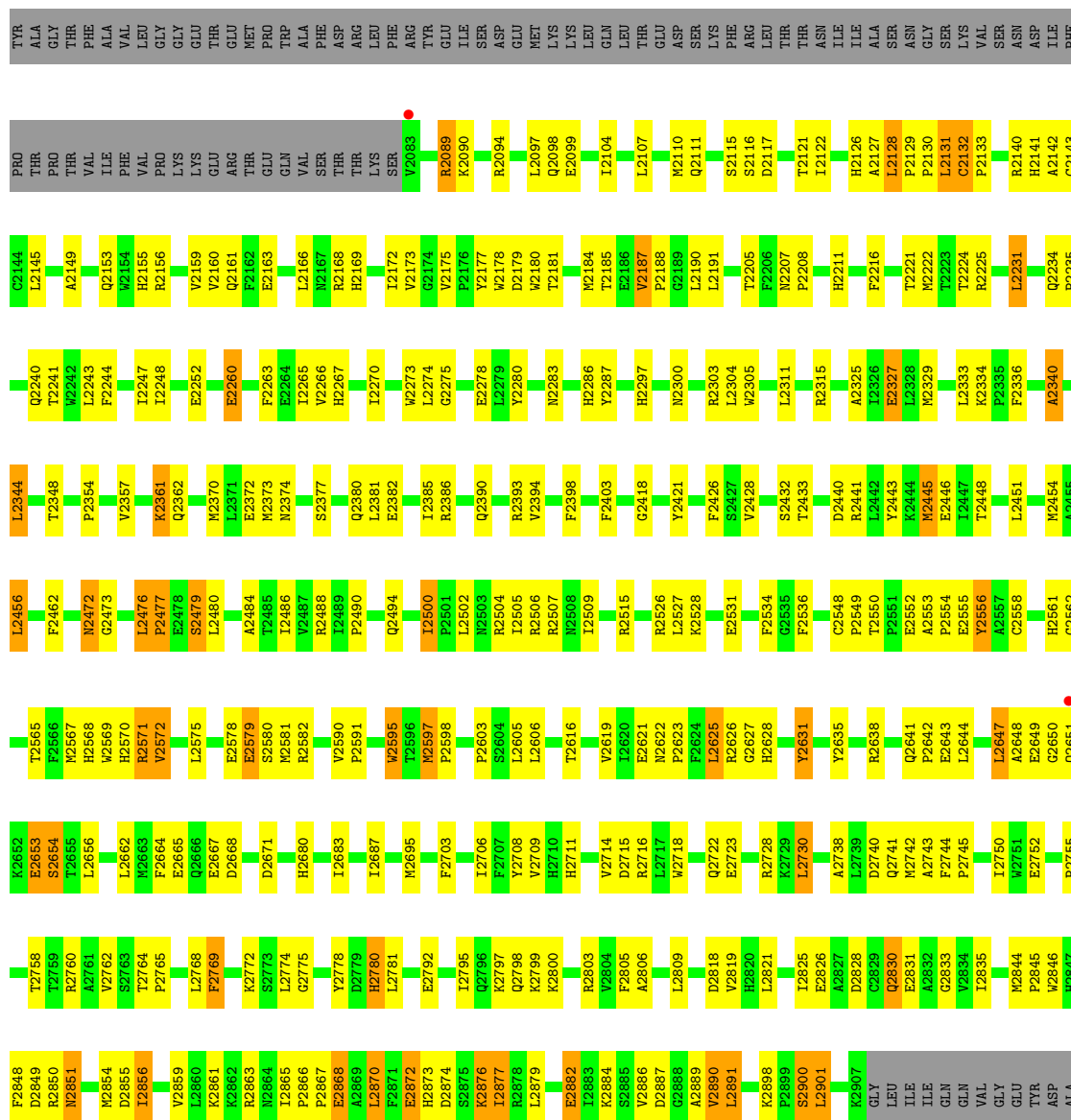
Chain K: 52% 32% 5% 10%





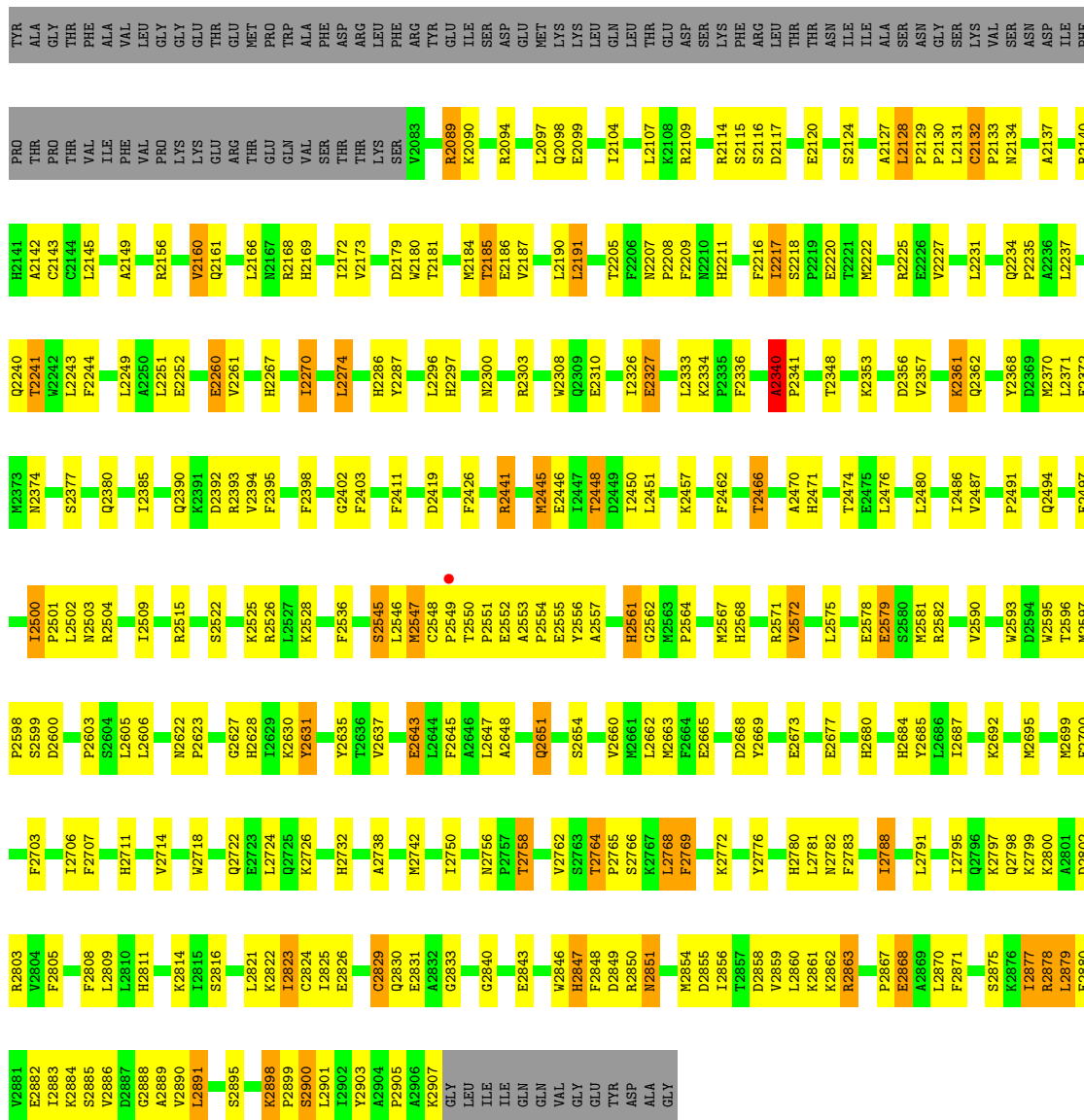
• Molecule 2: hemocyanin

Chain N:  55%  30%  5% 10%

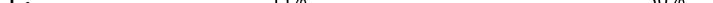


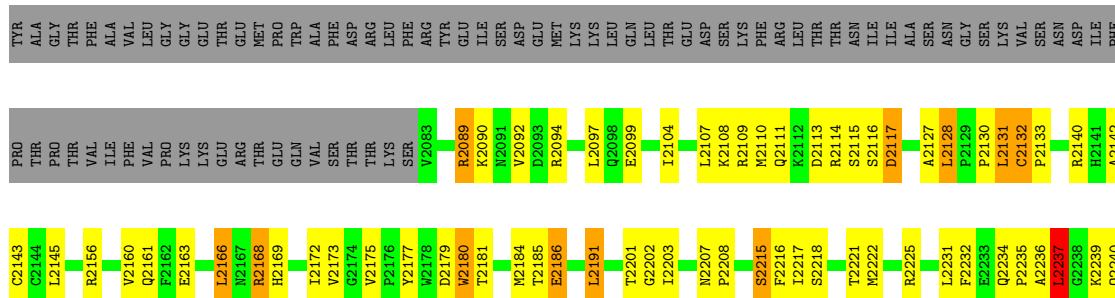
- Molecule 2: hemocyanin

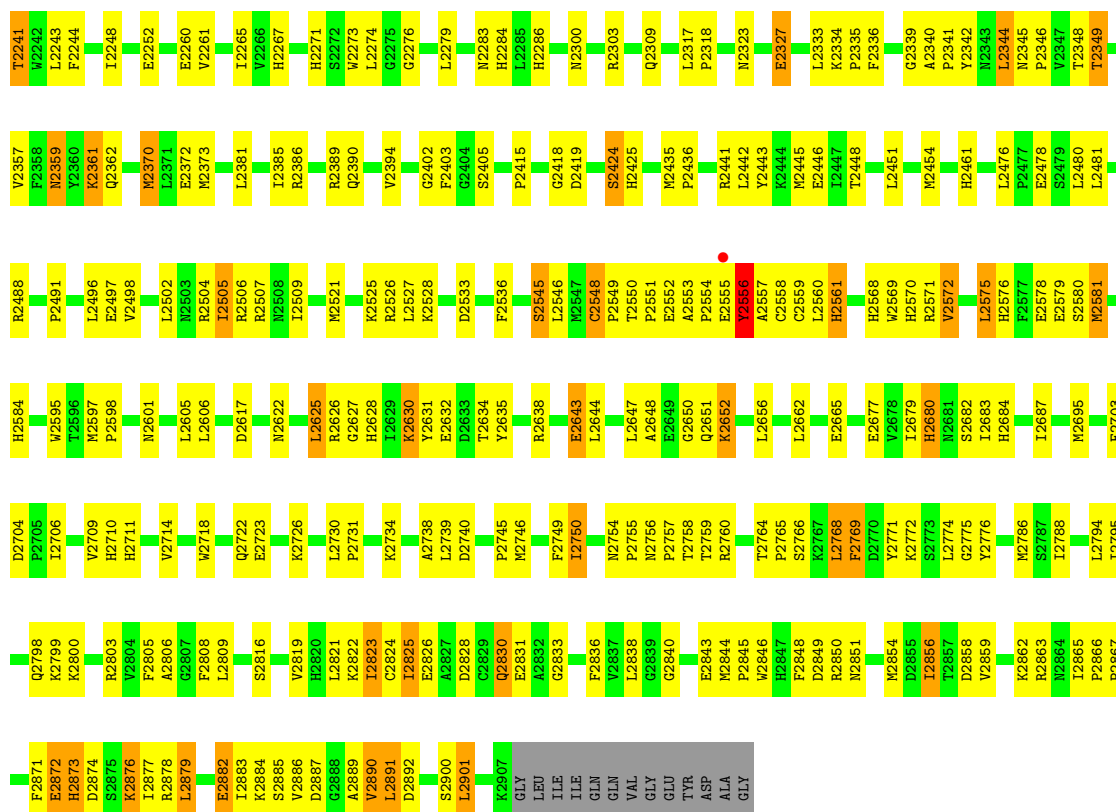
Chain Q:  56% 28% 5% 10%



- Molecule 2: hemocyanin

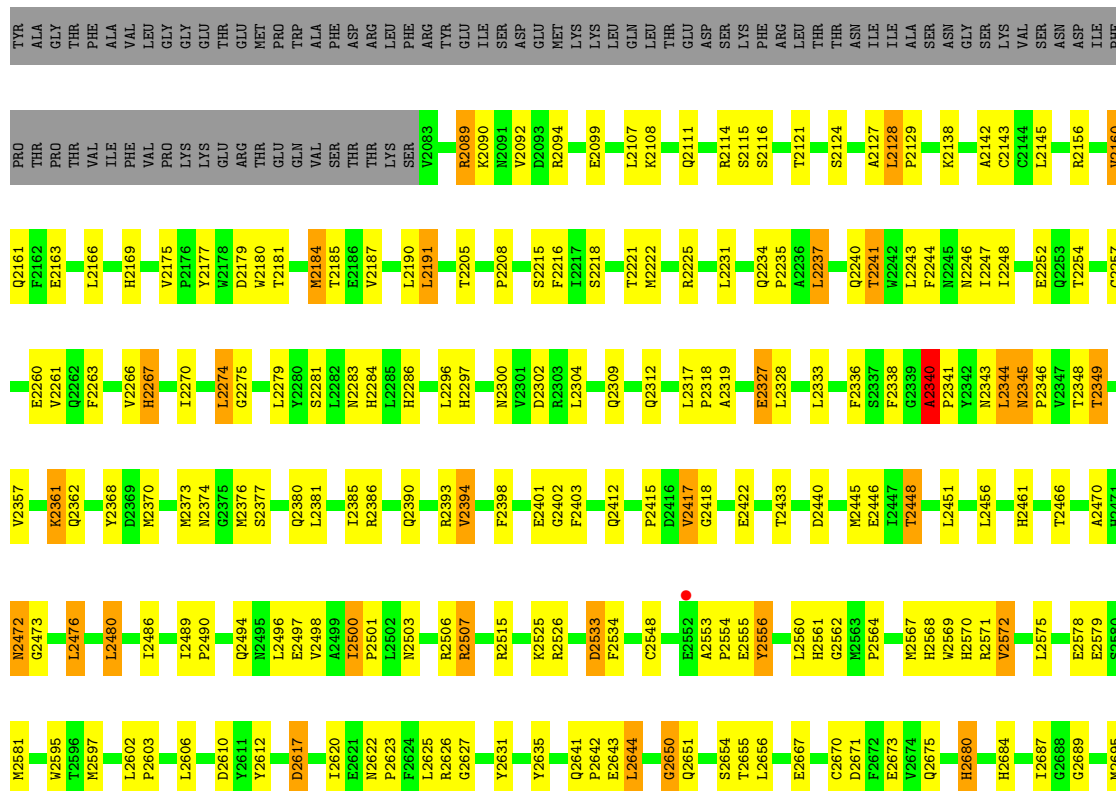
Chain T:  55% 30% 5% 10%



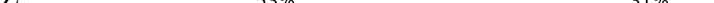


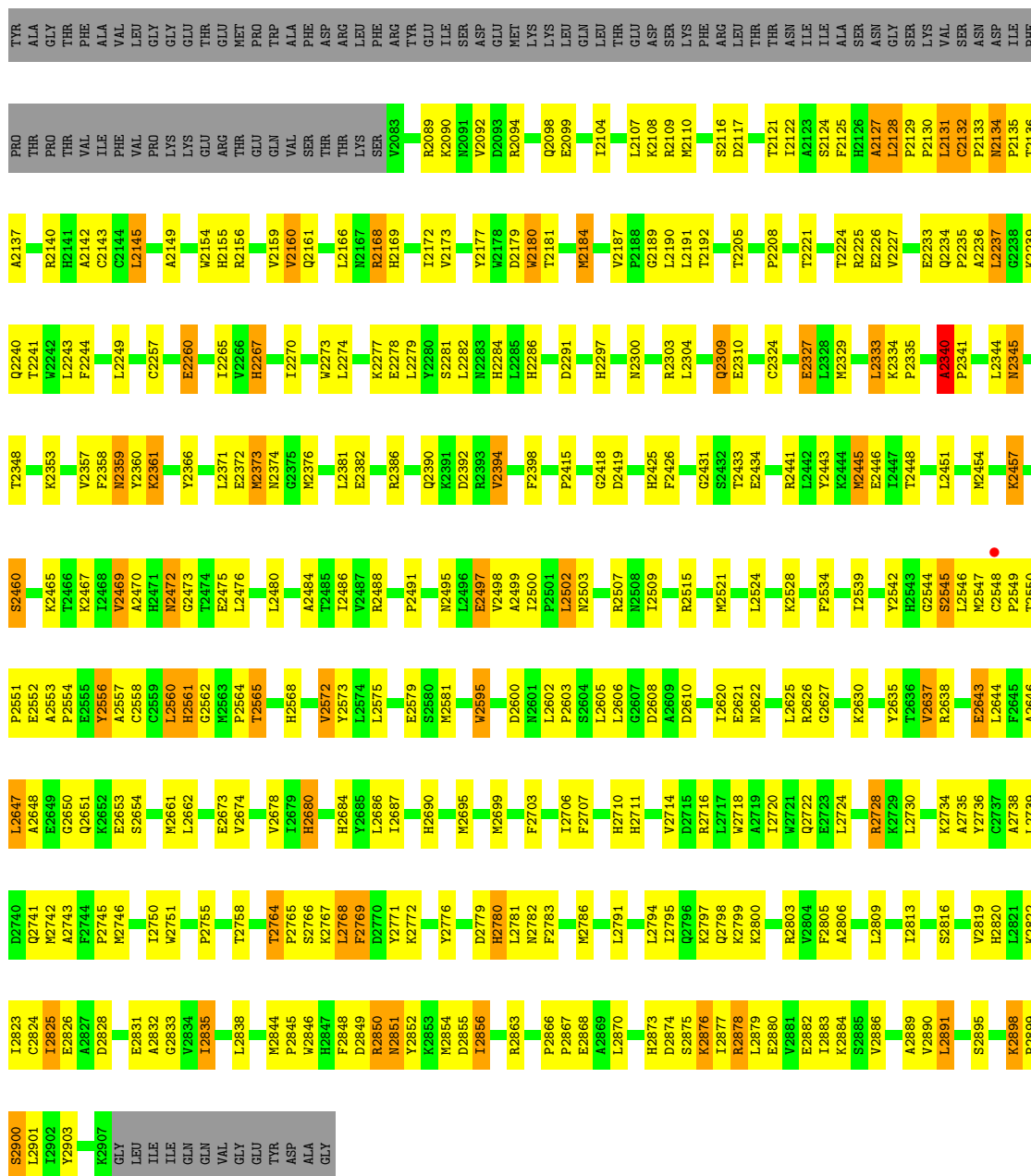
Chain W:

58% 27% 5% 10%



- Molecule 2: hemocyanin

Chain Z:  53% 31% 6% 10%



• Molecule 2: hemocyanin

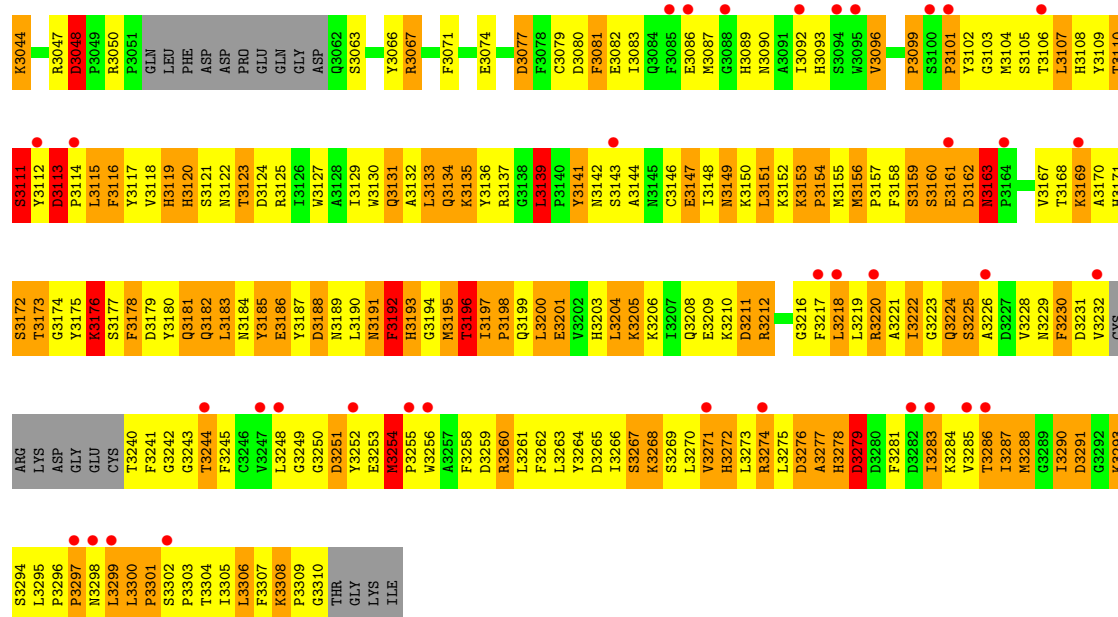
Chain c: 

Tyr	Ala	Pro	Thr	Phe	Val	Leu	Gly	Gly	Gly	Thr	Leu	Thr	Met	Pro	Trp	Ala	Phe	Asp	Arg	Leu	Phe	Ser	Tyr	Leu	Leu	Ser	Asp	Glu	Met	Lys	Lys	Leu	Gln	Leu	Leu	Thr	Glu	Asp	Ser	Lys	Phe	Arg	Leu	Thr	Thr	Asn	Thr	Leu	Thr	Leu	Thr	Leu	Ala	Ser	Asn	Asp	Thr	Phe																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
Pro	Thr	Thr	Thr	Val	Leu	Val	Pro	Gly	Gly	Val	Val	Arg	Leu	Thr	Glu	Val	Ser	Thr	Arg	Ser	Leu	Ser	V2083	R2089	K2090	L2097	Q2098	E2099	L2107	M2110	Q2111	R2114	S2115	S2116	E2120	T2121	A2122	S2124	A2127	L2128	P2129	P2130	L2131	C2132	P2133	R2140	H2141	A2142	C2143	V2145																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							

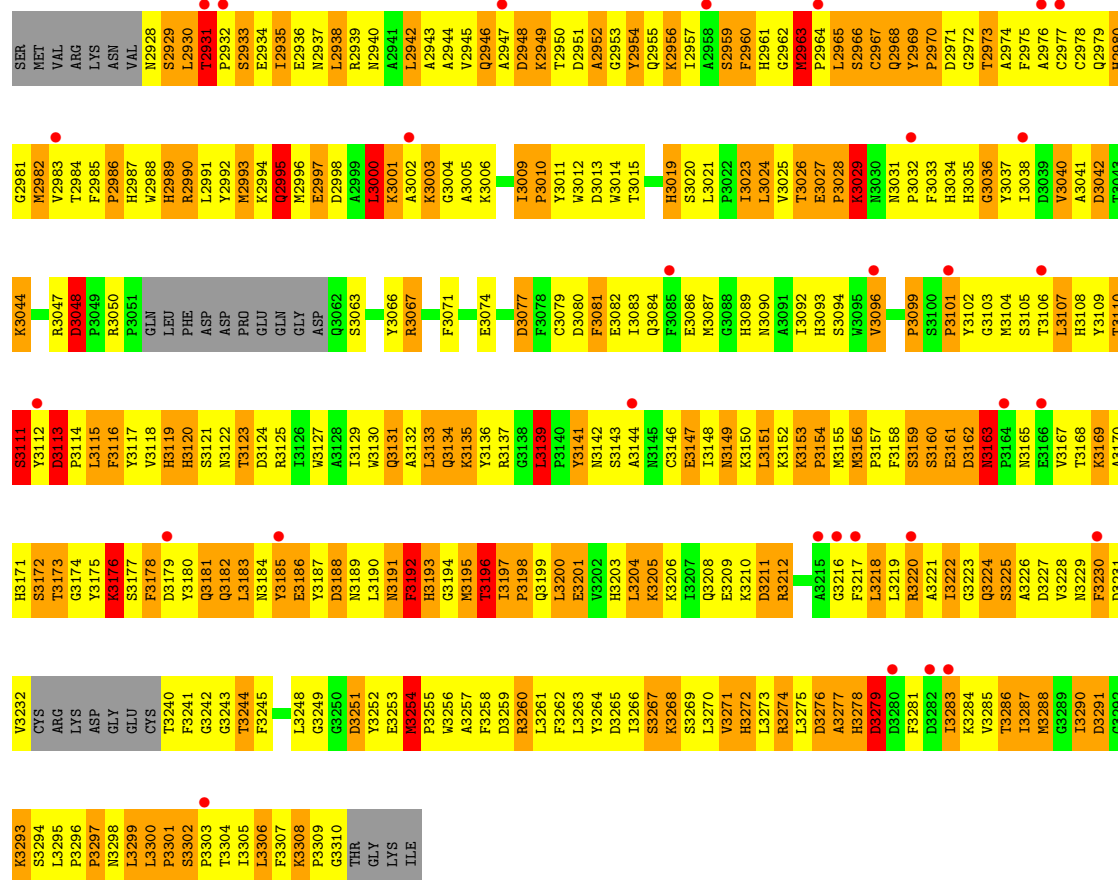
• Molecule 3: hemocyanin

Chain C: 

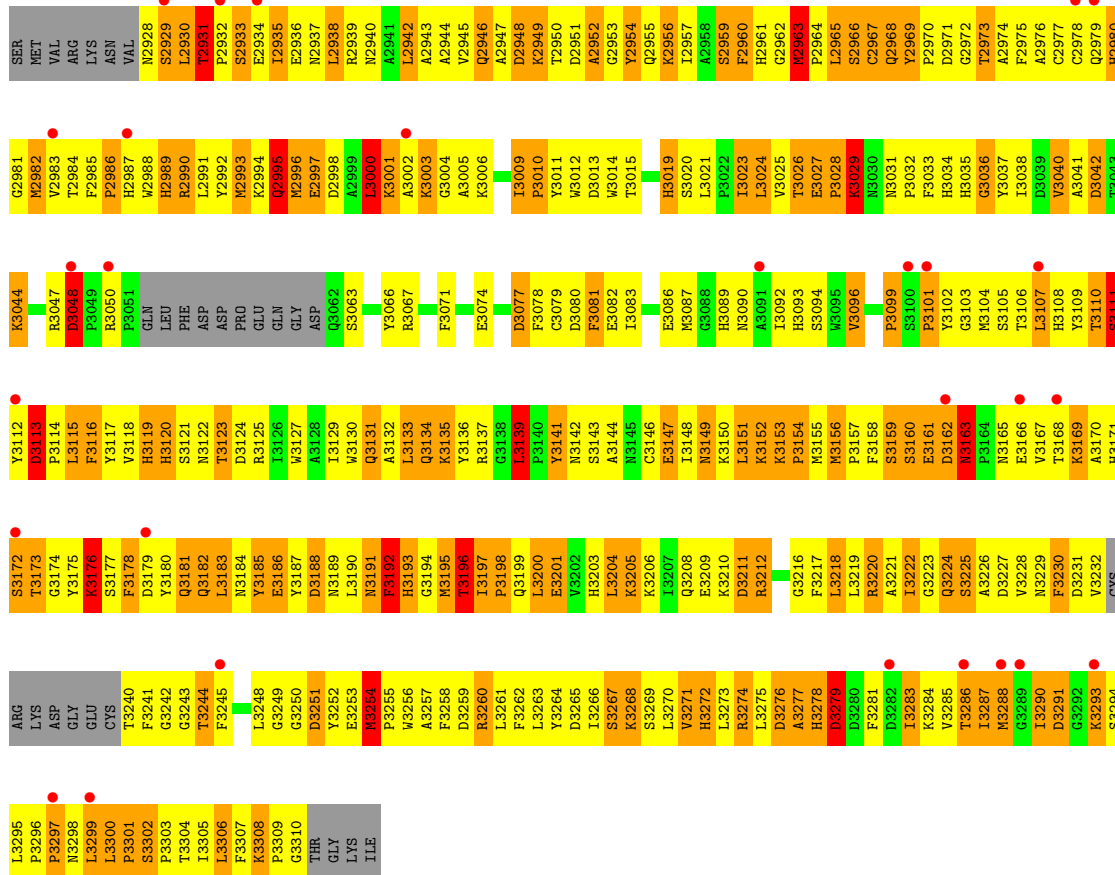
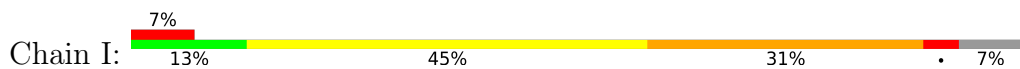
SER	MET	VAL	ARG	LYS	ASN	VAL	N2928	S2929	L2930	T2931	P2932	S2933	E2934	I2935	E2936	L2937	L2938	R2939	N2940	A2941	L2942	A2943	A2944	V2945	Q2946	A2947	D2948	K2949	T2950	L2951	D2952	G2953	Y2954	Q2955	K2956	I2957	A2958	S2959	F2960	H2961	G2962	K2963	P2964	L2965	S2966	C2967	Q2968	Y2969	P2970	D2971	G2972	T2973	A2974	F2975	A2976	C2977	C2978	Q2979	H2980
G2981	M2982	V2983	T2984	F2985	P2986	H2987	W2988	H2989	R2990	L2991	Y2992	M2993	K2994	Q2995	E2996	E2997	D2998	A2999	L3000	K3001	A3002	K3003	G3004	A3005	K3006	I3009	P3010	Y3011	K3012	D3013	W3014	T3015	H3019	S3020	L3021	F3022	I3023	L3024	H2961	V3025	T3026	E3027	P3028	K3029	N3030	N3031	P3032	F3033	H3034	G3035	G3036	Y3037	I3038	D3039	V3040	A3041	D3042	T3043	



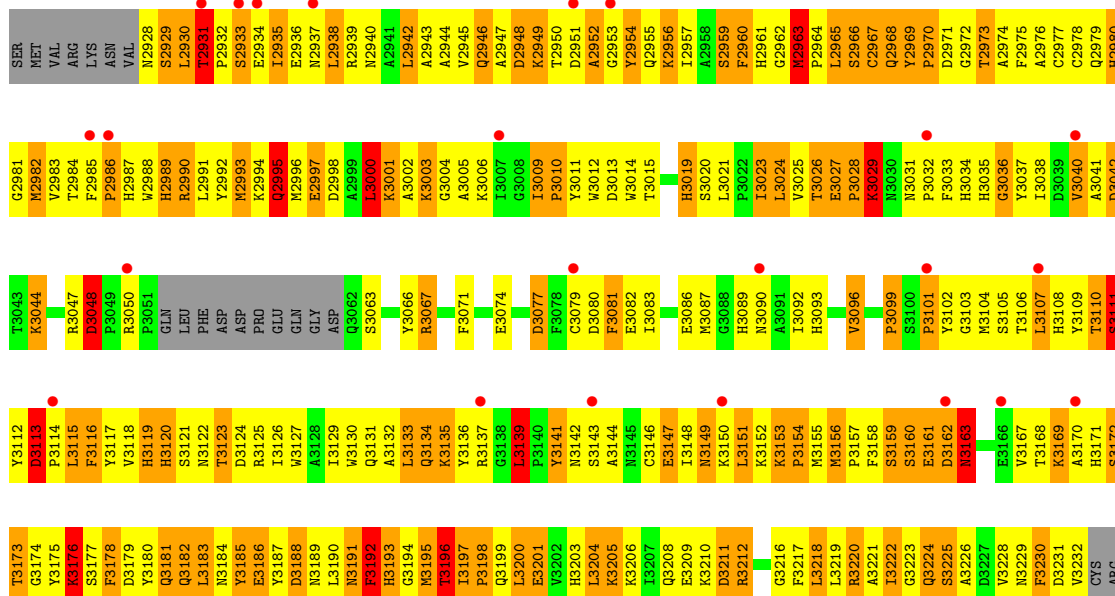
• Molecule 3: hemocyanin

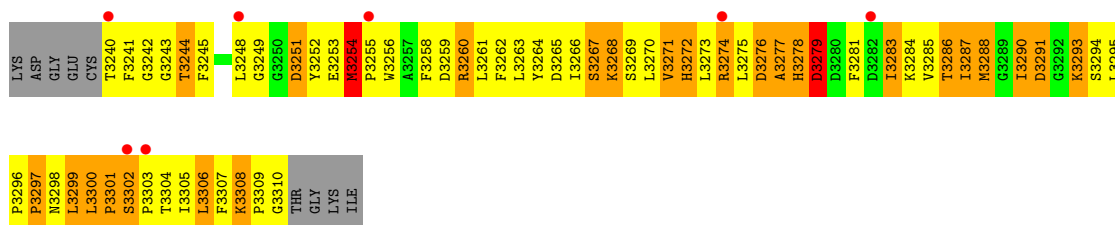


• Molecule 3: hemocyanin

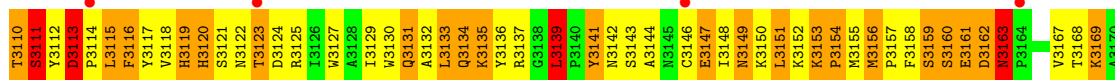
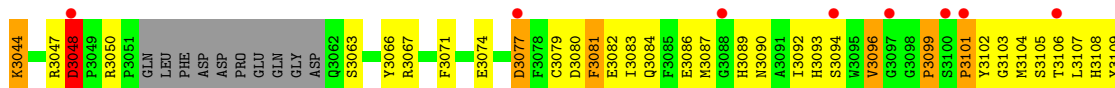
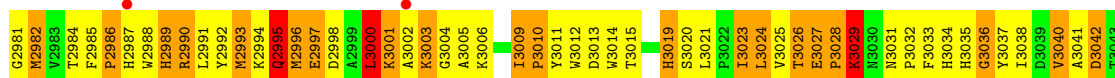
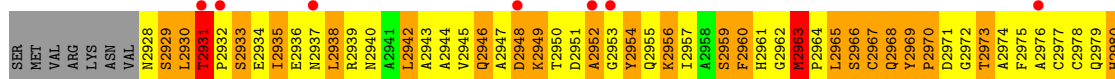
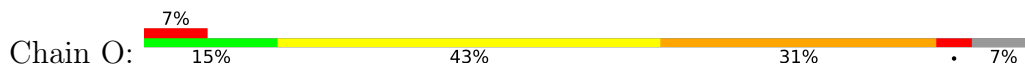


• Molecule 3: hemocyanin

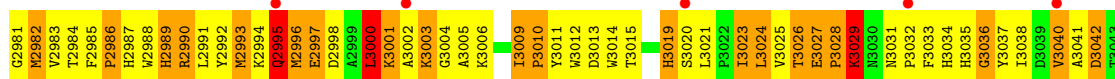
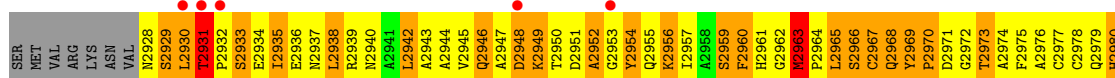
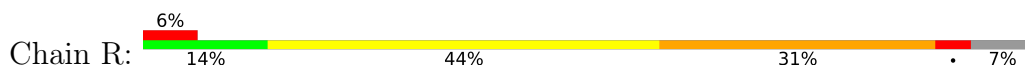


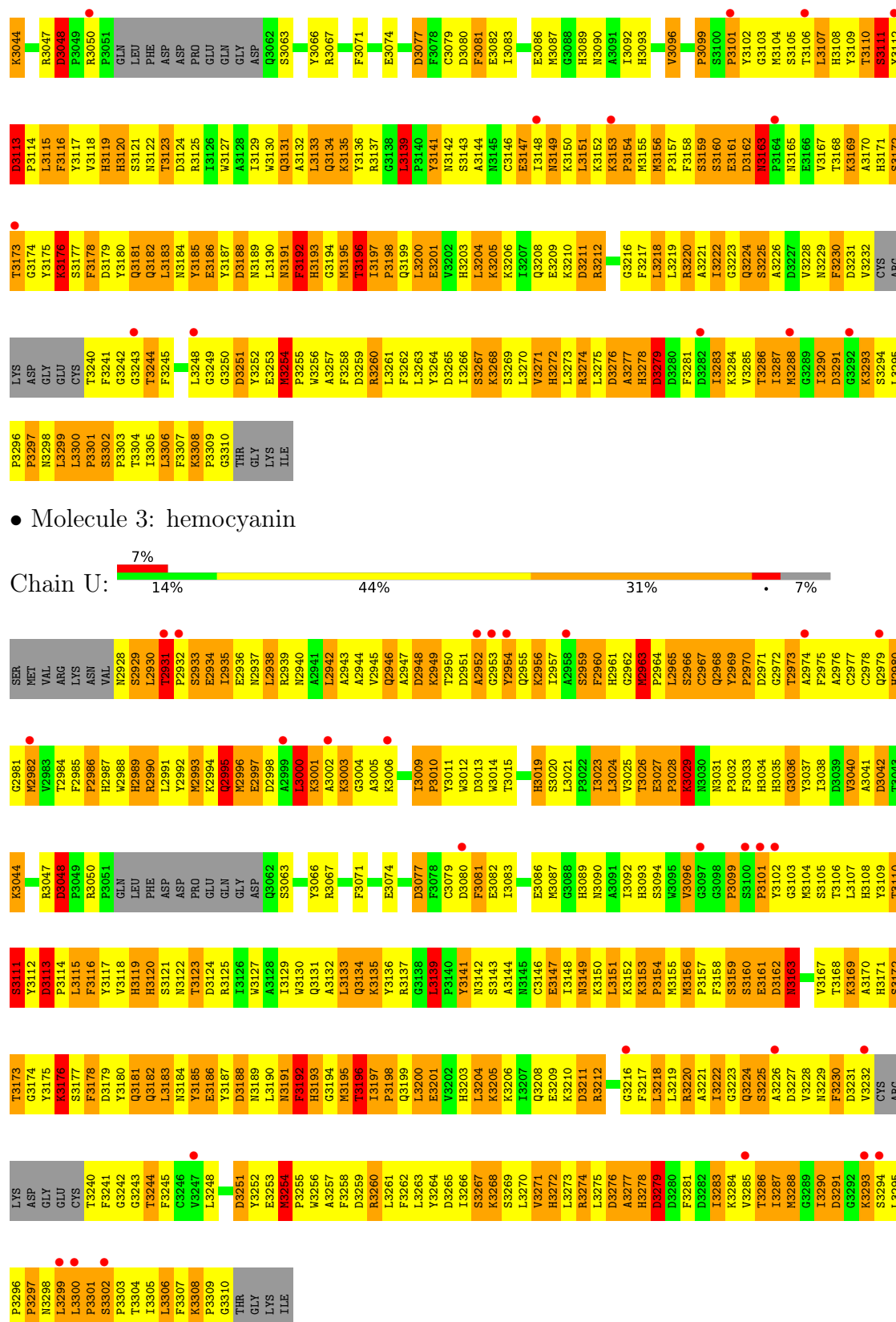


• Molecule 3: hemocyanin

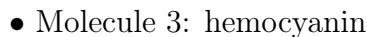


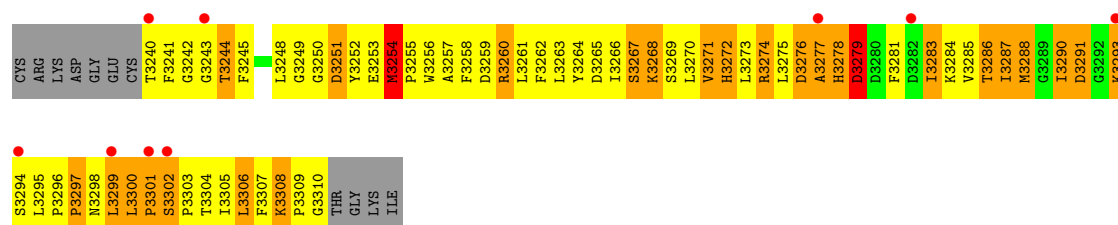
• Molecule 3: hemocyanin



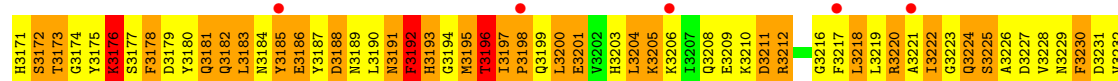
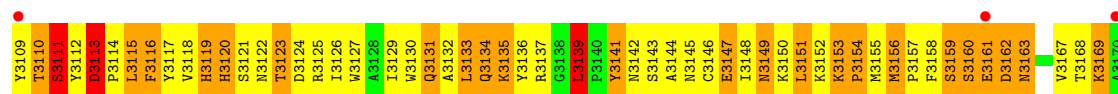
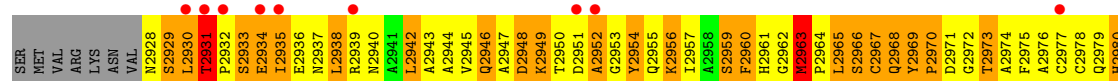


• Molecule 3: hemocyanin





• Molecule 3: hemocyanin



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:  100%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  50% 50%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:  50% 50%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:  50% 50%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:  100%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:  50% 50%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:  50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:  50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6:  50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA:  100%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain HA:  50% 50%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IA:  100%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JA:  50% 50%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain MA:  100%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain OA:  100%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain QA:  50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain RA:



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA:



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain KA:



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain PA:  25% 25% 50%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  67% 33%

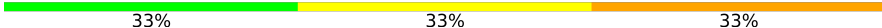


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  33% 67%

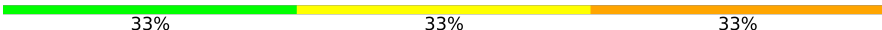


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  33% 33% 33%

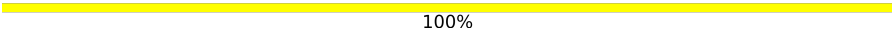


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:  33% 33% 33%

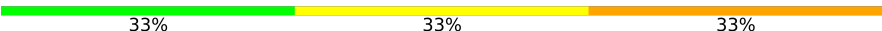


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:  100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:  33% 33% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5:



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA:



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA:



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA:



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain LA:



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain NA:  67% 33%

MAG1
MAG2
BMA3

- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:  20% 40% 40%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 8: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:  25% 75%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	171.37Å 538.66Å 310.92Å 90.00° 104.09° 90.00°	Depositor
Resolution (Å)	49.10 – 3.00 49.10 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.10-3.00) 89.6 (49.10-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.274 , 0.303 0.275 , 0.304	Depositor DCC
R_{free} test set	53588 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	261470	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.37	0/13698	0.89	40/18607 (0.2%)
1	D	0.37	0/13698	0.89	21/18607 (0.1%)
1	G	0.37	1/13698 (0.0%)	0.86	27/18607 (0.1%)
1	J	0.37	0/13698	0.87	22/18607 (0.1%)
1	M	0.35	0/13698	0.87	32/18607 (0.2%)
1	P	0.36	1/13698 (0.0%)	0.86	34/18607 (0.2%)
1	S	0.36	0/13698	0.86	32/18607 (0.2%)
1	V	0.36	0/13698	0.85	33/18607 (0.2%)
1	Y	0.34	0/13698	0.84	21/18607 (0.1%)
1	b	0.35	0/13698	0.87	26/18607 (0.1%)
2	B	0.34	0/6909	0.85	12/9383 (0.1%)
2	E	0.35	0/6909	0.87	17/9383 (0.2%)
2	H	0.35	0/6909	0.84	14/9383 (0.1%)
2	K	0.35	0/6909	0.85	13/9383 (0.1%)
2	N	0.35	0/6909	0.84	9/9383 (0.1%)
2	Q	0.34	0/6909	0.83	11/9383 (0.1%)
2	T	0.34	0/6909	0.82	9/9383 (0.1%)
2	W	0.33	0/6909	0.84	18/9383 (0.2%)
2	Z	0.33	0/6909	0.84	13/9383 (0.1%)
2	c	0.33	0/6909	0.82	9/9383 (0.1%)
3	C	1.08	36/6100 (0.6%)	1.39	120/8282 (1.4%)
3	F	1.08	36/6100 (0.6%)	1.40	120/8282 (1.4%)
3	I	1.08	34/6100 (0.6%)	1.40	120/8282 (1.4%)
3	L	1.08	36/6100 (0.6%)	1.39	120/8282 (1.4%)
3	O	1.08	36/6100 (0.6%)	1.39	120/8282 (1.4%)
3	R	1.08	36/6100 (0.6%)	1.40	120/8282 (1.4%)
3	U	1.08	36/6100 (0.6%)	1.40	122/8282 (1.5%)
3	X	1.08	38/6100 (0.6%)	1.40	116/8282 (1.4%)
3	a	1.08	34/6100 (0.6%)	1.39	120/8282 (1.4%)
3	d	1.08	38/6100 (0.6%)	1.40	122/8282 (1.5%)
All	All	0.60	362/267070 (0.1%)	1.01	1613/362720 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	3
1	G	0	1
1	J	0	2
1	M	0	1
1	S	0	3
1	Y	0	1
1	b	0	2
2	B	0	1
2	K	0	3
2	N	0	1
2	Q	0	1
2	T	0	2
2	W	0	1
2	Z	0	2
2	c	0	1
3	C	0	4
3	F	0	4
3	I	0	4
3	L	0	4
3	O	0	4
3	R	0	4
3	U	0	4
3	X	0	4
3	a	0	4
3	d	0	4
All	All	0	67

All (362) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	3296[A]	PRO	C-N	6.78	1.41	1.33
3	a	3296[B]	PRO	C-N	6.78	1.41	1.33
3	O	3296[A]	PRO	C-N	6.77	1.41	1.33
3	O	3296[B]	PRO	C-N	6.77	1.41	1.33
3	L	3296[A]	PRO	C-N	6.76	1.41	1.33
3	L	3296[B]	PRO	C-N	6.76	1.41	1.33
3	C	3296[A]	PRO	C-N	6.75	1.41	1.33
3	C	3296[B]	PRO	C-N	6.75	1.41	1.33

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	3296[A]	PRO	C-N	6.75	1.41	1.33
3	X	3296[B]	PRO	C-N	6.75	1.41	1.33
3	U	3296[A]	PRO	C-N	6.75	1.41	1.33
3	U	3296[B]	PRO	C-N	6.75	1.41	1.33
3	d	3296[A]	PRO	C-N	6.74	1.41	1.33
3	d	3296[B]	PRO	C-N	6.74	1.41	1.33
3	F	3296[A]	PRO	C-N	6.71	1.41	1.33
3	F	3296[B]	PRO	C-N	6.71	1.41	1.33
3	R	3296[A]	PRO	C-N	6.71	1.41	1.33
3	R	3296[B]	PRO	C-N	6.71	1.41	1.33
3	I	3296[A]	PRO	C-N	6.68	1.41	1.33
3	I	3296[B]	PRO	C-N	6.68	1.41	1.33
3	U	2989[A]	HIS	CA-C	-6.45	1.46	1.53
3	U	2989[B]	HIS	CA-C	-6.45	1.46	1.53
3	I	2989[A]	HIS	CA-C	-6.45	1.46	1.53
3	I	2989[B]	HIS	CA-C	-6.45	1.46	1.53
3	L	2989[A]	HIS	CA-C	-6.44	1.46	1.53
3	L	2989[B]	HIS	CA-C	-6.44	1.46	1.53
3	C	2989[A]	HIS	CA-C	-6.40	1.46	1.53
3	C	2989[B]	HIS	CA-C	-6.40	1.46	1.53
3	d	2989[A]	HIS	CA-C	-6.38	1.46	1.53
3	d	2989[B]	HIS	CA-C	-6.38	1.46	1.53
3	F	2989[A]	HIS	CA-C	-6.36	1.46	1.53
3	F	2989[B]	HIS	CA-C	-6.36	1.46	1.53
3	F	3308[A]	LYS	C-N	6.36	1.41	1.33
3	F	3308[B]	LYS	C-N	6.36	1.41	1.33
3	R	2989[A]	HIS	CA-C	-6.35	1.46	1.53
3	R	2989[B]	HIS	CA-C	-6.35	1.46	1.53
3	C	3308[A]	LYS	C-N	6.33	1.41	1.33
3	C	3308[B]	LYS	C-N	6.33	1.41	1.33
3	U	2963[A]	MET	C-N	6.33	1.41	1.33
3	U	2963[B]	MET	C-N	6.33	1.41	1.33
3	X	2989[A]	HIS	CA-C	-6.31	1.46	1.53
3	X	2989[B]	HIS	CA-C	-6.31	1.46	1.53
3	d	2963[A]	MET	C-N	6.31	1.41	1.33
3	d	2963[B]	MET	C-N	6.31	1.41	1.33
3	d	3308[A]	LYS	C-N	6.31	1.40	1.33
3	d	3308[B]	LYS	C-N	6.31	1.40	1.33
3	L	2963[A]	MET	C-N	6.31	1.41	1.33
3	L	2963[B]	MET	C-N	6.31	1.41	1.33
3	L	3308[A]	LYS	C-N	6.30	1.40	1.33
3	L	3308[B]	LYS	C-N	6.30	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	3308[A]	LYS	C-N	6.30	1.40	1.33
3	X	3308[B]	LYS	C-N	6.30	1.40	1.33
3	a	2989[A]	HIS	CA-C	-6.29	1.46	1.53
3	a	2989[B]	HIS	CA-C	-6.29	1.46	1.53
3	I	2963[A]	MET	C-N	6.29	1.41	1.33
3	I	2963[B]	MET	C-N	6.29	1.41	1.33
3	X	2963[A]	MET	C-N	6.29	1.41	1.33
3	X	2963[B]	MET	C-N	6.29	1.41	1.33
3	a	3308[A]	LYS	C-N	6.28	1.40	1.33
3	a	3308[B]	LYS	C-N	6.28	1.40	1.33
3	O	2989[A]	HIS	CA-C	-6.28	1.46	1.53
3	O	2989[B]	HIS	CA-C	-6.28	1.46	1.53
3	R	3308[A]	LYS	C-N	6.28	1.40	1.33
3	R	3308[B]	LYS	C-N	6.28	1.40	1.33
3	F	2963[A]	MET	C-N	6.27	1.41	1.33
3	F	2963[B]	MET	C-N	6.27	1.41	1.33
3	O	2963[A]	MET	C-N	6.27	1.41	1.33
3	O	2963[B]	MET	C-N	6.27	1.41	1.33
3	U	3308[A]	LYS	C-N	6.26	1.40	1.33
3	U	3308[B]	LYS	C-N	6.26	1.40	1.33
3	a	2963[A]	MET	C-N	6.25	1.41	1.33
3	a	2963[B]	MET	C-N	6.25	1.41	1.33
3	C	2963[A]	MET	C-N	6.23	1.41	1.33
3	C	2963[B]	MET	C-N	6.23	1.41	1.33
3	I	3308[A]	LYS	C-N	6.23	1.40	1.33
3	I	3308[B]	LYS	C-N	6.23	1.40	1.33
3	R	2963[A]	MET	C-N	6.22	1.41	1.33
3	R	2963[B]	MET	C-N	6.22	1.41	1.33
3	O	3308[A]	LYS	C-N	6.19	1.40	1.33
3	O	3308[B]	LYS	C-N	6.19	1.40	1.33
3	I	3153[A]	LYS	C-N	6.19	1.40	1.33
3	I	3153[B]	LYS	C-N	6.19	1.40	1.33
3	L	3153[A]	LYS	C-N	6.12	1.40	1.33
3	L	3153[B]	LYS	C-N	6.12	1.40	1.33
3	I	3048[A]	ASP	C-N	6.11	1.41	1.33
3	I	3048[B]	ASP	C-N	6.11	1.41	1.33
3	U	3153[A]	LYS	C-N	6.11	1.40	1.33
3	U	3153[B]	LYS	C-N	6.11	1.40	1.33
3	a	3048[A]	ASP	C-N	6.11	1.41	1.33
3	a	3048[B]	ASP	C-N	6.11	1.41	1.33
3	X	3153[A]	LYS	C-N	6.11	1.40	1.33
3	X	3153[B]	LYS	C-N	6.11	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	3048[A]	ASP	C-N	6.09	1.41	1.33
3	O	3048[B]	ASP	C-N	6.09	1.41	1.33
3	R	3048[A]	ASP	C-N	6.08	1.41	1.33
3	R	3048[B]	ASP	C-N	6.08	1.41	1.33
3	F	3153[A]	LYS	C-N	6.08	1.40	1.33
3	F	3153[B]	LYS	C-N	6.08	1.40	1.33
3	U	3048[A]	ASP	C-N	6.07	1.41	1.33
3	U	3048[B]	ASP	C-N	6.07	1.41	1.33
3	F	3048[A]	ASP	C-N	6.07	1.41	1.33
3	F	3048[B]	ASP	C-N	6.07	1.41	1.33
3	R	3153[A]	LYS	C-N	6.06	1.40	1.33
3	R	3153[B]	LYS	C-N	6.06	1.40	1.33
3	X	3048[A]	ASP	C-N	6.06	1.41	1.33
3	X	3048[B]	ASP	C-N	6.06	1.41	1.33
3	a	3153[A]	LYS	C-N	6.06	1.40	1.33
3	a	3153[B]	LYS	C-N	6.06	1.40	1.33
3	d	3153[A]	LYS	C-N	6.04	1.40	1.33
3	d	3153[B]	LYS	C-N	6.04	1.40	1.33
3	C	3153[A]	LYS	C-N	6.04	1.40	1.33
3	C	3153[B]	LYS	C-N	6.04	1.40	1.33
3	O	3153[A]	LYS	C-N	6.03	1.40	1.33
3	O	3153[B]	LYS	C-N	6.03	1.40	1.33
3	L	3048[A]	ASP	C-N	6.02	1.41	1.33
3	L	3048[B]	ASP	C-N	6.02	1.41	1.33
3	d	3048[A]	ASP	C-N	6.00	1.41	1.33
3	d	3048[B]	ASP	C-N	6.00	1.41	1.33
3	C	3048[A]	ASP	C-N	5.97	1.41	1.33
3	C	3048[B]	ASP	C-N	5.97	1.41	1.33
3	d	3254[A]	MET	C-N	5.91	1.40	1.33
3	d	3254[B]	MET	C-N	5.91	1.40	1.33
3	R	3254[A]	MET	C-N	5.88	1.40	1.33
3	R	3254[B]	MET	C-N	5.88	1.40	1.33
3	a	3254[A]	MET	C-N	5.88	1.40	1.33
3	a	3254[B]	MET	C-N	5.88	1.40	1.33
3	L	3254[A]	MET	C-N	5.88	1.40	1.33
3	L	3254[B]	MET	C-N	5.88	1.40	1.33
3	O	3254[A]	MET	C-N	5.87	1.40	1.33
3	O	3254[B]	MET	C-N	5.87	1.40	1.33
3	I	3254[A]	MET	C-N	5.86	1.40	1.33
3	I	3254[B]	MET	C-N	5.86	1.40	1.33
3	U	3254[A]	MET	C-N	5.86	1.40	1.33
3	U	3254[B]	MET	C-N	5.86	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	3254[A]	MET	C-N	5.85	1.40	1.33
3	X	3254[B]	MET	C-N	5.85	1.40	1.33
3	F	3254[A]	MET	C-N	5.85	1.40	1.33
3	F	3254[B]	MET	C-N	5.85	1.40	1.33
3	C	3254[A]	MET	C-N	5.76	1.40	1.33
3	C	3254[B]	MET	C-N	5.76	1.40	1.33
3	R	2931[A]	THR	C-N	5.66	1.41	1.33
3	R	2931[B]	THR	C-N	5.66	1.41	1.33
3	U	2931[A]	THR	C-N	5.60	1.40	1.33
3	U	2931[B]	THR	C-N	5.60	1.40	1.33
3	F	2931[A]	THR	C-N	5.59	1.40	1.33
3	F	2931[B]	THR	C-N	5.59	1.40	1.33
3	a	2931[A]	THR	C-N	5.59	1.40	1.33
3	a	2931[B]	THR	C-N	5.59	1.40	1.33
3	I	2931[A]	THR	C-N	5.58	1.40	1.33
3	I	2931[B]	THR	C-N	5.58	1.40	1.33
3	d	2931[A]	THR	C-N	5.57	1.40	1.33
3	d	2931[B]	THR	C-N	5.57	1.40	1.33
3	O	2931[A]	THR	C-N	5.56	1.40	1.33
3	O	2931[B]	THR	C-N	5.56	1.40	1.33
3	X	2931[A]	THR	C-N	5.56	1.40	1.33
3	X	2931[B]	THR	C-N	5.56	1.40	1.33
3	C	2931[A]	THR	C-N	5.55	1.40	1.33
3	C	2931[B]	THR	C-N	5.55	1.40	1.33
3	L	2931[A]	THR	C-N	5.54	1.40	1.33
3	L	2931[B]	THR	C-N	5.54	1.40	1.33
3	F	3009[A]	ILE	C-N	5.50	1.40	1.33
3	F	3009[B]	ILE	C-N	5.50	1.40	1.33
3	C	3009[A]	ILE	C-N	5.50	1.40	1.33
3	C	3009[B]	ILE	C-N	5.50	1.40	1.33
3	O	3009[A]	ILE	C-N	5.45	1.40	1.33
3	O	3009[B]	ILE	C-N	5.45	1.40	1.33
3	R	3009[A]	ILE	C-N	5.45	1.40	1.33
3	R	3009[B]	ILE	C-N	5.45	1.40	1.33
3	I	3009[A]	ILE	C-N	5.45	1.40	1.33
3	I	3009[B]	ILE	C-N	5.45	1.40	1.33
3	U	3009[A]	ILE	C-N	5.42	1.40	1.33
3	U	3009[B]	ILE	C-N	5.42	1.40	1.33
3	a	3009[A]	ILE	C-N	5.42	1.40	1.33
3	a	3009[B]	ILE	C-N	5.42	1.40	1.33
3	L	3009[A]	ILE	C-N	5.39	1.40	1.33
3	L	3009[B]	ILE	C-N	5.39	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	d	2969[A]	TYR	C-N	5.39	1.40	1.33
3	d	2969[B]	TYR	C-N	5.39	1.40	1.33
3	R	3139[A]	LEU	C-N	5.38	1.40	1.33
3	R	3139[B]	LEU	C-N	5.38	1.40	1.33
3	a	3139[A]	LEU	C-N	5.38	1.40	1.33
3	a	3139[B]	LEU	C-N	5.38	1.40	1.33
3	O	2969[A]	TYR	C-N	5.37	1.40	1.33
3	O	2969[B]	TYR	C-N	5.37	1.40	1.33
3	U	2969[A]	TYR	C-N	5.37	1.40	1.33
3	U	2969[B]	TYR	C-N	5.37	1.40	1.33
3	X	3009[A]	ILE	C-N	5.36	1.40	1.33
3	X	3009[B]	ILE	C-N	5.36	1.40	1.33
3	a	2969[A]	TYR	C-N	5.36	1.40	1.33
3	a	2969[B]	TYR	C-N	5.36	1.40	1.33
3	d	3139[A]	LEU	C-N	5.34	1.40	1.33
3	d	3139[B]	LEU	C-N	5.34	1.40	1.33
3	d	3009[A]	ILE	C-N	5.33	1.40	1.33
3	d	3009[B]	ILE	C-N	5.33	1.40	1.33
3	X	3154[A]	PRO	N-CD	5.33	1.55	1.47
3	X	3154[B]	PRO	N-CD	5.33	1.55	1.47
3	F	3139[A]	LEU	C-N	5.31	1.40	1.33
3	F	3139[B]	LEU	C-N	5.31	1.40	1.33
3	L	2969[A]	TYR	C-N	5.31	1.40	1.33
3	L	2969[B]	TYR	C-N	5.31	1.40	1.33
3	O	3154[A]	PRO	N-CD	5.31	1.55	1.47
3	O	3154[B]	PRO	N-CD	5.31	1.55	1.47
3	U	3139[A]	LEU	C-N	5.31	1.40	1.33
3	U	3139[B]	LEU	C-N	5.31	1.40	1.33
3	C	3154[A]	PRO	N-CD	5.31	1.55	1.47
3	C	3154[B]	PRO	N-CD	5.31	1.55	1.47
3	C	3139[A]	LEU	C-N	5.31	1.40	1.33
3	C	3139[B]	LEU	C-N	5.31	1.40	1.33
3	X	2969[A]	TYR	C-N	5.31	1.40	1.33
3	X	2969[B]	TYR	C-N	5.31	1.40	1.33
3	R	3154[A]	PRO	N-CD	5.30	1.55	1.47
3	R	3154[B]	PRO	N-CD	5.30	1.55	1.47
3	X	3139[A]	LEU	C-N	5.30	1.40	1.33
3	X	3139[B]	LEU	C-N	5.30	1.40	1.33
3	C	2969[A]	TYR	C-N	5.29	1.40	1.33
3	C	2969[B]	TYR	C-N	5.29	1.40	1.33
3	F	2969[A]	TYR	C-N	5.29	1.40	1.33
3	F	2969[B]	TYR	C-N	5.29	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	3139[A]	LEU	C-N	5.29	1.40	1.33
3	L	3139[B]	LEU	C-N	5.29	1.40	1.33
3	a	3154[A]	PRO	N-CD	5.29	1.55	1.47
3	a	3154[B]	PRO	N-CD	5.29	1.55	1.47
3	O	3139[A]	LEU	C-N	5.28	1.40	1.33
3	O	3139[B]	LEU	C-N	5.28	1.40	1.33
3	R	2969[A]	TYR	C-N	5.28	1.40	1.33
3	R	2969[B]	TYR	C-N	5.28	1.40	1.33
3	I	2969[A]	TYR	C-N	5.27	1.40	1.33
3	I	2969[B]	TYR	C-N	5.27	1.40	1.33
3	I	3139[A]	LEU	C-N	5.27	1.40	1.33
3	I	3139[B]	LEU	C-N	5.27	1.40	1.33
3	X	3028[A]	PRO	N-CD	5.25	1.55	1.47
3	X	3028[B]	PRO	N-CD	5.25	1.55	1.47
3	L	3154[A]	PRO	N-CD	5.24	1.55	1.47
3	L	3154[B]	PRO	N-CD	5.24	1.55	1.47
1	P	1339	SER	CA-C	5.24	1.58	1.53
3	d	3154[A]	PRO	N-CD	5.24	1.55	1.47
3	d	3154[B]	PRO	N-CD	5.24	1.55	1.47
3	R	3028[A]	PRO	N-CD	5.24	1.55	1.47
3	R	3028[B]	PRO	N-CD	5.24	1.55	1.47
3	a	3028[A]	PRO	N-CD	5.24	1.55	1.47
3	a	3028[B]	PRO	N-CD	5.24	1.55	1.47
3	I	3154[A]	PRO	N-CD	5.23	1.55	1.47
3	I	3154[B]	PRO	N-CD	5.23	1.55	1.47
3	U	3154[A]	PRO	N-CD	5.23	1.55	1.47
3	U	3154[B]	PRO	N-CD	5.23	1.55	1.47
3	F	3154[A]	PRO	N-CD	5.22	1.55	1.47
3	F	3154[B]	PRO	N-CD	5.22	1.55	1.47
3	O	3028[A]	PRO	N-CD	5.21	1.55	1.47
3	O	3028[B]	PRO	N-CD	5.21	1.55	1.47
3	L	3198[A]	PRO	N-CD	5.21	1.55	1.47
3	L	3198[B]	PRO	N-CD	5.21	1.55	1.47
3	U	2986[A]	PRO	N-CD	5.21	1.55	1.47
3	U	2986[B]	PRO	N-CD	5.21	1.55	1.47
3	a	2986[A]	PRO	N-CD	5.21	1.55	1.47
3	a	2986[B]	PRO	N-CD	5.21	1.55	1.47
3	C	3028[A]	PRO	N-CD	5.20	1.55	1.47
3	C	3028[B]	PRO	N-CD	5.20	1.55	1.47
3	F	3028[A]	PRO	N-CD	5.20	1.55	1.47
3	F	3028[B]	PRO	N-CD	5.20	1.55	1.47
3	O	2986[A]	PRO	N-CD	5.20	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	2986[B]	PRO	N-CD	5.20	1.55	1.47
3	U	3010[A]	PRO	N-CD	5.19	1.55	1.47
3	U	3010[B]	PRO	N-CD	5.19	1.55	1.47
3	I	3028[A]	PRO	N-CD	5.19	1.55	1.47
3	I	3028[B]	PRO	N-CD	5.19	1.55	1.47
3	L	2986[A]	PRO	N-CD	5.19	1.55	1.47
3	L	2986[B]	PRO	N-CD	5.19	1.55	1.47
3	X	3010[A]	PRO	N-CD	5.18	1.55	1.47
3	X	3010[B]	PRO	N-CD	5.18	1.55	1.47
3	C	3010[A]	PRO	N-CD	5.18	1.55	1.47
3	C	3010[B]	PRO	N-CD	5.18	1.55	1.47
3	a	3010[A]	PRO	N-CD	5.18	1.55	1.47
3	a	3010[B]	PRO	N-CD	5.18	1.55	1.47
3	d	3028[A]	PRO	N-CD	5.18	1.54	1.47
3	d	3028[B]	PRO	N-CD	5.18	1.54	1.47
3	L	3010[A]	PRO	N-CD	5.17	1.54	1.47
3	L	3010[B]	PRO	N-CD	5.17	1.54	1.47
3	L	3028[A]	PRO	N-CD	5.17	1.54	1.47
3	L	3028[B]	PRO	N-CD	5.17	1.54	1.47
3	I	3198[A]	PRO	N-CD	5.17	1.54	1.47
3	I	3198[B]	PRO	N-CD	5.17	1.54	1.47
3	O	3198[A]	PRO	N-CD	5.16	1.54	1.47
3	O	3198[B]	PRO	N-CD	5.16	1.54	1.47
3	X	2986[A]	PRO	N-CD	5.16	1.54	1.47
3	X	2986[B]	PRO	N-CD	5.16	1.54	1.47
3	I	2986[A]	PRO	N-CD	5.16	1.54	1.47
3	I	2986[B]	PRO	N-CD	5.16	1.54	1.47
3	R	3198[A]	PRO	N-CD	5.16	1.54	1.47
3	R	3198[B]	PRO	N-CD	5.16	1.54	1.47
3	F	2986[A]	PRO	N-CD	5.15	1.54	1.47
3	F	2986[B]	PRO	N-CD	5.15	1.54	1.47
3	R	3010[A]	PRO	N-CD	5.15	1.54	1.47
3	R	3010[B]	PRO	N-CD	5.15	1.54	1.47
3	d	3010[A]	PRO	N-CD	5.15	1.54	1.47
3	d	3010[B]	PRO	N-CD	5.15	1.54	1.47
3	C	2986[A]	PRO	N-CD	5.15	1.54	1.47
3	C	2986[B]	PRO	N-CD	5.15	1.54	1.47
3	O	3010[A]	PRO	N-CD	5.15	1.54	1.47
3	O	3010[B]	PRO	N-CD	5.15	1.54	1.47
3	U	3028[A]	PRO	N-CD	5.15	1.54	1.47
3	U	3028[B]	PRO	N-CD	5.15	1.54	1.47
3	I	3010[A]	PRO	N-CD	5.13	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3010[B]	PRO	N-CD	5.13	1.54	1.47
1	G	1339	SER	CA-C	5.13	1.58	1.53
3	d	3297[A]	PRO	N-CD	5.13	1.54	1.47
3	d	3297[B]	PRO	N-CD	5.13	1.54	1.47
3	d	2986[A]	PRO	N-CD	5.12	1.54	1.47
3	d	2986[B]	PRO	N-CD	5.12	1.54	1.47
3	a	3198[A]	PRO	N-CD	5.12	1.54	1.47
3	a	3198[B]	PRO	N-CD	5.12	1.54	1.47
3	C	3198[A]	PRO	N-CD	5.12	1.54	1.47
3	C	3198[B]	PRO	N-CD	5.12	1.54	1.47
3	R	2986[A]	PRO	N-CD	5.12	1.54	1.47
3	R	2986[B]	PRO	N-CD	5.12	1.54	1.47
3	I	3297[A]	PRO	N-CD	5.11	1.54	1.47
3	I	3297[B]	PRO	N-CD	5.11	1.54	1.47
3	R	2970[A]	PRO	N-CD	5.10	1.54	1.47
3	R	2970[B]	PRO	N-CD	5.10	1.54	1.47
3	a	3297[A]	PRO	N-CD	5.10	1.54	1.47
3	a	3297[B]	PRO	N-CD	5.10	1.54	1.47
3	d	3198[A]	PRO	N-CD	5.10	1.54	1.47
3	d	3198[B]	PRO	N-CD	5.10	1.54	1.47
3	X	3198[A]	PRO	N-CD	5.10	1.54	1.47
3	X	3198[B]	PRO	N-CD	5.10	1.54	1.47
3	L	3297[A]	PRO	N-CD	5.10	1.54	1.47
3	L	3297[B]	PRO	N-CD	5.10	1.54	1.47
3	R	3297[A]	PRO	N-CD	5.10	1.54	1.47
3	R	3297[B]	PRO	N-CD	5.10	1.54	1.47
3	F	3010[A]	PRO	N-CD	5.10	1.54	1.47
3	F	3010[B]	PRO	N-CD	5.10	1.54	1.47
3	U	3198[A]	PRO	N-CD	5.09	1.54	1.47
3	U	3198[B]	PRO	N-CD	5.09	1.54	1.47
3	F	2970[A]	PRO	N-CD	5.09	1.54	1.47
3	F	2970[B]	PRO	N-CD	5.09	1.54	1.47
3	F	3198[A]	PRO	N-CD	5.08	1.54	1.47
3	F	3198[B]	PRO	N-CD	5.08	1.54	1.47
3	F	3297[A]	PRO	N-CD	5.07	1.54	1.47
3	F	3297[B]	PRO	N-CD	5.07	1.54	1.47
3	X	3297[A]	PRO	N-CD	5.06	1.54	1.47
3	X	3297[B]	PRO	N-CD	5.06	1.54	1.47
3	U	3297[A]	PRO	N-CD	5.06	1.54	1.47
3	U	3297[B]	PRO	N-CD	5.06	1.54	1.47
3	L	2970[A]	PRO	N-CD	5.06	1.54	1.47
3	L	2970[B]	PRO	N-CD	5.06	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	d	2970[A]	PRO	N-CD	5.05	1.54	1.47
3	d	2970[B]	PRO	N-CD	5.05	1.54	1.47
3	C	3297[A]	PRO	N-CD	5.05	1.54	1.47
3	C	3297[B]	PRO	N-CD	5.05	1.54	1.47
3	O	2970[A]	PRO	N-CD	5.05	1.54	1.47
3	O	2970[B]	PRO	N-CD	5.05	1.54	1.47
3	O	3297[A]	PRO	N-CD	5.03	1.54	1.47
3	O	3297[B]	PRO	N-CD	5.03	1.54	1.47
3	C	2970[A]	PRO	N-CD	5.03	1.54	1.47
3	C	2970[B]	PRO	N-CD	5.03	1.54	1.47
3	d	3051[A]	PRO	N-CD	5.03	1.54	1.47
3	d	3051[B]	PRO	N-CD	5.03	1.54	1.47
3	X	3027[A]	GLU	C-N	5.02	1.40	1.34
3	X	3027[B]	GLU	C-N	5.02	1.40	1.34
3	X	2970[A]	PRO	N-CD	5.02	1.54	1.47
3	X	2970[B]	PRO	N-CD	5.02	1.54	1.47
3	U	2970[A]	PRO	N-CD	5.00	1.54	1.47
3	U	2970[B]	PRO	N-CD	5.00	1.54	1.47

All (1613) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	464	LEU	CA-C-N	-16.02	99.82	119.84
1	D	464	LEU	C-N-CA	-16.02	99.82	119.84
1	J	883	CYS	CA-C-N	-12.76	103.89	119.84
1	J	883	CYS	C-N-CA	-12.76	103.89	119.84
1	b	464	LEU	CA-C-N	-12.27	104.50	119.84
1	b	464	LEU	C-N-CA	-12.27	104.50	119.84
2	Z	2128	LEU	CA-C-N	-11.05	109.00	120.38
2	Z	2128	LEU	C-N-CA	-11.05	109.00	120.38
3	d	3120[A]	HIS	N-CA-C	10.77	122.99	111.03
3	d	3120[B]	HIS	N-CA-C	10.77	122.99	111.03
3	L	3120[A]	HIS	N-CA-C	10.76	122.97	111.03
3	L	3120[B]	HIS	N-CA-C	10.76	122.97	111.03
3	R	3120[A]	HIS	N-CA-C	10.73	122.94	111.03
3	R	3120[B]	HIS	N-CA-C	10.73	122.94	111.03
3	I	3120[A]	HIS	N-CA-C	10.72	122.93	111.03
3	I	3120[B]	HIS	N-CA-C	10.72	122.93	111.03
3	U	3120[A]	HIS	N-CA-C	10.72	122.92	111.03
3	U	3120[B]	HIS	N-CA-C	10.72	122.92	111.03
3	a	3120[A]	HIS	N-CA-C	10.70	122.91	111.03
3	a	3120[B]	HIS	N-CA-C	10.70	122.91	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3120[A]	HIS	N-CA-C	10.70	122.91	111.03
3	C	3120[B]	HIS	N-CA-C	10.70	122.91	111.03
3	F	3120[A]	HIS	N-CA-C	10.68	122.89	111.03
3	F	3120[B]	HIS	N-CA-C	10.68	122.89	111.03
3	O	3120[A]	HIS	N-CA-C	10.68	122.89	111.03
3	O	3120[B]	HIS	N-CA-C	10.68	122.89	111.03
3	X	3120[A]	HIS	N-CA-C	10.67	122.87	111.03
3	X	3120[B]	HIS	N-CA-C	10.67	122.87	111.03
1	Y	898	GLY	N-CA-C	10.57	127.05	114.48
2	N	2340	ALA	CA-C-N	-10.46	108.99	119.56
2	N	2340	ALA	C-N-CA	-10.46	108.99	119.56
1	D	898	GLY	N-CA-C	10.43	126.89	114.48
1	D	1286	ARG	N-CA-C	10.35	123.65	111.02
1	V	898	GLY	N-CA-C	9.98	126.36	114.48
1	M	464	LEU	CA-C-N	-9.82	109.96	120.47
1	M	464	LEU	C-N-CA	-9.82	109.96	120.47
3	a	3279[A]	ASP	N-CA-C	-9.80	97.02	110.35
3	a	3279[B]	ASP	N-CA-C	-9.80	97.02	110.35
3	L	3279[A]	ASP	N-CA-C	-9.80	97.02	110.35
3	L	3279[B]	ASP	N-CA-C	-9.80	97.02	110.35
3	R	3279[A]	ASP	N-CA-C	-9.79	97.03	110.35
3	R	3279[B]	ASP	N-CA-C	-9.79	97.03	110.35
3	O	3279[A]	ASP	N-CA-C	-9.79	97.04	110.35
3	O	3279[B]	ASP	N-CA-C	-9.79	97.04	110.35
1	A	1584	GLY	N-CA-C	9.78	124.73	111.03
3	C	3279[A]	ASP	N-CA-C	-9.78	97.04	110.35
3	C	3279[B]	ASP	N-CA-C	-9.78	97.04	110.35
3	U	3279[A]	ASP	N-CA-C	-9.78	97.05	110.35
3	U	3279[B]	ASP	N-CA-C	-9.78	97.05	110.35
3	F	3279[A]	ASP	N-CA-C	-9.77	97.06	110.35
3	F	3279[B]	ASP	N-CA-C	-9.77	97.06	110.35
3	d	3279[A]	ASP	N-CA-C	-9.76	97.07	110.35
3	d	3279[B]	ASP	N-CA-C	-9.76	97.07	110.35
3	X	3279[A]	ASP	N-CA-C	-9.75	97.09	110.35
3	X	3279[B]	ASP	N-CA-C	-9.75	97.09	110.35
3	I	3279[A]	ASP	N-CA-C	-9.74	97.11	110.35
3	I	3279[B]	ASP	N-CA-C	-9.74	97.11	110.35
1	b	883	CYS	CA-C-N	-9.37	107.60	120.25
1	b	883	CYS	C-N-CA	-9.37	107.60	120.25
1	M	898	GLY	N-CA-C	9.26	125.49	114.48
3	I	2948[A]	ASP	N-CA-C	-9.24	98.74	112.04
3	I	2948[B]	ASP	N-CA-C	-9.24	98.74	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	2948[A]	ASP	N-CA-C	-9.23	98.75	112.04
3	R	2948[B]	ASP	N-CA-C	-9.23	98.75	112.04
3	F	2948[A]	ASP	N-CA-C	-9.22	98.76	112.04
3	F	2948[B]	ASP	N-CA-C	-9.22	98.76	112.04
3	L	2948[A]	ASP	N-CA-C	-9.22	98.76	112.04
3	L	2948[B]	ASP	N-CA-C	-9.22	98.76	112.04
3	U	2948[A]	ASP	N-CA-C	-9.21	98.78	112.04
3	U	2948[B]	ASP	N-CA-C	-9.21	98.78	112.04
3	X	2948[A]	ASP	N-CA-C	-9.21	98.78	112.04
3	X	2948[B]	ASP	N-CA-C	-9.21	98.78	112.04
3	C	2948[A]	ASP	N-CA-C	-9.19	98.80	112.04
3	C	2948[B]	ASP	N-CA-C	-9.19	98.80	112.04
3	a	2948[A]	ASP	N-CA-C	-9.19	98.80	112.04
3	a	2948[B]	ASP	N-CA-C	-9.19	98.80	112.04
3	O	2948[A]	ASP	N-CA-C	-9.19	98.81	112.04
3	O	2948[B]	ASP	N-CA-C	-9.19	98.81	112.04
1	b	675	SER	CA-C-N	-9.19	109.45	119.19
1	b	675	SER	C-N-CA	-9.19	109.45	119.19
3	d	2948[A]	ASP	N-CA-C	-9.19	98.81	112.04
3	d	2948[B]	ASP	N-CA-C	-9.19	98.81	112.04
2	N	2128	LEU	CA-C-N	-9.05	111.06	120.38
2	N	2128	LEU	C-N-CA	-9.05	111.06	120.38
2	W	2128	LEU	CA-C-N	-8.97	111.14	120.38
2	W	2128	LEU	C-N-CA	-8.97	111.14	120.38
1	M	982	LYS	CA-C-N	-8.96	110.65	120.14
1	M	982	LYS	C-N-CA	-8.96	110.65	120.14
2	T	2128	LEU	CA-C-N	-8.76	111.36	120.38
2	T	2128	LEU	C-N-CA	-8.76	111.36	120.38
1	G	1584	GLY	N-CA-C	8.71	123.23	111.03
3	I	3176[A]	LYS	N-CA-C	-8.63	99.14	110.53
3	I	3176[B]	LYS	N-CA-C	-8.63	99.14	110.53
2	c	2128	LEU	CA-C-N	-8.62	111.51	120.38
2	c	2128	LEU	C-N-CA	-8.62	111.51	120.38
3	R	3176[A]	LYS	N-CA-C	-8.61	99.16	110.53
3	R	3176[B]	LYS	N-CA-C	-8.61	99.16	110.53
3	U	3176[A]	LYS	N-CA-C	-8.61	99.17	110.53
3	U	3176[B]	LYS	N-CA-C	-8.61	99.17	110.53
3	O	3176[A]	LYS	N-CA-C	-8.60	99.17	110.53
3	O	3176[B]	LYS	N-CA-C	-8.60	99.17	110.53
3	L	3176[A]	LYS	N-CA-C	-8.59	99.19	110.53
3	L	3176[B]	LYS	N-CA-C	-8.59	99.19	110.53
3	d	3176[A]	LYS	N-CA-C	-8.59	99.19	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	d	3176[B]	LYS	N-CA-C	-8.59	99.19	110.53
3	F	3176[A]	LYS	N-CA-C	-8.57	99.21	110.53
3	F	3176[B]	LYS	N-CA-C	-8.57	99.21	110.53
2	K	2128	LEU	CA-C-N	-8.57	111.55	120.38
2	K	2128	LEU	C-N-CA	-8.57	111.55	120.38
3	a	3176[A]	LYS	N-CA-C	-8.57	99.21	110.53
3	a	3176[B]	LYS	N-CA-C	-8.57	99.21	110.53
2	Q	2128	LEU	CA-C-N	-8.55	111.57	120.38
2	Q	2128	LEU	C-N-CA	-8.55	111.57	120.38
3	X	3176[A]	LYS	N-CA-C	-8.54	99.25	110.53
3	X	3176[B]	LYS	N-CA-C	-8.54	99.25	110.53
3	C	3176[A]	LYS	N-CA-C	-8.54	99.26	110.53
3	C	3176[B]	LYS	N-CA-C	-8.54	99.26	110.53
1	D	669	LYS	CA-C-N	-8.50	110.61	120.89
1	D	669	LYS	C-N-CA	-8.50	110.61	120.89
1	b	450	LYS	N-CA-C	8.46	121.20	109.18
1	A	898	GLY	N-CA-C	8.42	127.93	115.64
1	J	898	GLY	N-CA-C	8.42	126.43	114.64
3	X	2952[A]	ALA	N-CA-C	-8.31	100.99	112.12
3	X	2952[B]	ALA	N-CA-C	-8.31	100.99	112.12
3	d	2952[A]	ALA	N-CA-C	-8.29	101.01	112.12
3	d	2952[B]	ALA	N-CA-C	-8.29	101.01	112.12
3	a	2952[A]	ALA	N-CA-C	-8.29	101.01	112.12
3	a	2952[B]	ALA	N-CA-C	-8.29	101.01	112.12
3	L	2952[A]	ALA	N-CA-C	-8.27	101.04	112.12
3	L	2952[B]	ALA	N-CA-C	-8.27	101.04	112.12
3	R	2952[A]	ALA	N-CA-C	-8.26	101.05	112.12
3	R	2952[B]	ALA	N-CA-C	-8.26	101.05	112.12
3	U	2952[A]	ALA	N-CA-C	-8.26	101.06	112.12
3	U	2952[B]	ALA	N-CA-C	-8.26	101.06	112.12
3	O	2952[A]	ALA	N-CA-C	-8.24	101.08	112.12
3	O	2952[B]	ALA	N-CA-C	-8.24	101.08	112.12
3	F	2952[A]	ALA	N-CA-C	-8.23	101.09	112.12
3	F	2952[B]	ALA	N-CA-C	-8.23	101.09	112.12
1	D	1582	ASN	N-CA-C	8.22	121.01	108.52
3	I	2952[A]	ALA	N-CA-C	-8.22	101.11	112.12
3	I	2952[B]	ALA	N-CA-C	-8.22	101.11	112.12
3	C	2952[A]	ALA	N-CA-C	-8.21	101.12	112.12
3	C	2952[B]	ALA	N-CA-C	-8.21	101.12	112.12
1	D	982	LYS	CA-C-N	-8.18	111.31	119.90
1	D	982	LYS	C-N-CA	-8.18	111.31	119.90
1	b	898	GLY	N-CA-C	8.15	124.18	114.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	d	3003[A]	LYS	N-CA-C	-8.08	100.48	111.87
3	d	3003[B]	LYS	N-CA-C	-8.08	100.48	111.87
3	I	3003[A]	LYS	N-CA-C	-8.07	100.49	111.87
3	I	3003[B]	LYS	N-CA-C	-8.07	100.49	111.87
3	U	3003[A]	LYS	N-CA-C	-8.07	100.49	111.87
3	U	3003[B]	LYS	N-CA-C	-8.07	100.49	111.87
3	L	3003[A]	LYS	N-CA-C	-8.07	100.50	111.87
3	L	3003[B]	LYS	N-CA-C	-8.07	100.50	111.87
3	F	3003[A]	LYS	N-CA-C	-8.06	100.50	111.87
3	F	3003[B]	LYS	N-CA-C	-8.06	100.50	111.87
3	C	3003[A]	LYS	N-CA-C	-8.05	100.51	111.87
3	C	3003[B]	LYS	N-CA-C	-8.05	100.51	111.87
3	X	3003[A]	LYS	N-CA-C	-8.04	100.53	111.87
3	X	3003[B]	LYS	N-CA-C	-8.04	100.53	111.87
3	R	3003[A]	LYS	N-CA-C	-8.04	100.53	111.87
3	R	3003[B]	LYS	N-CA-C	-8.04	100.53	111.87
2	B	2128	LEU	CA-C-N	-8.04	112.10	120.38
2	B	2128	LEU	C-N-CA	-8.04	112.10	120.38
3	O	3003[A]	LYS	N-CA-C	-8.03	100.55	111.87
3	O	3003[B]	LYS	N-CA-C	-8.03	100.55	111.87
3	a	3003[A]	LYS	N-CA-C	-8.03	100.55	111.87
3	a	3003[B]	LYS	N-CA-C	-8.03	100.55	111.87
2	Q	2340	ALA	CA-C-N	-8.01	111.54	119.87
2	Q	2340	ALA	C-N-CA	-8.01	111.54	119.87
1	Y	85	SER	N-CA-C	7.88	119.02	108.38
2	H	2128	LEU	CA-C-N	-7.87	112.27	120.38
2	H	2128	LEU	C-N-CA	-7.87	112.27	120.38
2	Z	2340	ALA	CA-C-N	-7.82	111.74	119.87
2	Z	2340	ALA	C-N-CA	-7.82	111.74	119.87
2	E	2548	CYS	CA-C-N	-7.80	111.71	119.90
2	E	2548	CYS	C-N-CA	-7.80	111.71	119.90
1	A	464	LEU	CA-C-N	-7.78	111.63	121.04
1	A	464	LEU	C-N-CA	-7.78	111.63	121.04
2	W	2472	ASN	N-CA-C	7.72	119.77	111.36
1	M	1082	SER	CA-C-N	-7.69	110.23	119.84
1	M	1082	SER	C-N-CA	-7.69	110.23	119.84
3	I	2966[A]	SER	N-CA-C	7.66	119.71	111.36
3	I	2966[B]	SER	N-CA-C	7.66	119.71	111.36
3	a	3192[A]	PHE	N-CA-C	-7.65	100.46	110.33
3	a	3192[B]	PHE	N-CA-C	-7.65	100.46	110.33
3	R	2966[A]	SER	N-CA-C	7.65	119.69	111.36
3	R	2966[B]	SER	N-CA-C	7.65	119.69	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	2966[A]	SER	N-CA-C	7.64	119.69	111.36
3	U	2966[B]	SER	N-CA-C	7.64	119.69	111.36
3	R	3192[A]	PHE	N-CA-C	-7.64	100.48	110.33
3	R	3192[B]	PHE	N-CA-C	-7.64	100.48	110.33
3	U	3192[A]	PHE	N-CA-C	-7.64	100.48	110.33
3	U	3192[B]	PHE	N-CA-C	-7.64	100.48	110.33
3	d	2966[A]	SER	N-CA-C	7.64	119.69	111.36
3	d	2966[B]	SER	N-CA-C	7.64	119.69	111.36
3	F	3192[A]	PHE	N-CA-C	-7.64	100.48	110.33
3	F	3192[B]	PHE	N-CA-C	-7.64	100.48	110.33
3	C	2966[A]	SER	N-CA-C	7.63	119.68	111.36
3	C	2966[B]	SER	N-CA-C	7.63	119.68	111.36
3	I	3192[A]	PHE	N-CA-C	-7.62	100.49	110.33
3	I	3192[B]	PHE	N-CA-C	-7.62	100.49	110.33
3	C	3192[A]	PHE	N-CA-C	-7.62	100.50	110.33
3	C	3192[B]	PHE	N-CA-C	-7.62	100.50	110.33
3	F	2966[A]	SER	N-CA-C	7.61	119.66	111.36
3	F	2966[B]	SER	N-CA-C	7.61	119.66	111.36
3	d	3192[A]	PHE	N-CA-C	-7.61	100.51	110.33
3	d	3192[B]	PHE	N-CA-C	-7.61	100.51	110.33
3	L	2966[A]	SER	N-CA-C	7.60	119.65	111.36
3	L	2966[B]	SER	N-CA-C	7.60	119.65	111.36
3	X	3192[A]	PHE	N-CA-C	-7.60	100.53	110.33
3	X	3192[B]	PHE	N-CA-C	-7.60	100.53	110.33
3	O	3192[A]	PHE	N-CA-C	-7.60	100.53	110.33
3	O	3192[B]	PHE	N-CA-C	-7.60	100.53	110.33
3	X	2966[A]	SER	N-CA-C	7.60	119.64	111.36
3	X	2966[B]	SER	N-CA-C	7.60	119.64	111.36
3	a	2966[A]	SER	N-CA-C	7.60	119.64	111.36
3	a	2966[B]	SER	N-CA-C	7.60	119.64	111.36
1	b	830	ASN	N-CA-C	7.60	119.20	111.07
3	I	3009[A]	ILE	CA-C-N	-7.59	113.01	120.52
3	I	3009[A]	ILE	C-N-CA	-7.59	113.01	120.52
3	I	3009[B]	ILE	CA-C-N	-7.59	113.01	120.52
3	I	3009[B]	ILE	C-N-CA	-7.59	113.01	120.52
3	O	2966[A]	SER	N-CA-C	7.58	119.62	111.36
3	O	2966[B]	SER	N-CA-C	7.58	119.62	111.36
3	L	3192[A]	PHE	N-CA-C	-7.58	100.55	110.33
3	L	3192[B]	PHE	N-CA-C	-7.58	100.55	110.33
1	P	982	LYS	CA-C-N	-7.57	112.19	119.76
1	P	982	LYS	C-N-CA	-7.57	112.19	119.76
3	O	3009[A]	ILE	CA-C-N	-7.56	113.04	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	3009[A]	ILE	C-N-CA	-7.56	113.04	120.52
3	O	3009[B]	ILE	CA-C-N	-7.56	113.04	120.52
3	O	3009[B]	ILE	C-N-CA	-7.56	113.04	120.52
3	U	3009[A]	ILE	CA-C-N	-7.53	113.06	120.52
3	U	3009[A]	ILE	C-N-CA	-7.53	113.06	120.52
3	U	3009[B]	ILE	CA-C-N	-7.53	113.06	120.52
3	U	3009[B]	ILE	C-N-CA	-7.53	113.06	120.52
3	R	3009[A]	ILE	CA-C-N	-7.53	113.07	120.52
3	R	3009[A]	ILE	C-N-CA	-7.53	113.07	120.52
3	R	3009[B]	ILE	CA-C-N	-7.53	113.07	120.52
3	R	3009[B]	ILE	C-N-CA	-7.53	113.07	120.52
3	F	3009[A]	ILE	CA-C-N	-7.51	113.08	120.52
3	F	3009[A]	ILE	C-N-CA	-7.51	113.08	120.52
3	F	3009[B]	ILE	CA-C-N	-7.51	113.08	120.52
3	F	3009[B]	ILE	C-N-CA	-7.51	113.08	120.52
3	C	3009[A]	ILE	CA-C-N	-7.51	113.08	120.52
3	C	3009[A]	ILE	C-N-CA	-7.51	113.08	120.52
3	C	3009[B]	ILE	CA-C-N	-7.51	113.08	120.52
3	C	3009[B]	ILE	C-N-CA	-7.51	113.08	120.52
3	a	3009[A]	ILE	CA-C-N	-7.51	113.09	120.52
3	a	3009[A]	ILE	C-N-CA	-7.51	113.09	120.52
3	a	3009[B]	ILE	CA-C-N	-7.51	113.09	120.52
3	a	3009[B]	ILE	C-N-CA	-7.51	113.09	120.52
3	X	3009[A]	ILE	CA-C-N	-7.49	113.10	120.52
3	X	3009[A]	ILE	C-N-CA	-7.49	113.10	120.52
3	X	3009[B]	ILE	CA-C-N	-7.49	113.10	120.52
3	X	3009[B]	ILE	C-N-CA	-7.49	113.10	120.52
3	L	3009[A]	ILE	CA-C-N	-7.47	113.12	120.52
3	L	3009[A]	ILE	C-N-CA	-7.47	113.12	120.52
3	L	3009[B]	ILE	CA-C-N	-7.47	113.12	120.52
3	L	3009[B]	ILE	C-N-CA	-7.47	113.12	120.52
3	d	3009[A]	ILE	CA-C-N	-7.44	113.15	120.52
3	d	3009[A]	ILE	C-N-CA	-7.44	113.15	120.52
3	d	3009[B]	ILE	CA-C-N	-7.44	113.15	120.52
3	d	3009[B]	ILE	C-N-CA	-7.44	113.15	120.52
1	A	1195	ASP	CA-C-N	7.44	135.10	121.70
1	A	1195	ASP	C-N-CA	7.44	135.10	121.70
1	G	464	LEU	CA-C-N	-7.42	112.06	121.04
1	G	464	LEU	C-N-CA	-7.42	112.06	121.04
1	S	464	LEU	CA-C-N	-7.38	112.11	121.04
1	S	464	LEU	C-N-CA	-7.38	112.11	121.04
1	P	116	LYS	CB-CA-C	-7.34	108.10	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	883	CYS	CA-C-N	-7.32	110.69	119.84
1	G	883	CYS	C-N-CA	-7.32	110.69	119.84
2	E	2866	PRO	CA-C-N	7.31	127.32	119.28
2	E	2866	PRO	C-N-CA	7.31	127.32	119.28
3	d	3173[A]	THR	CA-C-N	7.28	128.02	119.94
3	d	3173[A]	THR	C-N-CA	7.28	128.02	119.94
3	d	3173[B]	THR	CA-C-N	7.28	128.02	119.94
3	d	3173[B]	THR	C-N-CA	7.28	128.02	119.94
3	F	3296[A]	PRO	CA-C-O	-7.26	115.67	120.90
3	F	3296[B]	PRO	CA-C-O	-7.26	115.67	120.90
3	I	3296[A]	PRO	CA-C-O	-7.26	115.67	120.90
3	I	3296[B]	PRO	CA-C-O	-7.26	115.67	120.90
3	R	3296[A]	PRO	CA-C-O	-7.26	115.67	120.90
3	R	3296[B]	PRO	CA-C-O	-7.26	115.67	120.90
3	X	3296[A]	PRO	CA-C-O	-7.26	115.67	120.90
3	X	3296[B]	PRO	CA-C-O	-7.26	115.67	120.90
1	b	228	GLY	N-CA-C	7.25	125.05	114.10
3	R	3173[A]	THR	CA-C-N	7.24	127.98	119.94
3	R	3173[A]	THR	C-N-CA	7.24	127.98	119.94
3	R	3173[B]	THR	CA-C-N	7.24	127.98	119.94
3	R	3173[B]	THR	C-N-CA	7.24	127.98	119.94
3	U	3296[A]	PRO	CA-C-O	-7.24	115.69	120.90
3	U	3296[B]	PRO	CA-C-O	-7.24	115.69	120.90
1	G	323	ILE	CA-C-N	7.22	127.26	119.89
1	G	323	ILE	C-N-CA	7.22	127.26	119.89
3	L	3173[A]	THR	CA-C-N	7.22	127.95	119.94
3	L	3173[A]	THR	C-N-CA	7.22	127.95	119.94
3	L	3173[B]	THR	CA-C-N	7.22	127.95	119.94
3	L	3173[B]	THR	C-N-CA	7.22	127.95	119.94
3	L	3296[A]	PRO	CA-C-O	-7.22	115.70	120.90
3	L	3296[B]	PRO	CA-C-O	-7.22	115.70	120.90
3	a	3296[A]	PRO	CA-C-O	-7.22	115.70	120.90
3	a	3296[B]	PRO	CA-C-O	-7.22	115.70	120.90
3	O	3173[A]	THR	CA-C-N	7.21	127.94	119.94
3	O	3173[A]	THR	C-N-CA	7.21	127.94	119.94
3	O	3173[B]	THR	CA-C-N	7.21	127.94	119.94
3	O	3173[B]	THR	C-N-CA	7.21	127.94	119.94
3	C	3173[A]	THR	CA-C-N	7.19	127.92	119.94
3	C	3173[A]	THR	C-N-CA	7.19	127.92	119.94
3	C	3173[B]	THR	CA-C-N	7.19	127.92	119.94
3	C	3173[B]	THR	C-N-CA	7.19	127.92	119.94
3	C	3296[A]	PRO	CA-C-O	-7.18	115.73	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3296[B]	PRO	CA-C-O	-7.18	115.73	120.90
3	F	3173[A]	THR	CA-C-N	7.18	127.91	119.94
3	F	3173[A]	THR	C-N-CA	7.18	127.91	119.94
3	F	3173[B]	THR	CA-C-N	7.18	127.91	119.94
3	F	3173[B]	THR	C-N-CA	7.18	127.91	119.94
3	I	3173[A]	THR	CA-C-N	7.18	127.91	119.94
3	I	3173[A]	THR	C-N-CA	7.18	127.91	119.94
3	I	3173[B]	THR	CA-C-N	7.18	127.91	119.94
3	I	3173[B]	THR	C-N-CA	7.18	127.91	119.94
3	U	3173[A]	THR	CA-C-N	7.17	127.90	119.94
3	U	3173[A]	THR	C-N-CA	7.17	127.90	119.94
3	U	3173[B]	THR	CA-C-N	7.17	127.90	119.94
3	U	3173[B]	THR	C-N-CA	7.17	127.90	119.94
3	F	3153[A]	LYS	CA-C-N	-7.17	113.29	120.31
3	F	3153[A]	LYS	C-N-CA	-7.17	113.29	120.31
3	F	3153[B]	LYS	CA-C-N	-7.17	113.29	120.31
3	F	3153[B]	LYS	C-N-CA	-7.17	113.29	120.31
3	U	3196[A]	THR	N-CA-C	-7.17	100.88	110.55
3	U	3196[B]	THR	N-CA-C	-7.17	100.88	110.55
3	a	3173[A]	THR	CA-C-N	7.17	127.89	119.94
3	a	3173[A]	THR	C-N-CA	7.17	127.89	119.94
3	a	3173[B]	THR	CA-C-N	7.17	127.89	119.94
3	a	3173[B]	THR	C-N-CA	7.17	127.89	119.94
3	X	3173[A]	THR	CA-C-N	7.16	127.89	119.94
3	X	3173[A]	THR	C-N-CA	7.16	127.89	119.94
3	X	3173[B]	THR	CA-C-N	7.16	127.89	119.94
3	X	3173[B]	THR	C-N-CA	7.16	127.89	119.94
3	d	3153[A]	LYS	CA-C-N	-7.16	113.30	120.31
3	d	3153[A]	LYS	C-N-CA	-7.16	113.30	120.31
3	d	3153[B]	LYS	CA-C-N	-7.16	113.30	120.31
3	d	3153[B]	LYS	C-N-CA	-7.16	113.30	120.31
3	U	3153[A]	LYS	CA-C-N	-7.15	113.30	120.31
3	U	3153[A]	LYS	C-N-CA	-7.15	113.30	120.31
3	U	3153[B]	LYS	CA-C-N	-7.15	113.30	120.31
3	U	3153[B]	LYS	C-N-CA	-7.15	113.30	120.31
3	R	3153[A]	LYS	CA-C-N	-7.14	113.31	120.31
3	R	3153[A]	LYS	C-N-CA	-7.14	113.31	120.31
3	R	3153[B]	LYS	CA-C-N	-7.14	113.31	120.31
3	R	3153[B]	LYS	C-N-CA	-7.14	113.31	120.31
1	S	1195	ASP	CA-C-N	7.14	134.56	121.70
1	S	1195	ASP	C-N-CA	7.14	134.56	121.70
1	M	417	MET	N-CA-C	7.14	119.60	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	3153[A]	LYS	CA-C-N	-7.13	113.32	120.31
3	L	3153[A]	LYS	C-N-CA	-7.13	113.32	120.31
3	L	3153[B]	LYS	CA-C-N	-7.13	113.32	120.31
3	L	3153[B]	LYS	C-N-CA	-7.13	113.32	120.31
3	d	3296[A]	PRO	CA-C-O	-7.13	115.76	120.90
3	d	3296[B]	PRO	CA-C-O	-7.13	115.76	120.90
3	X	3153[A]	LYS	CA-C-N	-7.13	113.32	120.31
3	X	3153[A]	LYS	C-N-CA	-7.13	113.32	120.31
3	X	3153[B]	LYS	CA-C-N	-7.13	113.32	120.31
3	X	3153[B]	LYS	C-N-CA	-7.13	113.32	120.31
3	a	3153[A]	LYS	CA-C-N	-7.13	113.32	120.31
3	a	3153[A]	LYS	C-N-CA	-7.13	113.32	120.31
3	a	3153[B]	LYS	CA-C-N	-7.13	113.32	120.31
3	a	3153[B]	LYS	C-N-CA	-7.13	113.32	120.31
3	O	3296[A]	PRO	CA-C-O	-7.13	115.77	120.90
3	O	3296[B]	PRO	CA-C-O	-7.13	115.77	120.90
3	O	3153[A]	LYS	CA-C-N	-7.13	113.33	120.31
3	O	3153[A]	LYS	C-N-CA	-7.13	113.33	120.31
3	O	3153[B]	LYS	CA-C-N	-7.13	113.33	120.31
3	O	3153[B]	LYS	C-N-CA	-7.13	113.33	120.31
3	I	3153[A]	LYS	CA-C-N	-7.12	113.33	120.31
3	I	3153[A]	LYS	C-N-CA	-7.12	113.33	120.31
3	I	3153[B]	LYS	CA-C-N	-7.12	113.33	120.31
3	I	3153[B]	LYS	C-N-CA	-7.12	113.33	120.31
3	I	3196[A]	THR	N-CA-C	-7.12	100.94	110.55
3	I	3196[B]	THR	N-CA-C	-7.12	100.94	110.55
3	O	3196[A]	THR	N-CA-C	-7.12	100.94	110.55
3	O	3196[B]	THR	N-CA-C	-7.12	100.94	110.55
3	L	3196[A]	THR	N-CA-C	-7.11	100.95	110.55
3	L	3196[B]	THR	N-CA-C	-7.11	100.95	110.55
3	R	3196[A]	THR	N-CA-C	-7.11	100.95	110.55
3	R	3196[B]	THR	N-CA-C	-7.11	100.95	110.55
3	d	3196[A]	THR	N-CA-C	-7.11	100.95	110.55
3	d	3196[B]	THR	N-CA-C	-7.11	100.95	110.55
3	F	3196[A]	THR	N-CA-C	-7.11	100.96	110.55
3	F	3196[B]	THR	N-CA-C	-7.11	100.96	110.55
3	C	3196[A]	THR	N-CA-C	-7.10	100.96	110.55
3	C	3196[B]	THR	N-CA-C	-7.10	100.96	110.55
2	E	2128	LEU	CA-C-N	-7.10	113.06	120.38
2	E	2128	LEU	C-N-CA	-7.10	113.06	120.38
3	X	3196[A]	THR	N-CA-C	-7.10	100.96	110.55
3	X	3196[B]	THR	N-CA-C	-7.10	100.96	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	3196[A]	THR	N-CA-C	-7.08	100.99	110.55
3	a	3196[B]	THR	N-CA-C	-7.08	100.99	110.55
3	C	3153[A]	LYS	CA-C-N	-7.05	113.40	120.31
3	C	3153[A]	LYS	C-N-CA	-7.05	113.40	120.31
3	C	3153[B]	LYS	CA-C-N	-7.05	113.40	120.31
3	C	3153[B]	LYS	C-N-CA	-7.05	113.40	120.31
1	M	897	HIS	N-CA-C	-7.00	99.17	108.34
3	I	3308[A]	LYS	CA-C-N	-6.98	113.47	120.31
3	I	3308[A]	LYS	C-N-CA	-6.98	113.47	120.31
3	I	3308[B]	LYS	CA-C-N	-6.98	113.47	120.31
3	I	3308[B]	LYS	C-N-CA	-6.98	113.47	120.31
1	P	418	ASP	N-CA-C	6.98	118.97	111.36
1	J	117	LYS	N-CA-C	6.93	117.64	108.07
3	R	3308[A]	LYS	CA-C-N	-6.93	113.52	120.31
3	R	3308[A]	LYS	C-N-CA	-6.93	113.52	120.31
3	R	3308[B]	LYS	CA-C-N	-6.93	113.52	120.31
3	R	3308[B]	LYS	C-N-CA	-6.93	113.52	120.31
3	C	3308[A]	LYS	CA-C-N	-6.93	113.52	120.31
3	C	3308[A]	LYS	C-N-CA	-6.93	113.52	120.31
3	C	3308[B]	LYS	CA-C-N	-6.93	113.52	120.31
3	C	3308[B]	LYS	C-N-CA	-6.93	113.52	120.31
1	P	1584	GLY	N-CA-C	6.93	123.34	111.15
1	S	1636	ASN	N-CA-C	-6.93	103.74	111.71
3	F	2931[A]	THR	CA-C-N	-6.90	112.65	119.76
3	F	2931[A]	THR	C-N-CA	-6.90	112.65	119.76
3	F	2931[B]	THR	CA-C-N	-6.90	112.65	119.76
3	F	2931[B]	THR	C-N-CA	-6.90	112.65	119.76
3	X	3308[A]	LYS	CA-C-N	-6.90	113.55	120.31
3	X	3308[A]	LYS	C-N-CA	-6.90	113.55	120.31
3	X	3308[B]	LYS	CA-C-N	-6.90	113.55	120.31
3	X	3308[B]	LYS	C-N-CA	-6.90	113.55	120.31
3	O	3308[A]	LYS	CA-C-N	-6.90	113.55	120.31
3	O	3308[A]	LYS	C-N-CA	-6.90	113.55	120.31
3	O	3308[B]	LYS	CA-C-N	-6.90	113.55	120.31
3	O	3308[B]	LYS	C-N-CA	-6.90	113.55	120.31
3	R	2931[A]	THR	CA-C-N	-6.90	112.66	119.76
3	R	2931[A]	THR	C-N-CA	-6.90	112.66	119.76
3	R	2931[B]	THR	CA-C-N	-6.90	112.66	119.76
3	R	2931[B]	THR	C-N-CA	-6.90	112.66	119.76
3	d	3308[A]	LYS	CA-C-N	-6.89	113.55	120.31
3	d	3308[A]	LYS	C-N-CA	-6.89	113.55	120.31
3	d	3308[B]	LYS	CA-C-N	-6.89	113.55	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	d	3308[B]	LYS	C-N-CA	-6.89	113.55	120.31
3	F	3308[A]	LYS	CA-C-N	-6.89	113.56	120.31
3	F	3308[A]	LYS	C-N-CA	-6.89	113.56	120.31
3	F	3308[B]	LYS	CA-C-N	-6.89	113.56	120.31
3	F	3308[B]	LYS	C-N-CA	-6.89	113.56	120.31
3	L	3308[A]	LYS	CA-C-N	-6.89	113.56	120.31
3	L	3308[A]	LYS	C-N-CA	-6.89	113.56	120.31
3	L	3308[B]	LYS	CA-C-N	-6.89	113.56	120.31
3	L	3308[B]	LYS	C-N-CA	-6.89	113.56	120.31
3	O	2931[A]	THR	CA-C-N	-6.89	112.67	119.76
3	O	2931[A]	THR	C-N-CA	-6.89	112.67	119.76
3	O	2931[B]	THR	CA-C-N	-6.89	112.67	119.76
3	O	2931[B]	THR	C-N-CA	-6.89	112.67	119.76
1	Y	957	ASN	CA-C-N	-6.89	113.60	120.21
1	Y	957	ASN	C-N-CA	-6.89	113.60	120.21
3	U	2931[A]	THR	CA-C-N	-6.89	112.67	119.76
3	U	2931[A]	THR	C-N-CA	-6.89	112.67	119.76
3	U	2931[B]	THR	CA-C-N	-6.89	112.67	119.76
3	U	2931[B]	THR	C-N-CA	-6.89	112.67	119.76
2	W	2650	GLY	N-CA-C	6.89	120.97	112.64
3	d	2931[A]	THR	CA-C-N	-6.89	112.67	119.76
3	d	2931[A]	THR	C-N-CA	-6.89	112.67	119.76
3	d	2931[B]	THR	CA-C-N	-6.89	112.67	119.76
3	d	2931[B]	THR	C-N-CA	-6.89	112.67	119.76
3	U	3308[A]	LYS	CA-C-N	-6.88	113.56	120.31
3	U	3308[A]	LYS	C-N-CA	-6.88	113.56	120.31
3	U	3308[B]	LYS	CA-C-N	-6.88	113.56	120.31
3	U	3308[B]	LYS	C-N-CA	-6.88	113.56	120.31
3	a	3308[A]	LYS	CA-C-N	-6.88	113.57	120.31
3	a	3308[A]	LYS	C-N-CA	-6.88	113.57	120.31
3	a	3308[B]	LYS	CA-C-N	-6.88	113.57	120.31
3	a	3308[B]	LYS	C-N-CA	-6.88	113.57	120.31
3	U	3197[A]	ILE	O-C-N	6.87	124.82	120.42
3	U	3197[B]	ILE	O-C-N	6.87	124.82	120.42
2	E	2340	ALA	CA-C-N	-6.86	112.71	119.64
2	E	2340	ALA	C-N-CA	-6.86	112.71	119.64
3	a	3197[A]	ILE	O-C-N	6.86	124.81	120.42
3	a	3197[B]	ILE	O-C-N	6.86	124.81	120.42
3	X	2931[A]	THR	CA-C-N	-6.85	112.70	119.76
3	X	2931[A]	THR	C-N-CA	-6.85	112.70	119.76
3	X	2931[B]	THR	CA-C-N	-6.85	112.70	119.76
3	X	2931[B]	THR	C-N-CA	-6.85	112.70	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	3197[A]	ILE	O-C-N	6.85	124.80	120.42
3	I	3197[B]	ILE	O-C-N	6.85	124.80	120.42
3	X	3197[A]	ILE	O-C-N	6.84	124.80	120.42
3	X	3197[B]	ILE	O-C-N	6.84	124.80	120.42
1	G	675	SER	CA-C-N	-6.83	111.30	119.84
1	G	675	SER	C-N-CA	-6.83	111.30	119.84
3	C	2931[A]	THR	CA-C-N	-6.83	112.72	119.76
3	C	2931[A]	THR	C-N-CA	-6.83	112.72	119.76
3	C	2931[B]	THR	CA-C-N	-6.83	112.72	119.76
3	C	2931[B]	THR	C-N-CA	-6.83	112.72	119.76
3	L	2931[A]	THR	CA-C-N	-6.83	112.72	119.76
3	L	2931[A]	THR	C-N-CA	-6.83	112.72	119.76
3	L	2931[B]	THR	CA-C-N	-6.83	112.72	119.76
3	L	2931[B]	THR	C-N-CA	-6.83	112.72	119.76
3	a	2931[A]	THR	CA-C-N	-6.83	112.73	119.76
3	a	2931[A]	THR	C-N-CA	-6.83	112.73	119.76
3	a	2931[B]	THR	CA-C-N	-6.83	112.73	119.76
3	a	2931[B]	THR	C-N-CA	-6.83	112.73	119.76
3	d	3197[A]	ILE	O-C-N	6.80	124.78	120.42
3	d	3197[B]	ILE	O-C-N	6.80	124.78	120.42
3	I	2931[A]	THR	CA-C-N	-6.80	112.76	119.76
3	I	2931[A]	THR	C-N-CA	-6.80	112.76	119.76
3	I	2931[B]	THR	CA-C-N	-6.80	112.76	119.76
3	I	2931[B]	THR	C-N-CA	-6.80	112.76	119.76
3	F	3197[A]	ILE	O-C-N	6.79	124.77	120.42
3	F	3197[B]	ILE	O-C-N	6.79	124.77	120.42
3	C	3197[A]	ILE	O-C-N	6.79	124.76	120.42
3	C	3197[B]	ILE	O-C-N	6.79	124.76	120.42
3	d	3000[A]	LEU	N-CA-C	-6.77	96.59	108.23
3	d	3000[B]	LEU	N-CA-C	-6.77	96.59	108.23
1	P	228	GLY	N-CA-C	6.76	124.11	114.64
3	O	3139[A]	LEU	CA-C-N	-6.76	113.00	119.76
3	O	3139[A]	LEU	C-N-CA	-6.76	113.00	119.76
3	O	3139[B]	LEU	CA-C-N	-6.76	113.00	119.76
3	O	3139[B]	LEU	C-N-CA	-6.76	113.00	119.76
3	U	3000[A]	LEU	N-CA-C	-6.75	96.62	108.23
3	U	3000[B]	LEU	N-CA-C	-6.75	96.62	108.23
3	C	3000[A]	LEU	N-CA-C	-6.74	96.64	108.23
3	C	3000[B]	LEU	N-CA-C	-6.74	96.64	108.23
3	R	3000[A]	LEU	N-CA-C	-6.74	96.64	108.23
3	R	3000[B]	LEU	N-CA-C	-6.74	96.64	108.23
3	F	3000[A]	LEU	N-CA-C	-6.74	96.64	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3000[B]	LEU	N-CA-C	-6.74	96.64	108.23
3	L	3000[A]	LEU	N-CA-C	-6.73	96.65	108.23
3	L	3000[B]	LEU	N-CA-C	-6.73	96.65	108.23
3	O	3000[A]	LEU	N-CA-C	-6.73	96.65	108.23
3	O	3000[B]	LEU	N-CA-C	-6.73	96.65	108.23
1	G	1486	LEU	CA-C-N	-6.73	112.76	119.56
1	G	1486	LEU	C-N-CA	-6.73	112.76	119.56
1	M	126	GLY	CA-C-N	6.73	133.81	121.70
1	M	126	GLY	C-N-CA	6.73	133.81	121.70
3	d	3139[A]	LEU	CA-C-N	-6.73	113.03	119.76
3	d	3139[A]	LEU	C-N-CA	-6.73	113.03	119.76
3	d	3139[B]	LEU	CA-C-N	-6.73	113.03	119.76
3	d	3139[B]	LEU	C-N-CA	-6.73	113.03	119.76
3	X	3000[A]	LEU	N-CA-C	-6.73	96.66	108.23
3	X	3000[B]	LEU	N-CA-C	-6.73	96.66	108.23
1	Y	669	LYS	CA-C-N	-6.72	112.75	120.89
1	Y	669	LYS	C-N-CA	-6.72	112.75	120.89
3	L	3197[A]	ILE	O-C-N	6.72	124.72	120.42
3	L	3197[B]	ILE	O-C-N	6.72	124.72	120.42
1	P	417	MET	N-CA-C	6.71	118.60	111.28
3	a	3139[A]	LEU	CA-C-N	-6.71	113.05	119.76
3	a	3139[A]	LEU	C-N-CA	-6.71	113.05	119.76
3	a	3139[B]	LEU	CA-C-N	-6.71	113.05	119.76
3	a	3139[B]	LEU	C-N-CA	-6.71	113.05	119.76
3	O	2967[A]	CYS	N-CA-C	6.71	116.91	108.45
3	O	2967[B]	CYS	N-CA-C	6.71	116.91	108.45
3	R	3139[A]	LEU	CA-C-N	-6.71	113.05	119.76
3	R	3139[A]	LEU	C-N-CA	-6.71	113.05	119.76
3	R	3139[B]	LEU	CA-C-N	-6.71	113.05	119.76
3	R	3139[B]	LEU	C-N-CA	-6.71	113.05	119.76
3	R	3197[A]	ILE	O-C-N	6.70	124.71	120.42
3	R	3197[B]	ILE	O-C-N	6.70	124.71	120.42
3	U	3139[A]	LEU	CA-C-N	-6.70	113.06	119.76
3	U	3139[A]	LEU	C-N-CA	-6.70	113.06	119.76
3	U	3139[B]	LEU	CA-C-N	-6.70	113.06	119.76
3	U	3139[B]	LEU	C-N-CA	-6.70	113.06	119.76
3	a	3000[A]	LEU	N-CA-C	-6.70	96.71	108.23
3	a	3000[B]	LEU	N-CA-C	-6.70	96.71	108.23
3	I	3000[A]	LEU	N-CA-C	-6.70	96.71	108.23
3	I	3000[B]	LEU	N-CA-C	-6.70	96.71	108.23
3	L	3139[A]	LEU	CA-C-N	-6.69	113.07	119.76
3	L	3139[A]	LEU	C-N-CA	-6.69	113.07	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	3139[B]	LEU	CA-C-N	-6.69	113.07	119.76
3	L	3139[B]	LEU	C-N-CA	-6.69	113.07	119.76
3	a	2967[A]	CYS	N-CA-C	6.68	116.87	108.45
3	a	2967[B]	CYS	N-CA-C	6.68	116.87	108.45
3	C	3139[A]	LEU	CA-C-N	-6.68	113.08	119.76
3	C	3139[A]	LEU	C-N-CA	-6.68	113.08	119.76
3	C	3139[B]	LEU	CA-C-N	-6.68	113.08	119.76
3	C	3139[B]	LEU	C-N-CA	-6.68	113.08	119.76
3	I	2967[A]	CYS	N-CA-C	6.68	116.86	108.45
3	I	2967[B]	CYS	N-CA-C	6.68	116.86	108.45
3	F	3139[A]	LEU	CA-C-N	-6.67	113.09	119.76
3	F	3139[A]	LEU	C-N-CA	-6.67	113.09	119.76
3	F	3139[B]	LEU	CA-C-N	-6.67	113.09	119.76
3	F	3139[B]	LEU	C-N-CA	-6.67	113.09	119.76
3	L	2967[A]	CYS	N-CA-C	6.67	116.86	108.45
3	L	2967[B]	CYS	N-CA-C	6.67	116.86	108.45
3	I	3139[A]	LEU	CA-C-N	-6.66	113.10	119.76
3	I	3139[A]	LEU	C-N-CA	-6.66	113.10	119.76
3	I	3139[B]	LEU	CA-C-N	-6.66	113.10	119.76
3	I	3139[B]	LEU	C-N-CA	-6.66	113.10	119.76
1	P	450	LYS	N-CA-C	6.66	120.00	109.81
3	R	2967[A]	CYS	N-CA-C	6.65	116.83	108.45
3	R	2967[B]	CYS	N-CA-C	6.65	116.83	108.45
1	P	1086	LEU	N-CA-C	6.64	119.13	111.02
3	X	2967[A]	CYS	N-CA-C	6.64	116.82	108.45
3	X	2967[B]	CYS	N-CA-C	6.64	116.82	108.45
3	X	3139[A]	LEU	CA-C-N	-6.64	113.12	119.76
3	X	3139[A]	LEU	C-N-CA	-6.64	113.12	119.76
3	X	3139[B]	LEU	CA-C-N	-6.64	113.12	119.76
3	X	3139[B]	LEU	C-N-CA	-6.64	113.12	119.76
3	O	3197[A]	ILE	O-C-N	6.64	124.67	120.42
3	O	3197[B]	ILE	O-C-N	6.64	124.67	120.42
3	C	2967[A]	CYS	N-CA-C	6.63	116.81	108.45
3	C	2967[B]	CYS	N-CA-C	6.63	116.81	108.45
3	L	3291[A]	ASP	N-CA-C	-6.63	102.25	110.41
3	L	3291[B]	ASP	N-CA-C	-6.63	102.25	110.41
3	d	2967[A]	CYS	N-CA-C	6.63	116.81	108.45
3	d	2967[B]	CYS	N-CA-C	6.63	116.81	108.45
3	F	2967[A]	CYS	N-CA-C	6.63	116.80	108.45
3	F	2967[B]	CYS	N-CA-C	6.63	116.80	108.45
3	a	3291[A]	ASP	N-CA-C	-6.63	102.26	110.41
3	a	3291[B]	ASP	N-CA-C	-6.63	102.26	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	3291[A]	ASP	N-CA-C	-6.62	102.27	110.41
3	R	3291[B]	ASP	N-CA-C	-6.62	102.27	110.41
3	F	3291[A]	ASP	N-CA-C	-6.61	102.28	110.41
3	F	3291[B]	ASP	N-CA-C	-6.61	102.28	110.41
3	U	2967[A]	CYS	N-CA-C	6.60	116.77	108.45
3	U	2967[B]	CYS	N-CA-C	6.60	116.77	108.45
3	C	3291[A]	ASP	N-CA-C	-6.59	102.30	110.41
3	C	3291[B]	ASP	N-CA-C	-6.59	102.30	110.41
3	L	3254[A]	MET	CA-C-N	-6.59	113.50	120.03
3	L	3254[A]	MET	C-N-CA	-6.59	113.50	120.03
3	L	3254[B]	MET	CA-C-N	-6.59	113.50	120.03
3	L	3254[B]	MET	C-N-CA	-6.59	113.50	120.03
3	O	3291[A]	ASP	N-CA-C	-6.59	102.30	110.41
3	O	3291[B]	ASP	N-CA-C	-6.59	102.30	110.41
3	X	3291[A]	ASP	N-CA-C	-6.59	102.30	110.41
3	X	3291[B]	ASP	N-CA-C	-6.59	102.30	110.41
3	d	3291[A]	ASP	N-CA-C	-6.59	102.30	110.41
3	d	3291[B]	ASP	N-CA-C	-6.59	102.30	110.41
3	U	3291[A]	ASP	N-CA-C	-6.58	102.31	110.41
3	U	3291[B]	ASP	N-CA-C	-6.58	102.31	110.41
3	I	3291[A]	ASP	N-CA-C	-6.58	102.32	110.41
3	I	3291[B]	ASP	N-CA-C	-6.58	102.32	110.41
1	G	1296	VAL	CA-C-N	-6.57	111.62	119.84
1	G	1296	VAL	C-N-CA	-6.57	111.62	119.84
3	I	3254[A]	MET	CA-C-N	-6.56	113.54	120.03
3	I	3254[A]	MET	C-N-CA	-6.56	113.54	120.03
3	I	3254[B]	MET	CA-C-N	-6.56	113.54	120.03
3	I	3254[B]	MET	C-N-CA	-6.56	113.54	120.03
1	J	823	VAL	CA-C-N	6.55	126.31	119.76
1	J	823	VAL	C-N-CA	6.55	126.31	119.76
3	O	3254[A]	MET	CA-C-N	-6.55	113.54	120.03
3	O	3254[A]	MET	C-N-CA	-6.55	113.54	120.03
3	O	3254[B]	MET	CA-C-N	-6.55	113.54	120.03
3	O	3254[B]	MET	C-N-CA	-6.55	113.54	120.03
3	d	3254[A]	MET	CA-C-N	-6.53	113.57	120.03
3	d	3254[A]	MET	C-N-CA	-6.53	113.57	120.03
3	d	3254[B]	MET	CA-C-N	-6.53	113.57	120.03
3	d	3254[B]	MET	C-N-CA	-6.53	113.57	120.03
3	U	2963[A]	MET	CA-C-N	-6.52	112.79	119.83
3	U	2963[A]	MET	C-N-CA	-6.52	112.79	119.83
3	U	2963[B]	MET	CA-C-N	-6.52	112.79	119.83
3	U	2963[B]	MET	C-N-CA	-6.52	112.79	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	3036[A]	GLY	N-CA-C	-6.52	102.16	111.42
3	L	3036[B]	GLY	N-CA-C	-6.52	102.16	111.42
3	U	3254[A]	MET	CA-C-N	-6.52	113.58	120.03
3	U	3254[A]	MET	C-N-CA	-6.52	113.58	120.03
3	U	3254[B]	MET	CA-C-N	-6.52	113.58	120.03
3	U	3254[B]	MET	C-N-CA	-6.52	113.58	120.03
3	a	3254[A]	MET	CA-C-N	-6.52	113.58	120.03
3	a	3254[A]	MET	C-N-CA	-6.52	113.58	120.03
3	a	3254[B]	MET	CA-C-N	-6.52	113.58	120.03
3	a	3254[B]	MET	C-N-CA	-6.52	113.58	120.03
3	X	3254[A]	MET	CA-C-N	-6.52	113.58	120.03
3	X	3254[A]	MET	C-N-CA	-6.52	113.58	120.03
3	X	3254[B]	MET	CA-C-N	-6.52	113.58	120.03
3	X	3254[B]	MET	C-N-CA	-6.52	113.58	120.03
3	F	3254[A]	MET	CA-C-N	-6.51	113.58	120.03
3	F	3254[A]	MET	C-N-CA	-6.51	113.58	120.03
3	F	3254[B]	MET	CA-C-N	-6.51	113.58	120.03
3	F	3254[B]	MET	C-N-CA	-6.51	113.58	120.03
3	U	3036[A]	GLY	N-CA-C	-6.51	102.17	111.42
3	U	3036[B]	GLY	N-CA-C	-6.51	102.17	111.42
3	R	3036[A]	GLY	N-CA-C	-6.51	102.18	111.42
3	R	3036[B]	GLY	N-CA-C	-6.51	102.18	111.42
3	R	3254[A]	MET	CA-C-N	-6.51	113.59	120.03
3	R	3254[A]	MET	C-N-CA	-6.51	113.59	120.03
3	R	3254[B]	MET	CA-C-N	-6.51	113.59	120.03
3	R	3254[B]	MET	C-N-CA	-6.51	113.59	120.03
3	C	3036[A]	GLY	N-CA-C	-6.50	102.19	111.42
3	C	3036[B]	GLY	N-CA-C	-6.50	102.19	111.42
1	A	404	ILE	CA-C-N	6.50	124.34	119.66
1	A	404	ILE	C-N-CA	6.50	124.34	119.66
3	a	3036[A]	GLY	N-CA-C	-6.50	102.19	111.42
3	a	3036[B]	GLY	N-CA-C	-6.50	102.19	111.42
3	I	3036[A]	GLY	N-CA-C	-6.50	102.19	111.42
3	I	3036[B]	GLY	N-CA-C	-6.50	102.19	111.42
3	L	2969[A]	TYR	N-CA-C	-6.49	99.35	109.87
3	L	2969[B]	TYR	N-CA-C	-6.49	99.35	109.87
3	L	2963[A]	MET	CA-C-N	-6.49	112.82	119.83
3	L	2963[A]	MET	C-N-CA	-6.49	112.82	119.83
3	L	2963[B]	MET	CA-C-N	-6.49	112.82	119.83
3	L	2963[B]	MET	C-N-CA	-6.49	112.82	119.83
3	O	3036[A]	GLY	N-CA-C	-6.49	102.21	111.42
3	O	3036[B]	GLY	N-CA-C	-6.49	102.21	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	d	3036[A]	GLY	N-CA-C	-6.49	102.21	111.42
3	d	3036[B]	GLY	N-CA-C	-6.49	102.21	111.42
3	F	2969[A]	TYR	N-CA-C	-6.48	99.37	109.87
3	F	2969[B]	TYR	N-CA-C	-6.48	99.37	109.87
3	U	2969[A]	TYR	N-CA-C	-6.48	99.37	109.87
3	U	2969[B]	TYR	N-CA-C	-6.48	99.37	109.87
3	d	2969[A]	TYR	N-CA-C	-6.48	99.38	109.87
3	d	2969[B]	TYR	N-CA-C	-6.48	99.38	109.87
3	C	2969[A]	TYR	N-CA-C	-6.47	99.38	109.87
3	C	2969[B]	TYR	N-CA-C	-6.47	99.38	109.87
3	O	2969[A]	TYR	N-CA-C	-6.47	99.38	109.87
3	O	2969[B]	TYR	N-CA-C	-6.47	99.38	109.87
1	G	1082	SER	CA-C-N	-6.47	111.75	119.84
1	G	1082	SER	C-N-CA	-6.47	111.75	119.84
3	a	2969[A]	TYR	N-CA-C	-6.47	99.38	109.87
3	a	2969[B]	TYR	N-CA-C	-6.47	99.38	109.87
3	F	3036[A]	GLY	N-CA-C	-6.47	102.23	111.42
3	F	3036[B]	GLY	N-CA-C	-6.47	102.23	111.42
3	X	2969[A]	TYR	N-CA-C	-6.47	99.39	109.87
3	X	2969[B]	TYR	N-CA-C	-6.47	99.39	109.87
1	V	1581	GLU	N-CA-C	6.47	116.39	107.73
3	X	3036[A]	GLY	N-CA-C	-6.47	102.24	111.42
3	X	3036[B]	GLY	N-CA-C	-6.47	102.24	111.42
2	c	2558	CYS	N-CA-C	6.46	121.30	113.41
3	C	3254[A]	MET	CA-C-N	-6.46	113.63	120.03
3	C	3254[A]	MET	C-N-CA	-6.46	113.63	120.03
3	C	3254[B]	MET	CA-C-N	-6.46	113.63	120.03
3	C	3254[B]	MET	C-N-CA	-6.46	113.63	120.03
3	R	2969[A]	TYR	N-CA-C	-6.46	99.40	109.87
3	R	2969[B]	TYR	N-CA-C	-6.46	99.40	109.87
3	I	2969[A]	TYR	N-CA-C	-6.46	99.40	109.87
3	I	2969[B]	TYR	N-CA-C	-6.46	99.40	109.87
3	O	2963[A]	MET	CA-C-N	-6.46	112.85	119.83
3	O	2963[A]	MET	C-N-CA	-6.46	112.85	119.83
3	O	2963[B]	MET	CA-C-N	-6.46	112.85	119.83
3	O	2963[B]	MET	C-N-CA	-6.46	112.85	119.83
3	a	2963[A]	MET	CA-C-N	-6.45	112.86	119.83
3	a	2963[A]	MET	C-N-CA	-6.45	112.86	119.83
3	a	2963[B]	MET	CA-C-N	-6.45	112.86	119.83
3	a	2963[B]	MET	C-N-CA	-6.45	112.86	119.83
3	X	2963[A]	MET	CA-C-N	-6.45	112.87	119.83
3	X	2963[A]	MET	C-N-CA	-6.45	112.87	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	2963[B]	MET	CA-C-N	-6.45	112.87	119.83
3	X	2963[B]	MET	C-N-CA	-6.45	112.87	119.83
3	F	2963[A]	MET	CA-C-N	-6.44	112.87	119.83
3	F	2963[A]	MET	C-N-CA	-6.44	112.87	119.83
3	F	2963[B]	MET	CA-C-N	-6.44	112.87	119.83
3	F	2963[B]	MET	C-N-CA	-6.44	112.87	119.83
3	I	2963[A]	MET	CA-C-N	-6.43	112.89	119.83
3	I	2963[A]	MET	C-N-CA	-6.43	112.89	119.83
3	I	2963[B]	MET	CA-C-N	-6.43	112.89	119.83
3	I	2963[B]	MET	C-N-CA	-6.43	112.89	119.83
3	R	2963[A]	MET	CA-C-N	-6.43	112.89	119.83
3	R	2963[A]	MET	C-N-CA	-6.43	112.89	119.83
3	R	2963[B]	MET	CA-C-N	-6.43	112.89	119.83
3	R	2963[B]	MET	C-N-CA	-6.43	112.89	119.83
1	b	758	GLY	N-CA-C	6.42	119.93	111.52
1	J	669	LYS	CA-C-N	-6.42	113.08	119.56
1	J	669	LYS	C-N-CA	-6.42	113.08	119.56
3	d	2963[A]	MET	CA-C-N	-6.41	112.91	119.83
3	d	2963[A]	MET	C-N-CA	-6.41	112.91	119.83
3	d	2963[B]	MET	CA-C-N	-6.41	112.91	119.83
3	d	2963[B]	MET	C-N-CA	-6.41	112.91	119.83
3	C	2963[A]	MET	CA-C-N	-6.41	112.91	119.83
3	C	2963[A]	MET	C-N-CA	-6.41	112.91	119.83
3	C	2963[B]	MET	CA-C-N	-6.41	112.91	119.83
3	C	2963[B]	MET	C-N-CA	-6.41	112.91	119.83
1	V	675	SER	CA-C-N	-6.39	111.86	119.84
1	V	675	SER	C-N-CA	-6.39	111.86	119.84
3	L	3178[A]	PHE	N-CA-C	-6.39	103.57	112.45
3	L	3178[B]	PHE	N-CA-C	-6.39	103.57	112.45
2	Z	2764	THR	CA-C-N	6.38	126.60	119.32
2	Z	2764	THR	C-N-CA	6.38	126.60	119.32
2	T	2340	ALA	CA-C-N	-6.37	111.87	119.84
2	T	2340	ALA	C-N-CA	-6.37	111.87	119.84
3	U	3178[A]	PHE	N-CA-C	-6.37	103.59	112.45
3	U	3178[B]	PHE	N-CA-C	-6.37	103.59	112.45
3	O	3178[A]	PHE	N-CA-C	-6.37	103.59	112.45
3	O	3178[B]	PHE	N-CA-C	-6.37	103.59	112.45
1	M	675	SER	CA-C-N	-6.37	111.88	119.84
1	M	675	SER	C-N-CA	-6.37	111.88	119.84
3	a	3178[A]	PHE	N-CA-C	-6.35	103.62	112.45
3	a	3178[B]	PHE	N-CA-C	-6.35	103.62	112.45
3	X	3178[A]	PHE	N-CA-C	-6.35	103.63	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	3178[B]	PHE	N-CA-C	-6.35	103.63	112.45
3	I	3048[A]	ASP	CA-C-N	-6.34	113.45	119.85
3	I	3048[A]	ASP	C-N-CA	-6.34	113.45	119.85
3	I	3048[B]	ASP	CA-C-N	-6.34	113.45	119.85
3	I	3048[B]	ASP	C-N-CA	-6.34	113.45	119.85
1	S	1639	LYS	N-CA-C	6.34	121.83	111.37
3	U	3048[A]	ASP	CA-C-N	-6.33	113.46	119.85
3	U	3048[A]	ASP	C-N-CA	-6.33	113.46	119.85
3	U	3048[B]	ASP	CA-C-N	-6.33	113.46	119.85
3	U	3048[B]	ASP	C-N-CA	-6.33	113.46	119.85
3	I	3178[A]	PHE	N-CA-C	-6.32	103.66	112.45
3	I	3178[B]	PHE	N-CA-C	-6.32	103.66	112.45
3	R	3178[A]	PHE	N-CA-C	-6.32	103.66	112.45
3	R	3178[B]	PHE	N-CA-C	-6.32	103.66	112.45
3	F	3048[A]	ASP	CA-C-N	-6.32	113.47	119.85
3	F	3048[A]	ASP	C-N-CA	-6.32	113.47	119.85
3	F	3048[B]	ASP	CA-C-N	-6.32	113.47	119.85
3	F	3048[B]	ASP	C-N-CA	-6.32	113.47	119.85
3	F	3178[A]	PHE	N-CA-C	-6.32	103.67	112.45
3	F	3178[B]	PHE	N-CA-C	-6.32	103.67	112.45
3	R	3048[A]	ASP	CA-C-N	-6.32	113.47	119.85
3	R	3048[A]	ASP	C-N-CA	-6.32	113.47	119.85
3	R	3048[B]	ASP	CA-C-N	-6.32	113.47	119.85
3	R	3048[B]	ASP	C-N-CA	-6.32	113.47	119.85
3	I	3296[A]	PRO	CA-C-N	-6.30	114.04	120.85
3	I	3296[A]	PRO	C-N-CA	-6.30	114.04	120.85
3	I	3296[B]	PRO	CA-C-N	-6.30	114.04	120.85
3	I	3296[B]	PRO	C-N-CA	-6.30	114.04	120.85
3	C	3178[A]	PHE	N-CA-C	-6.30	103.69	112.45
3	C	3178[B]	PHE	N-CA-C	-6.30	103.69	112.45
3	C	3048[A]	ASP	CA-C-N	-6.30	113.49	119.85
3	C	3048[A]	ASP	C-N-CA	-6.30	113.49	119.85
3	C	3048[B]	ASP	CA-C-N	-6.30	113.49	119.85
3	C	3048[B]	ASP	C-N-CA	-6.30	113.49	119.85
3	L	3048[A]	ASP	CA-C-N	-6.30	113.49	119.85
3	L	3048[A]	ASP	C-N-CA	-6.30	113.49	119.85
3	L	3048[B]	ASP	CA-C-N	-6.30	113.49	119.85
3	L	3048[B]	ASP	C-N-CA	-6.30	113.49	119.85
3	a	3197[A]	ILE	N-CA-C	-6.30	104.79	112.35
3	a	3197[B]	ILE	N-CA-C	-6.30	104.79	112.35
3	d	3178[A]	PHE	N-CA-C	-6.29	103.70	112.45
3	d	3178[B]	PHE	N-CA-C	-6.29	103.70	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	3048[A]	ASP	CA-C-N	-6.29	113.50	119.85
3	X	3048[A]	ASP	C-N-CA	-6.29	113.50	119.85
3	X	3048[B]	ASP	CA-C-N	-6.29	113.50	119.85
3	X	3048[B]	ASP	C-N-CA	-6.29	113.50	119.85
2	Z	2545	SER	CA-C-N	6.29	133.01	121.70
2	Z	2545	SER	C-N-CA	6.29	133.01	121.70
3	d	3048[A]	ASP	CA-C-N	-6.28	113.50	119.85
3	d	3048[A]	ASP	C-N-CA	-6.28	113.50	119.85
3	d	3048[B]	ASP	CA-C-N	-6.28	113.50	119.85
3	d	3048[B]	ASP	C-N-CA	-6.28	113.50	119.85
3	L	3116[A]	PHE	N-CA-C	6.28	118.13	111.28
3	L	3116[B]	PHE	N-CA-C	6.28	118.13	111.28
3	a	3296[A]	PRO	CA-C-N	-6.28	114.07	120.85
3	a	3296[A]	PRO	C-N-CA	-6.28	114.07	120.85
3	a	3296[B]	PRO	CA-C-N	-6.28	114.07	120.85
3	a	3296[B]	PRO	C-N-CA	-6.28	114.07	120.85
3	C	3296[A]	PRO	CA-C-N	-6.28	114.07	120.85
3	C	3296[A]	PRO	C-N-CA	-6.28	114.07	120.85
3	C	3296[B]	PRO	CA-C-N	-6.28	114.07	120.85
3	C	3296[B]	PRO	C-N-CA	-6.28	114.07	120.85
3	L	3197[A]	ILE	N-CA-C	-6.28	104.82	112.35
3	L	3197[B]	ILE	N-CA-C	-6.28	104.82	112.35
3	X	3296[A]	PRO	CA-C-N	-6.28	114.07	120.85
3	X	3296[A]	PRO	C-N-CA	-6.28	114.07	120.85
3	X	3296[B]	PRO	CA-C-N	-6.28	114.07	120.85
3	X	3296[B]	PRO	C-N-CA	-6.28	114.07	120.85
3	I	3197[A]	ILE	N-CA-C	-6.27	104.83	112.35
3	I	3197[B]	ILE	N-CA-C	-6.27	104.83	112.35
3	L	3296[A]	PRO	CA-C-N	-6.27	114.08	120.85
3	L	3296[A]	PRO	C-N-CA	-6.27	114.08	120.85
3	L	3296[B]	PRO	CA-C-N	-6.27	114.08	120.85
3	L	3296[B]	PRO	C-N-CA	-6.27	114.08	120.85
3	R	3197[A]	ILE	N-CA-C	-6.27	104.83	112.35
3	R	3197[B]	ILE	N-CA-C	-6.27	104.83	112.35
1	V	323	ILE	CA-C-N	6.26	126.29	119.90
1	V	323	ILE	C-N-CA	6.26	126.29	119.90
1	b	897	HIS	N-CA-C	-6.26	100.11	108.19
3	O	3296[A]	PRO	CA-C-N	-6.26	114.09	120.85
3	O	3296[A]	PRO	C-N-CA	-6.26	114.09	120.85
3	O	3296[B]	PRO	CA-C-N	-6.26	114.09	120.85
3	O	3296[B]	PRO	C-N-CA	-6.26	114.09	120.85
3	U	3197[A]	ILE	N-CA-C	-6.26	104.84	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	3197[B]	ILE	N-CA-C	-6.26	104.84	112.35
3	U	3296[A]	PRO	CA-C-N	-6.26	114.09	120.85
3	U	3296[A]	PRO	C-N-CA	-6.26	114.09	120.85
3	U	3296[B]	PRO	CA-C-N	-6.26	114.09	120.85
3	U	3296[B]	PRO	C-N-CA	-6.26	114.09	120.85
3	a	3048[A]	ASP	CA-C-N	-6.26	113.53	119.85
3	a	3048[A]	ASP	C-N-CA	-6.26	113.53	119.85
3	a	3048[B]	ASP	CA-C-N	-6.26	113.53	119.85
3	a	3048[B]	ASP	C-N-CA	-6.26	113.53	119.85
3	O	3048[A]	ASP	CA-C-N	-6.26	113.53	119.85
3	O	3048[A]	ASP	C-N-CA	-6.26	113.53	119.85
3	O	3048[B]	ASP	CA-C-N	-6.26	113.53	119.85
3	O	3048[B]	ASP	C-N-CA	-6.26	113.53	119.85
3	R	3296[A]	PRO	CA-C-N	-6.25	114.10	120.85
3	R	3296[A]	PRO	C-N-CA	-6.25	114.10	120.85
3	R	3296[B]	PRO	CA-C-N	-6.25	114.10	120.85
3	R	3296[B]	PRO	C-N-CA	-6.25	114.10	120.85
3	a	3116[A]	PHE	N-CA-C	6.25	118.09	111.28
3	a	3116[B]	PHE	N-CA-C	6.25	118.09	111.28
3	X	3197[A]	ILE	N-CA-C	-6.25	104.85	112.35
3	X	3197[B]	ILE	N-CA-C	-6.25	104.85	112.35
3	O	3197[A]	ILE	N-CA-C	-6.25	104.85	112.35
3	O	3197[B]	ILE	N-CA-C	-6.25	104.85	112.35
3	R	3116[A]	PHE	N-CA-C	6.25	118.09	111.28
3	R	3116[B]	PHE	N-CA-C	6.25	118.09	111.28
3	d	3296[A]	PRO	CA-C-N	-6.25	114.11	120.85
3	d	3296[A]	PRO	C-N-CA	-6.25	114.11	120.85
3	d	3296[B]	PRO	CA-C-N	-6.25	114.11	120.85
3	d	3296[B]	PRO	C-N-CA	-6.25	114.11	120.85
2	B	2345	ASN	CA-C-N	6.24	125.65	118.85
2	B	2345	ASN	C-N-CA	6.24	125.65	118.85
3	d	3197[A]	ILE	N-CA-C	-6.24	104.86	112.35
3	d	3197[B]	ILE	N-CA-C	-6.24	104.86	112.35
3	C	3197[A]	ILE	N-CA-C	-6.23	104.87	112.35
3	C	3197[B]	ILE	N-CA-C	-6.23	104.87	112.35
3	C	3116[A]	PHE	N-CA-C	6.21	118.05	111.28
3	C	3116[B]	PHE	N-CA-C	6.21	118.05	111.28
3	F	3116[A]	PHE	N-CA-C	6.21	118.05	111.28
3	F	3116[B]	PHE	N-CA-C	6.21	118.05	111.28
3	F	3197[A]	ILE	N-CA-C	-6.21	104.89	112.35
3	F	3197[B]	ILE	N-CA-C	-6.21	104.89	112.35
3	F	3296[A]	PRO	CA-C-N	-6.21	114.14	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3296[A]	PRO	C-N-CA	-6.21	114.14	120.85
3	F	3296[B]	PRO	CA-C-N	-6.21	114.14	120.85
3	F	3296[B]	PRO	C-N-CA	-6.21	114.14	120.85
1	b	296	ARG	N-CA-C	-6.21	105.75	113.38
2	T	2215	SER	N-CA-C	6.21	117.71	111.07
1	J	1296	VAL	CA-C-N	-6.20	112.09	119.84
1	J	1296	VAL	C-N-CA	-6.20	112.09	119.84
3	X	3116[A]	PHE	N-CA-C	6.19	118.03	111.28
3	X	3116[B]	PHE	N-CA-C	6.19	118.03	111.28
3	U	3116[A]	PHE	N-CA-C	6.18	118.02	111.28
3	U	3116[B]	PHE	N-CA-C	6.18	118.02	111.28
3	d	3116[A]	PHE	N-CA-C	6.17	118.01	111.28
3	d	3116[B]	PHE	N-CA-C	6.17	118.01	111.28
3	I	3116[A]	PHE	N-CA-C	6.17	118.00	111.28
3	I	3116[B]	PHE	N-CA-C	6.17	118.00	111.28
1	b	1296	VAL	CA-C-N	-6.17	112.13	119.84
1	b	1296	VAL	C-N-CA	-6.17	112.13	119.84
2	B	2489	ILE	CA-C-N	6.16	124.09	119.66
2	B	2489	ILE	C-N-CA	6.16	124.09	119.66
2	N	2831	GLU	N-CA-C	6.16	119.73	111.24
1	J	1637	GLY	N-CA-C	-6.15	100.49	110.95
2	H	2764	THR	CA-C-N	6.15	126.60	119.47
2	H	2764	THR	C-N-CA	6.15	126.60	119.47
2	K	2545	SER	CA-C-N	6.14	132.76	121.70
2	K	2545	SER	C-N-CA	6.14	132.76	121.70
1	Y	83	HIS	N-CA-C	6.13	121.04	113.50
3	O	3116[A]	PHE	N-CA-C	6.13	117.96	111.28
3	O	3116[B]	PHE	N-CA-C	6.13	117.96	111.28
1	P	669	LYS	CA-C-N	-6.12	113.92	120.47
1	P	669	LYS	C-N-CA	-6.12	113.92	120.47
1	S	1251	SER	CA-C-N	6.12	126.09	120.03
1	S	1251	SER	C-N-CA	6.12	126.09	120.03
2	E	2545	SER	CA-C-N	6.12	132.71	121.70
2	E	2545	SER	C-N-CA	6.12	132.71	121.70
2	W	2345	ASN	CA-C-N	6.11	127.48	119.84
2	W	2345	ASN	C-N-CA	6.11	127.48	119.84
1	A	1296	VAL	CA-C-N	-6.11	112.20	119.84
1	A	1296	VAL	C-N-CA	-6.11	112.20	119.84
1	V	1296	VAL	CA-C-N	-6.10	112.21	119.84
1	V	1296	VAL	C-N-CA	-6.10	112.21	119.84
2	T	2545	SER	CA-C-N	6.10	132.68	121.70
2	T	2545	SER	C-N-CA	6.10	132.68	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	1091	ASN	CA-C-N	6.09	126.62	120.04
1	S	1091	ASN	C-N-CA	6.09	126.62	120.04
1	D	1296	VAL	CA-C-N	-6.08	112.24	119.84
1	D	1296	VAL	C-N-CA	-6.08	112.24	119.84
1	A	1082	SER	CA-C-N	-6.08	112.25	119.84
1	A	1082	SER	C-N-CA	-6.08	112.25	119.84
1	D	953	GLU	N-CA-C	6.08	117.63	108.46
1	A	570	GLN	CA-C-N	-6.06	112.27	119.84
1	A	570	GLN	C-N-CA	-6.06	112.27	119.84
1	S	465	PRO	N-CA-C	-6.03	106.17	114.98
1	Y	323	ILE	CA-C-N	6.01	126.02	119.89
1	Y	323	ILE	C-N-CA	6.01	126.02	119.89
1	J	1237	GLU	CA-C-N	6.00	125.95	119.78
1	J	1237	GLU	C-N-CA	6.00	125.95	119.78
1	A	116	LYS	CB-CA-C	-5.99	109.09	117.23
1	V	669	LYS	CA-C-N	-5.99	112.36	119.84
1	V	669	LYS	C-N-CA	-5.99	112.36	119.84
2	c	2553	ALA	CA-C-N	5.98	126.48	120.14
2	c	2553	ALA	C-N-CA	5.98	126.48	120.14
2	N	2472	ASN	N-CA-C	5.97	117.79	111.28
1	A	388	GLY	N-CA-C	-5.97	107.59	114.69
1	P	1091	ASN	CA-C-N	5.97	126.48	120.04
1	P	1091	ASN	C-N-CA	5.97	126.48	120.04
1	J	323	ILE	CA-C-N	5.96	125.98	119.90
1	J	323	ILE	C-N-CA	5.96	125.98	119.90
1	S	296	ARG	N-CA-C	-5.96	105.84	113.23
1	Y	1296	VAL	CA-C-N	-5.95	112.41	119.84
1	Y	1296	VAL	C-N-CA	-5.95	112.41	119.84
1	G	1441	SER	N-CA-C	5.95	116.09	108.24
1	P	1039	ASP	CA-C-N	5.94	125.62	119.56
1	P	1039	ASP	C-N-CA	5.94	125.62	119.56
2	W	2340	ALA	CA-C-N	-5.93	113.54	120.12
2	W	2340	ALA	C-N-CA	-5.93	113.54	120.12
2	H	2472	ASN	N-CA-C	5.91	117.80	111.36
1	M	1296	VAL	CA-C-N	-5.89	112.47	119.84
1	M	1296	VAL	C-N-CA	-5.89	112.47	119.84
2	N	2418	GLY	N-CA-C	5.89	120.02	112.83
1	J	1039	ASP	CA-C-N	5.89	125.57	119.56
1	J	1039	ASP	C-N-CA	5.89	125.57	119.56
1	V	1209	ASP	N-CA-C	5.86	118.28	108.73
2	H	2340	ALA	CA-C-N	-5.86	113.78	119.87
2	H	2340	ALA	C-N-CA	-5.86	113.78	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	51	ASP	N-CA-C	5.85	118.13	111.11
3	O	2993[A]	MET	N-CA-C	-5.85	104.81	111.07
3	O	2993[B]	MET	N-CA-C	-5.85	104.81	111.07
2	Z	2127	ALA	CB-CA-C	-5.85	109.28	117.23
2	Q	2545	SER	CA-C-N	5.84	132.22	121.70
2	Q	2545	SER	C-N-CA	5.84	132.22	121.70
3	U	2993[A]	MET	N-CA-C	-5.82	104.84	111.07
3	U	2993[B]	MET	N-CA-C	-5.82	104.84	111.07
1	A	465	PRO	N-CA-C	-5.82	106.49	114.98
3	a	2993[A]	MET	N-CA-C	-5.81	104.86	111.07
3	a	2993[B]	MET	N-CA-C	-5.81	104.86	111.07
2	B	2556	TYR	N-CA-C	5.81	115.51	107.73
3	L	2993[A]	MET	N-CA-C	-5.80	104.86	111.07
3	L	2993[B]	MET	N-CA-C	-5.80	104.86	111.07
1	P	780	GLU	N-CA-C	5.79	119.53	112.23
3	d	2993[A]	MET	N-CA-C	-5.79	104.87	111.07
3	d	2993[B]	MET	N-CA-C	-5.79	104.87	111.07
1	P	1494	ARG	CA-C-N	-5.78	112.61	119.84
1	P	1494	ARG	C-N-CA	-5.78	112.61	119.84
3	I	2993[A]	MET	N-CA-C	-5.78	104.89	111.07
3	I	2993[B]	MET	N-CA-C	-5.78	104.89	111.07
3	R	2993[A]	MET	N-CA-C	-5.78	104.89	111.07
3	R	2993[B]	MET	N-CA-C	-5.78	104.89	111.07
3	C	2993[A]	MET	N-CA-C	-5.77	104.90	111.07
3	C	2993[B]	MET	N-CA-C	-5.77	104.90	111.07
3	U	2969[A]	TYR	CA-C-N	-5.77	112.93	119.28
3	U	2969[A]	TYR	C-N-CA	-5.77	112.93	119.28
3	U	2969[B]	TYR	CA-C-N	-5.77	112.93	119.28
3	U	2969[B]	TYR	C-N-CA	-5.77	112.93	119.28
1	A	1229	LYS	N-CA-C	5.76	118.17	109.41
2	Z	2472	ASN	N-CA-C	5.76	117.56	111.28
3	O	2969[A]	TYR	CA-C-N	-5.76	112.94	119.28
3	O	2969[A]	TYR	C-N-CA	-5.76	112.94	119.28
3	O	2969[B]	TYR	CA-C-N	-5.76	112.94	119.28
3	O	2969[B]	TYR	C-N-CA	-5.76	112.94	119.28
3	X	2993[A]	MET	N-CA-C	-5.76	104.91	111.07
3	X	2993[B]	MET	N-CA-C	-5.76	104.91	111.07
3	F	2993[A]	MET	N-CA-C	-5.75	104.92	111.07
3	F	2993[B]	MET	N-CA-C	-5.75	104.92	111.07
1	V	982	LYS	CA-C-N	-5.75	112.02	120.46
1	V	982	LYS	C-N-CA	-5.75	112.02	120.46
1	S	780	GLU	N-CA-C	5.74	118.48	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	125	SER	N-CA-C	5.74	117.96	108.49
2	E	2764	THR	CA-C-N	5.73	125.85	119.32
2	E	2764	THR	C-N-CA	5.73	125.85	119.32
3	a	2969[A]	TYR	CA-C-N	-5.73	112.97	119.28
3	a	2969[A]	TYR	C-N-CA	-5.73	112.97	119.28
3	a	2969[B]	TYR	CA-C-N	-5.73	112.97	119.28
3	a	2969[B]	TYR	C-N-CA	-5.73	112.97	119.28
3	d	2969[A]	TYR	CA-C-N	-5.73	112.98	119.28
3	d	2969[A]	TYR	C-N-CA	-5.73	112.98	119.28
3	d	2969[B]	TYR	CA-C-N	-5.73	112.98	119.28
3	d	2969[B]	TYR	C-N-CA	-5.73	112.98	119.28
3	C	2969[A]	TYR	CA-C-N	-5.73	112.98	119.28
3	C	2969[A]	TYR	C-N-CA	-5.73	112.98	119.28
3	C	2969[B]	TYR	CA-C-N	-5.73	112.98	119.28
3	C	2969[B]	TYR	C-N-CA	-5.73	112.98	119.28
1	Y	1227	ASP	N-CA-C	5.73	115.67	108.45
3	F	2969[A]	TYR	CA-C-N	-5.72	112.99	119.28
3	F	2969[A]	TYR	C-N-CA	-5.72	112.99	119.28
3	F	2969[B]	TYR	CA-C-N	-5.72	112.99	119.28
3	F	2969[B]	TYR	C-N-CA	-5.72	112.99	119.28
3	R	2969[A]	TYR	CA-C-N	-5.72	112.99	119.28
3	R	2969[A]	TYR	C-N-CA	-5.72	112.99	119.28
3	R	2969[B]	TYR	CA-C-N	-5.72	112.99	119.28
3	R	2969[B]	TYR	C-N-CA	-5.72	112.99	119.28
2	K	2617	ASP	N-CA-C	-5.72	105.89	112.92
3	L	2969[A]	TYR	CA-C-N	-5.71	112.99	119.28
3	L	2969[A]	TYR	C-N-CA	-5.71	112.99	119.28
3	L	2969[B]	TYR	CA-C-N	-5.71	112.99	119.28
3	L	2969[B]	TYR	C-N-CA	-5.71	112.99	119.28
1	P	1296	VAL	CA-C-N	-5.71	112.70	119.84
1	P	1296	VAL	C-N-CA	-5.71	112.70	119.84
2	c	2556	TYR	N-CA-C	5.71	116.92	107.73
3	O	2995[A]	GLN	N-CA-C	-5.70	104.06	111.02
3	O	2995[B]	GLN	N-CA-C	-5.70	104.06	111.02
1	G	1166	THR	N-CA-C	5.70	118.35	111.40
3	X	2969[A]	TYR	CA-C-N	-5.70	113.01	119.28
3	X	2969[A]	TYR	C-N-CA	-5.70	113.01	119.28
3	X	2969[B]	TYR	CA-C-N	-5.70	113.01	119.28
3	X	2969[B]	TYR	C-N-CA	-5.70	113.01	119.28
2	W	2865	ILE	CA-C-N	5.69	123.82	119.66
2	W	2865	ILE	C-N-CA	5.69	123.82	119.66
1	V	1494	ARG	CA-C-N	-5.69	113.16	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	1494	ARG	C-N-CA	-5.69	113.16	119.19
3	d	2995[A]	GLN	N-CA-C	-5.68	104.09	111.02
3	d	2995[B]	GLN	N-CA-C	-5.68	104.09	111.02
1	M	323	ILE	CA-C-N	5.67	125.60	119.76
1	M	323	ILE	C-N-CA	5.67	125.60	119.76
1	M	1210	LYS	CA-C-N	5.67	131.91	121.70
1	M	1210	LYS	C-N-CA	5.67	131.91	121.70
3	C	2995[A]	GLN	N-CA-C	-5.67	104.10	111.02
3	C	2995[B]	GLN	N-CA-C	-5.67	104.10	111.02
3	I	2969[A]	TYR	CA-C-N	-5.67	113.05	119.28
3	I	2969[A]	TYR	C-N-CA	-5.67	113.05	119.28
3	I	2969[B]	TYR	CA-C-N	-5.67	113.05	119.28
3	I	2969[B]	TYR	C-N-CA	-5.67	113.05	119.28
3	R	2995[A]	GLN	N-CA-C	-5.66	104.11	111.02
3	R	2995[B]	GLN	N-CA-C	-5.66	104.11	111.02
3	L	2995[A]	GLN	N-CA-C	-5.65	104.13	111.02
3	L	2995[B]	GLN	N-CA-C	-5.65	104.13	111.02
3	a	2995[A]	GLN	N-CA-C	-5.65	104.13	111.02
3	a	2995[B]	GLN	N-CA-C	-5.65	104.13	111.02
1	S	1339	SER	CA-C-N	5.65	131.86	121.70
1	S	1339	SER	C-N-CA	5.65	131.86	121.70
2	H	2134	ASN	N-CA-C	-5.64	103.14	108.22
1	V	1582	ASN	CA-C-N	5.64	131.85	121.70
1	V	1582	ASN	C-N-CA	5.64	131.85	121.70
1	M	758	GLY	N-CA-C	5.64	119.22	110.88
3	I	2995[A]	GLN	N-CA-C	-5.63	104.15	111.02
3	I	2995[B]	GLN	N-CA-C	-5.63	104.15	111.02
2	W	2689	GLY	N-CA-C	5.63	118.41	111.93
1	Y	823	VAL	CA-C-N	5.63	125.39	119.76
1	Y	823	VAL	C-N-CA	5.63	125.39	119.76
3	U	2995[A]	GLN	N-CA-C	-5.62	104.16	111.02
3	U	2995[B]	GLN	N-CA-C	-5.62	104.16	111.02
1	A	1251	SER	CA-C-N	5.62	125.56	119.78
1	A	1251	SER	C-N-CA	5.62	125.56	119.78
1	S	867	VAL	N-CA-C	5.61	118.92	111.17
3	F	2995[A]	GLN	N-CA-C	-5.61	104.17	111.02
3	F	2995[B]	GLN	N-CA-C	-5.61	104.17	111.02
3	U	3167[A]	VAL	N-CA-C	5.61	115.81	110.42
3	U	3167[B]	VAL	N-CA-C	5.61	115.81	110.42
1	P	1079	LYS	CA-C-N	5.61	125.54	119.76
1	P	1079	LYS	C-N-CA	5.61	125.54	119.76
3	X	2995[A]	GLN	N-CA-C	-5.60	104.19	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	2995[B]	GLN	N-CA-C	-5.60	104.19	111.02
1	A	557	VAL	N-CA-C	5.60	117.00	110.62
1	S	1296	VAL	CA-C-N	-5.60	112.84	119.84
1	S	1296	VAL	C-N-CA	-5.60	112.84	119.84
3	d	3167[A]	VAL	N-CA-C	5.59	115.79	110.42
3	d	3167[B]	VAL	N-CA-C	5.59	115.79	110.42
3	I	3167[A]	VAL	N-CA-C	5.57	115.77	110.42
3	I	3167[B]	VAL	N-CA-C	5.57	115.77	110.42
3	R	3167[A]	VAL	N-CA-C	5.57	115.76	110.42
3	R	3167[B]	VAL	N-CA-C	5.57	115.76	110.42
3	L	3167[A]	VAL	N-CA-C	5.56	115.76	110.42
3	L	3167[B]	VAL	N-CA-C	5.56	115.76	110.42
3	a	3167[A]	VAL	N-CA-C	5.56	115.75	110.42
3	a	3167[B]	VAL	N-CA-C	5.56	115.75	110.42
3	C	3167[A]	VAL	N-CA-C	5.55	115.75	110.42
3	C	3167[B]	VAL	N-CA-C	5.55	115.75	110.42
3	F	3167[A]	VAL	N-CA-C	5.54	115.74	110.42
3	F	3167[B]	VAL	N-CA-C	5.54	115.74	110.42
2	W	2764	THR	CA-C-N	5.54	125.64	119.32
2	W	2764	THR	C-N-CA	5.54	125.64	119.32
3	X	3167[A]	VAL	N-CA-C	5.54	115.74	110.42
3	X	3167[B]	VAL	N-CA-C	5.54	115.74	110.42
1	A	1286	ARG	N-CA-C	5.54	117.18	111.03
1	P	107	HIS	CA-C-N	5.54	125.21	119.56
1	P	107	HIS	C-N-CA	5.54	125.21	119.56
1	M	296	ARG	N-CA-C	-5.54	106.57	113.38
3	O	3167[A]	VAL	N-CA-C	5.53	115.73	110.42
3	O	3167[B]	VAL	N-CA-C	5.53	115.73	110.42
1	P	832	LYS	N-CA-C	5.53	115.58	108.34
2	E	2345	ASN	CA-C-N	5.52	124.87	118.85
2	E	2345	ASN	C-N-CA	5.52	124.87	118.85
2	Q	2207	ASN	CA-C-N	5.52	125.19	119.56
2	Q	2207	ASN	C-N-CA	5.52	125.19	119.56
1	G	465	PRO	N-CA-C	-5.52	106.92	114.98
1	M	669	LYS	CA-C-N	-5.52	114.07	119.64
1	M	669	LYS	C-N-CA	-5.52	114.07	119.64
1	D	229	LEU	CA-C-N	5.50	125.42	119.76
1	D	229	LEU	C-N-CA	5.50	125.42	119.76
2	K	2217	ILE	N-CA-C	-5.50	104.00	110.21
1	S	1494	ARG	CA-C-N	-5.50	112.97	119.84
1	S	1494	ARG	C-N-CA	-5.50	112.97	119.84
1	G	133	LYS	N-CA-C	5.50	117.54	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	1091	ASN	CA-C-N	5.50	125.19	119.64
1	b	1091	ASN	C-N-CA	5.50	125.19	119.64
2	N	2490	PRO	O-C-N	5.48	123.73	121.15
2	W	2489	ILE	CA-C-N	5.48	123.61	119.66
2	W	2489	ILE	C-N-CA	5.48	123.61	119.66
1	A	830	ASN	CA-C-N	5.47	131.55	121.70
1	A	830	ASN	C-N-CA	5.47	131.55	121.70
1	P	1339	SER	CA-C-N	5.47	131.54	121.70
1	P	1339	SER	C-N-CA	5.47	131.54	121.70
1	S	416	ASN	N-CA-C	5.46	117.66	111.11
2	Q	2237	LEU	CB-CA-C	-5.44	109.83	117.23
3	U	3005[A]	ALA	N-CA-C	-5.43	100.75	109.39
3	U	3005[B]	ALA	N-CA-C	-5.43	100.75	109.39
3	O	3101[A]	PRO	O-C-N	5.43	128.74	122.23
3	O	3101[B]	PRO	O-C-N	5.43	128.74	122.23
1	A	114	THR	CB-CA-C	-5.42	110.30	116.54
3	R	3005[A]	ALA	N-CA-C	-5.42	100.77	109.39
3	R	3005[B]	ALA	N-CA-C	-5.42	100.77	109.39
3	d	3119[A]	HIS	N-CA-C	-5.42	105.37	111.28
3	d	3119[B]	HIS	N-CA-C	-5.42	105.37	111.28
3	R	3119[A]	HIS	N-CA-C	-5.42	105.37	111.28
3	R	3119[B]	HIS	N-CA-C	-5.42	105.37	111.28
1	M	1339	SER	CA-C-N	5.42	131.46	121.70
1	M	1339	SER	C-N-CA	5.42	131.46	121.70
1	P	675	SER	CA-C-N	-5.42	113.07	119.84
1	P	675	SER	C-N-CA	-5.42	113.07	119.84
1	V	296	ARG	N-CA-C	-5.42	106.83	113.50
3	I	3005[A]	ALA	N-CA-C	-5.42	100.78	109.39
3	I	3005[B]	ALA	N-CA-C	-5.42	100.78	109.39
3	O	3005[A]	ALA	N-CA-C	-5.42	100.78	109.39
3	O	3005[B]	ALA	N-CA-C	-5.42	100.78	109.39
3	F	3005[A]	ALA	N-CA-C	-5.41	100.79	109.39
3	F	3005[B]	ALA	N-CA-C	-5.41	100.79	109.39
3	X	3101[A]	PRO	O-C-N	5.41	128.72	122.23
3	X	3101[B]	PRO	O-C-N	5.41	128.72	122.23
3	C	3101[A]	PRO	O-C-N	5.40	128.72	122.23
3	C	3101[B]	PRO	O-C-N	5.40	128.72	122.23
3	I	3101[A]	PRO	O-C-N	5.40	128.71	122.23
3	I	3101[B]	PRO	O-C-N	5.40	128.71	122.23
3	U	3119[A]	HIS	N-CA-C	-5.40	105.39	111.28
3	U	3119[B]	HIS	N-CA-C	-5.40	105.39	111.28
3	a	3101[A]	PRO	O-C-N	5.40	128.71	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	3101[B]	PRO	O-C-N	5.40	128.71	122.23
3	a	3113[A]	ASP	N-CA-C	5.40	116.47	109.72
3	a	3113[B]	ASP	N-CA-C	5.40	116.47	109.72
2	B	2764	THR	CA-C-N	5.40	125.48	119.32
2	B	2764	THR	C-N-CA	5.40	125.48	119.32
2	N	2553	ALA	N-CA-C	5.40	119.58	112.35
3	O	3119[A]	HIS	N-CA-C	-5.40	105.39	111.28
3	O	3119[B]	HIS	N-CA-C	-5.40	105.39	111.28
3	X	3005[A]	ALA	N-CA-C	-5.40	100.80	109.39
3	X	3005[B]	ALA	N-CA-C	-5.40	100.80	109.39
3	a	3119[A]	HIS	N-CA-C	-5.40	105.39	111.28
3	a	3119[B]	HIS	N-CA-C	-5.40	105.39	111.28
3	C	3005[A]	ALA	N-CA-C	-5.40	100.81	109.39
3	C	3005[B]	ALA	N-CA-C	-5.40	100.81	109.39
1	b	1494	ARG	CA-C-N	-5.40	113.09	119.84
1	b	1494	ARG	C-N-CA	-5.40	113.09	119.84
2	Q	2764	THR	CA-C-N	5.39	125.73	119.47
2	Q	2764	THR	C-N-CA	5.39	125.73	119.47
3	d	3005[A]	ALA	N-CA-C	-5.39	100.81	109.39
3	d	3005[B]	ALA	N-CA-C	-5.39	100.81	109.39
3	U	3101[A]	PRO	O-C-N	5.39	128.70	122.23
3	U	3101[B]	PRO	O-C-N	5.39	128.70	122.23
1	V	1082	SER	CA-C-N	-5.39	113.10	119.84
1	V	1082	SER	C-N-CA	-5.39	113.10	119.84
1	V	688	VAL	CA-C-N	5.39	126.58	119.84
1	V	688	VAL	C-N-CA	5.39	126.58	119.84
2	B	2490	PRO	O-C-N	5.39	123.68	121.15
3	C	3119[A]	HIS	N-CA-C	-5.39	105.41	111.28
3	C	3119[B]	HIS	N-CA-C	-5.39	105.41	111.28
2	B	2418	GLY	N-CA-C	5.38	119.19	112.73
3	R	3101[A]	PRO	O-C-N	5.38	128.69	122.23
3	R	3101[B]	PRO	O-C-N	5.38	128.69	122.23
3	R	3113[A]	ASP	N-CA-C	5.38	116.45	109.72
3	R	3113[B]	ASP	N-CA-C	5.38	116.45	109.72
3	U	3113[A]	ASP	N-CA-C	5.38	116.45	109.72
3	U	3113[B]	ASP	N-CA-C	5.38	116.45	109.72
1	V	551	GLU	N-CA-C	5.38	117.15	111.28
3	C	3113[A]	ASP	N-CA-C	5.38	116.44	109.72
3	C	3113[B]	ASP	N-CA-C	5.38	116.44	109.72
2	K	2418	GLY	N-CA-C	5.38	119.39	112.83
1	M	1286	ARG	N-CA-C	5.38	117.00	111.03
3	X	3113[A]	ASP	N-CA-C	5.37	116.44	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	3113[B]	ASP	N-CA-C	5.37	116.44	109.72
3	a	3005[A]	ALA	N-CA-C	-5.37	100.85	109.39
3	a	3005[B]	ALA	N-CA-C	-5.37	100.85	109.39
3	L	3101[A]	PRO	O-C-N	5.37	128.68	122.23
3	L	3101[B]	PRO	O-C-N	5.37	128.68	122.23
3	F	3119[A]	HIS	N-CA-C	-5.37	105.43	111.28
3	F	3119[B]	HIS	N-CA-C	-5.37	105.43	111.28
3	C	3300[A]	LEU	CA-C-N	-5.37	113.13	119.84
3	C	3300[A]	LEU	C-N-CA	-5.37	113.13	119.84
3	C	3300[B]	LEU	CA-C-N	-5.37	113.13	119.84
3	C	3300[B]	LEU	C-N-CA	-5.37	113.13	119.84
3	O	3113[A]	ASP	N-CA-C	5.37	116.43	109.72
3	O	3113[B]	ASP	N-CA-C	5.37	116.43	109.72
3	L	3005[A]	ALA	N-CA-C	-5.36	100.86	109.39
3	L	3005[B]	ALA	N-CA-C	-5.36	100.86	109.39
3	L	3119[A]	HIS	N-CA-C	-5.36	105.43	111.28
3	L	3119[B]	HIS	N-CA-C	-5.36	105.43	111.28
3	X	3119[A]	HIS	N-CA-C	-5.36	105.43	111.28
3	X	3119[B]	HIS	N-CA-C	-5.36	105.43	111.28
1	D	1512	ARG	CA-C-N	5.36	124.81	119.24
1	D	1512	ARG	C-N-CA	5.36	124.81	119.24
2	E	2558	CYS	N-CA-C	5.36	120.69	113.72
3	U	3300[A]	LEU	CA-C-N	-5.36	113.14	119.84
3	U	3300[A]	LEU	C-N-CA	-5.36	113.14	119.84
3	U	3300[B]	LEU	CA-C-N	-5.36	113.14	119.84
3	U	3300[B]	LEU	C-N-CA	-5.36	113.14	119.84
3	F	3113[A]	ASP	N-CA-C	5.36	116.42	109.72
3	F	3113[B]	ASP	N-CA-C	5.36	116.42	109.72
3	d	3300[A]	LEU	CA-C-N	-5.36	113.14	119.84
3	d	3300[A]	LEU	C-N-CA	-5.36	113.14	119.84
3	d	3300[B]	LEU	CA-C-N	-5.36	113.14	119.84
3	d	3300[B]	LEU	C-N-CA	-5.36	113.14	119.84
3	C	3277[A]	ALA	N-CA-C	-5.35	106.33	112.86
3	C	3277[B]	ALA	N-CA-C	-5.35	106.33	112.86
1	M	232	ARG	CA-C-N	5.35	125.61	119.83
1	M	232	ARG	C-N-CA	5.35	125.61	119.83
3	I	3119[A]	HIS	N-CA-C	-5.35	105.45	111.28
3	I	3119[B]	HIS	N-CA-C	-5.35	105.45	111.28
1	V	404	ILE	CA-C-N	5.35	123.56	119.66
1	V	404	ILE	C-N-CA	5.35	123.56	119.66
3	d	3113[A]	ASP	N-CA-C	5.35	116.40	109.72
3	d	3113[B]	ASP	N-CA-C	5.35	116.40	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	3300[A]	LEU	CA-C-N	-5.34	113.16	119.84
3	R	3300[A]	LEU	C-N-CA	-5.34	113.16	119.84
3	R	3300[B]	LEU	CA-C-N	-5.34	113.16	119.84
3	R	3300[B]	LEU	C-N-CA	-5.34	113.16	119.84
1	Y	1494	ARG	CA-C-N	-5.34	113.16	119.84
1	Y	1494	ARG	C-N-CA	-5.34	113.16	119.84
3	I	3113[A]	ASP	N-CA-C	5.34	116.40	109.72
3	I	3113[B]	ASP	N-CA-C	5.34	116.40	109.72
3	O	3277[A]	ALA	N-CA-C	-5.34	106.34	112.86
3	O	3277[B]	ALA	N-CA-C	-5.34	106.34	112.86
3	a	3277[A]	ALA	N-CA-C	-5.34	106.34	112.86
3	a	3277[B]	ALA	N-CA-C	-5.34	106.34	112.86
3	F	3101[A]	PRO	O-C-N	5.34	128.64	122.23
3	F	3101[B]	PRO	O-C-N	5.34	128.64	122.23
3	L	3300[A]	LEU	CA-C-N	-5.34	113.17	119.84
3	L	3300[A]	LEU	C-N-CA	-5.34	113.17	119.84
3	L	3300[B]	LEU	CA-C-N	-5.34	113.17	119.84
3	L	3300[B]	LEU	C-N-CA	-5.34	113.17	119.84
3	d	3101[A]	PRO	O-C-N	5.34	128.64	122.23
3	d	3101[B]	PRO	O-C-N	5.34	128.64	122.23
3	X	3277[A]	ALA	N-CA-C	-5.34	106.35	112.86
3	X	3277[B]	ALA	N-CA-C	-5.34	106.35	112.86
3	U	3027[A]	GLU	CA-C-N	-5.33	113.13	119.05
3	U	3027[A]	GLU	C-N-CA	-5.33	113.13	119.05
3	U	3027[B]	GLU	CA-C-N	-5.33	113.13	119.05
3	U	3027[B]	GLU	C-N-CA	-5.33	113.13	119.05
3	F	3277[A]	ALA	N-CA-C	-5.33	106.36	112.86
3	F	3277[B]	ALA	N-CA-C	-5.33	106.36	112.86
1	M	921	GLY	N-CA-C	5.33	121.26	113.48
3	L	3113[A]	ASP	N-CA-C	5.33	116.38	109.72
3	L	3113[B]	ASP	N-CA-C	5.33	116.38	109.72
1	S	463	GLY	N-CA-C	5.32	119.07	110.87
1	b	127	GLU	CA-CB-CG	5.32	124.75	114.10
3	O	3300[A]	LEU	CA-C-N	-5.32	113.19	119.84
3	O	3300[A]	LEU	C-N-CA	-5.32	113.19	119.84
3	O	3300[B]	LEU	CA-C-N	-5.32	113.19	119.84
3	O	3300[B]	LEU	C-N-CA	-5.32	113.19	119.84
3	R	3163[A]	ASN	CA-C-N	-5.32	113.19	119.84
3	R	3163[A]	ASN	C-N-CA	-5.32	113.19	119.84
3	R	3163[B]	ASN	CA-C-N	-5.32	113.19	119.84
3	R	3163[B]	ASN	C-N-CA	-5.32	113.19	119.84
2	E	2489	ILE	CA-C-N	5.32	125.86	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2489	ILE	C-N-CA	5.32	125.86	120.38
3	a	3300[A]	LEU	CA-C-N	-5.32	113.19	119.84
3	a	3300[A]	LEU	C-N-CA	-5.32	113.19	119.84
3	a	3300[B]	LEU	CA-C-N	-5.32	113.19	119.84
3	a	3300[B]	LEU	C-N-CA	-5.32	113.19	119.84
2	H	2558	CYS	N-CA-C	5.32	119.86	112.90
3	L	3163[A]	ASN	CA-C-N	-5.32	113.20	119.84
3	L	3163[A]	ASN	C-N-CA	-5.32	113.20	119.84
3	L	3163[B]	ASN	CA-C-N	-5.32	113.20	119.84
3	L	3163[B]	ASN	C-N-CA	-5.32	113.20	119.84
3	R	3277[A]	ALA	N-CA-C	-5.32	106.37	112.86
3	R	3277[B]	ALA	N-CA-C	-5.32	106.37	112.86
1	S	1582	ASN	CA-C-N	5.32	131.27	121.70
1	S	1582	ASN	C-N-CA	5.32	131.27	121.70
3	I	3027[A]	GLU	CA-C-N	-5.31	113.16	119.05
3	I	3027[A]	GLU	C-N-CA	-5.31	113.16	119.05
3	I	3027[B]	GLU	CA-C-N	-5.31	113.16	119.05
3	I	3027[B]	GLU	C-N-CA	-5.31	113.16	119.05
2	K	2489	ILE	CA-C-N	5.31	125.85	120.38
2	K	2489	ILE	C-N-CA	5.31	125.85	120.38
3	I	3277[A]	ALA	N-CA-C	-5.31	106.39	112.86
3	I	3277[B]	ALA	N-CA-C	-5.31	106.39	112.86
3	X	3300[A]	LEU	CA-C-N	-5.30	113.21	119.84
3	X	3300[A]	LEU	C-N-CA	-5.30	113.21	119.84
3	X	3300[B]	LEU	CA-C-N	-5.30	113.21	119.84
3	X	3300[B]	LEU	C-N-CA	-5.30	113.21	119.84
1	Y	1286	ARG	N-CA-C	5.30	116.75	110.97
3	F	3163[A]	ASN	CA-C-N	-5.30	113.21	119.84
3	F	3163[A]	ASN	C-N-CA	-5.30	113.21	119.84
3	F	3163[B]	ASN	CA-C-N	-5.30	113.21	119.84
3	F	3163[B]	ASN	C-N-CA	-5.30	113.21	119.84
3	U	3277[A]	ALA	N-CA-C	-5.30	106.39	112.86
3	U	3277[B]	ALA	N-CA-C	-5.30	106.39	112.86
3	F	3300[A]	LEU	CA-C-N	-5.30	113.22	119.84
3	F	3300[A]	LEU	C-N-CA	-5.30	113.22	119.84
3	F	3300[B]	LEU	CA-C-N	-5.30	113.22	119.84
3	F	3300[B]	LEU	C-N-CA	-5.30	113.22	119.84
2	c	2418	GLY	N-CA-C	5.30	120.18	113.24
1	J	450	LYS	N-CA-C	5.30	116.33	108.86
3	L	3027[A]	GLU	CA-C-N	-5.29	113.17	119.05
3	L	3027[A]	GLU	C-N-CA	-5.29	113.17	119.05
3	L	3027[B]	GLU	CA-C-N	-5.29	113.17	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	3027[B]	GLU	C-N-CA	-5.29	113.17	119.05
1	b	1286	ARG	N-CA-C	5.29	116.74	110.97
1	G	1512	ARG	CA-C-N	5.29	124.47	118.97
1	G	1512	ARG	C-N-CA	5.29	124.47	118.97
3	L	3277[A]	ALA	N-CA-C	-5.29	106.41	112.86
3	L	3277[B]	ALA	N-CA-C	-5.29	106.41	112.86
3	X	3027[A]	GLU	CA-C-N	-5.29	113.18	119.05
3	X	3027[A]	GLU	C-N-CA	-5.29	113.18	119.05
3	X	3027[B]	GLU	CA-C-N	-5.29	113.18	119.05
3	X	3027[B]	GLU	C-N-CA	-5.29	113.18	119.05
3	d	3027[A]	GLU	CA-C-N	-5.28	113.19	119.05
3	d	3027[A]	GLU	C-N-CA	-5.28	113.19	119.05
3	d	3027[B]	GLU	CA-C-N	-5.28	113.19	119.05
3	d	3027[B]	GLU	C-N-CA	-5.28	113.19	119.05
1	G	897	HIS	N-CA-C	-5.28	101.80	108.45
3	I	3163[A]	ASN	CA-C-N	-5.28	113.25	119.84
3	I	3163[A]	ASN	C-N-CA	-5.28	113.25	119.84
3	I	3163[B]	ASN	CA-C-N	-5.28	113.25	119.84
3	I	3163[B]	ASN	C-N-CA	-5.28	113.25	119.84
3	F	3027[A]	GLU	CA-C-N	-5.27	113.20	119.05
3	F	3027[A]	GLU	C-N-CA	-5.27	113.20	119.05
3	F	3027[B]	GLU	CA-C-N	-5.27	113.20	119.05
3	F	3027[B]	GLU	C-N-CA	-5.27	113.20	119.05
1	M	1637	GLY	N-CA-C	-5.27	100.68	113.18
3	d	3277[A]	ALA	N-CA-C	-5.27	106.43	112.86
3	d	3277[B]	ALA	N-CA-C	-5.27	106.43	112.86
3	I	3300[A]	LEU	CA-C-N	-5.27	113.25	119.84
3	I	3300[A]	LEU	C-N-CA	-5.27	113.25	119.84
3	I	3300[B]	LEU	CA-C-N	-5.27	113.25	119.84
3	I	3300[B]	LEU	C-N-CA	-5.27	113.25	119.84
3	X	3163[A]	ASN	CA-C-N	-5.27	113.25	119.84
3	X	3163[A]	ASN	C-N-CA	-5.27	113.25	119.84
3	X	3163[B]	ASN	CA-C-N	-5.27	113.25	119.84
3	X	3163[B]	ASN	C-N-CA	-5.27	113.25	119.84
3	O	3027[A]	GLU	CA-C-N	-5.26	113.21	119.05
3	O	3027[A]	GLU	C-N-CA	-5.26	113.21	119.05
3	O	3027[B]	GLU	CA-C-N	-5.26	113.21	119.05
3	O	3027[B]	GLU	C-N-CA	-5.26	113.21	119.05
3	C	3163[A]	ASN	CA-C-N	-5.26	113.26	119.84
3	C	3163[A]	ASN	C-N-CA	-5.26	113.26	119.84
3	C	3163[B]	ASN	CA-C-N	-5.26	113.26	119.84
3	C	3163[B]	ASN	C-N-CA	-5.26	113.26	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	3163[A]	ASN	CA-C-N	-5.26	113.27	119.84
3	O	3163[A]	ASN	C-N-CA	-5.26	113.27	119.84
3	O	3163[B]	ASN	CA-C-N	-5.26	113.27	119.84
3	O	3163[B]	ASN	C-N-CA	-5.26	113.27	119.84
3	U	3163[A]	ASN	CA-C-N	-5.26	113.27	119.84
3	U	3163[A]	ASN	C-N-CA	-5.26	113.27	119.84
3	U	3163[B]	ASN	CA-C-N	-5.26	113.27	119.84
3	U	3163[B]	ASN	C-N-CA	-5.26	113.27	119.84
3	a	3027[A]	GLU	CA-C-N	-5.26	113.21	119.05
3	a	3027[A]	GLU	C-N-CA	-5.26	113.21	119.05
3	a	3027[B]	GLU	CA-C-N	-5.26	113.21	119.05
3	a	3027[B]	GLU	C-N-CA	-5.26	113.21	119.05
3	a	3163[A]	ASN	CA-C-N	-5.26	113.27	119.84
3	a	3163[A]	ASN	C-N-CA	-5.26	113.27	119.84
3	a	3163[B]	ASN	CA-C-N	-5.26	113.27	119.84
3	a	3163[B]	ASN	C-N-CA	-5.26	113.27	119.84
1	J	1036	SER	N-CA-C	5.25	117.42	111.11
3	R	3027[A]	GLU	CA-C-N	-5.25	113.22	119.05
3	R	3027[A]	GLU	C-N-CA	-5.25	113.22	119.05
3	R	3027[B]	GLU	CA-C-N	-5.25	113.22	119.05
3	R	3027[B]	GLU	C-N-CA	-5.25	113.22	119.05
1	A	877	HIS	N-CA-C	-5.25	106.46	112.92
1	S	573	LYS	CA-C-N	5.25	131.15	121.70
1	S	573	LYS	C-N-CA	5.25	131.15	121.70
1	V	1584	GLY	N-CA-C	5.25	125.62	113.18
3	C	3027[A]	GLU	CA-C-N	-5.25	113.23	119.05
3	C	3027[A]	GLU	C-N-CA	-5.25	113.23	119.05
3	C	3027[B]	GLU	CA-C-N	-5.25	113.23	119.05
3	C	3027[B]	GLU	C-N-CA	-5.25	113.23	119.05
3	d	3163[A]	ASN	CA-C-N	-5.25	113.28	119.84
3	d	3163[A]	ASN	C-N-CA	-5.25	113.28	119.84
3	d	3163[B]	ASN	CA-C-N	-5.25	113.28	119.84
3	d	3163[B]	ASN	C-N-CA	-5.25	113.28	119.84
1	V	131	GLU	CB-CA-C	-5.24	110.52	116.54
3	F	3197[A]	ILE	CA-C-N	-5.24	113.24	119.05
3	F	3197[A]	ILE	C-N-CA	-5.24	113.24	119.05
3	F	3197[B]	ILE	CA-C-N	-5.24	113.24	119.05
3	F	3197[B]	ILE	C-N-CA	-5.24	113.24	119.05
1	G	50	ALA	CB-CA-C	-5.24	110.52	116.54
2	Z	2418	GLY	N-CA-C	5.23	120.09	113.24
1	P	1647	ASN	CA-C-N	5.23	125.53	119.93
1	P	1647	ASN	C-N-CA	5.23	125.53	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	1581	GLU	N-CA-C	5.23	115.25	107.88
1	A	565	GLU	N-CA-C	5.22	116.22	108.86
3	L	3029[A]	LYS	N-CA-C	5.22	117.48	109.07
3	L	3029[B]	LYS	N-CA-C	5.22	117.48	109.07
3	U	3197[A]	ILE	CA-C-N	-5.22	113.25	119.05
3	U	3197[A]	ILE	C-N-CA	-5.22	113.25	119.05
3	U	3197[B]	ILE	CA-C-N	-5.22	113.25	119.05
3	U	3197[B]	ILE	C-N-CA	-5.22	113.25	119.05
3	a	3197[A]	ILE	CA-C-N	-5.22	113.26	119.05
3	a	3197[A]	ILE	C-N-CA	-5.22	113.26	119.05
3	a	3197[B]	ILE	CA-C-N	-5.22	113.26	119.05
3	a	3197[B]	ILE	C-N-CA	-5.22	113.26	119.05
3	I	3197[A]	ILE	CA-C-N	-5.21	113.27	119.05
3	I	3197[A]	ILE	C-N-CA	-5.21	113.27	119.05
3	I	3197[B]	ILE	CA-C-N	-5.21	113.27	119.05
3	I	3197[B]	ILE	C-N-CA	-5.21	113.27	119.05
1	S	627	ASP	CA-C-N	5.21	124.87	119.56
1	S	627	ASP	C-N-CA	5.21	124.87	119.56
1	D	1316	MET	CA-C-N	5.21	124.82	119.56
1	D	1316	MET	C-N-CA	5.21	124.82	119.56
3	X	3197[A]	ILE	CA-C-N	-5.20	113.27	119.05
3	X	3197[A]	ILE	C-N-CA	-5.20	113.27	119.05
3	X	3197[B]	ILE	CA-C-N	-5.20	113.27	119.05
3	X	3197[B]	ILE	C-N-CA	-5.20	113.27	119.05
1	V	50	ALA	CB-CA-C	-5.20	110.16	117.23
1	b	465	PRO	N-CA-C	-5.20	101.76	112.47
3	C	3197[A]	ILE	CA-C-N	-5.20	113.28	119.05
3	C	3197[A]	ILE	C-N-CA	-5.20	113.28	119.05
3	C	3197[B]	ILE	CA-C-N	-5.20	113.28	119.05
3	C	3197[B]	ILE	C-N-CA	-5.20	113.28	119.05
1	V	985	PHE	CB-CA-C	-5.20	110.56	116.54
3	R	3197[A]	ILE	CA-C-N	-5.19	113.29	119.05
3	R	3197[A]	ILE	C-N-CA	-5.19	113.29	119.05
3	R	3197[B]	ILE	CA-C-N	-5.19	113.29	119.05
3	R	3197[B]	ILE	C-N-CA	-5.19	113.29	119.05
2	W	2490	PRO	O-C-N	5.19	123.59	121.15
3	X	3029[A]	LYS	N-CA-C	5.19	117.42	109.07
3	X	3029[B]	LYS	N-CA-C	5.19	117.42	109.07
3	a	3029[A]	LYS	N-CA-C	5.19	117.42	109.07
3	a	3029[B]	LYS	N-CA-C	5.19	117.42	109.07
1	P	897	HIS	N-CA-C	-5.19	101.58	108.74
2	Z	2728	ARG	N-CA-C	-5.19	104.03	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3029[A]	LYS	N-CA-C	5.18	117.42	109.07
3	C	3029[B]	LYS	N-CA-C	5.18	117.42	109.07
1	G	1339	SER	CA-C-N	5.18	131.02	121.70
1	G	1339	SER	C-N-CA	5.18	131.02	121.70
2	H	2237	LEU	CB-CA-C	-5.18	110.62	116.63
2	H	2489	ILE	CA-C-N	5.18	125.72	120.38
2	H	2489	ILE	C-N-CA	5.18	125.72	120.38
1	Y	758	GLY	N-CA-C	5.18	118.04	110.63
3	O	3029[A]	LYS	N-CA-C	5.18	117.41	109.07
3	O	3029[B]	LYS	N-CA-C	5.18	117.41	109.07
1	Y	1636	ASN	N-CA-C	-5.18	102.39	110.10
3	d	3029[A]	LYS	N-CA-C	5.17	117.40	109.07
3	d	3029[B]	LYS	N-CA-C	5.17	117.40	109.07
2	H	2132	CYS	CA-C-N	-5.17	113.38	119.84
2	H	2132	CYS	C-N-CA	-5.17	113.38	119.84
3	R	3029[A]	LYS	N-CA-C	5.17	117.39	109.07
3	R	3029[B]	LYS	N-CA-C	5.17	117.39	109.07
1	P	1441	SER	N-CA-C	5.16	115.06	108.24
3	U	3029[A]	LYS	N-CA-C	5.16	117.38	109.07
3	U	3029[B]	LYS	N-CA-C	5.16	117.38	109.07
2	T	2556	TYR	N-CA-C	5.16	115.15	107.88
1	M	1584	GLY	N-CA-C	5.15	125.40	113.18
3	d	3197[A]	ILE	CA-C-N	-5.15	113.33	119.05
3	d	3197[A]	ILE	C-N-CA	-5.15	113.33	119.05
3	d	3197[B]	ILE	CA-C-N	-5.15	113.33	119.05
3	d	3197[B]	ILE	C-N-CA	-5.15	113.33	119.05
3	F	3029[A]	LYS	N-CA-C	5.15	117.36	109.07
3	F	3029[B]	LYS	N-CA-C	5.15	117.36	109.07
1	S	562	GLN	N-CA-C	5.14	117.55	111.33
1	Y	296	ARG	N-CA-C	-5.14	106.85	113.23
1	D	675	SER	CA-C-N	-5.14	113.41	119.84
1	D	675	SER	C-N-CA	-5.14	113.41	119.84
3	I	3029[A]	LYS	N-CA-C	5.14	117.34	109.07
3	I	3029[B]	LYS	N-CA-C	5.14	117.34	109.07
3	L	3197[A]	ILE	CA-C-N	-5.13	113.35	119.05
3	L	3197[A]	ILE	C-N-CA	-5.13	113.35	119.05
3	L	3197[B]	ILE	CA-C-N	-5.13	113.35	119.05
3	L	3197[B]	ILE	C-N-CA	-5.13	113.35	119.05
1	A	99	THR	N-CA-C	-5.13	107.68	114.04
1	S	1486	LEU	CA-C-N	-5.13	114.50	120.04
1	S	1486	LEU	C-N-CA	-5.13	114.50	120.04
3	O	3197[A]	ILE	CA-C-N	-5.13	113.36	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	3197[A]	ILE	C-N-CA	-5.13	113.36	119.05
3	O	3197[B]	ILE	CA-C-N	-5.13	113.36	119.05
3	O	3197[B]	ILE	C-N-CA	-5.13	113.36	119.05
1	J	1582	ASN	CA-C-N	5.12	130.92	121.70
1	J	1582	ASN	C-N-CA	5.12	130.92	121.70
1	P	898	GLY	N-CA-C	5.12	125.31	113.18
1	J	1195	ASP	N-CA-C	5.11	116.93	111.36
3	F	3120[A]	HIS	CA-C-N	-5.09	111.83	121.54
3	F	3120[A]	HIS	C-N-CA	-5.09	111.83	121.54
3	F	3120[B]	HIS	CA-C-N	-5.09	111.83	121.54
3	F	3120[B]	HIS	C-N-CA	-5.09	111.83	121.54
2	B	2237	LEU	CB-CA-C	-5.08	110.32	117.23
3	L	3120[A]	HIS	CA-C-N	-5.07	111.85	121.54
3	L	3120[A]	HIS	C-N-CA	-5.07	111.85	121.54
3	L	3120[B]	HIS	CA-C-N	-5.07	111.85	121.54
3	L	3120[B]	HIS	C-N-CA	-5.07	111.85	121.54
2	c	2764	THR	CA-C-N	5.07	125.10	119.32
2	c	2764	THR	C-N-CA	5.07	125.10	119.32
3	I	3120[A]	HIS	CA-C-N	-5.07	111.86	121.54
3	I	3120[A]	HIS	C-N-CA	-5.07	111.86	121.54
3	I	3120[B]	HIS	CA-C-N	-5.07	111.86	121.54
3	I	3120[B]	HIS	C-N-CA	-5.07	111.86	121.54
2	K	2826	GLU	CB-CA-C	-5.07	110.75	116.63
1	Y	958	PRO	CA-C-O	-5.07	115.17	122.31
1	A	627	ASP	CA-C-N	5.06	125.09	119.32
1	A	627	ASP	C-N-CA	5.06	125.09	119.32
1	G	1581	GLU	N-CA-C	5.06	116.94	108.99
3	C	3120[A]	HIS	CA-C-N	-5.06	111.88	121.54
3	C	3120[A]	HIS	C-N-CA	-5.06	111.88	121.54
3	C	3120[B]	HIS	CA-C-N	-5.06	111.88	121.54
3	C	3120[B]	HIS	C-N-CA	-5.06	111.88	121.54
2	T	2418	GLY	N-CA-C	5.06	120.00	113.27
1	A	688	VAL	CA-C-N	5.06	126.16	119.84
1	A	688	VAL	C-N-CA	5.06	126.16	119.84
1	A	1295	GLY	N-CA-C	5.06	120.22	111.98
3	U	3120[A]	HIS	CA-C-N	-5.06	111.88	121.54
3	U	3120[A]	HIS	C-N-CA	-5.06	111.88	121.54
3	U	3120[B]	HIS	CA-C-N	-5.06	111.88	121.54
3	U	3120[B]	HIS	C-N-CA	-5.06	111.88	121.54
2	K	2558	CYS	N-CA-C	5.05	119.72	113.50
3	O	3120[A]	HIS	CA-C-N	-5.05	111.89	121.54
3	O	3120[A]	HIS	C-N-CA	-5.05	111.89	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	3120[B]	HIS	CA-C-N	-5.05	111.89	121.54
3	O	3120[B]	HIS	C-N-CA	-5.05	111.89	121.54
1	V	1295	GLY	N-CA-C	5.04	120.20	111.98
3	d	3120[A]	HIS	CA-C-N	-5.04	111.91	121.54
3	d	3120[A]	HIS	C-N-CA	-5.04	111.91	121.54
3	d	3120[B]	HIS	CA-C-N	-5.04	111.91	121.54
3	d	3120[B]	HIS	C-N-CA	-5.04	111.91	121.54
1	D	568	PHE	N-CA-C	5.04	117.43	111.33
1	V	566	ARG	CB-CA-C	-5.04	110.38	117.23
1	A	1486	LEU	CA-C-N	-5.03	114.64	119.87
1	A	1486	LEU	C-N-CA	-5.03	114.64	119.87
3	R	3120[A]	HIS	CA-C-N	-5.03	111.93	121.54
3	R	3120[A]	HIS	C-N-CA	-5.03	111.93	121.54
3	R	3120[B]	HIS	CA-C-N	-5.03	111.93	121.54
3	R	3120[B]	HIS	C-N-CA	-5.03	111.93	121.54
1	S	1537	ILE	CB-CA-C	-5.03	109.02	114.35
1	A	1300	CYS	CA-C-N	5.03	126.12	119.84
1	A	1300	CYS	C-N-CA	5.03	126.12	119.84
2	K	2704	ASP	CA-C-N	5.02	125.05	119.32
2	K	2704	ASP	C-N-CA	5.02	125.05	119.32
1	V	1441	SER	N-CA-C	5.02	114.78	108.45
3	a	3120[A]	HIS	CA-C-N	-5.02	111.95	121.54
3	a	3120[A]	HIS	C-N-CA	-5.02	111.95	121.54
3	a	3120[B]	HIS	CA-C-N	-5.02	111.95	121.54
3	a	3120[B]	HIS	C-N-CA	-5.02	111.95	121.54
1	A	675	SER	CA-C-N	-5.02	113.57	119.84
1	A	675	SER	C-N-CA	-5.02	113.57	119.84
1	b	823	VAL	CA-C-N	5.02	125.17	119.90
1	b	823	VAL	C-N-CA	5.02	125.17	119.90
1	A	296	ARG	N-CA-C	-5.01	107.17	113.28
1	b	323	ILE	CA-C-N	5.01	125.00	119.89
1	b	323	ILE	C-N-CA	5.01	125.00	119.89
3	U	2934[A]	GLU	N-CA-C	-5.01	105.82	111.28
3	U	2934[B]	GLU	N-CA-C	-5.01	105.82	111.28
3	d	2934[A]	GLU	N-CA-C	-5.01	105.82	111.28
3	d	2934[B]	GLU	N-CA-C	-5.01	105.82	111.28
2	Z	2128	LEU	N-CA-C	5.01	120.27	113.16
2	W	2476	LEU	CA-C-N	5.00	124.93	119.78
2	W	2476	LEU	C-N-CA	5.00	124.93	119.78

There are no chirality outliers.

All (67) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	464	LEU	Peptide
1	A	982	LYS	Peptide
2	B	2127	ALA	Peptide
3	C	3113[A]	ASP	Mainchain
3	C	3113[B]	ASP	Mainchain
3	C	3149[A]	ASN	Peptide
3	C	3149[B]	ASN	Peptide
1	D	464	LEU	Peptide
1	D	567	LEU	Peptide
1	D	883	CYS	Peptide
3	F	3113[A]	ASP	Mainchain
3	F	3113[B]	ASP	Mainchain
3	F	3149[A]	ASN	Peptide
3	F	3149[B]	ASN	Peptide
1	G	464	LEU	Peptide
3	I	3113[A]	ASP	Mainchain
3	I	3113[B]	ASP	Mainchain
3	I	3149[A]	ASN	Peptide
3	I	3149[B]	ASN	Peptide
1	J	1639	LYS	Peptide
1	J	464	LEU	Peptide
2	K	2127	ALA	Peptide
2	K	2830	GLN	Peptide
2	K	2889	ALA	Peptide
3	L	3113[A]	ASP	Mainchain
3	L	3113[B]	ASP	Mainchain
3	L	3149[A]	ASN	Peptide
3	L	3149[B]	ASN	Peptide
1	M	464	LEU	Peptide
2	N	2127	ALA	Peptide
3	O	3113[A]	ASP	Mainchain
3	O	3113[B]	ASP	Mainchain
3	O	3149[A]	ASN	Peptide
3	O	3149[B]	ASN	Peptide
2	Q	2127	ALA	Peptide
3	R	3113[A]	ASP	Mainchain
3	R	3113[B]	ASP	Mainchain
3	R	3149[A]	ASN	Peptide
3	R	3149[B]	ASN	Peptide
1	S	1638	SER	Peptide
1	S	464	LEU	Peptide
1	S	866	GLU	Peptide
2	T	2127	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	T	2548	CYS	Peptide
3	U	3113[A]	ASP	Mainchain
3	U	3113[B]	ASP	Mainchain
3	U	3149[A]	ASN	Peptide
3	U	3149[B]	ASN	Peptide
2	W	2127	ALA	Peptide
3	X	3113[A]	ASP	Mainchain
3	X	3113[B]	ASP	Mainchain
3	X	3149[A]	ASN	Peptide
3	X	3149[B]	ASN	Peptide
1	Y	464	LEU	Peptide
2	Z	2127	ALA	Peptide
2	Z	2497	GLU	Peptide
3	a	3113[A]	ASP	Mainchain
3	a	3113[B]	ASP	Mainchain
3	a	3149[A]	ASN	Peptide
3	a	3149[B]	ASN	Peptide
1	b	127	GLU	Peptide
1	b	464	LEU	Peptide
2	c	2127	ALA	Peptide
3	d	3113[A]	ASP	Mainchain
3	d	3113[B]	ASP	Mainchain
3	d	3149[A]	ASN	Peptide
3	d	3149[B]	ASN	Peptide

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	13318	0	12755	476	1
1	D	13318	0	12755	482	0
1	G	13318	0	12754	503	0
1	J	13318	0	12755	508	0
1	M	13318	0	12755	448	0
1	P	13318	0	12755	450	0
1	S	13318	0	12755	451	0
1	V	13318	0	12755	448	0
1	Y	13318	0	12744	528	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	13318	0	12754	452	1
2	B	6704	0	6445	213	0
2	E	6704	0	6445	245	0
2	H	6704	0	6445	243	0
2	K	6704	0	6445	218	0
2	N	6704	0	6445	203	0
2	Q	6704	0	6445	218	0
2	T	6704	0	6445	221	0
2	W	6704	0	6445	226	0
2	Z	6704	0	6444	238	0
2	c	6704	0	6445	224	0
3	C	5912	0	5607	2341	0
3	F	5912	0	5599	2386	0
3	I	5912	0	5601	2460	0
3	L	5912	0	5604	2354	0
3	O	5912	0	5604	2061	0
3	R	5912	0	5598	2438	0
3	U	5912	0	5612	2074	0
3	X	5912	0	5598	2059	0
3	a	5912	0	5594	2398	0
3	d	5912	0	5608	2177	0
4	1	28	0	25	1	0
4	2	28	0	25	1	0
4	4	28	0	25	0	0
4	6	28	0	25	2	0
4	7	28	0	25	6	0
4	8	28	0	25	0	0
4	9	28	0	25	2	0
4	BA	28	0	25	5	0
4	HA	28	0	25	6	0
4	IA	28	0	25	0	0
4	JA	28	0	25	2	0
4	MA	28	0	25	9	0
4	OA	28	0	25	2	0
4	QA	28	0	25	4	0
4	RA	28	0	25	1	0
4	e	28	0	25	0	0
4	f	28	0	25	2	0
4	i	28	0	25	3	0
4	j	28	0	25	4	0
4	m	28	0	25	9	0
4	n	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	o	28	0	25	3	0
4	p	28	0	25	0	0
4	q	28	0	25	7	0
4	s	28	0	25	2	0
4	t	28	0	25	1	0
4	u	28	0	25	6	0
4	v	28	0	25	2	0
4	x	28	0	25	0	0
5	AA	50	0	43	1	0
5	FA	50	0	43	2	0
5	KA	50	0	43	1	0
5	PA	50	0	43	1	0
5	g	50	0	43	0	0
5	l	50	0	43	2	0
6	3	39	0	34	3	0
6	5	39	0	34	2	0
6	CA	39	0	34	3	0
6	DA	39	0	34	2	0
6	EA	39	0	34	1	0
6	GA	39	0	34	9	0
6	LA	39	0	34	5	0
6	NA	39	0	34	3	0
6	h	39	0	34	1	0
6	k	39	0	34	4	0
6	r	39	0	34	8	0
6	w	39	0	34	2	0
6	y	39	0	34	0	0
7	z	61	0	52	2	0
8	0	50	0	43	8	0
9	A	24	0	0	2	0
9	B	8	0	0	0	0
9	C	8	0	0	7	0
9	D	24	0	0	2	0
9	E	8	0	0	0	0
9	F	8	0	0	7	0
9	G	24	0	0	1	0
9	H	8	0	0	0	0
9	I	8	0	0	6	0
9	J	24	0	0	2	0
9	K	8	0	0	0	0
9	L	8	0	0	7	0
9	M	24	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	N	8	0	0	0	0
9	O	8	0	0	10	0
9	P	24	0	0	0	0
9	Q	8	0	0	0	0
9	R	8	0	0	6	0
9	S	24	0	0	3	0
9	T	8	0	0	1	0
9	U	8	0	0	10	0
9	V	24	0	0	2	0
9	W	8	0	0	1	0
9	X	8	0	0	10	0
9	Y	24	0	0	3	0
9	Z	8	0	0	0	0
9	a	8	0	0	7	0
9	b	24	0	0	1	0
9	c	8	0	0	0	0
9	d	8	0	0	10	0
All	All	261470	0	249531	25303	1

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 50.

All (25303) 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)
3:F:2975[B]:PHE:CD1	3:a:3107[B]:LEU:HD11	1.20	1.69
3:F:2969[B]:TYR:HD1	3:a:2961[B]:HIS:CG	1.09	1.68
3:C:3079[B]:CYS:CB	3:L:3161[B]:GLU:HG2	1.22	1.65
3:C:2982[B]:MET:SD	3:L:3156[B]:MET:HB2	1.37	1.64
3:F:2970[B]:PRO:HD3	3:a:2989[B]:HIS:CD2	1.23	1.64
3:U:3256[B]:TRP:CG	3:d:2969[B]:TYR:HB2	1.33	1.63
3:U:3254[B]:MET:HE1	3:d:3254[B]:MET:CE	1.27	1.63
3:C:2975[B]:PHE:CD1	3:L:3107[B]:LEU:HD11	1.28	1.63
3:I:3174[B]:GLY:CA	3:R:3154[B]:PRO:HB3	1.17	1.62
3:U:2969[B]:TYR:CE1	3:d:3107[B]:LEU:CD1	1.82	1.61
2:Z:2867:PRO:CG	3:a:2932[A]:PRO:HG2	1.28	1.60
3:O:3153[B]:LYS:CD	3:X:3176[B]:LYS:HD3	1.31	1.60
3:F:3157[B]:PRO:HA	3:a:2982[B]:MET:SD	1.41	1.59
3:C:3156[B]:MET:CE	3:L:2979[B]:GLN:HG3	1.25	1.59
3:O:2963[B]:MET:HE1	3:X:2975[B]:PHE:CG	1.08	1.58
3:F:3155[B]:MET:CB	3:a:3153[B]:LYS:HD2	1.33	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3196[A]:THR:CG2	1:J:416:ASN:HD22	0.95	1.57
3:U:3256[B]:TRP:CB	3:d:2969[B]:TYR:HB2	1.22	1.57
3:O:2968[B]:GLN:NE2	3:X:2985[B]:PHE:CA	1.68	1.56
3:C:3156[B]:MET:HE2	3:L:2979[B]:GLN:CG	1.15	1.56
3:F:3153[B]:LYS:CG	3:a:3155[B]:MET:HB2	1.08	1.56
3:O:2968[B]:GLN:CB	3:X:2988[B]:TRP:HB2	1.29	1.56
3:C:2985[B]:PHE:CZ	3:L:2970[B]:PRO:HA	1.07	1.56
3:F:2975[B]:PHE:HD1	3:a:3107[B]:LEU:CD1	1.19	1.56
3:F:3155[B]:MET:HB2	3:a:3153[B]:LYS:CG	1.33	1.56
3:I:2989[B]:HIS:CG	3:R:2970[B]:PRO:HD3	1.37	1.55
3:I:3163[B]:ASN:CB	3:R:3150[B]:LYS:HE3	1.28	1.55
3:C:2985[B]:PHE:HZ	3:L:2970[B]:PRO:CA	0.91	1.55
3:F:2984[B]:THR:HG21	3:a:3159[B]:SER:CB	1.14	1.55
3:O:2970[B]:PRO:CD	3:X:2991[B]:LEU:HB2	1.37	1.54
3:O:2970[B]:PRO:HG2	3:X:2991[B]:LEU:CA	1.12	1.54
3:C:2965[B]:LEU:CD2	3:L:3253[B]:GLU:CD	1.79	1.54
3:C:3158[B]:PHE:CD2	3:L:3153[B]:LYS:CE	1.89	1.54
3:I:2975[B]:PHE:CD1	3:R:3107[B]:LEU:HD11	1.42	1.53
3:F:3149[B]:ASN:CB	3:a:3163[B]:ASN:ND2	1.68	1.53
3:C:2974[B]:ALA:CB	3:L:3249[B]:GLY:CA	1.83	1.53
3:F:2983[B]:VAL:CG2	3:a:3161[B]:GLU:N	1.70	1.53
3:F:3155[B]:MET:HB2	3:a:3153[B]:LYS:CD	1.06	1.53
3:U:3255[B]:PRO:HG2	3:d:3252[B]:TYR:C	1.29	1.53
1:Y:1546:LYS:CG	3:d:3001[B]:LYS:HE3	1.35	1.52
3:F:2970[B]:PRO:CD	3:a:2989[B]:HIS:CD2	1.91	1.52
3:O:2965[B]:LEU:HD12	3:X:2979[B]:GLN:CD	1.15	1.52
3:I:3150[B]:LYS:C	3:R:3159[B]:SER:HA	1.18	1.52
3:O:2970[B]:PRO:CG	3:X:2991[B]:LEU:N	1.69	1.52
3:C:2982[B]:MET:CG	3:L:3156[B]:MET:HB2	1.38	1.51
3:I:3159[B]:SER:C	3:R:3150[B]:LYS:HB3	1.31	1.51
3:O:3153[B]:LYS:HD3	3:X:3176[B]:LYS:CD	1.35	1.51
3:F:3154[B]:PRO:N	3:a:3155[B]:MET:CG	1.73	1.51
3:F:3159[B]:SER:HB3	3:a:2984[B]:THR:CG2	1.38	1.50
3:I:3251[B]:ASP:CB	3:R:3251[B]:ASP:HB3	1.07	1.50
3:I:3150[B]:LYS:HB3	3:R:3159[B]:SER:C	1.11	1.50
3:F:2966[B]:SER:C	3:a:3256[B]:TRP:CD1	1.87	1.49
3:O:2963[B]:MET:CE	3:X:2975[B]:PHE:CG	1.92	1.49
3:C:3150[B]:LYS:HZ3	3:L:3160[B]:SER:CB	1.22	1.49
3:I:2989[B]:HIS:CD2	3:R:2970[B]:PRO:HD3	1.48	1.49
1:Y:1546:LYS:HB2	3:d:3001[B]:LYS:NZ	1.21	1.49
3:O:3169[B]:LYS:CG	3:X:3148[B]:ILE:CG2	1.81	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3220[B]:ARG:HA	3:d:2973[B]:THR:CA	1.28	1.48
3:R:2956[A]:LYS:O	3:R:2960[A]:PHE:CE1	1.67	1.48
3:I:3149[B]:ASN:CB	3:R:3163[B]:ASN:ND2	1.74	1.48
3:L:2956[A]:LYS:O	3:L:2960[A]:PHE:CE1	1.67	1.48
3:U:3256[B]:TRP:HB2	3:d:2969[B]:TYR:CB	1.42	1.48
3:C:3090[B]:ASN:HD22	3:L:2972[B]:GLY:C	1.20	1.47
3:I:2956[B]:LYS:O	3:I:2960[B]:PHE:CE1	1.67	1.47
3:L:3089[B]:HIS:CE1	3:L:3119[B]:HIS:NE2	1.83	1.47
3:U:3089[B]:HIS:CE1	3:U:3119[B]:HIS:NE2	1.83	1.47
3:a:2956[B]:LYS:O	3:a:2960[B]:PHE:CE1	1.67	1.47
3:d:2956[A]:LYS:O	3:d:2960[A]:PHE:CE1	1.67	1.47
3:d:3089[A]:HIS:CE1	3:d:3119[A]:HIS:NE2	1.83	1.47
3:C:3160[B]:SER:CB	3:L:3150[B]:LYS:NZ	1.75	1.47
3:F:3150[B]:LYS:NZ	3:a:3160[B]:SER:HB3	1.26	1.47
3:I:3089[A]:HIS:CE1	3:I:3119[A]:HIS:NE2	1.83	1.47
3:U:3254[B]:MET:CE	3:d:3254[B]:MET:HE3	0.99	1.47
3:L:3089[A]:HIS:CE1	3:L:3119[A]:HIS:NE2	1.82	1.47
3:U:3089[A]:HIS:CE1	3:U:3119[A]:HIS:NE2	1.83	1.47
3:F:3160[B]:SER:HB3	3:a:3150[B]:LYS:NZ	1.21	1.47
3:L:2956[B]:LYS:O	3:L:2960[B]:PHE:CE1	1.67	1.47
3:O:2968[B]:GLN:NE2	3:X:2985[B]:PHE:N	1.63	1.47
3:U:2969[B]:TYR:CE1	3:d:3107[B]:LEU:HD11	1.44	1.47
3:X:3089[B]:HIS:CE1	3:X:3119[B]:HIS:NE2	1.82	1.47
3:C:3089[A]:HIS:CE1	3:C:3119[A]:HIS:NE2	1.83	1.46
3:X:3089[A]:HIS:CE1	3:X:3119[A]:HIS:NE2	1.83	1.46
3:C:2956[B]:LYS:O	3:C:2960[B]:PHE:CE1	1.67	1.46
3:C:3089[B]:HIS:CE1	3:C:3119[B]:HIS:NE2	1.83	1.46
3:O:3089[B]:HIS:CE1	3:O:3119[B]:HIS:NE2	1.83	1.46
3:d:3089[B]:HIS:CE1	3:d:3119[B]:HIS:NE2	1.82	1.46
3:F:2956[A]:LYS:O	3:F:2960[A]:PHE:CE1	1.67	1.46
1:S:416:ASN:CG	3:X:3196[A]:THR:HG21	1.41	1.46
3:a:3089[A]:HIS:CE1	3:a:3119[A]:HIS:NE2	1.83	1.46
3:F:2970[B]:PRO:HD3	3:a:2989[B]:HIS:CG	1.45	1.46
3:O:2956[A]:LYS:O	3:O:2960[A]:PHE:CE1	1.67	1.46
3:O:3153[B]:LYS:HG2	3:X:3176[B]:LYS:CE	1.41	1.46
3:d:2956[B]:LYS:O	3:d:2960[B]:PHE:CE1	1.67	1.46
3:F:2984[B]:THR:CG2	3:a:3159[B]:SER:HB3	0.98	1.45
3:I:3154[B]:PRO:HB3	3:R:3174[B]:GLY:CA	1.43	1.45
1:S:416:ASN:OD1	3:X:3196[A]:THR:CG2	1.64	1.45
3:a:2956[A]:LYS:O	3:a:2960[A]:PHE:CE1	1.67	1.45
3:F:3089[A]:HIS:CE1	3:F:3119[A]:HIS:NE2	1.83	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2956[A]:LYS:O	3:I:2960[A]:PHE:CE1	1.67	1.45
3:U:2956[B]:LYS:O	3:U:2960[B]:PHE:CE1	1.67	1.45
3:C:2956[A]:LYS:O	3:C:2960[A]:PHE:CE1	1.67	1.45
3:F:2982[B]:MET:CG	3:a:2967[B]:CYS:SG	2.05	1.45
3:O:3108[B]:HIS:HB3	3:X:2969[B]:TYR:C	1.05	1.45
3:F:3089[B]:HIS:CE1	3:F:3119[B]:HIS:NE2	1.83	1.45
3:F:3174[B]:GLY:N	3:a:3154[B]:PRO:HB3	1.19	1.44
3:I:2975[B]:PHE:HD1	3:R:3107[B]:LEU:CD1	1.28	1.44
3:O:2965[B]:LEU:CD1	3:X:2979[B]:GLN:NE2	1.75	1.44
3:U:2956[A]:LYS:O	3:U:2960[A]:PHE:CE1	1.67	1.44
3:U:3155[B]:MET:CA	3:d:3150[B]:LYS:HG2	1.45	1.44
3:C:3163[B]:ASN:ND2	3:L:3149[B]:ASN:CB	1.78	1.44
3:I:3089[B]:HIS:CE1	3:I:3119[B]:HIS:NE2	1.82	1.44
1:Y:1616:LYS:HD3	3:d:3187[B]:TYR:C	1.23	1.44
3:C:3079[B]:CYS:SG	3:L:3161[B]:GLU:CB	2.03	1.44
3:F:3155[B]:MET:CB	3:a:3153[B]:LYS:CD	1.84	1.44
3:F:3252[B]:TYR:N	3:a:3108[B]:HIS:NE2	1.63	1.44
3:I:3251[B]:ASP:HB3	3:R:3251[B]:ASP:CB	0.98	1.44
3:X:2956[B]:LYS:O	3:X:2960[B]:PHE:CE1	1.68	1.44
3:I:2959[B]:SER:CB	3:R:3255[B]:PRO:HB2	1.46	1.44
3:I:3150[B]:LYS:HE3	3:R:3163[B]:ASN:CB	1.46	1.44
3:O:2956[B]:LYS:O	3:O:2960[B]:PHE:CE1	1.67	1.44
3:R:3089[A]:HIS:CE1	3:R:3119[A]:HIS:NE2	1.83	1.44
3:C:3153[B]:LYS:CE	3:L:3158[B]:PHE:CD2	1.99	1.43
3:C:3154[B]:PRO:CD	3:L:3174[B]:GLY:HA2	1.46	1.43
3:O:3089[A]:HIS:CE1	3:O:3119[A]:HIS:NE2	1.83	1.43
3:R:2956[B]:LYS:O	3:R:2960[B]:PHE:CE1	1.67	1.43
3:F:2956[B]:LYS:O	3:F:2960[B]:PHE:CE1	1.67	1.43
3:F:2965[B]:LEU:N	3:a:3221[B]:ALA:CB	1.78	1.43
3:a:3089[B]:HIS:CE1	3:a:3119[B]:HIS:NE2	1.82	1.43
3:I:2969[B]:TYR:HD1	3:R:2961[B]:HIS:CG	1.35	1.43
3:I:3196[A]:THR:HG21	1:J:416:ASN:ND2	1.14	1.43
3:R:3089[B]:HIS:CE1	3:R:3119[B]:HIS:NE2	1.83	1.43
3:X:2956[A]:LYS:O	3:X:2960[A]:PHE:CE1	1.67	1.43
2:E:2868:GLU:CG	3:F:2932[A]:PRO:O	1.65	1.42
3:O:3108[B]:HIS:CB	3:X:2969[B]:TYR:C	1.92	1.42
3:U:3254[B]:MET:CB	3:d:3254[B]:MET:HA	1.45	1.42
3:U:2975[B]:PHE:CG	3:d:3256[B]:TRP:CD1	2.06	1.42
3:F:3251[B]:ASP:CB	3:a:3251[B]:ASP:HB3	0.96	1.42
3:U:2965[B]:LEU:N	3:d:3220[B]:ARG:NH1	1.66	1.42
3:F:3157[B]:PRO:O	3:a:3150[B]:LYS:CD	1.66	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3174[B]:GLY:CA	3:R:3154[B]:PRO:CB	1.94	1.41
3:I:3149[B]:ASN:HB2	3:R:3163[B]:ASN:ND2	1.09	1.41
3:U:3169[B]:LYS:C	3:d:3148[B]:ILE:HB	1.45	1.41
3:F:3153[B]:LYS:C	3:a:3155[B]:MET:HG3	1.45	1.41
3:C:2984[B]:THR:CG2	3:L:3159[B]:SER:OG	1.68	1.41
3:C:2988[B]:TRP:NE1	3:L:3153[B]:LYS:HZ3	1.19	1.41
3:F:2983[B]:VAL:HG21	3:a:3161[B]:GLU:N	1.08	1.41
3:I:2989[B]:HIS:CD2	3:R:2970[B]:PRO:CD	2.00	1.41
3:C:2972[B]:GLY:C	3:L:3090[B]:ASN:HD22	1.25	1.40
3:C:3158[B]:PHE:CD2	3:L:3153[B]:LYS:HE2	1.44	1.40
3:U:3254[B]:MET:HE3	3:d:3254[B]:MET:CB	1.50	1.40
3:F:2984[B]:THR:CG2	3:a:3159[B]:SER:CB	1.76	1.40
3:F:3161[B]:GLU:CG	3:a:3079[B]:CYS:SG	2.08	1.40
3:O:2968[B]:GLN:NE2	3:X:2985[B]:PHE:HA	1.22	1.40
3:U:2969[B]:TYR:CZ	3:d:3107[B]:LEU:HD12	1.53	1.40
3:C:2983[B]:VAL:CG2	3:L:3160[B]:SER:HA	1.50	1.40
3:C:2984[B]:THR:HG23	3:L:3159[B]:SER:CB	1.50	1.40
3:C:3150[B]:LYS:NZ	3:L:3160[B]:SER:CB	1.80	1.40
3:F:2966[B]:SER:CA	3:a:3256[B]:TRP:CD1	2.02	1.40
3:I:3169[B]:LYS:O	3:R:3152[B]:LYS:CG	1.68	1.40
3:U:3256[B]:TRP:CE3	3:d:2969[B]:TYR:HB3	1.56	1.40
3:C:2969[B]:TYR:CE2	3:L:3120[B]:HIS:NE2	1.82	1.40
3:C:3172[B]:SER:N	3:L:3152[B]:LYS:HB2	1.27	1.40
3:U:2965[B]:LEU:CA	3:d:3220[B]:ARG:NH1	1.85	1.40
3:C:2983[B]:VAL:HG21	3:L:3161[B]:GLU:N	1.15	1.40
3:C:3256[B]:TRP:CD2	3:L:2965[B]:LEU:O	1.72	1.39
3:C:2983[B]:VAL:HG23	3:L:3160[B]:SER:CA	1.49	1.39
3:F:3153[B]:LYS:CG	3:a:3155[B]:MET:CB	2.00	1.39
3:O:3038[B]:ILE:CG1	3:X:2969[B]:TYR:OH	1.69	1.39
3:F:2969[B]:TYR:HD1	3:a:2961[B]:HIS:CD2	1.08	1.39
3:O:3169[B]:LYS:CB	3:X:3148[B]:ILE:HG21	1.52	1.39
3:F:3153[B]:LYS:CD	3:a:3155[B]:MET:HB2	1.51	1.39
3:F:3174[B]:GLY:CA	3:a:3154[B]:PRO:HB3	1.53	1.39
3:I:2964[B]:PRO:C	3:R:3221[B]:ALA:HB1	1.45	1.38
3:U:3169[B]:LYS:HG2	3:d:3148[B]:ILE:N	1.10	1.38
3:C:2975[B]:PHE:CE1	3:L:3107[B]:LEU:HD11	1.57	1.38
3:O:3038[B]:ILE:HD13	3:X:2969[B]:TYR:CE2	1.59	1.38
3:C:2969[B]:TYR:C	3:L:2985[B]:PHE:CE2	1.80	1.37
3:C:2974[B]:ALA:HB3	3:L:3249[B]:GLY:CA	0.91	1.37
3:F:3152[B]:LYS:HB2	3:a:3172[B]:SER:N	1.30	1.37
3:U:2965[B]:LEU:N	3:d:3220[B]:ARG:HH12	1.19	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3169[B]:LYS:CG	3:d:3148[B]:ILE:H	1.36	1.37
3:U:2965[B]:LEU:HD11	3:d:3221[B]:ALA:N	1.39	1.37
3:C:2982[B]:MET:CB	3:L:3156[B]:MET:CB	2.02	1.37
3:C:3156[B]:MET:SD	3:L:2982[B]:MET:HB2	1.64	1.37
3:O:3169[B]:LYS:HG3	3:X:3148[B]:ILE:CG2	0.91	1.37
3:C:3155[B]:MET:CG	3:L:3153[B]:LYS:C	1.96	1.36
3:I:3154[B]:PRO:HG2	3:R:3155[B]:MET:SD	1.65	1.36
2:Z:2867:PRO:CG	3:a:2932[A]:PRO:CG	2.02	1.36
3:I:3174[B]:GLY:N	3:R:3154[B]:PRO:HB3	1.04	1.36
3:U:2970[B]:PRO:HA	3:d:3086[B]:GLU:CD	1.47	1.36
3:U:3155[B]:MET:C	3:d:3150[B]:LYS:CG	1.84	1.36
3:C:3154[B]:PRO:HD3	3:L:3174[B]:GLY:CA	1.53	1.36
3:O:2976[B]:ALA:HB2	3:X:3156[B]:MET:SD	1.63	1.36
3:F:3152[B]:LYS:CD	3:a:3170[B]:ALA:O	1.70	1.36
3:O:2976[B]:ALA:N	3:X:3156[B]:MET:HG2	1.07	1.36
3:F:3170[B]:ALA:C	3:a:3152[B]:LYS:HD2	1.36	1.36
3:U:2975[B]:PHE:CD1	3:d:3256[B]:TRP:CD1	2.12	1.36
3:U:3154[B]:PRO:HG3	3:d:2984[B]:THR:CG2	1.56	1.36
3:F:2975[B]:PHE:C	3:a:3253[B]:GLU:HB2	1.16	1.35
3:I:3221[B]:ALA:CB	3:R:2965[B]:LEU:N	1.86	1.35
3:O:2965[B]:LEU:CD1	3:X:2979[B]:GLN:HE22	1.30	1.35
3:C:2975[B]:PHE:CD1	3:L:3107[B]:LEU:CD1	2.09	1.35
3:F:2982[B]:MET:CE	3:a:2967[B]:CYS:SG	2.12	1.35
3:I:3155[B]:MET:HB2	3:R:3153[B]:LYS:CD	1.55	1.35
3:F:3173[B]:THR:C	3:a:3154[B]:PRO:HD3	1.50	1.35
3:I:2961[B]:HIS:CD2	3:R:2969[B]:TYR:HD1	1.35	1.35
3:X:2952[B]:ALA:HB3	3:X:2953[B]:GLY:C	1.52	1.35
3:I:3152[B]:LYS:CB	3:R:3172[B]:SER:H	1.18	1.35
3:O:2952[A]:ALA:HB3	3:O:2953[A]:GLY:C	1.52	1.35
3:O:2970[B]:PRO:HD2	3:X:2991[B]:LEU:CB	1.54	1.35
3:I:3154[B]:PRO:HB3	3:R:3174[B]:GLY:N	1.38	1.35
3:U:3255[B]:PRO:CG	3:d:3252[B]:TYR:C	1.98	1.35
3:U:3256[B]:TRP:CG	3:d:2969[B]:TYR:CB	2.08	1.35
3:F:2967[B]:CYS:SG	3:a:2982[B]:MET:CE	2.15	1.34
3:F:2984[B]:THR:HG21	3:a:3159[B]:SER:OG	1.19	1.34
3:I:2968[B]:GLN:HE21	3:R:3086[B]:GLU:CG	1.31	1.34
3:I:3107[B]:LEU:HD11	3:R:2975[B]:PHE:CD1	1.61	1.34
3:I:3159[B]:SER:HA	3:R:3150[B]:LYS:C	1.50	1.34
3:U:2952[A]:ALA:HB3	3:U:2953[A]:GLY:C	1.52	1.34
1:Y:1550:ARG:NH2	3:d:3008[B]:GLY:O	1.59	1.34
3:F:3161[B]:GLU:HG2	3:a:3079[B]:CYS:SG	1.67	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3221[B]:ALA:HB1	3:R:2965[B]:LEU:N	1.03	1.34
3:C:3147[B]:GLU:CG	3:L:3160[B]:SER:O	1.75	1.34
3:F:3159[B]:SER:CB	3:a:2984[B]:THR:CG2	2.02	1.34
3:U:3220[B]:ARG:CA	3:d:2973[B]:THR:HA	1.48	1.34
1:Y:1616:LYS:CD	3:d:3187[B]:TYR:C	1.94	1.34
3:F:3107[B]:LEU:HD11	3:a:2975[B]:PHE:CD1	1.62	1.34
3:U:2965[B]:LEU:HD12	3:d:3220[B]:ARG:CA	1.55	1.34
3:d:2952[B]:ALA:HB3	3:d:2953[B]:GLY:C	1.52	1.34
3:C:2979[B]:GLN:HG3	3:L:3156[B]:MET:CE	1.56	1.34
3:O:2952[B]:ALA:HB3	3:O:2953[B]:GLY:C	1.52	1.34
3:C:3150[B]:LYS:CA	3:L:3172[B]:SER:HB3	1.58	1.33
3:F:3147[B]:GLU:OE1	3:a:3163[B]:ASN:N	1.61	1.33
3:I:2965[B]:LEU:N	3:R:3221[B]:ALA:HB1	1.01	1.33
3:I:3174[B]:GLY:N	3:R:3154[B]:PRO:CB	1.89	1.33
3:U:3156[B]:MET:CE	3:d:2982[B]:MET:CG	2.06	1.33
2:W:2868:GLU:OE1	3:X:2933[A]:SER:N	1.60	1.33
3:C:3253[B]:GLU:HB2	3:L:2975[B]:PHE:C	1.51	1.33
3:I:3173[B]:THR:OG1	3:R:3173[B]:THR:CG2	1.75	1.33
3:R:2952[B]:ALA:HB3	3:R:2953[B]:GLY:C	1.52	1.33
3:U:3152[B]:LYS:CG	3:d:3154[B]:PRO:HB3	1.56	1.33
3:F:3153[B]:LYS:CB	3:a:3155[B]:MET:HB2	1.58	1.33
3:F:3253[B]:GLU:OE1	3:a:2974[B]:ALA:HB1	1.24	1.33
3:O:2963[B]:MET:CE	3:X:2975[B]:PHE:CD1	2.10	1.33
3:a:3089[B]:HIS:HE1	3:a:3119[B]:HIS:NE2	1.20	1.33
3:F:3157[B]:PRO:CA	3:a:2982[B]:MET:SD	2.14	1.33
3:F:3159[B]:SER:HA	3:a:3150[B]:LYS:C	1.30	1.33
3:I:2952[B]:ALA:HB3	3:I:2953[B]:GLY:C	1.52	1.33
3:I:2982[B]:MET:SD	3:R:3157[B]:PRO:CA	2.15	1.33
3:O:3108[B]:HIS:C	3:X:2970[B]:PRO:CD	1.86	1.33
3:a:3196[A]:THR:HG21	1:b:416:ASN:CG	1.53	1.33
3:C:2968[B]:GLN:NE2	3:L:3258[B]:PHE:HZ	1.27	1.33
3:O:2963[B]:MET:HE1	3:X:2975[B]:PHE:CD1	1.64	1.33
3:U:3252[B]:TYR:HE2	3:d:3222[B]:ILE:CD1	1.41	1.33
3:a:2952[A]:ALA:HB3	3:a:2953[A]:GLY:C	1.52	1.33
3:C:2952[B]:ALA:HB3	3:C:2953[B]:GLY:C	1.52	1.32
3:F:2952[B]:ALA:HB3	3:F:2953[B]:GLY:C	1.52	1.32
3:F:3159[B]:SER:CB	3:a:2984[B]:THR:HG21	1.56	1.32
3:F:3255[B]:PRO:HD3	3:a:2962[B]:GLY:O	1.29	1.32
3:I:2952[A]:ALA:HB3	3:I:2953[A]:GLY:C	1.52	1.32
3:L:2952[B]:ALA:HB3	3:L:2953[B]:GLY:C	1.52	1.32
3:O:2970[B]:PRO:HD2	3:X:2991[B]:LEU:CG	1.57	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3086[B]:GLU:OE2	3:d:2970[B]:PRO:HG3	1.15	1.32
3:d:2952[A]:ALA:HB3	3:d:2953[A]:GLY:C	1.52	1.32
3:I:2975[B]:PHE:C	3:R:3253[B]:GLU:HB2	1.51	1.32
3:I:3150[B]:LYS:CB	3:R:3159[B]:SER:C	2.00	1.32
3:L:2952[A]:ALA:HB3	3:L:2953[A]:GLY:C	1.52	1.32
3:O:3157[B]:PRO:O	3:X:3149[B]:ASN:C	1.71	1.32
3:a:2952[B]:ALA:HB3	3:a:2953[B]:GLY:C	1.52	1.32
3:F:3153[B]:LYS:CD	3:a:3155[B]:MET:CB	2.05	1.32
3:R:2952[A]:ALA:HB3	3:R:2953[A]:GLY:C	1.52	1.32
3:U:2979[B]:GLN:NE2	3:d:3153[B]:LYS:HZ1	1.27	1.32
3:F:2952[A]:ALA:HB3	3:F:2953[A]:GLY:C	1.52	1.32
3:U:2952[B]:ALA:HB3	3:U:2953[B]:GLY:C	1.52	1.32
3:C:2982[B]:MET:CB	3:L:3156[B]:MET:HB3	1.59	1.32
3:I:3163[B]:ASN:ND2	3:R:3150[B]:LYS:HG3	1.43	1.32
3:I:3255[B]:PRO:HB2	3:R:2959[B]:SER:CB	1.58	1.32
3:X:2952[A]:ALA:HB3	3:X:2953[A]:GLY:C	1.52	1.32
3:a:3196[A]:THR:HG21	1:b:416:ASN:OD1	1.30	1.32
3:C:2952[A]:ALA:HB3	3:C:2953[A]:GLY:C	1.52	1.31
3:I:2970[B]:PRO:HD3	3:R:2989[B]:HIS:CD2	1.64	1.31
3:U:2970[B]:PRO:CA	3:d:3086[B]:GLU:OE1	1.78	1.31
3:U:3154[B]:PRO:CG	3:d:2984[B]:THR:HG21	1.57	1.31
1:Y:1616:LYS:HD3	3:d:3188[B]:ASP:N	1.03	1.31
3:C:3159[B]:SER:CB	3:L:2984[B]:THR:HG23	1.58	1.31
3:I:3153[B]:LYS:O	3:R:3155[B]:MET:N	1.64	1.31
3:I:3169[B]:LYS:CE	3:R:3149[B]:ASN:OD1	1.76	1.31
3:C:3148[B]:ILE:O	3:L:3169[B]:LYS:C	1.71	1.31
3:C:3169[B]:LYS:C	3:L:3148[B]:ILE:O	1.63	1.31
3:F:3259[B]:ASP:CB	3:a:3162[B]:ASP:HB3	1.58	1.31
3:O:2963[B]:MET:SD	3:X:2975[B]:PHE:CD2	2.24	1.31
3:C:3160[B]:SER:OG	3:L:2983[B]:VAL:HG23	1.23	1.31
3:C:3162[B]:ASP:C	3:L:3147[B]:GLU:OE1	1.73	1.31
3:I:2982[B]:MET:SD	3:R:3157[B]:PRO:HA	1.70	1.31
3:I:3150[B]:LYS:O	3:R:3159[B]:SER:CA	1.78	1.31
3:O:2965[B]:LEU:CD1	3:X:2979[B]:GLN:OE1	1.72	1.31
3:L:3089[A]:HIS:HE1	3:L:3119[A]:HIS:NE2	1.20	1.30
3:O:2970[B]:PRO:CG	3:X:2991[B]:LEU:CA	2.02	1.30
3:C:2979[B]:GLN:CG	3:L:3156[B]:MET:HE2	1.30	1.30
3:F:3170[B]:ALA:O	3:a:3152[B]:LYS:CD	1.77	1.30
3:U:2969[B]:TYR:CZ	3:d:3107[B]:LEU:CD1	2.07	1.30
3:U:3089[A]:HIS:HE1	3:U:3119[A]:HIS:NE2	1.21	1.30
3:C:3160[B]:SER:HB2	3:L:3150[B]:LYS:NZ	1.33	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1546:LYS:HB2	3:d:3001[B]:LYS:CE	1.59	1.30
3:C:3160[B]:SER:CB	3:L:3150[B]:LYS:HZ3	1.32	1.30
3:C:3163[B]:ASN:N	3:L:3147[B]:GLU:OE1	1.62	1.30
3:I:2961[B]:HIS:HA	3:R:2975[B]:PHE:CZ	1.65	1.30
3:I:3150[B]:LYS:O	3:R:3159[B]:SER:HA	1.28	1.30
3:d:3089[B]:HIS:HE1	3:d:3119[B]:HIS:NE2	1.20	1.30
3:I:3150[B]:LYS:C	3:R:3159[B]:SER:CA	2.01	1.30
3:I:3161[B]:GLU:CG	3:R:3079[B]:CYS:SG	2.20	1.30
3:O:3169[B]:LYS:CG	3:X:3148[B]:ILE:HG21	1.41	1.30
3:U:3254[B]:MET:HB3	3:d:3254[B]:MET:CA	1.60	1.30
3:C:3153[B]:LYS:O	3:L:3154[B]:PRO:HA	1.31	1.29
3:F:2970[B]:PRO:CD	3:a:2989[B]:HIS:NE2	1.92	1.29
3:F:2975[B]:PHE:C	3:a:3253[B]:GLU:CB	1.93	1.29
3:F:3149[B]:ASN:HB2	3:a:3163[B]:ASN:ND2	0.98	1.29
3:I:3159[B]:SER:CA	3:R:3150[B]:LYS:HB3	1.55	1.29
3:O:2970[B]:PRO:HG2	3:X:2991[B]:LEU:N	0.98	1.29
3:O:3153[B]:LYS:CG	3:X:3176[B]:LYS:HD3	1.62	1.29
3:R:3089[A]:HIS:HE1	3:R:3119[A]:HIS:NE2	1.21	1.29
3:U:2971[B]:ASP:CA	3:d:3090[B]:ASN:HD22	1.45	1.29
3:U:2975[B]:PHE:CE2	3:d:3254[B]:MET:HG3	1.66	1.29
3:U:3256[B]:TRP:HB2	3:d:2969[B]:TYR:CA	1.60	1.29
3:F:3256[B]:TRP:HE1	3:a:2965[B]:LEU:CD1	1.45	1.29
3:I:2965[B]:LEU:N	3:R:3221[B]:ALA:CB	1.95	1.29
2:Z:2800:LYS:O	3:a:3023[A]:ILE:CD1	1.80	1.29
3:C:3156[B]:MET:HB2	3:L:2982[B]:MET:SD	1.70	1.29
3:F:3159[B]:SER:OG	3:a:2984[B]:THR:HG21	1.19	1.29
3:U:3254[B]:MET:CA	3:d:3254[B]:MET:HA	1.60	1.29
3:F:3173[B]:THR:O	3:a:3154[B]:PRO:HD3	1.30	1.29
3:F:3174[B]:GLY:N	3:a:3154[B]:PRO:CB	1.95	1.29
3:C:3161[B]:GLU:N	3:L:2983[B]:VAL:HG21	1.45	1.29
3:U:3255[B]:PRO:HG2	3:d:3252[B]:TYR:CA	1.62	1.29
3:X:3089[B]:HIS:HE1	3:X:3119[B]:HIS:NE2	1.20	1.29
3:C:2965[B]:LEU:CD2	3:L:3253[B]:GLU:OE1	1.74	1.28
3:I:2989[B]:HIS:CD2	3:R:2970[B]:PRO:N	2.00	1.28
3:O:3101[B]:PRO:CB	3:X:2971[B]:ASP:O	1.77	1.28
3:C:3147[B]:GLU:HG2	3:L:3161[B]:GLU:CA	1.52	1.28
3:C:3159[B]:SER:CB	3:L:2984[B]:THR:CG2	2.12	1.28
3:F:2969[B]:TYR:CD1	3:a:2961[B]:HIS:CG	1.98	1.28
3:F:2970[B]:PRO:N	3:a:2989[B]:HIS:NE2	1.82	1.28
2:W:2868:GLU:HG2	3:X:2932[A]:PRO:O	1.22	1.28
3:O:3141[A]:TYR:HD2	3:O:3142[A]:ASN:N	1.32	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3257[B]:ALA:H	3:d:2968[B]:GLN:CA	1.44	1.28
3:F:3153[B]:LYS:HD2	3:a:3155[B]:MET:CB	1.63	1.28
3:I:3196[A]:THR:CB	1:J:416:ASN:HD22	1.46	1.28
3:R:3141[B]:TYR:HD2	3:R:3142[B]:ASN:N	1.32	1.28
3:C:2982[B]:MET:CG	3:L:3156[B]:MET:CB	2.06	1.28
3:I:3221[B]:ALA:HB1	3:R:2964[B]:PRO:C	1.56	1.28
3:O:3038[B]:ILE:HG12	3:X:2969[B]:TYR:OH	1.22	1.28
3:U:3141[B]:TYR:HD2	3:U:3142[B]:ASN:N	1.32	1.28
3:F:3159[B]:SER:HA	3:a:3150[B]:LYS:O	1.34	1.27
3:I:3173[B]:THR:OG1	3:R:3173[B]:THR:HG23	1.16	1.27
3:U:3152[B]:LYS:HB2	3:d:3154[B]:PRO:CA	1.63	1.27
3:U:3152[B]:LYS:HA	3:d:3152[B]:LYS:O	1.21	1.27
3:X:3141[B]:TYR:HD2	3:X:3142[B]:ASN:N	1.32	1.27
3:C:2983[B]:VAL:CG2	3:L:3161[B]:GLU:H	1.46	1.27
3:C:3154[B]:PRO:CD	3:L:3174[B]:GLY:CA	2.10	1.27
3:I:2975[B]:PHE:O	3:R:3253[B]:GLU:HB2	1.13	1.27
3:I:3149[B]:ASN:OD1	3:R:3169[B]:LYS:CE	1.83	1.27
3:I:3173[B]:THR:CG2	3:R:3173[B]:THR:OG1	1.80	1.27
3:I:3248[B]:LEU:CB	3:R:2972[B]:GLY:O	1.81	1.27
3:O:3163[B]:ASN:HB2	3:X:3149[B]:ASN:CA	1.62	1.27
3:C:3154[B]:PRO:CG	3:L:3174[B]:GLY:HA2	1.64	1.27
3:F:3251[B]:ASP:HB3	3:a:3251[B]:ASP:CB	0.80	1.27
3:I:3150[B]:LYS:HB3	3:R:3159[B]:SER:CA	1.48	1.27
3:L:3141[B]:TYR:HD2	3:L:3142[B]:ASN:N	1.32	1.27
3:O:3141[B]:TYR:HD2	3:O:3142[B]:ASN:N	1.32	1.27
3:R:3141[A]:TYR:HD2	3:R:3142[A]:ASN:N	1.32	1.27
3:C:2972[B]:GLY:O	3:L:3090[B]:ASN:ND2	1.67	1.27
3:C:3089[A]:HIS:HE1	3:C:3119[A]:HIS:NE2	1.21	1.27
3:O:2967[B]:CYS:SG	3:X:3153[B]:LYS:HB3	1.74	1.27
3:I:3141[A]:TYR:HD2	3:I:3142[A]:ASN:N	1.32	1.27
3:U:2965[B]:LEU:CD1	3:d:3221[B]:ALA:H	1.47	1.27
3:U:3169[B]:LYS:CE	3:d:3147[B]:GLU:HA	1.64	1.27
3:U:3254[B]:MET:CE	3:d:3254[B]:MET:CE	1.92	1.27
3:F:3256[B]:TRP:CB	3:a:2966[B]:SER:HA	1.63	1.26
3:O:3158[B]:PHE:O	3:X:3148[B]:ILE:HG22	1.22	1.26
3:C:3154[B]:PRO:CB	3:L:3174[B]:GLY:HA3	1.65	1.26
3:L:3141[A]:TYR:HD2	3:L:3142[A]:ASN:N	1.32	1.26
1:S:416:ASN:OD1	3:X:3196[A]:THR:HG21	1.18	1.26
3:U:3082[B]:GLU:OE1	3:d:2970[B]:PRO:HB3	1.29	1.26
3:C:3141[A]:TYR:HD2	3:C:3142[A]:ASN:N	1.32	1.26
3:C:3149[B]:ASN:HD22	3:L:3163[B]:ASN:ND2	1.34	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3163[B]:ASN:ND2	3:R:3149[B]:ASN:HB2	1.50	1.26
3:O:3040[B]:VAL:HG21	3:X:2969[B]:TYR:CD1	1.68	1.26
3:U:3141[A]:TYR:HD2	3:U:3142[A]:ASN:N	1.32	1.26
3:a:3141[A]:TYR:HD2	3:a:3142[A]:ASN:N	1.32	1.26
3:C:2982[B]:MET:HG3	3:L:3156[B]:MET:SD	1.75	1.26
3:C:3090[B]:ASN:ND2	3:L:2972[B]:GLY:HA3	1.46	1.26
3:C:3147[B]:GLU:OE1	3:L:3163[B]:ASN:N	1.67	1.26
3:I:3153[B]:LYS:CG	3:R:3155[B]:MET:HB2	1.64	1.26
3:O:2976[B]:ALA:O	3:X:3154[B]:PRO:CG	1.83	1.26
3:O:3272[A]:HIS:NE2	1:P:1542:ARG:NH2	1.84	1.26
3:C:2978[B]:CYS:N	3:L:3254[B]:MET:CB	1.95	1.26
3:C:3024[A]:LEU:HD12	3:C:3025[A]:VAL:N	1.51	1.26
3:C:3159[B]:SER:OG	3:L:2984[B]:THR:CG2	1.83	1.26
3:I:2975[B]:PHE:CZ	3:R:2961[B]:HIS:HA	1.69	1.26
3:I:3221[B]:ALA:CB	3:R:2964[B]:PRO:C	2.08	1.26
3:O:2965[B]:LEU:CB	3:X:3254[B]:MET:HE1	1.65	1.26
3:O:2969[B]:TYR:CG	3:X:3158[B]:PHE:CE1	2.24	1.26
3:O:3109[B]:TYR:CD1	3:X:2970[B]:PRO:N	2.03	1.26
3:a:3024[B]:LEU:HD12	3:a:3025[B]:VAL:N	1.51	1.26
3:d:3141[A]:TYR:HD2	3:d:3142[A]:ASN:N	1.32	1.26
3:d:3141[B]:TYR:HD2	3:d:3142[B]:ASN:N	1.32	1.26
3:F:3120[B]:HIS:NE2	3:a:2969[B]:TYR:CE2	2.04	1.25
3:I:2961[B]:HIS:CG	3:R:2969[B]:TYR:HD1	1.52	1.25
3:I:2982[B]:MET:SD	3:R:3157[B]:PRO:HB3	1.75	1.25
3:O:3163[B]:ASN:HB3	3:X:3149[B]:ASN:N	1.51	1.25
3:C:3152[B]:LYS:HB2	3:L:3172[B]:SER:N	1.49	1.25
3:C:3153[B]:LYS:HZ3	3:L:2988[B]:TRP:CD1	1.53	1.25
3:F:2965[B]:LEU:CD1	3:a:3256[B]:TRP:HE1	1.48	1.25
3:F:3141[B]:TYR:HD2	3:F:3142[B]:ASN:N	1.32	1.25
3:I:3024[A]:LEU:HD12	3:I:3025[A]:VAL:N	1.51	1.25
3:O:3024[A]:LEU:HD12	3:O:3025[A]:VAL:N	1.51	1.25
3:X:3141[A]:TYR:HD2	3:X:3142[A]:ASN:N	1.32	1.25
3:a:3024[A]:LEU:HD12	3:a:3025[A]:VAL:N	1.51	1.25
3:F:3169[B]:LYS:O	3:a:3152[B]:LYS:HG3	1.35	1.25
3:L:3089[B]:HIS:HE1	3:L:3119[B]:HIS:NE2	1.21	1.25
3:O:3024[B]:LEU:HD12	3:O:3025[B]:VAL:N	1.51	1.25
3:C:3255[B]:PRO:HB2	3:L:2959[B]:SER:O	1.19	1.25
3:F:3174[B]:GLY:HA2	3:a:3154[B]:PRO:CG	1.65	1.25
3:F:3256[B]:TRP:CE2	3:a:2965[B]:LEU:HB3	1.70	1.25
3:I:3172[B]:SER:N	3:R:3152[B]:LYS:HB2	1.41	1.25
3:O:2963[B]:MET:HE1	3:X:2975[B]:PHE:CB	1.65	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2965[B]:LEU:O	3:L:3256[B]:TRP:O	1.55	1.25
3:C:3169[B]:LYS:O	3:L:3152[B]:LYS:HG3	1.37	1.25
3:F:3113[A]:ASP:OD2	3:F:3114[A]:PRO:HD2	1.07	1.25
3:F:3113[B]:ASP:OD2	3:F:3114[B]:PRO:HD2	1.07	1.25
3:F:3259[B]:ASP:HB3	3:a:3162[B]:ASP:CB	1.65	1.25
3:I:3108[B]:HIS:CE1	3:R:3251[B]:ASP:OD1	1.88	1.25
3:I:3174[B]:GLY:HA2	3:R:3154[B]:PRO:CG	1.67	1.25
3:O:2970[B]:PRO:CD	3:X:2991[B]:LEU:CB	2.07	1.25
3:O:3038[B]:ILE:HG21	3:X:2969[B]:TYR:CZ	1.72	1.25
3:O:3101[B]:PRO:HB2	3:X:2971[B]:ASP:C	1.60	1.25
3:O:3102[B]:TYR:N	3:X:2971[B]:ASP:HA	1.51	1.25
3:R:3113[A]:ASP:OD2	3:R:3114[A]:PRO:HD2	1.07	1.25
3:R:3113[B]:ASP:OD2	3:R:3114[B]:PRO:HD2	1.07	1.25
3:U:3160[B]:SER:OG	3:d:3259[B]:ASP:HB3	1.24	1.25
3:a:3089[A]:HIS:HE1	3:a:3119[A]:HIS:NE2	1.21	1.25
3:a:3113[A]:ASP:OD2	3:a:3114[A]:PRO:HD2	1.07	1.25
3:d:3089[A]:HIS:HE1	3:d:3119[A]:HIS:NE2	1.21	1.25
3:C:2988[B]:TRP:CD1	3:L:3153[B]:LYS:HZ3	1.54	1.25
3:C:3159[B]:SER:OG	3:L:2984[B]:THR:HG21	1.14	1.25
3:F:3141[A]:TYR:HD2	3:F:3142[A]:ASN:N	1.32	1.25
3:O:2965[B]:LEU:CD1	3:X:2979[B]:GLN:CD	1.92	1.25
3:U:3113[A]:ASP:OD2	3:U:3114[A]:PRO:HD2	1.07	1.25
3:U:3155[B]:MET:C	3:d:3150[B]:LYS:HG3	1.42	1.25
3:U:3252[B]:TYR:CE2	3:d:3222[B]:ILE:HD13	1.71	1.25
1:Y:1616:LYS:CD	3:d:3187[B]:TYR:CA	2.15	1.25
3:C:3113[B]:ASP:OD2	3:C:3114[B]:PRO:HD2	1.07	1.24
3:I:3135[A]:LYS:CG	3:I:3141[A]:TYR:HE1	1.50	1.24
3:I:3135[B]:LYS:CG	3:I:3141[B]:TYR:HE1	1.51	1.24
3:I:3141[B]:TYR:HD2	3:I:3142[B]:ASN:N	1.32	1.24
3:L:3113[A]:ASP:OD2	3:L:3114[A]:PRO:HD2	1.07	1.24
3:O:2970[B]:PRO:HD2	3:X:2991[B]:LEU:CD1	1.66	1.24
3:O:3158[B]:PHE:O	3:X:3148[B]:ILE:CG2	1.85	1.24
3:C:3162[B]:ASP:OD2	3:L:3259[B]:ASP:N	1.68	1.24
3:F:2967[B]:CYS:SG	3:a:2982[B]:MET:HE2	1.71	1.24
3:I:3113[B]:ASP:OD2	3:I:3114[B]:PRO:HD2	1.07	1.24
3:I:3169[B]:LYS:CD	3:R:3149[B]:ASN:OD1	1.85	1.24
3:I:3196[A]:THR:CB	1:J:416:ASN:ND2	1.98	1.24
3:O:3135[B]:LYS:CG	3:O:3141[B]:TYR:HE1	1.50	1.24
3:R:3024[B]:LEU:HD12	3:R:3025[B]:VAL:N	1.51	1.24
1:Y:1546:LYS:CB	3:d:3001[B]:LYS:HE3	1.66	1.24
3:F:2966[B]:SER:O	3:a:3256[B]:TRP:HB3	1.25	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3154[B]:PRO:HG2	3:a:3155[B]:MET:SD	1.78	1.24
3:L:3135[B]:LYS:CG	3:L:3141[B]:TYR:HE1	1.51	1.24
3:U:3153[B]:LYS:CE	3:d:2979[B]:GLN:HE22	1.48	1.24
3:U:3230[B]:PHE:HB2	3:U:3243[B]:GLY:CA	1.68	1.24
3:X:3089[A]:HIS:HE1	3:X:3119[A]:HIS:NE2	1.21	1.24
3:C:3153[B]:LYS:HE2	3:L:3158[B]:PHE:CD2	1.66	1.24
3:I:2964[B]:PRO:C	3:R:3221[B]:ALA:CB	2.08	1.24
3:I:3089[B]:HIS:HE1	3:I:3119[B]:HIS:NE2	1.20	1.24
3:I:3230[A]:PHE:HB2	3:I:3243[A]:GLY:CA	1.68	1.24
2:Q:2868:GLU:OE2	3:R:2932[A]:PRO:C	1.80	1.24
3:R:3135[A]:LYS:CG	3:R:3141[A]:TYR:HE1	1.50	1.24
3:X:3230[B]:PHE:HB2	3:X:3243[B]:GLY:CA	1.68	1.24
3:a:3135[B]:LYS:CG	3:a:3141[B]:TYR:HE1	1.51	1.24
3:C:3024[B]:LEU:HD12	3:C:3025[B]:VAL:N	1.51	1.24
3:C:3160[B]:SER:HA	3:L:2983[B]:VAL:CG2	1.67	1.24
3:F:3024[B]:LEU:HD12	3:F:3025[B]:VAL:N	1.51	1.24
3:F:3157[B]:PRO:O	3:a:3150[B]:LYS:HD3	1.14	1.24
3:I:3163[B]:ASN:CB	3:R:3150[B]:LYS:CE	2.14	1.24
3:L:3135[A]:LYS:CG	3:L:3141[A]:TYR:HE1	1.50	1.24
3:U:2971[B]:ASP:HA	3:d:3090[B]:ASN:ND2	1.52	1.24
1:Y:1616:LYS:CD	3:d:3188[B]:ASP:N	1.97	1.24
3:C:3090[B]:ASN:ND2	3:L:2972[B]:GLY:CA	2.01	1.23
3:F:3174[B]:GLY:CA	3:a:3154[B]:PRO:CB	2.15	1.23
3:I:3161[B]:GLU:HB3	3:R:3079[B]:CYS:SG	1.79	1.23
3:U:2965[B]:LEU:CB	3:d:3220[B]:ARG:NH1	2.00	1.23
3:U:3135[A]:LYS:CG	3:U:3141[A]:TYR:HE1	1.50	1.23
3:C:3135[B]:LYS:CG	3:C:3141[B]:TYR:HE1	1.50	1.23
3:C:3248[B]:LEU:HD22	3:L:2971[B]:ASP:OD1	1.38	1.23
3:F:3089[A]:HIS:HE1	3:F:3119[A]:HIS:NE2	1.21	1.23
3:F:3256[B]:TRP:NE1	3:a:2965[B]:LEU:CB	1.90	1.23
3:I:2961[B]:HIS:CG	3:R:2975[B]:PHE:CZ	2.26	1.23
3:I:3155[B]:MET:CB	3:R:3153[B]:LYS:HD2	1.66	1.23
3:I:3160[B]:SER:OG	3:R:2983[B]:VAL:N	1.71	1.23
3:O:2969[B]:TYR:CD1	3:X:3158[B]:PHE:CD1	2.25	1.23
3:O:3113[B]:ASP:OD2	3:O:3114[B]:PRO:HD2	1.07	1.23
3:X:3113[B]:ASP:OD2	3:X:3114[B]:PRO:HD2	1.07	1.23
3:a:3141[B]:TYR:HD2	3:a:3142[B]:ASN:N	1.32	1.23
3:d:3024[B]:LEU:HD12	3:d:3025[B]:VAL:N	1.51	1.23
3:F:3298[A]:ASN:CB	3:F:3300[A]:LEU:HD23	1.69	1.23
3:I:2982[B]:MET:CG	3:R:2967[B]:CYS:SG	2.27	1.23
3:I:3113[A]:ASP:OD2	3:I:3114[A]:PRO:HD2	1.07	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3173[B]:THR:O	3:R:3154[B]:PRO:HD3	1.34	1.23
3:L:3024[A]:LEU:HD12	3:L:3025[A]:VAL:N	1.51	1.23
3:L:3024[B]:LEU:HD12	3:L:3025[B]:VAL:N	1.51	1.23
3:L:3217[A]:PHE:HE1	3:L:3230[A]:PHE:CZ	1.57	1.23
3:X:3024[A]:LEU:HD12	3:X:3025[A]:VAL:N	1.51	1.23
3:X:3298[A]:ASN:CB	3:X:3300[A]:LEU:HD23	1.69	1.23
3:d:3230[B]:PHE:HB2	3:d:3243[B]:GLY:CA	1.68	1.23
3:C:2969[B]:TYR:OH	3:L:3120[B]:HIS:CD2	1.91	1.23
3:C:3141[B]:TYR:HD2	3:C:3142[B]:ASN:N	1.32	1.23
3:F:2966[B]:SER:O	3:a:3256[B]:TRP:CB	1.84	1.23
3:F:3256[B]:TRP:HE1	3:a:2965[B]:LEU:CB	1.49	1.23
3:F:3256[B]:TRP:HB3	3:a:2966[B]:SER:CA	1.69	1.23
3:I:2969[B]:TYR:HD1	3:R:2961[B]:HIS:CD2	1.50	1.23
3:I:2970[B]:PRO:HD3	3:R:2989[B]:HIS:CG	1.71	1.23
3:I:3107[B]:LEU:CD1	3:R:2975[B]:PHE:HD1	1.50	1.23
3:I:3163[B]:ASN:HB2	3:R:3150[B]:LYS:CE	1.67	1.23
3:O:3135[A]:LYS:CG	3:O:3141[A]:TYR:HE1	1.51	1.23
3:O:3298[B]:ASN:CB	3:O:3300[B]:LEU:HD23	1.69	1.23
3:R:3217[A]:PHE:HE1	3:R:3230[A]:PHE:CZ	1.57	1.23
3:R:3217[B]:PHE:HE1	3:R:3230[B]:PHE:CZ	1.57	1.23
3:U:3298[B]:ASN:CB	3:U:3300[B]:LEU:HD23	1.69	1.23
3:X:3024[B]:LEU:HD12	3:X:3025[B]:VAL:N	1.51	1.23
3:X:3135[A]:LYS:CG	3:X:3141[A]:TYR:HE1	1.51	1.23
3:C:2965[B]:LEU:HD21	3:L:3253[B]:GLU:CD	1.41	1.23
3:C:2970[B]:PRO:HD2	9:C:3401[B]:CUO:O1	1.36	1.23
3:C:3113[A]:ASP:OD2	3:C:3114[A]:PRO:HD2	1.07	1.23
3:F:2975[B]:PHE:CD1	3:a:3107[B]:LEU:CD1	2.02	1.23
3:F:3157[B]:PRO:O	3:a:3150[B]:LYS:CE	1.87	1.23
3:L:3113[B]:ASP:OD2	3:L:3114[B]:PRO:HD2	1.07	1.23
3:O:3113[A]:ASP:OD2	3:O:3114[A]:PRO:HD2	1.07	1.23
3:R:3298[B]:ASN:CB	3:R:3300[B]:LEU:HD23	1.69	1.23
3:d:3135[B]:LYS:CG	3:d:3141[B]:TYR:HE1	1.50	1.23
3:C:2982[B]:MET:HB2	3:L:3156[B]:MET:SD	1.79	1.22
3:F:2966[B]:SER:C	3:a:3256[B]:TRP:CG	2.17	1.22
3:O:3108[B]:HIS:C	3:X:2970[B]:PRO:HD3	1.32	1.22
3:R:2979[B]:GLN:HG2	3:R:3155[B]:MET:CE	1.69	1.22
3:a:2979[A]:GLN:HG2	3:a:3155[A]:MET:CE	1.69	1.22
3:d:3135[A]:LYS:CG	3:d:3141[A]:TYR:HE1	1.50	1.22
3:C:3154[B]:PRO:HB3	3:L:3174[B]:GLY:CA	1.69	1.22
3:C:3156[B]:MET:HE2	3:L:2979[B]:GLN:CB	1.64	1.22
3:F:3024[A]:LEU:HD12	3:F:3025[A]:VAL:N	1.51	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3230[A]:PHE:HB2	3:F:3243[A]:GLY:CA	1.68	1.22
3:I:2979[A]:GLN:HG2	3:I:3155[A]:MET:CE	1.69	1.22
3:I:3163[B]:ASN:N	3:R:3147[B]:GLU:OE1	1.69	1.22
3:L:3298[B]:ASN:CB	3:L:3300[B]:LEU:HD23	1.69	1.22
3:O:3135[B]:LYS:CG	3:O:3141[B]:TYR:CE1	2.23	1.22
3:O:3217[B]:PHE:HE1	3:O:3230[B]:PHE:CZ	1.57	1.22
3:R:3135[B]:LYS:CG	3:R:3141[B]:TYR:HE1	1.50	1.22
3:U:3024[A]:LEU:HD12	3:U:3025[A]:VAL:N	1.51	1.22
3:a:2979[B]:GLN:HG2	3:a:3155[B]:MET:CE	1.69	1.22
3:a:3217[B]:PHE:HE1	3:a:3230[B]:PHE:CZ	1.57	1.22
3:d:3113[B]:ASP:OD2	3:d:3114[B]:PRO:HD2	1.07	1.22
3:d:3230[A]:PHE:HB2	3:d:3243[A]:GLY:CA	1.68	1.22
3:d:3298[A]:ASN:CB	3:d:3300[A]:LEU:HD23	1.69	1.22
3:C:2979[A]:GLN:HG2	3:C:3155[A]:MET:CE	1.69	1.22
3:C:3153[B]:LYS:NZ	3:L:3158[B]:PHE:CD2	2.07	1.22
3:F:2979[A]:GLN:HG2	3:F:3155[A]:MET:CE	1.69	1.22
3:I:2969[B]:TYR:CD1	3:R:2961[B]:HIS:CG	2.27	1.22
3:I:3024[B]:LEU:HD12	3:I:3025[B]:VAL:N	1.51	1.22
3:I:3149[B]:ASN:CB	3:R:3163[B]:ASN:HD21	1.41	1.22
3:I:3259[B]:ASP:CB	3:R:3162[B]:ASP:HB3	1.70	1.22
3:I:3298[B]:ASN:CB	3:I:3300[B]:LEU:HD23	1.69	1.22
3:L:2979[B]:GLN:HG2	3:L:3155[B]:MET:CE	1.69	1.22
3:L:3230[B]:PHE:HB2	3:L:3243[B]:GLY:CA	1.68	1.22
3:O:3160[B]:SER:HB3	3:X:3149[B]:ASN:OD1	1.31	1.22
3:O:3217[A]:PHE:HE1	3:O:3230[A]:PHE:CZ	1.57	1.22
3:O:3230[A]:PHE:HB2	3:O:3243[A]:GLY:CA	1.68	1.22
3:O:3230[B]:PHE:HB2	3:O:3243[B]:GLY:CA	1.68	1.22
3:U:2979[B]:GLN:HG2	3:U:3155[B]:MET:CE	1.69	1.22
3:U:3135[A]:LYS:CG	3:U:3141[A]:TYR:CE1	2.23	1.22
3:X:3217[B]:PHE:HE1	3:X:3230[B]:PHE:CZ	1.57	1.22
3:a:3135[A]:LYS:CG	3:a:3141[A]:TYR:HE1	1.50	1.22
3:d:3024[A]:LEU:HD12	3:d:3025[A]:VAL:N	1.51	1.22
3:C:2972[B]:GLY:C	3:L:3090[B]:ASN:ND2	1.96	1.22
3:C:3298[A]:ASN:CB	3:C:3300[A]:LEU:HD23	1.69	1.22
3:F:3230[B]:PHE:HB2	3:F:3243[B]:GLY:CA	1.68	1.22
3:I:3135[A]:LYS:CG	3:I:3141[A]:TYR:CE1	2.23	1.22
3:O:3298[A]:ASN:CB	3:O:3300[A]:LEU:HD23	1.69	1.22
3:U:3135[B]:LYS:CG	3:U:3141[B]:TYR:HE1	1.51	1.22
3:U:3173[B]:THR:HG23	3:d:3152[B]:LYS:C	1.56	1.22
3:X:3135[B]:LYS:CG	3:X:3141[B]:TYR:HE1	1.50	1.22
3:C:2974[B]:ALA:CB	3:L:3249[B]:GLY:HA2	1.52	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3090[B]:ASN:CG	3:L:2972[B]:GLY:HA3	1.61	1.22
3:C:3135[A]:LYS:CG	3:C:3141[A]:TYR:HE1	1.50	1.22
3:C:3135[B]:LYS:CG	3:C:3141[B]:TYR:CE1	2.23	1.22
3:F:3160[B]:SER:CB	3:a:3150[B]:LYS:NZ	2.03	1.22
3:F:3217[A]:PHE:HE1	3:F:3230[A]:PHE:CZ	1.57	1.22
3:I:3169[B]:LYS:CG	3:R:3149[B]:ASN:OD1	1.87	1.22
3:L:3217[B]:PHE:HE1	3:L:3230[B]:PHE:CZ	1.57	1.22
3:O:2976[B]:ALA:N	3:X:3156[B]:MET:CG	2.00	1.22
2:Q:2868:GLU:OE2	3:R:2932[A]:PRO:O	1.58	1.22
3:R:2979[A]:GLN:HG2	3:R:3155[A]:MET:CE	1.69	1.22
3:R:3135[A]:LYS:CG	3:R:3141[A]:TYR:CE1	2.23	1.22
3:U:2979[A]:GLN:HG2	3:U:3155[A]:MET:CE	1.69	1.22
3:a:3113[B]:ASP:OD2	3:a:3114[B]:PRO:HD2	1.07	1.22
3:a:3230[A]:PHE:HB2	3:a:3243[A]:GLY:CA	1.68	1.22
3:a:3298[A]:ASN:CB	3:a:3300[A]:LEU:HD23	1.69	1.22
3:C:2964[B]:PRO:O	3:L:3255[B]:PRO:CB	1.86	1.21
3:C:3135[A]:LYS:CG	3:C:3141[A]:TYR:CE1	2.23	1.21
3:F:3135[A]:LYS:CG	3:F:3141[A]:TYR:HE1	1.51	1.21
3:I:2982[B]:MET:SD	3:R:3157[B]:PRO:CB	2.28	1.21
3:I:3217[B]:PHE:HE1	3:I:3230[B]:PHE:CZ	1.57	1.21
3:I:3230[B]:PHE:HB2	3:I:3243[B]:GLY:CA	1.68	1.21
3:O:3163[B]:ASN:CB	3:X:3149[B]:ASN:CA	2.18	1.21
3:R:3024[A]:LEU:HD12	3:R:3025[A]:VAL:N	1.51	1.21
3:U:3113[B]:ASP:OD2	3:U:3114[B]:PRO:HD2	1.07	1.21
3:U:3176[B]:LYS:CD	3:d:3152[B]:LYS:HD2	1.68	1.21
3:U:3217[A]:PHE:HE1	3:U:3230[A]:PHE:CZ	1.57	1.21
3:U:3230[A]:PHE:HB2	3:U:3243[A]:GLY:CA	1.68	1.21
3:X:3230[A]:PHE:HB2	3:X:3243[A]:GLY:CA	1.68	1.21
3:a:3230[B]:PHE:HB2	3:a:3243[B]:GLY:CA	1.68	1.21
3:d:3217[B]:PHE:HE1	3:d:3230[B]:PHE:CZ	1.57	1.21
3:I:2961[B]:HIS:CD2	3:R:2969[B]:TYR:CD1	2.13	1.21
3:L:3135[B]:LYS:CG	3:L:3141[B]:TYR:CE1	2.23	1.21
3:R:3230[A]:PHE:HB2	3:R:3243[A]:GLY:CA	1.68	1.21
3:U:3024[B]:LEU:HD12	3:U:3025[B]:VAL:N	1.51	1.21
3:U:3155[B]:MET:N	3:d:3150[B]:LYS:HG2	1.55	1.21
3:a:3135[B]:LYS:CG	3:a:3141[B]:TYR:CE1	2.23	1.21
3:a:3217[A]:PHE:HE1	3:a:3230[A]:PHE:CZ	1.57	1.21
3:F:2982[B]:MET:HE3	3:a:2977[B]:CYS:CB	1.69	1.21
3:F:3089[B]:HIS:HE1	3:F:3119[B]:HIS:NE2	1.21	1.21
3:F:3135[B]:LYS:CG	3:F:3141[B]:TYR:CE1	2.23	1.21
3:F:3298[B]:ASN:CB	3:F:3300[B]:LEU:HD23	1.69	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3150[B]:LYS:HG2	3:R:3158[B]:PHE:CA	1.45	1.21
3:L:3298[A]:ASN:CB	3:L:3300[A]:LEU:HD23	1.69	1.21
3:R:3230[B]:PHE:HB2	3:R:3243[B]:GLY:CA	1.68	1.21
3:X:3135[B]:LYS:CG	3:X:3141[B]:TYR:CE1	2.23	1.21
3:d:3217[A]:PHE:HE1	3:d:3230[A]:PHE:CZ	1.57	1.21
3:d:3298[B]:ASN:CB	3:d:3300[B]:LEU:HD23	1.69	1.21
3:F:3135[A]:LYS:CG	3:F:3141[A]:TYR:CE1	2.23	1.21
3:F:3135[B]:LYS:CG	3:F:3141[B]:TYR:HE1	1.51	1.21
3:I:2975[B]:PHE:CZ	3:R:2961[B]:HIS:CG	2.29	1.21
3:I:2989[B]:HIS:CE1	3:R:2969[B]:TYR:HA	1.74	1.21
3:O:3089[B]:HIS:HE1	3:O:3119[B]:HIS:NE2	1.21	1.21
3:U:3298[A]:ASN:CB	3:U:3300[A]:LEU:HD23	1.69	1.21
3:X:2979[A]:GLN:HG2	3:X:3155[A]:MET:CE	1.69	1.21
3:a:3293[B]:LYS:CB	3:a:3294[B]:SER:HB2	1.71	1.21
3:a:3298[B]:ASN:CB	3:a:3300[B]:LEU:HD23	1.69	1.21
3:C:2969[B]:TYR:CZ	3:L:3120[B]:HIS:NE2	1.92	1.21
3:C:2979[B]:GLN:HG2	3:C:3155[B]:MET:CE	1.69	1.21
3:C:2984[B]:THR:CG2	3:L:3159[B]:SER:CB	2.15	1.21
3:C:3150[B]:LYS:CA	3:L:3172[B]:SER:CB	2.18	1.21
3:C:3217[B]:PHE:HE1	3:C:3230[B]:PHE:CZ	1.57	1.21
3:C:3252[B]:TYR:CZ	3:L:3223[B]:GLY:O	1.94	1.21
3:C:3293[A]:LYS:CB	3:C:3294[A]:SER:HB2	1.71	1.21
3:F:3108[B]:HIS:CE1	3:a:3251[B]:ASP:OD1	1.94	1.21
3:I:2982[B]:MET:CE	3:R:2966[B]:SER:HB3	1.68	1.21
3:I:3217[A]:PHE:HE1	3:I:3230[A]:PHE:CZ	1.57	1.21
3:L:3230[A]:PHE:HB2	3:L:3243[A]:GLY:CA	1.68	1.21
3:O:2979[A]:GLN:HG2	3:O:3155[A]:MET:CE	1.69	1.21
3:O:3135[A]:LYS:CG	3:O:3141[A]:TYR:CE1	2.23	1.21
1:S:1617:LYS:HE2	3:X:3135[B]:LYS:NZ	1.56	1.21
3:X:3113[A]:ASP:OD2	3:X:3114[A]:PRO:HD2	1.07	1.21
3:d:2979[B]:GLN:HG2	3:d:3155[B]:MET:CE	1.69	1.21
3:d:3113[A]:ASP:OD2	3:d:3114[A]:PRO:HD2	1.07	1.21
3:d:3135[A]:LYS:CG	3:d:3141[A]:TYR:CE1	2.23	1.21
3:C:3230[B]:PHE:HB2	3:C:3243[B]:GLY:CA	1.68	1.20
3:C:3293[B]:LYS:CB	3:C:3294[B]:SER:HB2	1.71	1.20
3:F:3147[B]:GLU:OE1	3:a:3162[B]:ASP:CA	1.85	1.20
3:F:3217[B]:PHE:HE1	3:F:3230[B]:PHE:CZ	1.57	1.20
3:F:3293[A]:LYS:CB	3:F:3294[A]:SER:HB2	1.71	1.20
3:I:2979[B]:GLN:HG2	3:I:3155[B]:MET:CE	1.69	1.20
3:O:2970[B]:PRO:CD	3:X:2991[B]:LEU:HD13	1.69	1.20
3:O:3160[B]:SER:HA	3:X:3151[B]:LEU:CD1	1.70	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3217[B]:PHE:HE1	3:U:3230[B]:PHE:CZ	1.57	1.20
3:U:3255[B]:PRO:CG	3:d:3252[B]:TYR:CA	2.20	1.20
3:d:2979[A]:GLN:HG2	3:d:3155[A]:MET:CE	1.69	1.20
3:C:3217[A]:PHE:HE1	3:C:3230[A]:PHE:CZ	1.57	1.20
3:C:3256[B]:TRP:CZ2	3:L:2965[B]:LEU:HB3	1.75	1.20
3:C:3298[B]:ASN:CB	3:C:3300[B]:LEU:HD23	1.69	1.20
3:F:2979[B]:GLN:HG2	3:F:3155[B]:MET:CE	1.69	1.20
3:I:3293[B]:LYS:CB	3:I:3294[B]:SER:HB2	1.71	1.20
3:I:3298[A]:ASN:CB	3:I:3300[A]:LEU:HD23	1.69	1.20
3:O:2979[B]:GLN:HG2	3:O:3155[B]:MET:CE	1.69	1.20
3:R:3089[B]:HIS:HE1	3:R:3119[B]:HIS:NE2	1.20	1.20
3:U:3104[B]:MET:HA	3:U:3110[B]:THR:HG23	1.23	1.20
3:U:3293[B]:LYS:CB	3:U:3294[B]:SER:HB2	1.71	1.20
1:Y:1616:LYS:O	3:d:3187[B]:TYR:HB2	1.03	1.20
3:C:2982[B]:MET:SD	3:L:3156[B]:MET:CB	2.29	1.20
3:C:3230[A]:PHE:HB2	3:C:3243[A]:GLY:CA	1.68	1.20
3:I:3135[B]:LYS:CG	3:I:3141[B]:TYR:CE1	2.23	1.20
3:I:3293[A]:LYS:CB	3:I:3294[A]:SER:HB2	1.71	1.20
3:L:3135[A]:LYS:CG	3:L:3141[A]:TYR:CE1	2.23	1.20
3:O:3163[B]:ASN:CB	3:X:3149[B]:ASN:HA	1.71	1.20
3:O:3293[B]:LYS:CB	3:O:3294[B]:SER:HB2	1.71	1.20
3:R:3135[B]:LYS:CG	3:R:3141[B]:TYR:CE1	2.23	1.20
3:U:3089[B]:HIS:HE1	3:U:3119[B]:HIS:NE2	1.21	1.20
3:U:3135[B]:LYS:CG	3:U:3141[B]:TYR:CE1	2.23	1.20
3:U:3253[B]:GLU:CA	3:d:3255[B]:PRO:HG2	1.69	1.20
3:X:3217[A]:PHE:HE1	3:X:3230[A]:PHE:CZ	1.57	1.20
2:Z:2800:LYS:O	3:a:3023[A]:ILE:HD11	1.33	1.20
3:a:3135[A]:LYS:CG	3:a:3141[A]:TYR:CE1	2.23	1.20
3:C:3169[B]:LYS:HG3	3:L:3149[B]:ASN:OD1	1.04	1.20
3:I:3120[B]:HIS:NE2	3:R:2969[B]:TYR:CE2	2.10	1.20
3:I:3155[B]:MET:HG3	3:R:3153[B]:LYS:C	1.67	1.20
3:I:3160[B]:SER:CA	3:R:2983[B]:VAL:H	1.52	1.20
3:L:2979[A]:GLN:HG2	3:L:3155[A]:MET:CE	1.69	1.20
3:O:3293[A]:LYS:CB	3:O:3294[A]:SER:HB2	1.71	1.20
2:E:2868:GLU:HG3	3:F:2932[A]:PRO:O	1.15	1.20
1:G:1636:ASN:OD1	6:r:1:NAG:H82	1.42	1.20
3:I:3150[B]:LYS:HD2	3:R:3160[B]:SER:N	1.53	1.20
3:I:3163[B]:ASN:HD22	3:R:3150[B]:LYS:CG	1.55	1.20
3:I:3255[B]:PRO:HD3	3:R:2962[B]:GLY:O	1.41	1.20
3:R:3298[A]:ASN:CB	3:R:3300[A]:LEU:HD23	1.69	1.20
3:X:3135[A]:LYS:CG	3:X:3141[A]:TYR:CE1	2.23	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3293[B]:LYS:CB	3:X:3294[B]:SER:HB2	1.71	1.20
3:X:3298[B]:ASN:CB	3:X:3300[B]:LEU:HD23	1.69	1.20
3:d:3135[B]:LYS:CG	3:d:3141[B]:TYR:CE1	2.23	1.20
3:F:3163[B]:ASN:CB	3:a:3150[B]:LYS:HE3	1.70	1.19
3:F:3293[B]:LYS:HB2	3:F:3294[B]:SER:CB	1.72	1.19
3:I:3293[B]:LYS:HB2	3:I:3294[B]:SER:CB	1.72	1.19
3:L:3293[A]:LYS:CB	3:L:3294[A]:SER:HB2	1.71	1.19
3:O:3293[A]:LYS:HB2	3:O:3294[A]:SER:CB	1.72	1.19
3:U:3257[B]:ALA:N	3:d:2968[B]:GLN:HA	1.37	1.19
3:U:3293[A]:LYS:CB	3:U:3294[A]:SER:HB2	1.71	1.19
3:d:3293[A]:LYS:HB2	3:d:3294[A]:SER:CB	1.72	1.19
3:O:2968[B]:GLN:HB2	3:X:2988[B]:TRP:CB	1.71	1.19
3:O:3161[B]:GLU:OE2	3:X:3151[B]:LEU:CD1	1.88	1.19
3:O:3255[B]:PRO:HG2	3:X:3163[B]:ASN:HB3	1.22	1.19
3:R:3293[A]:LYS:CB	3:R:3294[A]:SER:HB2	1.71	1.19
3:C:3090[B]:ASN:ND2	3:L:2972[B]:GLY:C	1.99	1.19
3:O:3109[B]:TYR:CD1	3:X:2970[B]:PRO:CD	2.08	1.19
3:R:3293[B]:LYS:CB	3:R:3294[B]:SER:HB2	1.71	1.19
3:U:3255[B]:PRO:HG2	3:d:3252[B]:TYR:O	1.37	1.19
3:d:3293[B]:LYS:CB	3:d:3294[B]:SER:HB2	1.71	1.19
3:C:3217[B]:PHE:CZ	3:C:3230[B]:PHE:HE1	1.61	1.19
3:F:3293[B]:LYS:CB	3:F:3294[B]:SER:HB2	1.71	1.19
3:I:3150[B]:LYS:CD	3:R:3160[B]:SER:N	2.05	1.19
3:R:3104[A]:MET:HA	3:R:3110[A]:THR:HG23	1.23	1.19
3:d:3293[A]:LYS:CB	3:d:3294[A]:SER:HB2	1.71	1.19
3:C:3174[B]:GLY:HA2	3:L:3154[B]:PRO:HD3	1.20	1.19
3:L:3217[A]:PHE:CZ	3:L:3230[A]:PHE:HE1	1.61	1.19
3:O:3159[B]:SER:O	3:X:3148[B]:ILE:HA	1.39	1.19
3:U:3153[B]:LYS:HE2	3:d:2979[B]:GLN:NE2	1.58	1.19
3:U:3256[B]:TRP:CD2	3:d:2969[B]:TYR:CB	2.25	1.19
3:X:3293[A]:LYS:HB2	3:X:3294[A]:SER:CB	1.72	1.19
1:Y:1546:LYS:CB	3:d:3001[B]:LYS:NZ	2.06	1.19
3:a:3217[B]:PHE:CZ	3:a:3230[B]:PHE:HE1	1.61	1.19
3:a:3293[B]:LYS:HB2	3:a:3294[B]:SER:CB	1.72	1.19
3:d:3217[B]:PHE:CZ	3:d:3230[B]:PHE:HE1	1.61	1.19
3:C:3251[B]:ASP:OD1	3:L:3108[B]:HIS:HE1	1.26	1.18
3:F:3163[B]:ASN:ND2	3:a:3149[B]:ASN:HB2	1.57	1.18
3:F:3217[A]:PHE:CZ	3:F:3230[A]:PHE:HE1	1.61	1.18
3:I:3160[B]:SER:N	3:R:3150[B]:LYS:CD	2.04	1.18
3:L:3217[B]:PHE:CZ	3:L:3230[B]:PHE:HE1	1.61	1.18
3:U:3153[B]:LYS:HB2	3:d:3154[B]:PRO:O	1.39	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3169[B]:LYS:O	3:d:3148[B]:ILE:CB	1.91	1.18
3:U:3255[B]:PRO:HG3	3:d:3252[B]:TYR:HA	1.22	1.18
3:a:3293[A]:LYS:CB	3:a:3294[A]:SER:HB2	1.71	1.18
3:C:2985[B]:PHE:CZ	3:L:2970[B]:PRO:CA	1.80	1.18
3:C:3104[B]:MET:HA	3:C:3110[B]:THR:HG23	1.23	1.18
3:C:3156[B]:MET:HB2	3:L:2982[B]:MET:CG	1.73	1.18
3:C:3293[A]:LYS:HB2	3:C:3294[A]:SER:CB	1.72	1.18
3:L:3293[B]:LYS:CB	3:L:3294[B]:SER:HB2	1.71	1.18
3:O:2969[B]:TYR:OH	3:X:2994[B]:LYS:CB	1.92	1.18
3:O:3104[B]:MET:HA	3:O:3110[B]:THR:HG23	1.23	1.18
3:R:3217[A]:PHE:CZ	3:R:3230[A]:PHE:HE1	1.61	1.18
3:X:3293[A]:LYS:CB	3:X:3294[A]:SER:HB2	1.71	1.18
3:F:2965[B]:LEU:N	3:a:3221[B]:ALA:HB1	0.86	1.18
3:F:2982[B]:MET:CE	3:a:2966[B]:SER:HB3	1.73	1.18
3:I:3159[B]:SER:HA	3:R:3150[B]:LYS:O	1.38	1.18
3:R:3293[A]:LYS:HB2	3:R:3294[A]:SER:CB	1.72	1.18
1:S:416:ASN:OD1	3:X:3196[A]:THR:CB	1.90	1.18
3:U:3156[B]:MET:HE1	3:d:2982[B]:MET:CG	1.71	1.18
3:U:3217[A]:PHE:CZ	3:U:3230[A]:PHE:HE1	1.61	1.18
3:a:3104[B]:MET:HA	3:a:3110[B]:THR:HG23	1.24	1.18
3:C:3255[B]:PRO:HB3	3:L:2964[B]:PRO:O	1.40	1.18
3:C:3255[B]:PRO:CB	3:L:2959[B]:SER:O	1.90	1.18
3:C:3293[B]:LYS:HB2	3:C:3294[B]:SER:CB	1.72	1.18
3:F:3152[B]:LYS:CB	3:a:3172[B]:SER:H	1.57	1.18
3:F:3217[B]:PHE:CZ	3:F:3230[B]:PHE:HE1	1.61	1.18
3:I:3256[B]:TRP:HE1	3:R:2965[B]:LEU:CB	1.44	1.18
3:O:3153[B]:LYS:HG2	3:X:3176[B]:LYS:HE3	1.20	1.18
3:O:3154[B]:PRO:CG	3:X:3175[B]:TYR:HB3	1.74	1.18
3:R:3293[B]:LYS:HB2	3:R:3294[B]:SER:CB	1.72	1.18
3:d:3293[B]:LYS:HB2	3:d:3294[B]:SER:CB	1.73	1.18
3:C:3160[B]:SER:OG	3:L:2983[B]:VAL:CG2	1.92	1.18
3:F:2968[B]:GLN:HE21	3:a:3086[B]:GLU:CG	1.51	1.18
3:F:3160[B]:SER:CB	3:a:3150[B]:LYS:HZ3	1.54	1.18
3:I:3163[B]:ASN:HB3	3:R:3150[B]:LYS:HE3	1.24	1.18
3:L:3293[A]:LYS:HB2	3:L:3294[A]:SER:CB	1.72	1.18
2:Z:2867:PRO:HG3	3:a:2932[A]:PRO:CG	1.66	1.18
3:d:3217[A]:PHE:CZ	3:d:3230[A]:PHE:HE1	1.61	1.18
3:C:3135[B]:LYS:HG3	3:C:3141[B]:TYR:CE1	1.80	1.17
3:C:3217[A]:PHE:CZ	3:C:3230[A]:PHE:HE1	1.61	1.17
3:F:2982[B]:MET:HE3	3:a:2977[B]:CYS:SG	1.84	1.17
3:I:2989[B]:HIS:NE2	3:R:2969[B]:TYR:C	2.01	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3135[B]:LYS:HG3	3:I:3141[B]:TYR:CE1	1.80	1.17
3:I:3221[B]:ALA:HB3	3:R:2964[B]:PRO:CB	1.74	1.17
3:I:3248[B]:LEU:HB3	3:R:2972[B]:GLY:O	1.38	1.17
3:O:3217[A]:PHE:CZ	3:O:3230[A]:PHE:HE1	1.61	1.17
3:O:3217[B]:PHE:CZ	3:O:3230[B]:PHE:HE1	1.61	1.17
3:O:3293[B]:LYS:HB2	3:O:3294[B]:SER:CB	1.72	1.17
3:U:3293[A]:LYS:HB2	3:U:3294[A]:SER:CB	1.72	1.17
3:U:3293[B]:LYS:HB2	3:U:3294[B]:SER:CB	1.72	1.17
3:d:3217[B]:PHE:CE1	3:d:3230[B]:PHE:CZ	2.32	1.17
3:C:2974[B]:ALA:O	3:L:3107[B]:LEU:HD13	1.42	1.17
3:I:3293[A]:LYS:HB2	3:I:3294[A]:SER:CB	1.72	1.17
3:R:3217[B]:PHE:CZ	3:R:3230[B]:PHE:HE1	1.61	1.17
3:U:3217[B]:PHE:CZ	3:U:3230[B]:PHE:HE1	1.61	1.17
3:X:3217[B]:PHE:CE1	3:X:3230[B]:PHE:CZ	2.32	1.17
1:Y:1546:LYS:CB	3:d:3001[B]:LYS:CE	2.19	1.17
3:a:3293[A]:LYS:HB2	3:a:3294[A]:SER:CB	1.73	1.17
3:C:3154[B]:PRO:CG	3:L:3174[B]:GLY:CA	2.23	1.17
3:C:3160[B]:SER:CB	3:L:2983[B]:VAL:HG23	1.72	1.17
3:C:3253[B]:GLU:HB2	3:L:2976[B]:ALA:N	1.22	1.17
3:F:2970[B]:PRO:HA	3:a:2985[B]:PHE:CZ	1.79	1.17
3:F:2989[B]:HIS:CE1	3:a:2969[B]:TYR:HA	1.59	1.17
3:F:3253[B]:GLU:HB2	3:a:2975[B]:PHE:C	1.68	1.17
3:I:3153[B]:LYS:C	3:R:3155[B]:MET:HG3	1.37	1.17
3:I:3217[B]:PHE:CZ	3:I:3230[B]:PHE:HE1	1.61	1.17
3:L:2970[B]:PRO:HD2	9:L:3401[B]:CUO:O1	1.02	1.17
3:L:3217[B]:PHE:CE1	3:L:3230[B]:PHE:CZ	2.32	1.17
3:O:3038[B]:ILE:HD13	3:X:2969[B]:TYR:CZ	1.79	1.17
3:O:3158[B]:PHE:N	3:X:3152[B]:LYS:HB2	1.60	1.17
3:R:3217[A]:PHE:CE1	3:R:3230[A]:PHE:CZ	2.32	1.17
3:U:2970[B]:PRO:HA	3:d:3086[B]:GLU:OE1	1.00	1.17
3:X:3104[A]:MET:HA	3:X:3110[A]:THR:HG23	1.23	1.17
3:a:3217[A]:PHE:CZ	3:a:3230[A]:PHE:HE1	1.61	1.17
3:a:3217[B]:PHE:CE1	3:a:3230[B]:PHE:CZ	2.32	1.17
3:C:3159[B]:SER:OG	3:L:3150[B]:LYS:O	1.61	1.17
3:C:3163[B]:ASN:HB3	3:L:3149[B]:ASN:ND2	1.59	1.17
3:C:3217[B]:PHE:CE1	3:C:3230[B]:PHE:CZ	2.32	1.17
3:F:3217[B]:PHE:CE1	3:F:3230[B]:PHE:CZ	2.32	1.17
3:I:3089[A]:HIS:HE1	3:I:3119[A]:HIS:NE2	1.21	1.17
3:I:3160[B]:SER:N	3:R:3150[B]:LYS:HD2	1.58	1.17
3:I:3160[B]:SER:HA	3:R:2983[B]:VAL:H	1.03	1.17
3:O:3255[B]:PRO:CG	3:X:3163[B]:ASN:HB3	1.73	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3253[B]:GLU:CA	3:d:3255[B]:PRO:CG	2.20	1.17
3:X:3217[B]:PHE:CZ	3:X:3230[B]:PHE:HE1	1.61	1.17
3:a:3135[A]:LYS:HG3	3:a:3141[A]:TYR:CE1	1.80	1.17
3:F:3135[B]:LYS:HG3	3:F:3141[B]:TYR:CE1	1.79	1.17
3:I:2966[B]:SER:CB	3:R:3254[B]:MET:HG3	1.73	1.17
3:O:2970[B]:PRO:N	3:X:2991[B]:LEU:HB2	1.59	1.17
3:O:3135[B]:LYS:HG3	3:O:3141[B]:TYR:CE1	1.80	1.17
3:X:3293[B]:LYS:HB2	3:X:3294[B]:SER:CB	1.72	1.17
3:C:3090[B]:ASN:ND2	3:L:2972[B]:GLY:O	1.75	1.16
3:C:3217[A]:PHE:CE1	3:C:3230[A]:PHE:CZ	2.32	1.16
3:F:2961[B]:HIS:HA	3:a:2975[B]:PHE:HZ	1.10	1.16
3:F:3293[A]:LYS:HB2	3:F:3294[A]:SER:CB	1.72	1.16
3:I:2969[B]:TYR:CD1	3:R:2961[B]:HIS:CD2	2.20	1.16
3:L:3217[A]:PHE:CE1	3:L:3230[A]:PHE:CZ	2.32	1.16
3:O:2968[B]:GLN:CB	3:X:2988[B]:TRP:CB	2.22	1.16
3:O:3217[B]:PHE:CE1	3:O:3230[B]:PHE:CZ	2.32	1.16
3:U:3135[A]:LYS:HG3	3:U:3141[A]:TYR:CE1	1.79	1.16
3:U:3135[B]:LYS:HG3	3:U:3141[B]:TYR:CE1	1.80	1.16
3:U:3153[B]:LYS:HB3	3:d:3153[B]:LYS:CD	1.73	1.16
3:X:3217[A]:PHE:CE1	3:X:3230[A]:PHE:CZ	2.33	1.16
3:X:3217[A]:PHE:CZ	3:X:3230[A]:PHE:HE1	1.61	1.16
2:Z:2472:ASN:HB3	4:MA:1:NAG:H82	1.27	1.16
3:d:3217[A]:PHE:CE1	3:d:3230[A]:PHE:CZ	2.32	1.16
3:C:2982[B]:MET:HG3	3:L:3156[B]:MET:CG	1.75	1.16
3:F:3173[B]:THR:C	3:a:3154[B]:PRO:CD	2.17	1.16
2:H:2800:LYS:O	3:I:3023[A]:ILE:HD11	1.42	1.16
3:I:3152[B]:LYS:HB2	3:R:3172[B]:SER:N	1.15	1.16
3:O:3217[A]:PHE:CE1	3:O:3230[A]:PHE:CZ	2.32	1.16
3:R:3217[B]:PHE:CE1	3:R:3230[B]:PHE:CZ	2.32	1.16
3:U:3152[B]:LYS:CA	3:d:3152[B]:LYS:O	1.92	1.16
3:U:3170[B]:ALA:HA	3:d:3148[B]:ILE:CG2	1.74	1.16
3:U:3217[A]:PHE:CE1	3:U:3230[A]:PHE:CZ	2.32	1.16
3:U:3219[B]:LEU:O	3:d:2971[B]:ASP:O	1.62	1.16
3:U:3254[B]:MET:CB	3:d:3254[B]:MET:CA	2.18	1.16
3:C:2984[B]:THR:HG21	3:L:3159[B]:SER:OG	1.01	1.16
3:C:3169[B]:LYS:CG	3:L:3149[B]:ASN:OD1	1.94	1.16
3:F:2975[B]:PHE:O	3:a:3253[B]:GLU:HB2	1.01	1.16
3:F:2983[B]:VAL:HG21	3:a:3161[B]:GLU:CA	1.73	1.16
3:F:3196[B]:THR:N	3:F:3199[B]:GLN:OE1	1.79	1.16
3:I:3169[B]:LYS:O	3:R:3152[B]:LYS:HG3	1.01	1.16
3:I:3217[A]:PHE:CE1	3:I:3230[A]:PHE:CZ	2.32	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3293[B]:LYS:HB2	3:L:3294[B]:SER:CB	1.72	1.16
3:O:2969[B]:TYR:OH	3:X:2994[B]:LYS:HB3	0.99	1.16
3:O:2970[B]:PRO:CB	3:X:2991[B]:LEU:N	2.09	1.16
3:O:3101[B]:PRO:C	3:X:2971[B]:ASP:HA	1.68	1.16
3:R:2960[B]:PHE:HD2	3:R:3157[B]:PRO:HG3	1.10	1.16
3:U:3170[B]:ALA:CA	3:d:3148[B]:ILE:HG21	1.75	1.16
3:a:3135[B]:LYS:HG3	3:a:3141[B]:TYR:CE1	1.80	1.16
3:a:3217[A]:PHE:CE1	3:a:3230[A]:PHE:CZ	2.32	1.16
3:C:2985[B]:PHE:CE2	3:L:2969[B]:TYR:C	2.23	1.16
3:F:3255[B]:PRO:CD	3:a:2962[B]:GLY:O	1.94	1.16
3:I:3149[B]:ASN:CG	3:R:3163[B]:ASN:ND2	2.04	1.16
3:R:2937[A]:ASN:HB2	3:R:3006[A]:LYS:HE2	1.28	1.16
3:U:2937[B]:ASN:HB2	3:U:3006[B]:LYS:HE2	1.28	1.16
3:a:3196[B]:THR:N	3:a:3199[B]:GLN:OE1	1.79	1.16
3:C:2968[B]:GLN:O	3:L:2985[B]:PHE:CD2	1.98	1.16
3:F:3154[B]:PRO:HA	3:a:3153[B]:LYS:O	1.46	1.16
3:F:3196[A]:THR:N	3:F:3199[A]:GLN:OE1	1.79	1.16
3:I:3155[B]:MET:HG3	3:R:3154[B]:PRO:N	1.38	1.16
3:O:3153[B]:LYS:CG	3:X:3176[B]:LYS:CD	2.22	1.16
3:R:3196[A]:THR:N	3:R:3199[A]:GLN:OE1	1.79	1.16
3:R:3196[B]:THR:N	3:R:3199[B]:GLN:OE1	1.79	1.16
3:U:3196[A]:THR:N	3:U:3199[A]:GLN:OE1	1.79	1.16
3:U:3217[B]:PHE:CE1	3:U:3230[B]:PHE:CZ	2.32	1.16
3:d:2937[A]:ASN:HB2	3:d:3006[A]:LYS:HE2	1.28	1.16
3:C:3079[B]:CYS:SG	3:L:3161[B]:GLU:CD	2.27	1.15
3:C:3104[A]:MET:HA	3:C:3110[A]:THR:HG23	1.23	1.15
3:F:3135[A]:LYS:HG3	3:F:3141[A]:TYR:CE1	1.80	1.15
3:F:3154[B]:PRO:CD	3:a:3155[B]:MET:SD	2.34	1.15
3:F:3217[A]:PHE:CE1	3:F:3230[A]:PHE:CZ	2.32	1.15
3:I:3104[B]:MET:HA	3:I:3110[B]:THR:HG23	1.23	1.15
3:I:3217[A]:PHE:CZ	3:I:3230[A]:PHE:HE1	1.61	1.15
3:O:3135[A]:LYS:HG3	3:O:3141[A]:TYR:CE1	1.80	1.15
3:R:3217[A]:PHE:CZ	3:R:3230[A]:PHE:CE1	2.35	1.15
3:U:2960[A]:PHE:HD2	3:U:3157[A]:PRO:HG3	1.10	1.15
3:U:3162[B]:ASP:N	3:d:3260[B]:ARG:NH1	1.93	1.15
3:d:3196[B]:THR:N	3:d:3199[B]:GLN:OE1	1.79	1.15
3:d:3217[B]:PHE:CZ	3:d:3230[B]:PHE:CE1	2.35	1.15
6:GA:1:NAG:H4	6:GA:2:NAG:O7	1.46	1.15
3:C:3253[B]:GLU:CB	3:L:2976[B]:ALA:N	1.95	1.15
3:C:3256[B]:TRP:CE2	3:L:2965[B]:LEU:HB3	1.77	1.15
3:I:3135[A]:LYS:HG3	3:I:3141[A]:TYR:CE1	1.79	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3196[B]:THR:N	3:L:3199[B]:GLN:OE1	1.79	1.15
3:O:3089[A]:HIS:HE1	3:O:3119[A]:HIS:NE2	1.21	1.15
2:Q:2868:GLU:OE2	3:R:2933[A]:SER:N	1.77	1.15
3:R:3135[B]:LYS:HG3	3:R:3141[B]:TYR:CE1	1.80	1.15
3:U:3217[A]:PHE:CZ	3:U:3230[A]:PHE:CE1	2.35	1.15
3:X:2937[A]:ASN:HB2	3:X:3006[A]:LYS:HE2	1.28	1.15
3:X:3196[A]:THR:N	3:X:3199[A]:GLN:OE1	1.79	1.15
1:Y:1616:LYS:O	3:d:3187[B]:TYR:CB	1.93	1.15
3:I:3150[B]:LYS:HG3	3:R:3163[B]:ASN:ND2	1.61	1.15
3:I:3154[B]:PRO:CG	3:R:3155[B]:MET:SD	2.34	1.15
3:L:3217[A]:PHE:CZ	3:L:3230[A]:PHE:CE1	2.35	1.15
3:L:3217[B]:PHE:CZ	3:L:3230[B]:PHE:CE1	2.35	1.15
3:U:3160[B]:SER:OG	3:d:3259[B]:ASP:CB	1.93	1.15
3:C:2937[B]:ASN:HB2	3:C:3006[B]:LYS:HE2	1.28	1.15
3:C:3196[A]:THR:N	3:C:3199[A]:GLN:OE1	1.79	1.15
3:C:3222[B]:ILE:HD12	3:L:2963[B]:MET:HE1	1.27	1.15
3:F:3217[A]:PHE:CZ	3:F:3230[A]:PHE:CE1	2.35	1.15
3:I:3161[B]:GLU:CB	3:R:3079[B]:CYS:SG	2.35	1.15
3:I:3217[B]:PHE:CZ	3:I:3230[B]:PHE:CE1	2.35	1.15
3:L:3135[B]:LYS:HG3	3:L:3141[B]:TYR:CE1	1.80	1.15
3:L:3196[A]:THR:N	3:L:3199[A]:GLN:OE1	1.79	1.15
3:R:3135[A]:LYS:HG3	3:R:3141[A]:TYR:CE1	1.80	1.15
3:R:3217[B]:PHE:CZ	3:R:3230[B]:PHE:CE1	2.35	1.15
3:U:3086[B]:GLU:OE2	3:d:2970[B]:PRO:CG	1.95	1.15
3:F:2961[B]:HIS:HA	3:a:2975[B]:PHE:CZ	1.82	1.15
3:F:3217[B]:PHE:CZ	3:F:3230[B]:PHE:CE1	2.35	1.15
3:O:2976[B]:ALA:C	3:X:3154[B]:PRO:HG2	1.64	1.15
3:O:3253[B]:GLU:OE1	3:X:3161[B]:GLU:OE1	1.62	1.15
3:X:3217[B]:PHE:CZ	3:X:3230[B]:PHE:CE1	2.35	1.15
3:a:3217[B]:PHE:CZ	3:a:3230[B]:PHE:CE1	2.35	1.15
3:d:2937[B]:ASN:HB2	3:d:3006[B]:LYS:HE2	1.28	1.15
3:d:3135[B]:LYS:HG3	3:d:3141[B]:TYR:CE1	1.79	1.15
3:C:2983[B]:VAL:HG23	3:L:3160[B]:SER:CB	1.78	1.14
3:F:2937[A]:ASN:HB2	3:F:3006[A]:LYS:HE2	1.28	1.14
3:F:2960[B]:PHE:HD2	3:F:3157[B]:PRO:HG3	1.10	1.14
3:I:3256[B]:TRP:CE2	3:R:2965[B]:LEU:HB3	1.81	1.14
3:L:3135[A]:LYS:HG3	3:L:3141[A]:TYR:CE1	1.79	1.14
3:O:2973[B]:THR:HB	3:X:3158[B]:PHE:HE2	1.11	1.14
3:U:2979[B]:GLN:NE2	3:d:3153[B]:LYS:NZ	1.95	1.14
3:d:3196[A]:THR:N	3:d:3199[A]:GLN:OE1	1.79	1.14
3:C:2959[B]:SER:O	3:L:3255[B]:PRO:HB2	1.43	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3093[B]:HIS:CE1	3:L:2971[B]:ASP:HB3	1.42	1.14
3:F:3108[B]:HIS:NE2	3:a:3252[B]:TYR:N	1.93	1.14
3:F:3155[B]:MET:HG3	3:a:3154[B]:PRO:N	1.53	1.14
3:I:3150[B]:LYS:CE	3:R:3163[B]:ASN:HB2	1.77	1.14
3:I:3173[B]:THR:HG23	3:R:3173[B]:THR:OG1	1.42	1.14
3:I:3217[B]:PHE:CE1	3:I:3230[B]:PHE:CZ	2.32	1.14
3:O:3154[B]:PRO:HD2	3:X:3176[B]:LYS:CE	1.77	1.14
3:O:3196[B]:THR:N	3:O:3199[B]:GLN:OE1	1.79	1.14
3:U:2965[B]:LEU:CD1	3:d:3220[B]:ARG:CA	2.26	1.14
3:U:3149[B]:ASN:C	3:d:3154[B]:PRO:HB2	1.70	1.14
3:U:3217[B]:PHE:CZ	3:U:3230[B]:PHE:CE1	2.35	1.14
3:C:2976[B]:ALA:N	3:L:3253[B]:GLU:HB2	1.62	1.14
3:C:2979[B]:GLN:CG	3:L:3156[B]:MET:CE	2.14	1.14
3:C:3135[A]:LYS:HG3	3:C:3141[A]:TYR:CE1	1.79	1.14
3:C:3149[B]:ASN:O	3:L:3168[B]:THR:O	1.62	1.14
2:E:2868:GLU:OE2	3:F:2932[A]:PRO:C	1.89	1.14
3:F:3256[B]:TRP:HE1	3:a:2965[B]:LEU:CG	1.60	1.14
3:O:3217[B]:PHE:CZ	3:O:3230[B]:PHE:CE1	2.35	1.14
3:R:2937[B]:ASN:HB2	3:R:3006[B]:LYS:HE2	1.28	1.14
3:U:3196[B]:THR:N	3:U:3199[B]:GLN:OE1	1.79	1.14
3:a:3104[A]:MET:HA	3:a:3110[A]:THR:HG23	1.23	1.14
3:d:3217[A]:PHE:CZ	3:d:3230[A]:PHE:CE1	2.35	1.14
3:C:3217[A]:PHE:CZ	3:C:3230[A]:PHE:CE1	2.35	1.14
3:C:3217[B]:PHE:CZ	3:C:3230[B]:PHE:CE1	2.35	1.14
3:F:3152[B]:LYS:CB	3:a:3172[B]:SER:N	2.07	1.14
3:I:2966[B]:SER:HA	3:R:3256[B]:TRP:CB	1.74	1.14
3:I:2970[B]:PRO:CD	3:R:2989[B]:HIS:CD2	2.29	1.14
3:L:3230[B]:PHE:HB2	3:L:3243[B]:GLY:HA2	1.14	1.14
3:O:2965[B]:LEU:CB	3:X:3254[B]:MET:CE	2.25	1.14
3:O:2968[B]:GLN:NE2	3:X:2984[B]:THR:C	2.00	1.14
3:U:2975[B]:PHE:HE2	3:d:3254[B]:MET:CG	1.58	1.14
3:U:3159[B]:SER:HB2	3:d:3150[B]:LYS:CD	1.73	1.14
3:X:3135[B]:LYS:HG3	3:X:3141[B]:TYR:CE1	1.79	1.14
3:X:3196[B]:THR:N	3:X:3199[B]:GLN:OE1	1.79	1.14
3:C:3149[B]:ASN:ND2	3:L:3163[B]:ASN:ND2	1.94	1.14
3:C:3154[B]:PRO:HA	3:L:3153[B]:LYS:O	1.48	1.14
3:I:3159[B]:SER:C	3:R:3150[B]:LYS:CB	2.20	1.14
3:I:3254[B]:MET:HG3	3:R:2966[B]:SER:CB	1.76	1.14
3:O:3196[A]:THR:N	3:O:3199[A]:GLN:OE1	1.79	1.14
3:O:3217[A]:PHE:CZ	3:O:3230[A]:PHE:CE1	2.35	1.14
3:U:3155[B]:MET:O	3:d:3150[B]:LYS:HG3	1.47	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3169[B]:LYS:CD	3:d:3147[B]:GLU:HA	1.76	1.14
3:a:3217[A]:PHE:CZ	3:a:3230[A]:PHE:CE1	2.35	1.14
3:C:3156[B]:MET:CB	3:L:2982[B]:MET:CB	2.24	1.13
3:C:3196[B]:THR:N	3:C:3199[B]:GLN:OE1	1.79	1.13
3:F:2959[B]:SER:HB2	3:a:3255[B]:PRO:HB2	1.17	1.13
3:F:2966[B]:SER:CA	3:a:3256[B]:TRP:HD1	1.33	1.13
3:F:2985[B]:PHE:CZ	3:a:2970[B]:PRO:HA	1.80	1.13
2:H:2797:LYS:NZ	3:I:3028[A]:PRO:HD3	1.60	1.13
3:I:3156[B]:MET:HB2	3:R:2982[B]:MET:HG3	1.14	1.13
3:O:2960[B]:PHE:HD2	3:O:3157[B]:PRO:HG3	1.10	1.13
3:O:3108[B]:HIS:O	3:X:2970[B]:PRO:CD	1.88	1.13
3:O:3153[B]:LYS:CD	3:X:3176[B]:LYS:CD	2.04	1.13
3:R:3293[B]:LYS:HD3	3:R:3294[B]:SER:HB3	1.14	1.13
3:U:3256[B]:TRP:HB2	3:d:2969[B]:TYR:N	1.62	1.13
3:X:3217[A]:PHE:CZ	3:X:3230[A]:PHE:CE1	2.35	1.13
3:X:3230[B]:PHE:HB2	3:X:3243[B]:GLY:HA2	1.14	1.13
2:Z:2867:PRO:HG3	3:a:2932[A]:PRO:HG3	1.26	1.13
3:a:3196[A]:THR:N	3:a:3199[A]:GLN:OE1	1.79	1.13
3:a:3293[B]:LYS:HD3	3:a:3294[B]:SER:HB3	1.14	1.13
3:d:3230[B]:PHE:HB2	3:d:3243[B]:GLY:HA2	1.14	1.13
3:C:2983[B]:VAL:CG2	3:L:3160[B]:SER:CA	2.14	1.13
3:F:3154[B]:PRO:HD2	3:a:3155[B]:MET:SD	1.86	1.13
3:F:3293[B]:LYS:HD3	3:F:3294[B]:SER:HB3	1.13	1.13
3:I:2982[B]:MET:HE3	3:R:2977[B]:CYS:CB	1.78	1.13
3:I:3217[A]:PHE:CZ	3:I:3230[A]:PHE:CE1	2.35	1.13
3:U:3293[A]:LYS:HD3	3:U:3294[A]:SER:HB3	1.13	1.13
3:X:2979[B]:GLN:HG2	3:X:3155[B]:MET:CE	1.69	1.13
3:X:3135[A]:LYS:HG3	3:X:3141[A]:TYR:CE1	1.80	1.13
3:d:3135[A]:LYS:HG3	3:d:3141[A]:TYR:CE1	1.79	1.13
3:C:2965[B]:LEU:HD23	3:L:3253[B]:GLU:OE2	1.44	1.13
3:C:2975[B]:PHE:HD1	3:L:3107[B]:LEU:CD1	1.52	1.13
3:C:3230[B]:PHE:HB2	3:C:3243[B]:GLY:HA2	1.14	1.13
3:I:2966[B]:SER:HB2	3:R:3254[B]:MET:CG	1.79	1.13
3:I:3155[B]:MET:HB2	3:R:3153[B]:LYS:CG	1.76	1.13
3:U:3256[B]:TRP:CD2	3:d:2969[B]:TYR:HB3	1.80	1.13
3:F:2965[B]:LEU:CA	3:a:3221[B]:ALA:HB1	1.77	1.13
3:F:2981[B]:GLY:HA2	3:a:2968[B]:GLN:OE1	1.45	1.13
3:F:3169[B]:LYS:O	3:a:3152[B]:LYS:CG	1.97	1.13
3:I:2972[B]:GLY:CA	3:R:3090[B]:ASN:HB3	1.77	1.13
3:I:3160[B]:SER:OG	3:R:2982[B]:MET:CA	1.96	1.13
3:I:3196[A]:THR:N	3:I:3199[A]:GLN:OE1	1.79	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2937[A]:ASN:HB2	3:L:3006[A]:LYS:HE2	1.28	1.13
3:O:3108[B]:HIS:HB3	3:X:2970[B]:PRO:N	1.63	1.13
3:O:3153[B]:LYS:CG	3:X:3176[B]:LYS:CE	2.27	1.13
3:U:3154[B]:PRO:CD	3:d:2984[B]:THR:HG21	1.78	1.13
3:U:3170[B]:ALA:O	3:d:3152[B]:LYS:NZ	1.80	1.13
3:U:3253[B]:GLU:HA	3:d:3255[B]:PRO:CG	1.77	1.13
3:C:2968[B]:GLN:NE2	3:L:3258[B]:PHE:CZ	2.17	1.13
3:C:3284[B]:LYS:HD3	3:C:3285[B]:VAL:N	1.64	1.13
3:C:3149[B]:ASN:CB	3:L:3163[B]:ASN:ND2	2.12	1.12
3:C:3163[B]:ASN:HD22	3:L:3149[B]:ASN:CG	1.56	1.12
3:C:3169[B]:LYS:O	3:L:3148[B]:ILE:O	1.65	1.13
2:E:2800:LYS:O	3:F:3023[A]:ILE:CD1	1.97	1.12
3:F:3153[B]:LYS:HG2	3:a:3155[B]:MET:HB2	1.23	1.13
3:F:3284[B]:LYS:HD3	3:F:3285[B]:VAL:N	1.64	1.13
3:I:3174[B]:GLY:HA2	3:R:3154[B]:PRO:HG3	1.29	1.13
3:C:3252[B]:TYR:CE1	3:L:3223[B]:GLY:O	2.01	1.12
2:E:2868:GLU:OE2	3:F:2933[A]:SER:N	1.80	1.12
3:F:3154[B]:PRO:CD	3:a:3155[B]:MET:HG3	1.79	1.12
3:I:2982[B]:MET:HE2	3:R:2966[B]:SER:HB3	1.15	1.12
3:I:3196[B]:THR:N	3:I:3199[B]:GLN:OE1	1.79	1.12
3:I:3254[B]:MET:C	3:R:2966[B]:SER:OG	1.92	1.12
3:R:3284[A]:LYS:HD3	3:R:3285[A]:VAL:N	1.64	1.12
3:U:3152[B]:LYS:O	3:d:3152[B]:LYS:C	1.92	1.12
3:a:3135[A]:LYS:HG2	3:a:3141[A]:TYR:HE1	1.14	1.12
3:a:3284[B]:LYS:HD3	3:a:3285[B]:VAL:N	1.64	1.12
3:d:2960[B]:PHE:HD2	3:d:3157[B]:PRO:HG3	1.10	1.12
3:C:3174[B]:GLY:HA2	3:L:3154[B]:PRO:CD	1.79	1.12
3:F:3256[B]:TRP:HB3	3:a:2966[B]:SER:C	1.73	1.12
3:I:3153[B]:LYS:CD	3:R:3155[B]:MET:HB2	1.79	1.12
3:O:2973[B]:THR:HB	3:X:3158[B]:PHE:CE2	1.84	1.12
3:O:2975[B]:PHE:HE2	3:X:3172[B]:SER:CB	1.61	1.12
3:R:2960[A]:PHE:HD2	3:R:3157[A]:PRO:HG3	1.10	1.12
3:U:2969[B]:TYR:CE1	3:d:3107[B]:LEU:HD13	1.84	1.12
3:d:3293[B]:LYS:HD3	3:d:3294[B]:SER:HB3	1.13	1.12
3:C:2982[B]:MET:CG	3:L:3156[B]:MET:SD	2.36	1.12
3:F:2974[B]:ALA:HB1	3:a:3253[B]:GLU:OE1	1.48	1.12
3:F:2977[B]:CYS:O	3:a:3254[B]:MET:CE	1.81	1.12
3:F:3150[B]:LYS:NZ	3:a:3160[B]:SER:CB	2.11	1.12
3:I:2975[B]:PHE:HZ	3:R:2961[B]:HIS:CA	1.60	1.12
3:L:2937[B]:ASN:HB2	3:L:3006[B]:LYS:HE2	1.28	1.12
3:O:2963[B]:MET:SD	3:X:2975[B]:PHE:CE2	2.43	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3230[B]:PHE:HB2	3:O:3243[B]:GLY:HA2	1.14	1.12
3:O:3284[B]:LYS:HD3	3:O:3285[B]:VAL:N	1.64	1.12
3:U:3252[B]:TYR:HE2	3:d:3222[B]:ILE:HD13	1.00	1.12
4:j:1:NAG:H61	4:j:2:NAG:HN2	1.08	1.12
3:C:2964[B]:PRO:O	3:L:3255[B]:PRO:HB3	1.43	1.12
3:C:3154[B]:PRO:HB3	3:L:3151[B]:LEU:O	1.47	1.12
3:C:3156[B]:MET:SD	3:L:2982[B]:MET:CB	2.38	1.12
3:C:3254[B]:MET:O	3:L:2976[B]:ALA:CA	1.91	1.12
3:F:3153[B]:LYS:NZ	3:a:3157[B]:PRO:HD2	1.64	1.12
3:I:2963[B]:MET:HE1	3:R:3223[B]:GLY:HA3	1.29	1.12
3:I:3153[B]:LYS:HB2	3:R:3158[B]:PHE:HB2	1.29	1.12
3:I:3165[B]:ASN:O	3:R:3149[B]:ASN:HB3	1.49	1.12
3:U:3155[B]:MET:N	3:d:3150[B]:LYS:CA	2.13	1.12
3:a:2960[B]:PHE:HD2	3:a:3157[B]:PRO:HG3	1.10	1.12
3:d:3293[A]:LYS:HD3	3:d:3294[A]:SER:HB3	1.14	1.12
3:C:3089[B]:HIS:HE1	3:C:3119[B]:HIS:NE2	1.21	1.12
3:C:3173[B]:THR:OG1	3:L:3152[B]:LYS:HA	1.42	1.12
3:F:2960[A]:PHE:HD2	3:F:3157[A]:PRO:HG3	1.10	1.12
3:F:3154[B]:PRO:CG	3:a:3155[B]:MET:SD	2.38	1.12
3:I:2977[B]:CYS:SG	3:R:2978[B]:CYS:O	2.08	1.12
3:L:3293[A]:LYS:HD3	3:L:3294[A]:SER:HB3	1.14	1.12
3:L:3293[B]:LYS:HD3	3:L:3294[B]:SER:HB3	1.13	1.12
3:O:3040[B]:VAL:CG2	3:X:2969[B]:TYR:CD1	2.31	1.12
3:R:3104[B]:MET:HA	3:R:3110[B]:THR:HG23	1.23	1.12
3:U:3254[B]:MET:HE3	3:d:3254[B]:MET:HB2	1.22	1.12
3:U:3255[B]:PRO:HD3	3:d:3253[B]:GLU:C	1.73	1.12
3:a:3230[B]:PHE:HB2	3:a:3243[B]:GLY:HA2	1.14	1.12
3:C:3284[A]:LYS:HD3	3:C:3285[A]:VAL:N	1.64	1.11
3:F:3230[B]:PHE:HB2	3:F:3243[B]:GLY:HA2	1.14	1.11
3:L:3104[A]:MET:HA	3:L:3110[A]:THR:HG23	1.23	1.11
3:L:3104[B]:MET:HA	3:L:3110[B]:THR:HG23	1.24	1.11
3:O:3153[B]:LYS:HD3	3:X:3176[B]:LYS:HD2	1.28	1.11
3:O:3251[B]:ASP:HB2	3:X:2968[B]:GLN:OE1	1.47	1.11
3:U:2965[B]:LEU:CB	3:d:3220[B]:ARG:HH11	1.61	1.11
3:X:2960[A]:PHE:HD2	3:X:3157[A]:PRO:HG3	1.10	1.11
3:X:3284[A]:LYS:HD3	3:X:3285[A]:VAL:N	1.64	1.11
3:X:3284[B]:LYS:HD3	3:X:3285[B]:VAL:N	1.64	1.11
3:d:3284[B]:LYS:HD3	3:d:3285[B]:VAL:N	1.64	1.11
3:C:3147[B]:GLU:CG	3:L:3161[B]:GLU:HA	1.78	1.11
3:C:3256[B]:TRP:O	3:L:2965[B]:LEU:O	1.68	1.11
3:I:3284[A]:LYS:HD3	3:I:3285[A]:VAL:N	1.64	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3284[A]:LYS:HD3	3:L:3285[A]:VAL:N	1.64	1.11
3:U:3284[A]:LYS:HD3	3:U:3285[A]:VAL:N	1.64	1.11
3:d:3104[B]:MET:HA	3:d:3110[B]:THR:HG23	1.23	1.11
3:C:2969[B]:TYR:C	3:L:2985[B]:PHE:HE2	1.23	1.11
3:C:3158[B]:PHE:HD2	3:L:3153[B]:LYS:CE	1.39	1.11
3:C:3163[B]:ASN:CG	3:L:3149[B]:ASN:HD22	1.56	1.11
3:C:3163[B]:ASN:CB	3:L:3149[B]:ASN:HD22	1.63	1.11
3:F:3154[B]:PRO:HB3	3:a:3174[B]:GLY:N	1.65	1.11
3:F:3284[A]:LYS:HD3	3:F:3285[A]:VAL:N	1.64	1.11
3:I:2937[A]:ASN:HB2	3:I:3006[A]:LYS:HE2	1.28	1.11
3:I:3174[B]:GLY:HA2	3:R:3154[B]:PRO:CB	1.71	1.11
3:O:3253[B]:GLU:HG3	3:X:3160[B]:SER:HA	1.20	1.11
1:Y:1616:LYS:HD2	3:d:3187[B]:TYR:HA	1.17	1.11
3:a:3284[A]:LYS:HD3	3:a:3285[A]:VAL:N	1.64	1.11
3:a:3293[A]:LYS:HD3	3:a:3294[A]:SER:HB3	1.13	1.11
3:d:3284[A]:LYS:HD3	3:d:3285[A]:VAL:N	1.64	1.11
3:C:2968[B]:GLN:CD	3:L:3258[B]:PHE:HZ	1.56	1.11
3:C:3256[B]:TRP:CD2	3:L:2965[B]:LEU:C	2.22	1.11
3:F:3254[B]:MET:HG3	3:a:2966[B]:SER:HB2	1.19	1.11
3:I:2989[B]:HIS:NE2	3:R:2970[B]:PRO:N	1.96	1.11
3:I:3160[B]:SER:HB3	3:R:3150[B]:LYS:HZ3	1.12	1.11
3:I:3223[B]:GLY:HA3	3:R:2963[B]:MET:HE1	1.23	1.11
3:I:3293[B]:LYS:HD3	3:I:3294[B]:SER:HB3	1.13	1.11
3:O:3104[A]:MET:HA	3:O:3110[A]:THR:HG23	1.23	1.11
3:R:3284[B]:LYS:HD3	3:R:3285[B]:VAL:N	1.64	1.11
3:U:3293[B]:LYS:HD3	3:U:3294[B]:SER:HB3	1.13	1.11
3:C:3160[B]:SER:CA	3:L:2983[B]:VAL:HG23	1.79	1.11
3:C:3163[B]:ASN:ND2	3:L:3149[B]:ASN:HD22	1.48	1.11
3:C:3293[B]:LYS:HD3	3:C:3294[B]:SER:HB3	1.13	1.11
3:F:2937[B]:ASN:HB2	3:F:3006[B]:LYS:HE2	1.28	1.11
3:F:2964[B]:PRO:C	3:a:3221[B]:ALA:HB1	1.75	1.11
3:I:3104[A]:MET:HA	3:I:3110[A]:THR:HG23	1.24	1.11
3:I:3252[B]:TYR:HB2	3:R:3251[B]:ASP:O	1.34	1.11
3:I:3252[B]:TYR:CB	3:R:3251[B]:ASP:O	1.74	1.11
3:L:3135[A]:LYS:HG2	3:L:3141[A]:TYR:HE1	1.14	1.11
3:U:3153[B]:LYS:HB3	3:d:3153[B]:LYS:HD2	1.18	1.11
3:U:3230[A]:PHE:HB2	3:U:3243[A]:GLY:HA2	1.14	1.11
3:U:3230[B]:PHE:HB2	3:U:3243[B]:GLY:HA2	1.14	1.11
3:U:3284[B]:LYS:HD3	3:U:3285[B]:VAL:N	1.64	1.11
3:F:2981[B]:GLY:H	3:a:2968[B]:GLN:HG2	1.12	1.10
3:F:2982[B]:MET:HG3	3:a:2967[B]:CYS:SG	1.79	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2800:LYS:O	3:I:3023[A]:ILE:CD1	1.97	1.10
3:I:2937[B]:ASN:HB2	3:I:3006[B]:LYS:HE2	1.28	1.10
3:I:3153[B]:LYS:NZ	3:R:3157[B]:PRO:HD2	1.65	1.10
3:O:2965[B]:LEU:HB2	3:X:3254[B]:MET:SD	1.90	1.10
3:O:3038[B]:ILE:CG2	3:X:2969[B]:TYR:CZ	2.33	1.10
3:O:3161[B]:GLU:OE2	3:X:3151[B]:LEU:HD11	0.95	1.10
3:U:3220[B]:ARG:CB	3:d:2973[B]:THR:HA	1.81	1.10
3:C:2974[B]:ALA:CB	3:L:3249[B]:GLY:HA3	1.53	1.10
3:C:3150[B]:LYS:C	3:L:3172[B]:SER:HB2	1.74	1.10
3:F:2964[B]:PRO:C	3:a:3221[B]:ALA:CB	2.23	1.10
3:I:2961[B]:HIS:CG	3:R:2975[B]:PHE:HZ	1.64	1.10
3:I:3090[B]:ASN:HA	3:R:2971[B]:ASP:O	1.48	1.10
3:I:3251[B]:ASP:HB3	3:R:3251[B]:ASP:HB2	1.16	1.10
3:I:3284[B]:LYS:HD3	3:I:3285[B]:VAL:N	1.64	1.10
3:O:3293[A]:LYS:HD3	3:O:3294[A]:SER:HB3	1.13	1.10
3:U:2971[B]:ASP:O	3:d:3247[B]:VAL:HA	1.49	1.10
3:a:2960[A]:PHE:HD2	3:a:3157[A]:PRO:HG3	1.10	1.10
3:C:3163[B]:ASN:ND2	3:L:3149[B]:ASN:HB3	1.52	1.10
3:F:3150[B]:LYS:HE3	3:a:3163[B]:ASN:HB2	1.32	1.10
3:F:3153[B]:LYS:HB3	3:a:3155[B]:MET:O	1.52	1.10
3:F:3154[B]:PRO:N	3:a:3155[B]:MET:HG3	1.00	1.10
3:I:3256[B]:TRP:CB	3:R:2966[B]:SER:HA	1.65	1.10
3:L:2960[A]:PHE:HD2	3:L:3157[A]:PRO:HG3	1.10	1.10
3:L:3284[B]:LYS:HD3	3:L:3285[B]:VAL:N	1.64	1.10
3:R:3230[B]:PHE:HB2	3:R:3243[B]:GLY:HA2	1.14	1.10
3:U:3162[B]:ASP:CG	3:d:3259[B]:ASP:HB2	1.51	1.10
3:F:3251[B]:ASP:CA	3:a:3251[B]:ASP:HB3	1.81	1.10
3:I:3120[B]:HIS:CD2	3:R:2969[B]:TYR:CE2	2.40	1.10
3:I:3253[B]:GLU:HB2	3:R:2975[B]:PHE:O	1.47	1.10
3:R:3230[A]:PHE:HB2	3:R:3243[A]:GLY:HA2	1.14	1.10
3:U:2960[B]:PHE:HD2	3:U:3157[B]:PRO:HG3	1.10	1.10
3:U:3169[B]:LYS:O	3:d:3148[B]:ILE:C	1.93	1.10
3:U:3169[B]:LYS:HE2	3:d:3146[B]:CYS:HA	1.16	1.10
3:U:3254[B]:MET:HE3	3:d:3254[B]:MET:HB3	1.23	1.10
3:d:3135[A]:LYS:HG2	3:d:3141[A]:TYR:HE1	1.14	1.10
3:C:2988[B]:TRP:NE1	3:L:3153[B]:LYS:NZ	1.99	1.10
3:F:3107[B]:LEU:CD1	3:a:2975[B]:PHE:HD1	1.62	1.10
3:I:2975[B]:PHE:C	3:R:3253[B]:GLU:CB	2.25	1.10
3:I:3160[B]:SER:OG	3:R:2982[B]:MET:C	1.95	1.10
3:I:3169[B]:LYS:O	3:R:3152[B]:LYS:CB	2.00	1.10
3:I:3254[B]:MET:CG	3:R:2966[B]:SER:HB2	1.82	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2960[A]:PHE:HD2	3:O:3157[A]:PRO:HG3	1.10	1.10
3:R:3135[A]:LYS:HG2	3:R:3141[A]:TYR:HE1	1.14	1.10
3:C:3107[B]:LEU:HD13	3:L:2974[B]:ALA:O	1.50	1.09
3:C:3149[B]:ASN:ND2	3:L:3163[B]:ASN:HD22	1.49	1.09
3:C:3174[B]:GLY:CA	3:L:3154[B]:PRO:HB3	1.82	1.09
3:I:2959[B]:SER:CB	3:R:3255[B]:PRO:CB	2.29	1.09
3:I:2975[B]:PHE:CD1	3:R:3107[B]:LEU:CD1	2.14	1.09
3:I:3149[B]:ASN:OD1	3:R:3169[B]:LYS:HE3	1.48	1.09
3:I:3160[B]:SER:HA	3:R:2983[B]:VAL:N	1.65	1.09
3:O:2967[B]:CYS:HB2	3:X:3155[B]:MET:HG2	1.10	1.09
3:O:3109[B]:TYR:CD1	3:X:2970[B]:PRO:HD2	1.80	1.09
3:O:3154[B]:PRO:HG2	3:X:3175[B]:TYR:CB	1.81	1.09
3:O:3284[A]:LYS:HD3	3:O:3285[A]:VAL:N	1.64	1.09
3:U:2937[A]:ASN:HB2	3:U:3006[A]:LYS:HE2	1.28	1.09
2:c:2867:PRO:HG3	3:d:2932[A]:PRO:HG2	1.22	1.09
3:C:2937[A]:ASN:HB2	3:C:3006[A]:LYS:HE2	1.28	1.09
3:C:2975[B]:PHE:CE1	3:L:3107[B]:LEU:CD1	2.33	1.09
3:F:2968[B]:GLN:HG2	3:a:2981[B]:GLY:H	1.16	1.09
3:F:3104[A]:MET:HA	3:F:3110[A]:THR:HG23	1.23	1.09
3:F:3104[B]:MET:HA	3:F:3110[B]:THR:HG23	1.23	1.09
3:F:3154[B]:PRO:HB3	3:a:3174[B]:GLY:CA	1.83	1.09
3:F:3248[B]:LEU:HB3	3:a:2972[B]:GLY:O	1.50	1.09
3:I:2975[B]:PHE:HD1	3:R:3107[B]:LEU:CG	1.65	1.09
3:I:3252[B]:TYR:HB2	3:R:3251[B]:ASP:C	1.73	1.09
3:I:3293[A]:LYS:HD3	3:I:3294[A]:SER:HB3	1.14	1.09
3:O:3230[A]:PHE:HB2	3:O:3243[A]:GLY:HA2	1.14	1.09
3:R:3293[A]:LYS:HD3	3:R:3294[A]:SER:HB3	1.14	1.09
3:U:3155[B]:MET:N	3:d:3150[B]:LYS:HA	1.31	1.09
3:U:3162[B]:ASP:CA	3:d:3260[B]:ARG:HH12	1.65	1.09
3:X:3135[A]:LYS:HG2	3:X:3141[A]:TYR:HE1	1.14	1.09
3:F:2982[B]:MET:HE3	3:a:2967[B]:CYS:SG	1.86	1.09
3:F:2982[B]:MET:HG2	3:a:2967[B]:CYS:SG	1.79	1.09
3:I:3163[B]:ASN:ND2	3:R:3149[B]:ASN:CB	2.14	1.09
3:L:3135[B]:LYS:HG2	3:L:3141[B]:TYR:HE1	1.14	1.09
3:O:3154[B]:PRO:CG	3:X:3175[B]:TYR:CB	2.28	1.09
3:O:3255[B]:PRO:HD2	3:X:3169[B]:LYS:HG3	1.33	1.09
2:W:2800:LYS:O	3:X:3023[A]:ILE:CD1	2.01	1.09
3:X:3293[A]:LYS:HD3	3:X:3294[A]:SER:HB3	1.13	1.09
2:E:2868:GLU:CD	3:F:2932[A]:PRO:O	1.95	1.09
3:F:3172[B]:SER:H	3:a:3152[B]:LYS:HB2	1.05	1.09
3:L:3230[A]:PHE:HB2	3:L:3243[A]:GLY:HA2	1.14	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3038[B]:ILE:CD1	3:X:2969[B]:TYR:OH	2.01	1.09
3:O:3108[B]:HIS:O	3:X:2970[B]:PRO:HD3	0.92	1.09
3:O:3251[B]:ASP:HB3	3:X:2967[B]:CYS:CA	1.83	1.09
3:U:2930[B]:LEU:H	3:U:2930[B]:LEU:HD22	1.18	1.09
1:Y:1546:LYS:HG3	3:d:3001[B]:LYS:HE3	1.20	1.09
3:C:3163[B]:ASN:ND2	3:L:3149[B]:ASN:ND2	2.01	1.09
3:C:3174[B]:GLY:HA3	3:L:3154[B]:PRO:HB3	1.14	1.09
3:C:3258[B]:PHE:HZ	3:L:2968[B]:GLN:NE2	1.49	1.09
3:C:3293[A]:LYS:HD3	3:C:3294[A]:SER:HB3	1.13	1.09
3:F:2967[B]:CYS:HA	3:a:2981[B]:GLY:HA3	1.27	1.09
3:F:2982[B]:MET:CE	3:a:2977[B]:CYS:CB	2.31	1.09
3:I:3135[A]:LYS:HG2	3:I:3141[A]:TYR:HE1	1.14	1.09
3:I:3154[B]:PRO:CB	3:R:3174[B]:GLY:CA	2.29	1.09
3:O:2930[B]:LEU:HD22	3:O:2930[B]:LEU:H	1.18	1.09
3:O:2937[A]:ASN:HB2	3:O:3006[A]:LYS:HE2	1.28	1.09
3:X:3104[B]:MET:HA	3:X:3110[B]:THR:HG23	1.23	1.09
3:X:3135[B]:LYS:HG2	3:X:3141[B]:TYR:HE1	1.14	1.09
3:X:3217[B]:PHE:CE1	3:X:3230[B]:PHE:HZ	1.71	1.09
3:d:2960[A]:PHE:HD2	3:d:3157[A]:PRO:HG3	1.10	1.09
3:C:2971[B]:ASP:HB3	3:L:3093[B]:HIS:CE1	1.64	1.08
3:C:2982[B]:MET:HB3	3:L:3156[B]:MET:HB3	1.10	1.08
3:C:2983[B]:VAL:CG2	3:L:3161[B]:GLU:OE2	1.68	1.08
3:F:3162[B]:ASP:HB3	3:a:3259[B]:ASP:HB3	1.21	1.08
3:F:3256[B]:TRP:NE1	3:a:2965[B]:LEU:CD1	2.16	1.08
3:I:2960[B]:PHE:HD2	3:I:3157[B]:PRO:HG3	1.10	1.08
3:O:2965[B]:LEU:CB	3:X:3254[B]:MET:SD	2.41	1.08
3:O:2965[B]:LEU:CA	3:X:3254[B]:MET:HE1	1.80	1.08
3:O:3196[A]:THR:HG21	1:P:416:ASN:ND2	1.68	1.08
3:R:2930[B]:LEU:HD22	3:R:2930[B]:LEU:H	1.18	1.08
3:U:3252[B]:TYR:CE2	3:d:3222[B]:ILE:CD1	2.33	1.08
3:U:3254[B]:MET:HB3	3:d:3254[B]:MET:CB	1.80	1.08
3:U:3255[B]:PRO:CG	3:d:3252[B]:TYR:HA	1.79	1.08
3:X:2930[A]:LEU:HD22	3:X:2930[A]:LEU:H	1.18	1.08
3:a:2937[B]:ASN:HB2	3:a:3006[B]:LYS:HE2	1.28	1.08
3:d:3104[A]:MET:HA	3:d:3110[A]:THR:HG23	1.23	1.08
3:C:3160[B]:SER:CA	3:L:2983[B]:VAL:CG2	2.29	1.08
3:C:3161[B]:GLU:OE2	3:L:2983[B]:VAL:HG21	1.53	1.08
3:F:3154[B]:PRO:CD	3:a:3155[B]:MET:CG	2.32	1.08
3:I:3255[B]:PRO:HB2	3:R:2959[B]:SER:HB2	1.26	1.08
3:O:3160[B]:SER:HA	3:X:3151[B]:LEU:CG	1.82	1.08
3:O:3162[B]:ASP:OD2	3:X:3150[B]:LYS:HD2	1.51	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3217[A]:PHE:CE1	3:O:3230[A]:PHE:HZ	1.71	1.08
3:O:3293[B]:LYS:HD3	3:O:3294[B]:SER:HB3	1.13	1.08
3:U:2930[A]:LEU:HD22	3:U:2930[A]:LEU:H	1.18	1.08
3:U:3104[A]:MET:HA	3:U:3110[A]:THR:HG23	1.23	1.08
3:X:2937[B]:ASN:HB2	3:X:3006[B]:LYS:HE2	1.28	1.08
3:a:2937[A]:ASN:HB2	3:a:3006[A]:LYS:HE2	1.28	1.08
3:a:3217[B]:PHE:CE1	3:a:3230[B]:PHE:HZ	1.71	1.08
3:C:2982[B]:MET:CB	3:L:3156[B]:MET:SD	2.41	1.08
3:C:2985[B]:PHE:CE1	3:L:2970[B]:PRO:HA	1.88	1.08
3:C:3152[B]:LYS:CA	3:L:3173[B]:THR:OG1	1.98	1.08
3:C:3217[A]:PHE:CE1	3:C:3230[A]:PHE:HZ	1.71	1.08
3:F:2982[B]:MET:SD	3:a:3157[B]:PRO:HA	1.92	1.08
3:F:3155[B]:MET:CA	3:a:3153[B]:LYS:HD2	1.82	1.08
3:F:3163[B]:ASN:HB3	3:a:3150[B]:LYS:HE3	1.25	1.08
3:O:2930[A]:LEU:H	3:O:2930[A]:LEU:HD22	1.18	1.08
3:O:2937[B]:ASN:HB2	3:O:3006[B]:LYS:HE2	1.28	1.08
3:O:2969[B]:TYR:CD1	3:X:3158[B]:PHE:CE1	2.40	1.08
3:U:3156[B]:MET:HE2	3:d:2982[B]:MET:CG	1.74	1.08
3:a:3230[A]:PHE:HB2	3:a:3243[A]:GLY:HA2	1.14	1.08
3:C:2960[A]:PHE:HD2	3:C:3157[A]:PRO:HG3	1.10	1.08
3:C:3120[B]:HIS:NE2	3:L:2969[B]:TYR:CE2	2.15	1.08
3:F:2966[B]:SER:C	3:a:3256[B]:TRP:HB3	1.77	1.08
3:I:3253[B]:GLU:HB2	3:R:2975[B]:PHE:C	1.79	1.08
3:O:2970[B]:PRO:CD	3:X:2991[B]:LEU:CD1	2.29	1.08
3:O:3025[B]:VAL:HG22	3:O:3047[B]:ARG:HH12	1.19	1.08
3:O:3135[A]:LYS:HG2	3:O:3141[A]:TYR:HE1	1.14	1.08
3:O:3154[B]:PRO:HG2	3:X:3175[B]:TYR:HB2	1.30	1.08
3:R:2930[A]:LEU:H	3:R:2930[A]:LEU:HD22	1.18	1.08
3:U:3113[B]:ASP:OD2	3:U:3114[B]:PRO:CD	2.02	1.08
3:a:2930[A]:LEU:H	3:a:2930[A]:LEU:HD22	1.18	1.08
2:c:2867:PRO:CG	3:d:2932[A]:PRO:HG2	1.81	1.08
3:C:3152[B]:LYS:HG3	3:L:3169[B]:LYS:O	1.53	1.08
3:F:3155[B]:MET:C	3:a:3153[B]:LYS:HD2	1.79	1.08
3:F:3174[B]:GLY:CA	3:a:3154[B]:PRO:CG	2.30	1.08
3:F:3251[B]:ASP:HB3	3:a:3251[B]:ASP:HB2	1.29	1.08
3:O:3113[A]:ASP:OD2	3:O:3114[A]:PRO:CD	2.02	1.08
3:O:3135[B]:LYS:HG2	3:O:3141[B]:TYR:HE1	1.14	1.08
3:X:3113[B]:ASP:OD2	3:X:3114[B]:PRO:CD	2.02	1.08
3:X:3185[A]:TYR:O	3:X:3186[A]:GLU:OE2	1.72	1.08
3:X:3230[A]:PHE:HB2	3:X:3243[A]:GLY:HA2	1.14	1.08
3:C:2960[B]:PHE:HD2	3:C:3157[B]:PRO:HG3	1.10	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2985[B]:PHE:CZ	3:L:2970[B]:PRO:N	2.22	1.07
3:C:3148[B]:ILE:O	3:L:3169[B]:LYS:O	1.71	1.07
3:C:3156[B]:MET:CB	3:L:2982[B]:MET:HB3	1.84	1.07
3:F:2930[A]:LEU:H	3:F:2930[A]:LEU:HD22	1.18	1.07
3:F:2966[B]:SER:HA	3:a:3256[B]:TRP:CB	1.83	1.07
3:F:3230[A]:PHE:HB2	3:F:3243[A]:GLY:HA2	1.14	1.07
3:I:3169[B]:LYS:C	3:R:3152[B]:LYS:HG3	1.65	1.07
3:L:3025[B]:VAL:HG22	3:L:3047[B]:ARG:HH12	1.19	1.07
3:O:3113[B]:ASP:OD2	3:O:3114[B]:PRO:CD	2.02	1.07
3:O:3154[B]:PRO:HG3	3:X:3175[B]:TYR:HB3	1.17	1.07
3:U:3113[A]:ASP:OD2	3:U:3114[A]:PRO:CD	2.02	1.07
3:U:3254[B]:MET:HA	3:d:3254[B]:MET:HA	1.27	1.07
3:a:3217[A]:PHE:CE1	3:a:3230[A]:PHE:HZ	1.71	1.07
3:d:3113[B]:ASP:OD2	3:d:3114[B]:PRO:CD	2.02	1.07
3:C:2930[B]:LEU:HD22	3:C:2930[B]:LEU:H	1.18	1.07
3:C:3113[B]:ASP:OD2	3:C:3114[B]:PRO:CD	2.02	1.07
3:C:3150[B]:LYS:NZ	3:L:3160[B]:SER:HB3	1.56	1.07
3:C:3163[B]:ASN:HD22	3:L:3149[B]:ASN:ND2	1.51	1.07
3:C:3256[B]:TRP:CG	3:L:2965[B]:LEU:O	2.01	1.07
3:F:2972[B]:GLY:HA3	3:a:3090[B]:ASN:HB3	1.27	1.07
3:F:3113[A]:ASP:OD2	3:F:3114[A]:PRO:CD	2.02	1.07
3:F:3159[B]:SER:CA	3:a:3150[B]:LYS:C	2.27	1.07
3:F:3293[A]:LYS:HD3	3:F:3294[A]:SER:HB3	1.13	1.07
3:I:2971[B]:ASP:O	3:R:3090[B]:ASN:HA	1.54	1.07
3:I:3113[B]:ASP:OD2	3:I:3114[B]:PRO:CD	2.02	1.07
3:I:3256[B]:TRP:HB3	3:R:2966[B]:SER:HA	1.10	1.07
3:L:3025[A]:VAL:HG22	3:L:3047[A]:ARG:HH12	1.19	1.07
3:O:2968[B]:GLN:CA	3:X:2988[B]:TRP:HB2	1.82	1.07
3:O:3161[B]:GLU:OE2	3:O:3161[B]:GLU:N	1.88	1.07
3:O:3185[B]:TYR:O	3:O:3186[B]:GLU:OE2	1.72	1.07
3:R:3025[A]:VAL:HG22	3:R:3047[A]:ARG:HH12	1.19	1.07
3:U:2965[B]:LEU:HB2	3:d:3220[B]:ARG:NH1	1.66	1.07
3:U:3025[B]:VAL:HG22	3:U:3047[B]:ARG:HH12	1.19	1.07
3:U:3154[B]:PRO:CG	3:d:2984[B]:THR:CG2	2.25	1.07
3:U:3162[B]:ASP:CG	3:d:3259[B]:ASP:CB	2.17	1.07
3:U:3185[A]:TYR:O	3:U:3186[A]:GLU:OE2	1.72	1.07
3:X:3293[B]:LYS:HD3	3:X:3294[B]:SER:HB3	1.13	1.07
3:C:2965[B]:LEU:O	3:L:3256[B]:TRP:C	1.97	1.07
3:C:3113[A]:ASP:OD2	3:C:3114[A]:PRO:CD	2.02	1.07
3:C:3150[B]:LYS:NZ	3:L:3160[B]:SER:HB2	1.49	1.07
3:C:3172[B]:SER:HB3	3:L:3150[B]:LYS:CA	1.84	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3230[A]:PHE:HB2	3:C:3243[A]:GLY:HA2	1.14	1.07
3:C:3255[B]:PRO:CB	3:L:2964[B]:PRO:O	2.02	1.07
3:F:2946[B]:GLN:OE1	3:F:2947[B]:ALA:N	1.88	1.07
3:F:3159[B]:SER:CA	3:a:3150[B]:LYS:O	2.02	1.07
3:F:3185[A]:TYR:O	3:F:3186[A]:GLU:OE2	1.72	1.07
2:H:2868:GLU:HG2	3:I:2932[A]:PRO:O	1.54	1.07
3:I:3113[A]:ASP:OD2	3:I:3114[A]:PRO:CD	2.02	1.07
3:I:3161[A]:GLU:N	3:I:3161[A]:GLU:OE2	1.88	1.07
3:L:2960[B]:PHE:HD2	3:L:3157[B]:PRO:HG3	1.10	1.07
3:L:3113[A]:ASP:OD2	3:L:3114[A]:PRO:CD	2.02	1.07
3:L:3161[B]:GLU:N	3:L:3161[B]:GLU:OE2	1.88	1.07
3:O:2946[B]:GLN:OE1	3:O:2947[B]:ALA:N	1.88	1.07
3:O:3161[A]:GLU:OE2	3:O:3161[A]:GLU:N	1.88	1.07
3:R:3025[B]:VAL:HG22	3:R:3047[B]:ARG:HH12	1.19	1.07
3:R:3113[B]:ASP:OD2	3:R:3114[B]:PRO:CD	2.02	1.07
3:R:3185[B]:TYR:O	3:R:3186[B]:GLU:OE2	1.72	1.07
3:U:3152[B]:LYS:HG3	3:d:3154[B]:PRO:CB	1.82	1.07
3:d:2930[B]:LEU:H	3:d:2930[B]:LEU:HD22	1.18	1.07
3:d:3113[A]:ASP:OD2	3:d:3114[A]:PRO:CD	2.02	1.07
3:C:2988[B]:TRP:HD1	3:L:3153[B]:LYS:HD3	1.18	1.07
3:C:3093[B]:HIS:CE1	3:L:2971[B]:ASP:CB	2.33	1.07
3:C:3154[B]:PRO:HD3	3:L:3174[B]:GLY:N	1.69	1.07
3:C:3154[B]:PRO:CB	3:L:3174[B]:GLY:CA	2.25	1.07
3:I:2961[B]:HIS:CG	3:R:2969[B]:TYR:CD1	2.40	1.07
3:I:3025[B]:VAL:HG22	3:I:3047[B]:ARG:HH12	1.19	1.07
3:I:3160[B]:SER:H	3:R:3150[B]:LYS:HD3	1.19	1.07
3:I:3172[B]:SER:H	3:R:3152[B]:LYS:CB	1.51	1.07
3:I:3230[A]:PHE:HB2	3:I:3243[A]:GLY:HA2	1.14	1.07
3:L:3113[B]:ASP:OD2	3:L:3114[B]:PRO:CD	2.02	1.07
3:L:3185[A]:TYR:O	3:L:3186[A]:GLU:OE2	1.72	1.07
3:L:3185[B]:TYR:O	3:L:3186[B]:GLU:OE2	1.72	1.07
3:O:2976[B]:ALA:O	3:X:3154[B]:PRO:HG2	0.90	1.07
3:O:3160[B]:SER:N	3:X:3148[B]:ILE:O	1.88	1.07
1:Y:1546:LYS:CG	3:d:3001[B]:LYS:CE	2.31	1.07
3:a:3025[A]:VAL:HG22	3:a:3047[A]:ARG:HH12	1.19	1.07
3:a:3113[A]:ASP:OD2	3:a:3114[A]:PRO:CD	2.02	1.07
3:a:3185[A]:TYR:O	3:a:3186[A]:GLU:OE2	1.72	1.07
3:F:2946[A]:GLN:OE1	3:F:2947[A]:ALA:N	1.88	1.07
3:F:3135[B]:LYS:HG2	3:F:3141[B]:TYR:HE1	1.14	1.07
3:I:2956[B]:LYS:HD2	3:R:3257[B]:ALA:HB3	1.32	1.07
3:I:2982[B]:MET:HG2	3:R:2967[B]:CYS:SG	1.91	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3160[B]:SER:CB	3:R:2983[B]:VAL:H	1.66	1.07
3:I:3217[B]:PHE:CE1	3:I:3230[B]:PHE:HZ	1.71	1.07
3:I:3230[B]:PHE:HB2	3:I:3243[B]:GLY:HA2	1.14	1.07
3:L:3135[B]:LYS:HG2	3:L:3141[B]:TYR:CE1	1.89	1.07
3:L:3161[A]:GLU:N	3:L:3161[A]:GLU:OE2	1.88	1.07
3:O:2975[B]:PHE:C	3:X:3156[B]:MET:HG2	1.78	1.07
3:O:3185[A]:TYR:O	3:O:3186[A]:GLU:OE2	1.72	1.07
3:U:2965[B]:LEU:HB2	3:d:3220[B]:ARG:CZ	1.69	1.07
3:U:3161[A]:GLU:N	3:U:3161[A]:GLU:OE2	1.88	1.07
3:U:3185[B]:TYR:O	3:U:3186[B]:GLU:OE2	1.72	1.07
3:U:3256[B]:TRP:CB	3:d:2969[B]:TYR:CB	2.00	1.07
3:X:2946[B]:GLN:OE1	3:X:2947[B]:ALA:N	1.88	1.07
3:X:3025[A]:VAL:HG22	3:X:3047[A]:ARG:HH12	1.19	1.07
3:X:3217[A]:PHE:CE1	3:X:3230[A]:PHE:HZ	1.71	1.07
3:a:3113[B]:ASP:OD2	3:a:3114[B]:PRO:CD	2.02	1.07
3:d:3230[A]:PHE:HB2	3:d:3243[A]:GLY:HA2	1.14	1.07
3:C:3185[B]:TYR:O	3:C:3186[B]:GLU:OE2	1.72	1.06
3:F:3162[B]:ASP:HB3	3:a:3259[B]:ASP:CB	1.85	1.06
3:I:3135[B]:LYS:HG2	3:I:3141[B]:TYR:HE1	1.14	1.06
3:I:3152[B]:LYS:CB	3:R:3172[B]:SER:N	1.77	1.06
3:L:2946[B]:GLN:OE1	3:L:2947[B]:ALA:N	1.88	1.06
3:O:3251[B]:ASP:CB	3:X:2967[B]:CYS:HA	1.83	1.06
3:R:3113[A]:ASP:OD2	3:R:3114[A]:PRO:CD	2.02	1.06
3:U:2946[A]:GLN:OE1	3:U:2947[A]:ALA:N	1.88	1.06
3:X:3113[A]:ASP:OD2	3:X:3114[A]:PRO:CD	2.02	1.06
3:X:3161[A]:GLU:N	3:X:3161[A]:GLU:OE2	1.88	1.06
3:C:2983[B]:VAL:CG2	3:L:3161[B]:GLU:N	2.08	1.06
3:C:3149[B]:ASN:HD22	3:L:3163[B]:ASN:CG	1.63	1.06
3:C:3150[B]:LYS:HA	3:L:3172[B]:SER:HB3	1.10	1.06
3:C:3153[B]:LYS:HZ3	3:L:2988[B]:TRP:NE1	1.53	1.06
3:C:3161[A]:GLU:OE2	3:C:3161[A]:GLU:N	1.88	1.06
3:F:3135[A]:LYS:HG2	3:F:3141[A]:TYR:HE1	1.14	1.06
3:I:2946[B]:GLN:OE1	3:I:2947[B]:ALA:N	1.88	1.06
3:I:3153[B]:LYS:C	3:R:3155[B]:MET:CG	2.22	1.06
3:I:3153[B]:LYS:CB	3:R:3155[B]:MET:HB2	1.84	1.06
3:I:3259[B]:ASP:HB3	3:R:3162[B]:ASP:CB	1.84	1.06
3:R:2946[B]:GLN:OE1	3:R:2947[B]:ALA:N	1.88	1.06
3:R:3135[B]:LYS:HG2	3:R:3141[B]:TYR:CE1	1.89	1.06
3:R:3185[A]:TYR:O	3:R:3186[A]:GLU:OE2	1.72	1.06
3:U:3217[A]:PHE:CE1	3:U:3230[A]:PHE:HZ	1.71	1.06
3:X:3135[B]:LYS:HG2	3:X:3141[B]:TYR:CE1	1.89	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:2930[B]:LEU:H	3:a:2930[B]:LEU:HD22	1.18	1.06
3:d:2946[B]:GLN:OE1	3:d:2947[B]:ALA:N	1.88	1.06
3:C:2985[B]:PHE:HE2	3:L:2969[B]:TYR:C	1.60	1.06
3:C:3135[A]:LYS:HG2	3:C:3141[A]:TYR:HE1	1.14	1.06
3:F:2966[B]:SER:HB2	3:a:3254[B]:MET:HG3	1.09	1.06
3:F:3150[B]:LYS:HE3	3:a:3163[B]:ASN:CB	1.84	1.06
3:F:3157[B]:PRO:O	3:a:3150[B]:LYS:HE2	1.49	1.06
3:I:2956[B]:LYS:C	3:I:2960[B]:PHE:HE1	1.63	1.06
3:I:2975[B]:PHE:HZ	3:R:2961[B]:HIS:CG	1.66	1.06
3:I:3150[B]:LYS:NZ	3:R:3160[B]:SER:HB3	1.70	1.06
3:I:3160[B]:SER:OG	3:R:2982[B]:MET:HA	1.52	1.06
3:I:3185[B]:TYR:O	3:I:3186[B]:GLU:OE2	1.72	1.06
3:I:3251[B]:ASP:O	3:R:3252[B]:TYR:CB	1.88	1.06
3:O:2969[B]:TYR:CB	3:X:3158[B]:PHE:CE1	2.39	1.06
3:R:3217[A]:PHE:CE1	3:R:3230[A]:PHE:HZ	1.71	1.06
3:U:3025[A]:VAL:HG22	3:U:3047[A]:ARG:HH12	1.19	1.06
3:a:2956[A]:LYS:C	3:a:2960[A]:PHE:HE1	1.64	1.06
2:c:2867:PRO:HG3	3:d:2932[A]:PRO:CG	1.85	1.06
3:d:2961[A]:HIS:NE2	3:d:2980[A]:HIS:NE2	2.04	1.06
3:d:2961[B]:HIS:NE2	3:d:2980[B]:HIS:NE2	2.04	1.06
3:C:3024[B]:LEU:HD12	3:C:3025[B]:VAL:H	0.89	1.06
3:C:3154[B]:PRO:CA	3:L:3153[B]:LYS:O	2.04	1.06
3:C:3172[B]:SER:CB	3:L:3152[B]:LYS:H	1.68	1.06
3:F:2967[B]:CYS:N	3:a:3256[B]:TRP:CD1	2.21	1.06
3:F:2970[B]:PRO:HD3	3:a:2989[B]:HIS:NE2	1.59	1.06
3:F:3222[B]:ILE:HD12	3:F:3223[B]:GLY:H	1.20	1.06
3:I:3155[B]:MET:SD	3:R:3154[B]:PRO:HG2	1.96	1.06
3:I:3162[B]:ASP:HB3	3:R:3259[B]:ASP:CB	1.86	1.06
3:O:2970[B]:PRO:C	3:X:2989[B]:HIS:N	1.96	1.06
3:O:3108[B]:HIS:CB	3:X:2969[B]:TYR:O	2.00	1.06
3:U:2956[A]:LYS:C	3:U:2960[A]:PHE:HE1	1.64	1.06
3:U:2961[A]:HIS:NE2	3:U:2980[A]:HIS:NE2	2.04	1.06
3:U:2961[B]:HIS:NE2	3:U:2980[B]:HIS:NE2	2.03	1.06
3:U:3161[B]:GLU:OE2	3:U:3161[B]:GLU:N	1.88	1.06
3:X:2946[A]:GLN:OE1	3:X:2947[A]:ALA:N	1.88	1.06
3:X:3185[B]:TYR:O	3:X:3186[B]:GLU:OE2	1.72	1.06
3:d:3161[A]:GLU:N	3:d:3161[A]:GLU:OE2	1.88	1.06
3:C:2946[B]:GLN:OE1	3:C:2947[B]:ALA:N	1.88	1.06
3:C:2963[B]:MET:HE1	3:L:3223[B]:GLY:H	1.21	1.06
3:C:3135[B]:LYS:HG2	3:C:3141[B]:TYR:HE1	1.14	1.06
3:F:2975[B]:PHE:O	3:a:3253[B]:GLU:CB	1.94	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3113[B]:ASP:OD2	3:F:3114[B]:PRO:CD	2.02	1.06
3:I:2961[A]:HIS:NE2	3:I:2980[A]:HIS:NE2	2.03	1.06
3:I:2975[B]:PHE:CZ	3:R:2961[B]:HIS:CA	2.37	1.06
3:I:3135[A]:LYS:HG2	3:I:3141[A]:TYR:CE1	1.89	1.06
3:L:2930[A]:LEU:HD22	3:L:2930[A]:LEU:H	1.18	1.06
3:O:2961[A]:HIS:NE2	3:O:2980[A]:HIS:NE2	2.04	1.06
3:O:3135[A]:LYS:HG2	3:O:3141[A]:TYR:CE1	1.89	1.06
3:O:3252[B]:TYR:HB3	3:X:3156[B]:MET:HB2	1.31	1.06
3:R:3161[A]:GLU:OE2	3:R:3161[A]:GLU:N	1.88	1.06
3:U:3217[B]:PHE:CE1	3:U:3230[B]:PHE:HZ	1.71	1.06
3:C:2946[A]:GLN:OE1	3:C:2947[A]:ALA:N	1.88	1.05
3:C:2956[A]:LYS:C	3:C:2960[A]:PHE:HE1	1.64	1.05
3:C:2983[B]:VAL:HG21	3:L:3161[B]:GLU:OE2	1.26	1.05
3:C:3024[A]:LEU:HD12	3:C:3025[A]:VAL:H	0.89	1.05
3:C:3222[B]:ILE:HD12	3:C:3223[B]:GLY:H	1.20	1.05
3:F:2956[B]:LYS:C	3:F:2960[B]:PHE:HE1	1.64	1.05
3:F:3024[B]:LEU:HD12	3:F:3025[B]:VAL:H	0.89	1.05
3:F:3153[B]:LYS:HZ1	3:a:3157[B]:PRO:CD	1.68	1.05
3:I:2961[B]:HIS:CA	3:R:2975[B]:PHE:HZ	1.69	1.05
3:I:3256[B]:TRP:HB3	3:R:2966[B]:SER:CA	1.86	1.05
3:R:2956[A]:LYS:C	3:R:2960[A]:PHE:HE1	1.63	1.05
3:R:3024[A]:LEU:HD12	3:R:3025[A]:VAL:H	0.89	1.05
3:R:3222[A]:ILE:HD12	3:R:3223[A]:GLY:H	1.20	1.05
3:U:2975[B]:PHE:CD2	3:d:3256[B]:TRP:HD1	1.72	1.05
3:U:3024[A]:LEU:HD12	3:U:3025[A]:VAL:H	0.89	1.05
3:X:3222[A]:ILE:HD12	3:X:3223[A]:GLY:H	1.20	1.05
3:a:2956[B]:LYS:C	3:a:2960[B]:PHE:HE1	1.64	1.05
3:a:3135[A]:LYS:HG2	3:a:3141[A]:TYR:CE1	1.89	1.05
3:d:3161[B]:GLU:OE2	3:d:3161[B]:GLU:N	1.88	1.05
3:d:3185[A]:TYR:O	3:d:3186[A]:GLU:OE2	1.72	1.05
3:C:3155[B]:MET:SD	3:L:3154[B]:PRO:HD2	1.96	1.05
3:C:3156[B]:MET:SD	3:L:2982[B]:MET:HG3	1.96	1.05
3:C:3161[B]:GLU:N	3:C:3161[B]:GLU:OE2	1.88	1.05
3:C:3185[A]:TYR:O	3:C:3186[A]:GLU:OE2	1.72	1.05
3:F:3217[A]:PHE:CE1	3:F:3230[A]:PHE:HZ	1.71	1.05
3:I:2960[A]:PHE:HD2	3:I:3157[A]:PRO:HG3	1.10	1.05
3:I:2989[B]:HIS:NE2	3:R:2969[B]:TYR:CA	2.20	1.05
3:I:3150[B]:LYS:HG2	3:R:3158[B]:PHE:HA	1.29	1.05
3:L:2930[B]:LEU:H	3:L:2930[B]:LEU:HD22	1.18	1.05
3:O:3160[B]:SER:CB	3:X:3151[B]:LEU:H	1.67	1.05
3:R:3222[B]:ILE:HD12	3:R:3223[B]:GLY:H	1.20	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2956[B]:LYS:C	3:U:2960[B]:PHE:HE1	1.64	1.05
3:U:3135[B]:LYS:HG2	3:U:3141[B]:TYR:HE1	1.14	1.05
3:X:2960[B]:PHE:HD2	3:X:3157[B]:PRO:HG3	1.10	1.05
3:a:2946[A]:GLN:OE1	3:a:2947[A]:ALA:N	1.88	1.05
1:A:416:ASN:CG	3:F:3196[A]:THR:HG21	1.81	1.05
3:C:2930[A]:LEU:H	3:C:2930[A]:LEU:HD22	1.18	1.05
3:C:2961[A]:HIS:NE2	3:C:2980[A]:HIS:NE2	2.04	1.05
3:C:3174[B]:GLY:CA	3:L:3154[B]:PRO:HD3	1.86	1.05
3:C:3222[A]:ILE:HD12	3:C:3223[A]:GLY:H	1.20	1.05
3:F:2982[B]:MET:CE	3:a:2977[B]:CYS:HB2	1.85	1.05
3:I:2969[B]:TYR:OH	3:R:3116[B]:PHE:CD1	0.78	1.05
3:I:3149[B]:ASN:ND2	3:R:3163[B]:ASN:CG	2.14	1.05
3:I:3156[B]:MET:HB2	3:R:2982[B]:MET:CG	1.86	1.05
3:I:3251[B]:ASP:HB2	3:R:3251[B]:ASP:HB3	1.36	1.05
3:O:2946[A]:GLN:OE1	3:O:2947[A]:ALA:N	1.88	1.05
3:O:3156[B]:MET:CG	3:X:3173[B]:THR:HG23	1.86	1.05
3:O:3160[B]:SER:HA	3:X:3151[B]:LEU:HD12	1.34	1.05
3:R:2961[A]:HIS:NE2	3:R:2980[A]:HIS:NE2	2.04	1.05
3:U:3135[A]:LYS:HG2	3:U:3141[A]:TYR:CE1	1.89	1.05
3:U:3169[B]:LYS:HE2	3:d:3146[B]:CYS:CA	1.84	1.05
3:U:3220[B]:ARG:HG2	3:d:2973[B]:THR:HG22	1.36	1.05
3:X:2948[A]:ASP:HB3	3:X:2953[A]:GLY:HA3	1.39	1.05
3:X:2961[B]:HIS:NE2	3:X:2980[B]:HIS:NE2	2.04	1.05
3:X:3161[B]:GLU:N	3:X:3161[B]:GLU:OE2	1.88	1.05
3:a:2946[B]:GLN:OE1	3:a:2947[B]:ALA:N	1.88	1.05
3:a:3161[B]:GLU:N	3:a:3161[B]:GLU:OE2	1.88	1.05
3:C:2988[B]:TRP:HE1	3:L:3153[B]:LYS:NZ	1.55	1.05
3:C:3135[A]:LYS:HG2	3:C:3141[A]:TYR:CE1	1.89	1.05
3:C:3150[B]:LYS:C	3:L:3172[B]:SER:CB	2.29	1.05
3:C:3153[B]:LYS:O	3:L:3154[B]:PRO:CA	2.05	1.05
3:C:3160[B]:SER:HB3	3:L:3150[B]:LYS:NZ	1.53	1.05
3:F:3185[B]:TYR:O	3:F:3186[B]:GLU:OE2	1.72	1.05
3:F:3251[B]:ASP:CB	3:a:3251[B]:ASP:CB	1.76	1.05
3:I:2956[A]:LYS:C	3:I:2960[A]:PHE:HE1	1.64	1.05
3:I:3024[A]:LEU:HD12	3:I:3025[A]:VAL:H	0.89	1.05
3:I:3135[B]:LYS:HG2	3:I:3141[B]:TYR:CE1	1.89	1.05
3:I:3259[B]:ASP:HB3	3:R:3162[B]:ASP:HB3	1.07	1.05
3:O:2961[B]:HIS:NE2	3:O:2980[B]:HIS:NE2	2.03	1.05
3:O:2963[B]:MET:HE3	3:X:2975[B]:PHE:CD1	1.86	1.05
3:O:3158[B]:PHE:N	3:X:3152[B]:LYS:CB	2.19	1.05
3:O:3163[B]:ASN:CA	3:X:3149[B]:ASN:HB3	1.84	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3135[A]:LYS:HG2	3:U:3141[A]:TYR:HE1	1.14	1.05
3:a:3161[A]:GLU:N	3:a:3161[A]:GLU:OE2	1.88	1.05
3:a:3185[B]:TYR:O	3:a:3186[B]:GLU:OE2	1.72	1.05
3:d:3025[A]:VAL:HG22	3:d:3047[A]:ARG:HH12	1.19	1.05
3:d:3141[B]:TYR:CD2	3:d:3142[B]:ASN:N	2.24	1.05
3:d:3217[A]:PHE:CE1	3:d:3230[A]:PHE:HZ	1.71	1.05
3:C:2948[B]:ASP:HB3	3:C:2953[B]:GLY:HA3	1.39	1.05
3:F:2959[B]:SER:CB	3:a:3255[B]:PRO:HB2	1.87	1.05
3:F:2961[A]:HIS:NE2	3:F:2980[A]:HIS:NE2	2.03	1.05
3:F:2981[B]:GLY:CA	3:a:2968[B]:GLN:OE1	2.05	1.05
3:F:3170[B]:ALA:O	3:a:3152[B]:LYS:HD2	0.89	1.05
3:F:3256[B]:TRP:HB3	3:a:2966[B]:SER:HA	1.09	1.05
3:I:2959[B]:SER:CA	3:R:3255[B]:PRO:HB2	1.80	1.05
3:I:2964[B]:PRO:CB	3:R:3221[B]:ALA:HB3	1.86	1.05
3:I:2971[B]:ASP:OD2	3:R:3110[B]:THR:HG21	1.56	1.05
3:I:3141[B]:TYR:CD2	3:I:3142[B]:ASN:N	2.24	1.05
3:L:2956[B]:LYS:C	3:L:2960[B]:PHE:HE1	1.64	1.05
3:L:3024[B]:LEU:HD12	3:L:3025[B]:VAL:H	0.89	1.05
3:O:3101[B]:PRO:HB2	3:X:2971[B]:ASP:O	0.87	1.05
3:O:3141[A]:TYR:CD2	3:O:3142[A]:ASN:N	2.23	1.05
3:O:3253[B]:GLU:CD	3:X:3161[B]:GLU:OE1	1.99	1.05
3:R:2948[A]:ASP:HB3	3:R:2953[A]:GLY:HA3	1.39	1.05
3:d:2946[A]:GLN:OE1	3:d:2947[A]:ALA:N	1.88	1.05
3:d:3025[B]:VAL:HG22	3:d:3047[B]:ARG:HH12	1.19	1.05
3:d:3135[A]:LYS:HG2	3:d:3141[A]:TYR:CE1	1.89	1.05
3:d:3185[B]:TYR:O	3:d:3186[B]:GLU:OE2	1.72	1.05
3:C:2978[B]:CYS:N	3:L:3254[B]:MET:HB3	1.19	1.04
3:C:3147[B]:GLU:CG	3:L:3161[B]:GLU:CA	2.29	1.04
3:C:3154[B]:PRO:C	3:L:3153[B]:LYS:O	2.00	1.04
3:C:3163[B]:ASN:ND2	3:L:3149[B]:ASN:HB2	1.68	1.04
3:C:3163[B]:ASN:HD21	3:L:3149[B]:ASN:HB3	1.09	1.04
3:C:3169[B]:LYS:HE3	3:L:3149[B]:ASN:OD1	1.51	1.04
3:C:3172[B]:SER:OG	3:L:3152[B]:LYS:HG3	1.57	1.04
3:F:2930[B]:LEU:H	3:F:2930[B]:LEU:HD22	1.18	1.04
3:F:2948[B]:ASP:HB3	3:F:2953[B]:GLY:HA3	1.39	1.04
3:F:2956[A]:LYS:C	3:F:2960[A]:PHE:HE1	1.64	1.04
3:F:3150[B]:LYS:HZ3	3:a:3160[B]:SER:CB	1.66	1.04
3:I:2946[A]:GLN:OE1	3:I:2947[A]:ALA:N	1.88	1.04
3:I:3090[B]:ASN:HB3	3:R:2972[B]:GLY:HA3	1.37	1.04
3:I:3141[A]:TYR:CD2	3:I:3142[A]:ASN:N	2.24	1.04
3:L:2946[A]:GLN:OE1	3:L:2947[A]:ALA:N	1.88	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2956[A]:LYS:C	3:L:2960[A]:PHE:HE1	1.64	1.04
3:L:2961[A]:HIS:NE2	3:L:2980[A]:HIS:NE2	2.04	1.04
3:L:2966[B]:SER:HB2	3:L:2977[B]:CYS:HB2	1.39	1.04
3:L:3135[A]:LYS:HG2	3:L:3141[A]:TYR:CE1	1.89	1.04
3:O:2948[A]:ASP:HB3	3:O:2953[A]:GLY:HA3	1.39	1.04
3:O:2956[A]:LYS:C	3:O:2960[A]:PHE:HE1	1.64	1.04
3:O:2970[B]:PRO:HG2	3:X:2991[B]:LEU:HA	1.32	1.04
3:R:2956[B]:LYS:C	3:R:2960[B]:PHE:HE1	1.64	1.04
3:R:2966[A]:SER:HB2	3:R:2977[A]:CYS:HB2	1.39	1.04
3:R:3135[B]:LYS:HG2	3:R:3141[B]:TYR:HE1	1.14	1.04
3:U:2946[B]:GLN:OE1	3:U:2947[B]:ALA:N	1.88	1.04
3:U:3176[B]:LYS:HD2	3:d:3152[B]:LYS:HD2	1.07	1.04
3:a:3025[B]:VAL:HG22	3:a:3047[B]:ARG:HH12	1.19	1.04
3:C:2956[B]:LYS:C	3:C:2960[B]:PHE:HE1	1.64	1.04
3:F:3155[B]:MET:CB	3:a:3153[B]:LYS:CG	2.21	1.04
3:F:3161[A]:GLU:N	3:F:3161[A]:GLU:OE2	1.88	1.04
3:I:3025[A]:VAL:HG22	3:I:3047[A]:ARG:HH12	1.19	1.04
3:I:3038[B]:ILE:HG12	3:I:3112[B]:TYR:CD2	1.93	1.04
3:I:3196[A]:THR:HG21	1:J:416:ASN:CG	1.81	1.04
3:U:3255[B]:PRO:HB2	3:d:2975[B]:PHE:HA	1.37	1.04
3:X:2948[B]:ASP:HB3	3:X:2953[B]:GLY:HA3	1.39	1.04
3:X:2961[A]:HIS:NE2	3:X:2980[A]:HIS:NE2	2.04	1.04
3:X:3024[A]:LEU:HD12	3:X:3025[A]:VAL:H	0.89	1.04
1:Y:1616:LYS:CD	3:d:3187[B]:TYR:HA	1.79	1.04
3:a:2948[A]:ASP:HB3	3:a:2953[A]:GLY:HA3	1.39	1.04
3:C:2985[B]:PHE:CE2	3:L:2970[B]:PRO:N	2.26	1.04
3:C:3147[B]:GLU:HG3	3:L:3160[B]:SER:O	0.87	1.04
3:C:3160[B]:SER:HB3	3:L:3150[B]:LYS:HZ2	1.00	1.04
3:C:3169[B]:LYS:HG3	3:L:3149[B]:ASN:CG	1.67	1.04
3:C:3259[B]:ASP:CG	3:L:3162[B]:ASP:OD1	1.98	1.04
3:F:3147[B]:GLU:OE1	3:a:3162[B]:ASP:C	1.99	1.04
3:I:3153[B]:LYS:HD2	3:R:3155[B]:MET:CB	1.86	1.04
3:I:3185[A]:TYR:O	3:I:3186[A]:GLU:OE2	1.72	1.04
3:I:3256[B]:TRP:NE1	3:R:2965[B]:LEU:HB3	1.41	1.04
3:R:2946[A]:GLN:OE1	3:R:2947[A]:ALA:N	1.88	1.04
3:R:2966[B]:SER:HB2	3:R:2977[B]:CYS:HB2	1.39	1.04
3:R:3038[A]:ILE:HG12	3:R:3112[A]:TYR:CD2	1.93	1.04
3:R:3135[A]:LYS:HG2	3:R:3141[A]:TYR:CE1	1.89	1.04
3:R:3141[A]:TYR:CD2	3:R:3142[A]:ASN:N	2.24	1.04
3:U:2965[B]:LEU:CD1	3:d:3256[B]:TRP:O	2.06	1.04
3:U:2969[B]:TYR:N	3:d:3256[B]:TRP:CE2	2.02	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2956[A]:LYS:C	3:d:2960[A]:PHE:HE1	1.64	1.04
3:C:3038[B]:ILE:HG12	3:C:3112[B]:TYR:CD2	1.93	1.04
3:C:3153[B]:LYS:NZ	3:L:3158[B]:PHE:HD2	1.49	1.04
3:C:3156[B]:MET:CE	3:L:2979[B]:GLN:CG	1.93	1.04
3:F:2966[B]:SER:HA	3:a:3255[B]:PRO:C	1.82	1.04
3:F:3038[B]:ILE:HG12	3:F:3112[B]:TYR:CD2	1.93	1.04
3:F:3161[B]:GLU:HA	3:a:3147[B]:GLU:CG	1.87	1.04
3:F:3163[B]:ASN:HD22	3:a:3150[B]:LYS:HG3	1.17	1.04
2:H:2868:GLU:OE2	3:I:2932[A]:PRO:O	1.75	1.04
3:I:2930[B]:LEU:H	3:I:2930[B]:LEU:HD22	1.18	1.04
3:I:3024[B]:LEU:HD12	3:I:3025[B]:VAL:H	0.89	1.04
3:I:3149[B]:ASN:HD22	3:R:3163[B]:ASN:CG	1.65	1.04
3:L:2948[B]:ASP:HB3	3:L:2953[B]:GLY:HA3	1.39	1.04
3:O:2956[B]:LYS:C	3:O:2960[B]:PHE:HE1	1.64	1.04
3:O:3106[B]:THR:HG21	3:X:2970[B]:PRO:O	1.57	1.04
3:U:2973[B]:THR:HG22	3:d:3222[B]:ILE:CG2	1.87	1.04
3:U:3169[B]:LYS:CG	3:d:3148[B]:ILE:N	2.05	1.04
3:X:2956[A]:LYS:C	3:X:2960[A]:PHE:HE1	1.64	1.04
3:a:2961[A]:HIS:NE2	3:a:2980[A]:HIS:NE2	2.04	1.04
3:a:3024[B]:LEU:HD12	3:a:3025[B]:VAL:H	0.89	1.04
3:d:2930[A]:LEU:HD22	3:d:2930[A]:LEU:H	1.18	1.04
3:d:3024[B]:LEU:HD12	3:d:3025[B]:VAL:H	0.89	1.04
3:d:3038[A]:ILE:HG12	3:d:3112[A]:TYR:CD2	1.93	1.04
3:d:3141[A]:TYR:CD2	3:d:3142[A]:ASN:N	2.24	1.04
3:C:2963[B]:MET:HE1	3:L:3222[B]:ILE:HD12	1.38	1.04
3:C:3038[A]:ILE:HG12	3:C:3112[A]:TYR:CD2	1.93	1.04
3:C:3141[A]:TYR:CD2	3:C:3142[A]:ASN:N	2.24	1.04
3:F:3153[B]:LYS:HB2	3:a:3158[B]:PHE:HB2	1.38	1.04
3:I:2968[B]:GLN:NE2	3:R:3086[B]:GLU:HG2	1.21	1.04
3:I:3156[B]:MET:CB	3:R:2982[B]:MET:HG3	1.87	1.04
3:L:3038[A]:ILE:HG12	3:L:3112[A]:TYR:CD2	1.93	1.04
3:L:3307[A]:PHE:HE1	3:L:3309[A]:PRO:HG3	1.23	1.04
3:O:3025[A]:VAL:HG22	3:O:3047[A]:ARG:HH12	1.19	1.04
3:O:3135[B]:LYS:HG2	3:O:3141[B]:TYR:CE1	1.89	1.04
3:U:2971[B]:ASP:O	3:d:3247[B]:VAL:CA	2.05	1.04
3:U:3307[B]:PHE:HE1	3:U:3309[B]:PRO:HG3	1.23	1.04
3:X:2930[B]:LEU:H	3:X:2930[B]:LEU:HD22	1.18	1.04
3:a:3038[A]:ILE:HG12	3:a:3112[A]:TYR:CD2	1.93	1.04
3:d:3024[A]:LEU:HD12	3:d:3025[A]:VAL:H	0.89	1.04
3:C:2961[B]:HIS:NE2	3:C:2980[B]:HIS:NE2	2.03	1.03
3:C:2966[A]:SER:HB2	3:C:2977[A]:CYS:HB2	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3141[B]:TYR:CD2	3:C:3142[B]:ASN:N	2.24	1.03
3:C:3158[B]:PHE:CE2	3:L:3153[B]:LYS:HE2	1.92	1.03
3:F:3024[A]:LEU:HD12	3:F:3025[A]:VAL:H	0.89	1.03
3:F:3253[B]:GLU:HB2	3:a:2975[B]:PHE:O	1.55	1.03
1:G:1636:ASN:OD1	6:r:1:NAG:C8	2.05	1.03
2:H:2868:GLU:CD	3:I:2932[A]:PRO:O	2.01	1.03
3:I:2959[B]:SER:HB2	3:R:3255[B]:PRO:CB	1.86	1.03
3:I:3038[A]:ILE:HG12	3:I:3112[A]:TYR:CD2	1.93	1.03
3:L:3307[B]:PHE:HE1	3:L:3309[B]:PRO:HG3	1.23	1.03
3:O:2969[B]:TYR:CB	3:X:3158[B]:PHE:CZ	2.40	1.03
3:O:2975[B]:PHE:HE2	3:X:3172[B]:SER:CA	1.71	1.03
1:S:416:ASN:OD1	3:X:3196[A]:THR:OG1	1.74	1.03
3:X:3025[B]:VAL:HG22	3:X:3047[B]:ARG:HH12	1.19	1.03
3:a:2966[A]:SER:HB2	3:a:2977[A]:CYS:HB2	1.39	1.03
3:a:3038[B]:ILE:HG12	3:a:3112[B]:TYR:CD2	1.93	1.03
3:a:3135[B]:LYS:HG2	3:a:3141[B]:TYR:CE1	1.89	1.03
3:a:3135[B]:LYS:HG2	3:a:3141[B]:TYR:HE1	1.14	1.03
3:a:3307[A]:PHE:HE1	3:a:3309[A]:PRO:HG3	1.23	1.03
3:d:3222[A]:ILE:HD12	3:d:3223[A]:GLY:H	1.20	1.03
3:C:3154[B]:PRO:CD	3:L:3174[B]:GLY:N	2.21	1.03
3:C:3161[B]:GLU:OE2	3:L:2983[B]:VAL:CG2	2.07	1.03
3:F:2948[B]:ASP:H	3:F:2949[B]:LYS:HA	1.23	1.03
3:F:3153[B]:LYS:CD	3:a:3155[B]:MET:HB3	1.88	1.03
3:F:3161[B]:GLU:HG3	3:a:3079[B]:CYS:SG	1.93	1.03
3:I:2948[A]:ASP:H	3:I:2949[A]:LYS:HA	1.23	1.03
3:I:3159[B]:SER:CA	3:R:3150[B]:LYS:O	2.05	1.03
3:I:3162[B]:ASP:HB3	3:R:3259[B]:ASP:HB3	1.37	1.03
3:I:3251[B]:ASP:O	3:R:3252[B]:TYR:HB2	1.54	1.03
3:L:3217[A]:PHE:CE1	3:L:3230[A]:PHE:HZ	1.71	1.03
3:O:2965[B]:LEU:HD12	3:X:2979[B]:GLN:OE1	0.86	1.03
3:R:3307[B]:PHE:HE1	3:R:3309[B]:PRO:HG3	1.23	1.03
3:U:2965[B]:LEU:O	3:d:3257[B]:ALA:HB1	1.56	1.03
3:U:3024[B]:LEU:HD12	3:U:3025[B]:VAL:H	0.89	1.03
3:X:2956[B]:LYS:C	3:X:2960[B]:PHE:HE1	1.64	1.03
3:X:3038[A]:ILE:HG12	3:X:3112[A]:TYR:CD2	1.93	1.03
1:Y:1656:ASP:O	3:d:2937[B]:ASN:ND2	1.91	1.03
3:C:2975[B]:PHE:C	3:L:3253[B]:GLU:HB2	1.84	1.03
3:C:3025[B]:VAL:HG22	3:C:3047[B]:ARG:HH12	1.19	1.03
3:C:3163[B]:ASN:H	3:L:3147[B]:GLU:CD	1.66	1.03
3:F:2968[B]:GLN:HG2	3:a:2981[B]:GLY:N	1.72	1.03
3:I:2982[B]:MET:HG3	3:R:2967[B]:CYS:SG	1.94	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3150[B]:LYS:HD3	3:R:3160[B]:SER:H	1.20	1.03
3:I:3154[B]:PRO:HB3	3:R:3174[B]:GLY:HA2	1.40	1.03
3:I:3222[A]:ILE:HD12	3:I:3223[A]:GLY:H	1.20	1.03
3:L:2948[A]:ASP:HB3	3:L:2953[A]:GLY:HA3	1.39	1.03
3:L:3222[B]:ILE:HD12	3:L:3223[B]:GLY:H	1.20	1.03
3:O:2975[B]:PHE:C	3:X:3156[B]:MET:CG	2.31	1.03
3:O:3040[B]:VAL:CG2	3:X:2969[B]:TYR:CE1	2.42	1.03
3:O:3222[A]:ILE:HD12	3:O:3223[A]:GLY:H	1.20	1.03
3:R:2951[B]:ASP:O	3:R:2956[B]:LYS:NZ	1.92	1.03
3:R:3038[B]:ILE:HG12	3:R:3112[B]:TYR:CD2	1.93	1.03
3:U:2966[B]:SER:HB2	3:U:2977[B]:CYS:HB2	1.39	1.03
3:U:3154[B]:PRO:HG3	3:d:2984[B]:THR:HG21	1.20	1.03
3:a:3024[A]:LEU:HD12	3:a:3025[A]:VAL:H	0.89	1.03
3:a:3307[B]:PHE:HE1	3:a:3309[B]:PRO:HG3	1.23	1.03
3:d:2956[B]:LYS:C	3:d:2960[B]:PHE:HE1	1.64	1.03
3:d:3298[B]:ASN:ND2	3:d:3301[B]:PRO:HA	1.74	1.03
3:C:2951[B]:ASP:O	3:C:2956[B]:LYS:NZ	1.92	1.03
3:C:2969[B]:TYR:CA	3:L:2985[B]:PHE:HE2	1.71	1.03
3:F:3025[A]:VAL:HG22	3:F:3047[A]:ARG:HH12	1.19	1.03
3:F:3162[B]:ASP:CB	3:a:3259[B]:ASP:HB3	1.88	1.03
3:F:3217[B]:PHE:CE1	3:F:3230[B]:PHE:HZ	1.71	1.03
3:F:3298[B]:ASN:ND2	3:F:3301[B]:PRO:HA	1.74	1.03
3:I:2951[B]:ASP:O	3:I:2956[B]:LYS:NZ	1.92	1.03
3:L:3298[A]:ASN:ND2	3:L:3301[A]:PRO:HA	1.74	1.03
3:O:3038[B]:ILE:HG12	3:O:3112[B]:TYR:CD2	1.93	1.03
3:O:3217[B]:PHE:CE1	3:O:3230[B]:PHE:HZ	1.71	1.03
3:R:2948[B]:ASP:HB3	3:R:2953[B]:GLY:HA3	1.39	1.03
3:U:2948[A]:ASP:HB3	3:U:2953[A]:GLY:HA3	1.39	1.03
3:U:2965[B]:LEU:HD12	3:d:3220[B]:ARG:HA	1.04	1.03
3:U:2969[B]:TYR:OH	3:d:3107[B]:LEU:HD12	1.58	1.03
3:U:3038[A]:ILE:HG12	3:U:3112[A]:TYR:CD2	1.93	1.03
3:U:3169[B]:LYS:C	3:d:3148[B]:ILE:CB	2.30	1.03
3:X:3135[A]:LYS:HG2	3:X:3141[A]:TYR:CE1	1.89	1.03
3:d:2951[A]:ASP:O	3:d:2956[A]:LYS:NZ	1.92	1.03
3:C:2961[B]:HIS:CE1	3:C:2980[B]:HIS:HE2	1.77	1.03
3:C:2982[B]:MET:HB3	3:L:3156[B]:MET:CB	1.74	1.03
3:C:2983[B]:VAL:HG21	3:L:3160[B]:SER:C	1.83	1.03
3:C:3156[B]:MET:HB3	3:L:2982[B]:MET:HB3	1.39	1.03
3:F:2948[A]:ASP:H	3:F:2949[A]:LYS:HA	1.23	1.03
3:F:2966[B]:SER:HB2	3:a:3254[B]:MET:CG	1.87	1.03
3:F:2982[B]:MET:HE2	3:a:2967[B]:CYS:SG	1.91	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3141[B]:TYR:CD2	3:F:3142[B]:ASN:N	2.23	1.03
3:F:3172[B]:SER:N	3:a:3152[B]:LYS:HB2	1.72	1.03
3:I:2930[A]:LEU:HD22	3:I:2930[A]:LEU:H	1.18	1.03
3:I:2975[B]:PHE:HA	3:R:3107[B]:LEU:CD2	1.88	1.03
3:I:2979[B]:GLN:HA	3:R:2977[B]:CYS:SG	1.98	1.03
3:I:3155[B]:MET:HB2	3:R:3153[B]:LYS:HD2	1.07	1.03
3:L:3151[A]:LEU:HB2	3:L:3175[A]:TYR:CE2	1.94	1.03
3:L:3298[B]:ASN:ND2	3:L:3301[B]:PRO:HA	1.74	1.03
3:O:2948[A]:ASP:H	3:O:2949[A]:LYS:HA	1.23	1.03
3:O:3024[B]:LEU:HD12	3:O:3025[B]:VAL:H	0.89	1.03
3:R:3217[B]:PHE:CE1	3:R:3230[B]:PHE:HZ	1.71	1.03
3:U:3151[A]:LEU:HB2	3:U:3175[A]:TYR:CE2	1.94	1.03
3:X:2948[A]:ASP:H	3:X:2949[A]:LYS:HA	1.24	1.03
3:X:2951[B]:ASP:O	3:X:2956[B]:LYS:NZ	1.92	1.03
3:X:2966[A]:SER:HB2	3:X:2977[A]:CYS:HB2	1.39	1.03
3:X:3298[A]:ASN:ND2	3:X:3301[A]:PRO:HA	1.74	1.03
1:Y:1401:ARG:CD	3:d:3182[B]:GLN:OE1	2.07	1.03
3:a:3151[A]:LEU:HB2	3:a:3175[A]:TYR:CE2	1.94	1.03
3:a:3298[B]:ASN:ND2	3:a:3301[B]:PRO:HA	1.74	1.03
3:C:3147[B]:GLU:HG3	3:L:3160[B]:SER:C	1.82	1.02
3:C:3153[B]:LYS:HB3	3:L:3155[B]:MET:N	1.71	1.02
3:C:3298[B]:ASN:HB3	3:C:3300[B]:LEU:HD23	1.41	1.02
3:F:2974[B]:ALA:H	3:a:3249[B]:GLY:N	1.46	1.02
3:F:3038[A]:ILE:HG12	3:F:3112[A]:TYR:CD2	1.93	1.02
3:F:3151[A]:LEU:HB2	3:F:3175[A]:TYR:CE2	1.94	1.02
3:I:2948[B]:ASP:H	3:I:2949[B]:LYS:HA	1.23	1.02
3:I:2961[B]:HIS:NE2	3:I:2980[B]:HIS:NE2	2.04	1.02
3:I:3222[B]:ILE:HD12	3:I:3223[B]:GLY:H	1.20	1.02
3:I:3255[B]:PRO:CD	3:R:2962[B]:GLY:O	2.07	1.02
3:L:3038[B]:ILE:HG12	3:L:3112[B]:TYR:CD2	1.93	1.02
3:O:2961[A]:HIS:CE1	3:O:2980[A]:HIS:HE2	1.77	1.02
3:O:2969[B]:TYR:HB3	3:X:3158[B]:PHE:CZ	1.95	1.02
3:O:3038[A]:ILE:HG12	3:O:3112[A]:TYR:CD2	1.93	1.02
3:O:3038[B]:ILE:CG2	3:X:2969[B]:TYR:CE1	2.42	1.02
3:O:3151[A]:LEU:HB2	3:O:3175[A]:TYR:CE2	1.94	1.02
3:O:3160[B]:SER:N	3:X:3148[B]:ILE:C	2.16	1.02
3:U:2968[B]:GLN:N	3:d:3256[B]:TRP:HB2	1.70	1.02
3:U:3220[B]:ARG:CA	3:d:2973[B]:THR:CA	2.12	1.02
3:X:2948[B]:ASP:H	3:X:2949[B]:LYS:HA	1.23	1.02
3:X:3222[B]:ILE:HD12	3:X:3223[B]:GLY:H	1.20	1.02
3:d:2948[A]:ASP:H	3:d:2949[A]:LYS:HA	1.24	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2951[B]:ASP:O	3:F:2956[B]:LYS:NZ	1.92	1.02
3:F:2975[B]:PHE:HD1	3:a:3107[B]:LEU:CG	1.71	1.02
3:F:2982[B]:MET:HE2	3:a:2966[B]:SER:HB3	1.39	1.02
3:F:3293[B]:LYS:HD3	3:F:3294[B]:SER:CB	1.90	1.02
3:I:2961[B]:HIS:CA	3:R:2975[B]:PHE:CZ	2.41	1.02
3:I:3151[B]:LEU:HB2	3:I:3175[B]:TYR:CE2	1.94	1.02
3:I:3153[B]:LYS:CB	3:R:3158[B]:PHE:HB2	1.89	1.02
3:L:2961[A]:HIS:CE1	3:L:2980[A]:HIS:HE2	1.77	1.02
3:L:2961[B]:HIS:CE1	3:L:2980[B]:HIS:HE2	1.77	1.02
3:O:2968[B]:GLN:HB3	3:X:2988[B]:TRP:HB2	1.41	1.02
3:O:3253[B]:GLU:CD	3:X:3161[B]:GLU:CD	2.26	1.02
3:O:3293[B]:LYS:HD3	3:O:3294[B]:SER:CB	1.90	1.02
3:R:3024[B]:LEU:HD12	3:R:3025[B]:VAL:H	0.89	1.02
3:R:3151[A]:LEU:HB2	3:R:3175[A]:TYR:CE2	1.94	1.02
3:U:3159[B]:SER:CB	3:d:3150[B]:LYS:HD2	1.87	1.02
1:Y:1546:LYS:HE3	3:d:3001[B]:LYS:O	1.27	1.02
3:d:2948[A]:ASP:HB3	3:d:2953[A]:GLY:HA3	1.39	1.02
3:d:3038[B]:ILE:HG12	3:d:3112[B]:TYR:CD2	1.93	1.02
3:d:3135[B]:LYS:HG2	3:d:3141[B]:TYR:HE1	1.14	1.02
3:C:2966[B]:SER:HB2	3:C:2977[B]:CYS:HB2	1.39	1.02
3:C:3135[B]:LYS:HG2	3:C:3141[B]:TYR:CE1	1.89	1.02
3:C:3158[B]:PHE:HD2	3:L:3153[B]:LYS:HE3	1.22	1.02
3:F:2961[A]:HIS:CE1	3:F:2980[A]:HIS:HE2	1.77	1.02
3:F:2971[B]:ASP:O	3:a:3090[B]:ASN:HA	1.58	1.02
3:F:3161[B]:GLU:HA	3:a:3147[B]:GLU:HG2	1.41	1.02
3:I:2948[B]:ASP:HB3	3:I:2953[B]:GLY:HA3	1.39	1.02
3:I:3173[B]:THR:HG21	3:R:3173[B]:THR:OG1	1.55	1.02
3:I:3217[A]:PHE:CE1	3:I:3230[A]:PHE:HZ	1.71	1.02
3:I:3298[A]:ASN:ND2	3:I:3301[A]:PRO:HA	1.74	1.02
3:L:3024[A]:LEU:HD12	3:L:3025[A]:VAL:H	0.89	1.02
3:L:3141[A]:TYR:CD2	3:L:3142[A]:ASN:N	2.24	1.02
3:O:2951[B]:ASP:O	3:O:2956[B]:LYS:NZ	1.92	1.02
3:O:2970[B]:PRO:O	3:X:2990[B]:ARG:N	1.63	1.02
3:O:3254[B]:MET:HE3	3:X:3172[B]:SER:OG	1.58	1.02
3:R:3298[B]:ASN:HB3	3:R:3300[B]:LEU:HD23	1.41	1.02
3:U:3038[B]:ILE:HG12	3:U:3112[B]:TYR:CD2	1.93	1.02
3:U:3151[B]:LEU:HB2	3:U:3175[B]:TYR:CE2	1.94	1.02
3:U:3153[B]:LYS:HD2	3:d:3153[B]:LYS:HD2	1.39	1.02
3:X:3038[B]:ILE:HG12	3:X:3112[B]:TYR:CD2	1.93	1.02
3:X:3307[A]:PHE:HE1	3:X:3309[A]:PRO:HG3	1.23	1.02
3:a:2961[A]:HIS:CE1	3:a:2980[A]:HIS:HE2	1.78	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3293[A]:LYS:HD3	3:d:3294[A]:SER:CB	1.90	1.02
3:d:3293[B]:LYS:HD3	3:d:3294[B]:SER:CB	1.90	1.02
3:C:2951[A]:ASP:O	3:C:2956[A]:LYS:NZ	1.92	1.02
3:C:2972[B]:GLY:CA	3:L:3090[B]:ASN:ND2	2.22	1.02
3:C:3151[B]:LEU:HB2	3:C:3175[B]:TYR:CE2	1.94	1.02
3:F:2966[B]:SER:HB2	3:F:2977[B]:CYS:HB2	1.39	1.02
3:F:2967[B]:CYS:SG	3:a:2982[B]:MET:HE3	1.98	1.02
3:F:3298[A]:ASN:HB3	3:F:3300[A]:LEU:HD23	1.42	1.02
3:I:2961[A]:HIS:CE1	3:I:2980[A]:HIS:HE2	1.77	1.02
3:L:2966[A]:SER:HB2	3:L:2977[A]:CYS:HB2	1.39	1.02
3:L:3217[B]:PHE:CE1	3:L:3230[B]:PHE:HZ	1.71	1.02
3:O:2948[B]:ASP:H	3:O:2949[B]:LYS:HA	1.23	1.02
3:O:2966[A]:SER:CB	3:O:2977[A]:CYS:HB2	1.90	1.02
3:O:3228[A]:VAL:HG21	3:O:3245[A]:PHE:CZ	1.95	1.02
3:R:2961[A]:HIS:CE1	3:R:2980[A]:HIS:HE2	1.77	1.02
3:R:2966[A]:SER:CB	3:R:2977[A]:CYS:HB2	1.90	1.02
3:U:2961[A]:HIS:CE1	3:U:2980[A]:HIS:HE2	1.78	1.02
3:U:3293[A]:LYS:HD3	3:U:3294[A]:SER:CB	1.90	1.02
1:V:1582:ASN:HB3	1:V:1583:CYS:HB2	1.41	1.02
3:X:2961[B]:HIS:CE1	3:X:2980[B]:HIS:HE2	1.77	1.02
3:X:2966[B]:SER:HB2	3:X:2977[B]:CYS:HB2	1.39	1.02
3:X:3024[B]:LEU:HD12	3:X:3025[B]:VAL:H	0.89	1.02
3:X:3141[B]:TYR:CD2	3:X:3142[B]:ASN:N	2.24	1.02
4:BA:1:NAG:O3	4:BA:2:NAG:N2	1.92	1.02
3:C:2983[B]:VAL:HG23	3:L:3160[B]:SER:OG	1.57	1.02
3:C:3079[B]:CYS:SG	3:L:3161[B]:GLU:CG	0.92	1.02
3:C:3159[B]:SER:HB3	3:L:2984[B]:THR:HG23	1.03	1.02
3:F:3155[B]:MET:N	3:a:3153[B]:LYS:O	1.91	1.02
3:I:2948[A]:ASP:HB3	3:I:2953[A]:GLY:HA3	1.39	1.02
3:I:3169[B]:LYS:HE3	3:R:3149[B]:ASN:OD1	1.60	1.02
3:I:3248[B]:LEU:HB2	3:R:2972[B]:GLY:O	1.53	1.02
3:L:2966[A]:SER:CB	3:L:2977[A]:CYS:HB2	1.90	1.02
3:L:3228[B]:VAL:HG21	3:L:3245[B]:PHE:CZ	1.95	1.02
3:L:3293[A]:LYS:HD3	3:L:3294[A]:SER:CB	1.90	1.02
3:L:3293[B]:LYS:HD3	3:L:3294[B]:SER:CB	1.90	1.02
3:O:2951[A]:ASP:O	3:O:2956[A]:LYS:NZ	1.92	1.02
3:O:2961[B]:HIS:CE1	3:O:2980[B]:HIS:HE2	1.77	1.02
3:O:2968[B]:GLN:HB2	3:X:2988[B]:TRP:HB2	1.04	1.02
3:O:2973[B]:THR:OG1	3:X:3158[B]:PHE:HZ	1.41	1.02
3:O:2974[B]:ALA:CB	3:X:2977[B]:CYS:C	2.33	1.02
3:O:3024[A]:LEU:HD12	3:O:3025[A]:VAL:H	0.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3141[B]:TYR:CD2	3:R:3142[B]:ASN:N	2.23	1.02
3:R:3151[B]:LEU:HB2	3:R:3175[B]:TYR:CE2	1.94	1.02
3:U:2951[B]:ASP:O	3:U:2956[B]:LYS:NZ	1.92	1.02
3:U:2966[B]:SER:CB	3:U:2977[B]:CYS:HB2	1.90	1.02
3:U:2970[B]:PRO:HB3	3:d:2985[B]:PHE:CE2	1.93	1.02
3:U:3222[A]:ILE:HD12	3:U:3223[A]:GLY:H	1.20	1.02
3:U:3298[A]:ASN:ND2	3:U:3301[A]:PRO:HA	1.74	1.02
3:U:3298[B]:ASN:ND2	3:U:3301[B]:PRO:HA	1.74	1.02
2:W:2868:GLU:CG	3:X:2932[A]:PRO:O	2.07	1.02
3:X:2966[A]:SER:CB	3:X:2977[A]:CYS:HB2	1.90	1.02
3:X:3151[A]:LEU:HB2	3:X:3175[A]:TYR:CE2	1.94	1.02
3:X:3307[B]:PHE:HE1	3:X:3309[B]:PRO:HG3	1.23	1.02
1:Y:1546:LYS:CE	3:d:3001[B]:LYS:O	2.02	1.02
3:a:2966[A]:SER:CB	3:a:2977[A]:CYS:HB2	1.90	1.02
3:a:3141[A]:TYR:CD2	3:a:3142[A]:ASN:N	2.24	1.02
3:d:2966[A]:SER:CB	3:d:2977[A]:CYS:HB2	1.90	1.02
3:d:3151[A]:LEU:HB2	3:d:3175[A]:TYR:CE2	1.94	1.02
3:d:3151[B]:LEU:HB2	3:d:3175[B]:TYR:CE2	1.94	1.02
3:d:3222[B]:ILE:HD12	3:d:3223[B]:GLY:H	1.20	1.02
3:C:3151[A]:LEU:HB2	3:C:3175[A]:TYR:CE2	1.94	1.01
3:C:3172[B]:SER:N	3:L:3152[B]:LYS:CB	2.22	1.01
3:F:2989[B]:HIS:CE1	3:a:2969[B]:TYR:CA	2.38	1.01
3:F:3151[B]:LEU:HB2	3:F:3175[B]:TYR:CE2	1.94	1.01
3:F:3153[B]:LYS:HE3	3:a:3158[B]:PHE:H	1.23	1.01
3:F:3222[A]:ILE:HD12	3:F:3223[A]:GLY:H	1.20	1.01
3:F:3256[B]:TRP:HB3	3:a:2966[B]:SER:O	1.59	1.01
3:I:2951[A]:ASP:O	3:I:2956[A]:LYS:NZ	1.92	1.01
3:O:2970[B]:PRO:CG	3:X:2991[B]:LEU:CB	2.36	1.01
3:O:2971[B]:ASP:N	3:X:2988[B]:TRP:C	1.93	1.01
3:O:3151[B]:LEU:HB2	3:O:3175[B]:TYR:CE2	1.94	1.01
3:O:3157[B]:PRO:C	3:X:3152[B]:LYS:HG3	1.84	1.01
3:O:3253[B]:GLU:CG	3:X:3160[B]:SER:HA	1.90	1.01
3:R:2951[A]:ASP:O	3:R:2956[A]:LYS:NZ	1.92	1.01
3:R:3293[A]:LYS:HD3	3:R:3294[A]:SER:CB	1.90	1.01
3:U:2951[A]:ASP:O	3:U:2956[A]:LYS:NZ	1.92	1.01
3:U:2961[B]:HIS:CE1	3:U:2980[B]:HIS:HE2	1.77	1.01
3:U:2966[A]:SER:HB2	3:U:2977[A]:CYS:HB2	1.39	1.01
3:X:3151[B]:LEU:HB2	3:X:3175[B]:TYR:CE2	1.94	1.01
3:X:3293[A]:LYS:HD3	3:X:3294[A]:SER:CB	1.90	1.01
3:a:2951[A]:ASP:O	3:a:2956[A]:LYS:NZ	1.92	1.01
3:a:3151[B]:LEU:HB2	3:a:3175[B]:TYR:CE2	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3228[B]:VAL:HG21	3:a:3245[B]:PHE:CZ	1.95	1.01
3:a:3298[A]:ASN:ND2	3:a:3301[A]:PRO:HA	1.74	1.01
3:d:3228[B]:VAL:HG21	3:d:3245[B]:PHE:CZ	1.95	1.01
3:d:3307[A]:PHE:HE1	3:d:3309[A]:PRO:HG3	1.23	1.01
3:C:3155[B]:MET:HE3	3:L:3154[B]:PRO:O	1.59	1.01
3:C:3228[A]:VAL:HG21	3:C:3245[A]:PHE:CZ	1.95	1.01
3:C:3248[B]:LEU:HD22	3:L:2971[B]:ASP:CG	1.83	1.01
3:C:3259[B]:ASP:OD2	3:L:3162[B]:ASP:OD1	1.78	1.01
3:C:3307[A]:PHE:HE1	3:C:3309[A]:PRO:HG3	1.23	1.01
3:F:2966[A]:SER:CB	3:F:2977[A]:CYS:HB2	1.90	1.01
3:F:3025[B]:VAL:HG22	3:F:3047[B]:ARG:HH12	1.19	1.01
3:F:3153[B]:LYS:HB3	3:a:3155[B]:MET:C	1.86	1.01
3:F:3256[B]:TRP:NE1	3:a:2965[B]:LEU:HB3	1.29	1.01
3:I:2966[B]:SER:CB	3:I:2977[B]:CYS:HB2	1.90	1.01
3:I:3150[B]:LYS:HD2	3:R:3160[B]:SER:CA	1.90	1.01
3:I:3228[B]:VAL:HG21	3:I:3245[B]:PHE:CZ	1.95	1.01
3:I:3256[B]:TRP:NE1	3:R:2965[B]:LEU:CB	1.99	1.01
3:O:2948[B]:ASP:HB3	3:O:2953[B]:GLY:HA3	1.39	1.01
3:R:3298[B]:ASN:ND2	3:R:3301[B]:PRO:HA	1.74	1.01
3:U:3189[A]:ASN:OD1	3:U:3191[A]:ASN:ND2	1.94	1.01
3:U:3293[B]:LYS:HD3	3:U:3294[B]:SER:CB	1.90	1.01
3:a:2966[B]:SER:CB	3:a:2977[B]:CYS:HB2	1.90	1.01
3:d:3298[A]:ASN:ND2	3:d:3301[A]:PRO:HA	1.74	1.01
3:d:3307[B]:PHE:HE1	3:d:3309[B]:PRO:HG3	1.23	1.01
3:C:2961[A]:HIS:CE1	3:C:2980[A]:HIS:HE2	1.77	1.01
3:C:3248[B]:LEU:CD2	3:L:2971[B]:ASP:OD1	2.08	1.01
3:C:3293[B]:LYS:HD3	3:C:3294[B]:SER:CB	1.90	1.01
3:F:2951[A]:ASP:O	3:F:2956[A]:LYS:NZ	1.92	1.01
3:F:2966[A]:SER:HB2	3:F:2977[A]:CYS:HB2	1.40	1.01
3:F:2966[B]:SER:CB	3:F:2977[B]:CYS:HB2	1.90	1.01
3:F:2983[B]:VAL:N	3:a:3160[B]:SER:OG	1.91	1.01
3:F:3228[B]:VAL:HG21	3:F:3245[B]:PHE:CZ	1.95	1.01
3:F:3251[B]:ASP:HB3	3:a:3251[B]:ASP:CG	1.85	1.01
3:F:3293[A]:LYS:HD3	3:F:3294[A]:SER:CB	1.90	1.01
3:I:2961[B]:HIS:CD2	3:R:2975[B]:PHE:CZ	2.48	1.01
3:I:2982[B]:MET:HE2	3:R:2966[B]:SER:CB	1.89	1.01
3:I:3150[B]:LYS:HG3	3:R:3163[B]:ASN:HD22	0.85	1.01
3:I:3293[B]:LYS:HD3	3:I:3294[B]:SER:CB	1.90	1.01
3:I:3298[B]:ASN:ND2	3:I:3301[B]:PRO:HA	1.74	1.01
3:L:2951[A]:ASP:O	3:L:2956[A]:LYS:NZ	1.92	1.01
3:L:3151[B]:LEU:HB2	3:L:3175[B]:TYR:CE2	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3228[A]:VAL:HG21	3:L:3245[A]:PHE:CZ	1.95	1.01
3:O:2975[B]:PHE:CE2	3:X:3172[B]:SER:CB	2.43	1.01
3:O:3293[A]:LYS:HD3	3:O:3294[A]:SER:CB	1.90	1.01
3:R:2948[B]:ASP:H	3:R:2949[B]:LYS:HA	1.24	1.01
3:R:3189[B]:ASN:OD1	3:R:3191[B]:ASN:ND2	1.94	1.01
3:U:2948[B]:ASP:H	3:U:2949[B]:LYS:HA	1.23	1.01
3:U:2965[B]:LEU:H	3:d:3220[B]:ARG:NH1	1.54	1.01
3:U:2967[B]:CYS:O	3:d:3256[B]:TRP:CE3	1.88	1.01
3:U:2970[B]:PRO:O	3:d:3090[B]:ASN:ND2	1.92	1.01
3:U:3222[B]:ILE:HD12	3:U:3223[B]:GLY:H	1.20	1.01
3:U:3228[B]:VAL:HG21	3:U:3245[B]:PHE:CZ	1.95	1.01
3:X:2951[A]:ASP:O	3:X:2956[A]:LYS:NZ	1.92	1.01
3:a:2948[B]:ASP:HB3	3:a:2953[B]:GLY:HA3	1.39	1.01
3:a:3293[B]:LYS:HD3	3:a:3294[B]:SER:CB	1.90	1.01
3:C:3155[B]:MET:HG2	3:L:3153[B]:LYS:C	1.81	1.01
3:F:3248[B]:LEU:CB	3:a:2972[B]:GLY:O	2.07	1.01
3:I:2966[B]:SER:HB2	3:I:2977[B]:CYS:HB2	1.39	1.01
3:I:3154[B]:PRO:CD	3:R:3155[B]:MET:SD	2.49	1.01
3:I:3162[B]:ASP:HB3	3:R:3259[B]:ASP:N	1.75	1.01
3:L:2951[B]:ASP:O	3:L:2956[B]:LYS:NZ	1.92	1.01
3:L:3222[A]:ILE:HD12	3:L:3223[A]:GLY:H	1.20	1.01
3:O:3189[B]:ASN:OD1	3:O:3191[B]:ASN:ND2	1.94	1.01
3:O:3298[A]:ASN:ND2	3:O:3301[A]:PRO:HA	1.74	1.01
2:Q:2867:PRO:CG	3:R:2932[A]:PRO:HG2	1.90	1.01
3:R:2952[B]:ALA:H	3:R:2953[B]:GLY:HA2	1.26	1.01
3:R:3228[B]:VAL:HG21	3:R:3245[B]:PHE:CZ	1.95	1.01
3:R:3298[A]:ASN:ND2	3:R:3301[A]:PRO:HA	1.74	1.01
1:S:1617:LYS:HE2	3:X:3135[B]:LYS:HZ1	1.21	1.01
3:U:2952[B]:ALA:H	3:U:2953[B]:GLY:HA2	1.26	1.01
3:U:3228[A]:VAL:HG21	3:U:3245[A]:PHE:CZ	1.95	1.01
3:X:2966[B]:SER:CB	3:X:2977[B]:CYS:HB2	1.90	1.01
3:X:2969[A]:TYR:HD2	3:X:2971[A]:ASP:H	1.02	1.01
3:X:2979[A]:GLN:HG2	3:X:3155[A]:MET:HE1	1.01	1.01
3:X:3228[A]:VAL:HG21	3:X:3245[A]:PHE:CZ	1.95	1.01
3:X:3228[B]:VAL:HG21	3:X:3245[B]:PHE:CZ	1.95	1.01
3:X:3293[B]:LYS:HD3	3:X:3294[B]:SER:CB	1.90	1.01
3:a:2951[B]:ASP:O	3:a:2956[B]:LYS:NZ	1.92	1.01
3:a:3222[A]:ILE:HD12	3:a:3223[A]:GLY:H	1.20	1.01
3:a:3293[A]:LYS:HD3	3:a:3294[A]:SER:CB	1.90	1.01
3:d:2948[B]:ASP:HB3	3:d:2953[B]:GLY:HA3	1.39	1.01
3:d:2951[B]:ASP:O	3:d:2956[B]:LYS:NZ	1.92	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2961[A]:HIS:CE1	3:d:2980[A]:HIS:HE2	1.77	1.01
3:d:2979[B]:GLN:HG2	3:d:3155[B]:MET:HE1	1.01	1.01
3:d:3298[B]:ASN:HB3	3:d:3300[B]:LEU:HD23	1.41	1.01
3:C:2948[A]:ASP:H	3:C:2949[A]:LYS:HA	1.24	1.01
3:C:2966[A]:SER:CB	3:C:2977[A]:CYS:HB2	1.90	1.01
3:C:3158[B]:PHE:CD2	3:L:3153[B]:LYS:NZ	2.27	1.01
3:C:3217[B]:PHE:CE1	3:C:3230[B]:PHE:HZ	1.71	1.01
3:C:3298[A]:ASN:ND2	3:C:3301[A]:PRO:HA	1.74	1.01
3:F:3174[B]:GLY:CA	3:a:3154[B]:PRO:HG3	1.91	1.01
3:F:3298[A]:ASN:ND2	3:F:3301[A]:PRO:HA	1.74	1.01
3:I:3228[A]:VAL:HG21	3:I:3245[A]:PHE:CZ	1.95	1.01
3:I:3293[A]:LYS:HD3	3:I:3294[A]:SER:CB	1.90	1.01
3:L:3298[A]:ASN:HB3	3:L:3300[A]:LEU:HD23	1.41	1.01
3:O:3228[B]:VAL:HG21	3:O:3245[B]:PHE:CZ	1.95	1.01
3:R:2969[A]:TYR:HD2	3:R:2971[A]:ASP:H	1.02	1.01
3:R:2979[B]:GLN:HG2	3:R:3155[B]:MET:HE1	1.01	1.01
3:R:3189[A]:ASN:OD1	3:R:3191[A]:ASN:ND2	1.94	1.01
3:U:2979[A]:GLN:HG2	3:U:3155[A]:MET:HE1	1.01	1.01
3:U:3189[B]:ASN:OD1	3:U:3191[B]:ASN:ND2	1.94	1.01
3:X:2961[A]:HIS:CE1	3:X:2980[A]:HIS:HE2	1.77	1.01
3:a:3222[B]:ILE:HD12	3:a:3223[B]:GLY:H	1.20	1.01
3:F:2948[A]:ASP:HB3	3:F:2953[A]:GLY:HA3	1.39	1.00
3:F:2968[B]:GLN:HE21	3:a:3086[B]:GLU:HG2	0.87	1.00
3:F:2970[B]:PRO:HD3	3:a:2989[B]:HIS:CE1	1.95	1.00
3:F:2979[B]:GLN:HG2	3:F:3155[B]:MET:HE1	1.01	1.00
3:F:3149[B]:ASN:ND2	3:a:3163[B]:ASN:HB3	1.74	1.00
3:F:3253[B]:GLU:HA	3:a:2976[B]:ALA:N	1.75	1.00
3:I:2983[B]:VAL:HG23	3:R:3160[B]:SER:CB	1.90	1.00
3:I:3151[A]:LEU:HB2	3:I:3175[A]:TYR:CE2	1.94	1.00
3:L:2979[A]:GLN:HG2	3:L:3155[A]:MET:HE1	1.01	1.00
3:O:2968[B]:GLN:OE1	3:X:2984[B]:THR:OG1	1.78	1.00
3:O:3109[B]:TYR:CZ	3:X:2969[B]:TYR:C	2.30	1.00
3:O:3298[B]:ASN:ND2	3:O:3301[B]:PRO:HA	1.74	1.00
2:Q:2800:LYS:O	3:R:3023[A]:ILE:CD1	2.08	1.00
3:R:3228[A]:VAL:HG21	3:R:3245[A]:PHE:CZ	1.95	1.00
3:U:2952[A]:ALA:H	3:U:2953[A]:GLY:HA2	1.26	1.00
3:U:3149[B]:ASN:O	3:d:3154[B]:PRO:HB2	1.61	1.00
3:U:3152[B]:LYS:CB	3:d:3154[B]:PRO:HA	1.79	1.00
3:U:3155[B]:MET:HE3	3:d:3153[B]:LYS:HE2	1.43	1.00
3:U:3298[A]:ASN:HB3	3:U:3300[A]:LEU:HD23	1.42	1.00
3:X:2979[A]:GLN:HE21	3:X:3155[A]:MET:CE	1.74	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3298[B]:ASN:ND2	3:X:3301[B]:PRO:HA	1.74	1.00
3:d:2961[B]:HIS:CE1	3:d:2980[B]:HIS:HE2	1.77	1.00
3:d:2979[A]:GLN:HE21	3:d:3155[A]:MET:CE	1.74	1.00
3:C:2966[B]:SER:CB	3:C:2977[B]:CYS:HB2	1.90	1.00
3:C:2968[B]:GLN:CD	3:L:3258[B]:PHE:CZ	2.38	1.00
3:C:2979[B]:GLN:HG2	3:C:3155[B]:MET:HE1	1.01	1.00
3:C:3152[B]:LYS:HA	3:L:3173[B]:THR:OG1	1.20	1.00
3:C:3189[B]:ASN:OD1	3:C:3191[B]:ASN:ND2	1.94	1.00
3:C:3298[B]:ASN:ND2	3:C:3301[B]:PRO:HA	1.74	1.00
2:E:2868:GLU:OE2	3:F:2932[A]:PRO:O	1.79	1.00
3:F:2979[B]:GLN:HE21	3:F:3155[B]:MET:CE	1.74	1.00
3:F:3135[B]:LYS:HG2	3:F:3141[B]:TYR:CE1	1.89	1.00
3:F:3307[A]:PHE:HE1	3:F:3309[A]:PRO:HG3	1.23	1.00
3:I:2979[A]:GLN:HG2	3:I:3155[A]:MET:HE1	1.01	1.00
3:I:3149[B]:ASN:ND2	3:R:3163[B]:ASN:O	1.94	1.00
3:I:3150[B]:LYS:CE	3:R:3163[B]:ASN:CB	2.35	1.00
3:I:3163[B]:ASN:HD21	3:R:3149[B]:ASN:CB	1.71	1.00
3:L:3298[B]:ASN:HB3	3:L:3300[B]:LEU:HD23	1.42	1.00
3:O:3222[B]:ILE:HD12	3:O:3223[B]:GLY:H	1.20	1.00
3:O:3307[A]:PHE:HE1	3:O:3309[A]:PRO:HG3	1.23	1.00
3:R:2979[A]:GLN:HG2	3:R:3155[A]:MET:HE1	1.01	1.00
3:R:3293[B]:LYS:HD3	3:R:3294[B]:SER:CB	1.90	1.00
2:T:2800:LYS:O	3:U:3023[A]:ILE:HD11	1.60	1.00
3:U:2973[B]:THR:OG1	3:d:3248[B]:LEU:O	1.79	1.00
3:U:3169[B]:LYS:HG2	3:d:3147[B]:GLU:C	1.87	1.00
3:X:2952[A]:ALA:H	3:X:2953[A]:GLY:HA2	1.26	1.00
3:a:3228[A]:VAL:HG21	3:a:3245[A]:PHE:CZ	1.95	1.00
3:a:3298[A]:ASN:HB3	3:a:3300[A]:LEU:HD23	1.41	1.00
3:d:2948[B]:ASP:H	3:d:2949[B]:LYS:HA	1.24	1.00
3:d:2966[B]:SER:CB	3:d:2977[B]:CYS:HB2	1.90	1.00
3:C:2948[A]:ASP:HB3	3:C:2953[A]:GLY:HA3	1.39	1.00
3:C:2979[A]:GLN:HG2	3:C:3155[A]:MET:HE1	1.01	1.00
3:C:3113[B]:ASP:CG	3:C:3114[B]:PRO:HD2	1.87	1.00
3:C:3256[B]:TRP:CE2	3:L:2965[B]:LEU:CB	2.31	1.00
3:C:3293[A]:LYS:HD3	3:C:3294[A]:SER:CB	1.90	1.00
3:I:2966[B]:SER:HA	3:R:3256[B]:TRP:HB3	1.39	1.00
3:I:3154[B]:PRO:CB	3:R:3174[B]:GLY:HA2	1.92	1.00
3:I:3189[A]:ASN:OD1	3:I:3191[A]:ASN:ND2	1.94	1.00
3:I:3254[B]:MET:HB2	3:R:2966[B]:SER:OG	1.60	1.00
3:I:3255[B]:PRO:HB2	3:R:2959[B]:SER:CA	1.90	1.00
3:I:3307[A]:PHE:HE1	3:I:3309[A]:PRO:HG3	1.23	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2948[A]:ASP:H	3:L:2949[A]:LYS:HA	1.23	1.00
3:L:2960[A]:PHE:CD2	3:L:3157[A]:PRO:HG3	1.97	1.00
3:L:2966[B]:SER:CB	3:L:2977[B]:CYS:HB2	1.90	1.00
3:L:2979[B]:GLN:HG2	3:L:3155[B]:MET:HE1	1.01	1.00
3:O:2965[B]:LEU:HD13	3:X:2979[B]:GLN:HE22	0.84	1.00
3:O:2972[B]:GLY:O	3:X:2979[B]:GLN:HB3	1.62	1.00
3:O:2979[B]:GLN:HE21	3:O:3155[B]:MET:CE	1.74	1.00
3:R:3307[A]:PHE:HE1	3:R:3309[A]:PRO:HG3	1.23	1.00
3:U:2948[A]:ASP:H	3:U:2949[A]:LYS:HA	1.24	1.00
3:U:2979[A]:GLN:HE21	3:U:3155[A]:MET:CE	1.74	1.00
3:U:3159[B]:SER:CB	3:d:3150[B]:LYS:CD	2.35	1.00
3:U:3257[B]:ALA:N	3:d:2969[B]:TYR:H	1.60	1.00
3:X:3113[B]:ASP:CG	3:X:3114[B]:PRO:HD2	1.87	1.00
3:X:3298[A]:ASN:HB3	3:X:3300[A]:LEU:HD23	1.42	1.00
3:a:3113[A]:ASP:CG	3:a:3114[A]:PRO:HD2	1.87	1.00
3:a:3113[B]:ASP:CG	3:a:3114[B]:PRO:HD2	1.87	1.00
3:C:3113[A]:ASP:CG	3:C:3114[A]:PRO:HD2	1.87	1.00
3:C:3228[B]:VAL:HG21	3:C:3245[B]:PHE:CZ	1.95	1.00
3:C:3248[B]:LEU:HB2	3:L:2973[B]:THR:N	1.50	1.00
3:F:2983[B]:VAL:HG23	3:a:3160[B]:SER:OG	1.59	1.00
3:I:2966[A]:SER:CB	3:I:2977[A]:CYS:HB2	1.90	1.00
3:O:3255[B]:PRO:HG2	3:X:3163[B]:ASN:CB	1.90	1.00
3:R:2966[B]:SER:CB	3:R:2977[B]:CYS:HB2	1.90	1.00
3:R:2979[B]:GLN:HE21	3:R:3155[B]:MET:CE	1.74	1.00
3:U:2966[A]:SER:CB	3:U:2977[A]:CYS:HB2	1.90	1.00
3:a:2979[A]:GLN:HE21	3:a:3155[A]:MET:CE	1.74	1.00
3:d:2966[A]:SER:HB2	3:d:2977[A]:CYS:HB2	1.39	1.00
3:d:3113[B]:ASP:CG	3:d:3114[B]:PRO:HD2	1.87	1.00
3:d:3189[B]:ASN:OD1	3:d:3191[B]:ASN:ND2	1.94	1.00
3:F:2952[B]:ALA:H	3:F:2953[B]:GLY:HA2	1.26	1.00
3:F:3174[B]:GLY:HA2	3:a:3154[B]:PRO:HG3	1.02	1.00
3:F:3228[A]:VAL:HG21	3:F:3245[A]:PHE:CZ	1.95	1.00
3:I:3113[A]:ASP:CG	3:I:3114[A]:PRO:HD2	1.87	1.00
3:I:3150[B]:LYS:CG	3:R:3163[B]:ASN:HD22	1.74	1.00
3:I:3255[B]:PRO:HB3	3:R:2964[B]:PRO:HB2	1.42	1.00
3:I:3307[B]:PHE:HE1	3:I:3309[B]:PRO:HG3	1.23	1.00
3:L:2948[B]:ASP:H	3:L:2949[B]:LYS:HA	1.23	1.00
3:O:3141[B]:TYR:CD2	3:O:3142[B]:ASN:N	2.23	1.00
3:O:3307[B]:PHE:HE1	3:O:3309[B]:PRO:HG3	1.23	1.00
3:R:3298[A]:ASN:HB3	3:R:3300[A]:LEU:HD23	1.41	1.00
3:U:3298[B]:ASN:HB3	3:U:3300[B]:LEU:HD23	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3135[B]:LYS:HG2	3:d:3141[B]:TYR:CE1	1.89	1.00
3:C:3025[A]:VAL:HG22	3:C:3047[A]:ARG:HH12	1.19	1.00
3:F:2981[B]:GLY:H	3:a:2968[B]:GLN:CG	1.74	1.00
3:F:3113[B]:ASP:CG	3:F:3114[B]:PRO:HD2	1.87	1.00
3:I:2960[A]:PHE:CD2	3:I:3157[A]:PRO:HG3	1.97	1.00
3:I:3150[B]:LYS:O	3:R:3159[B]:SER:N	1.94	1.00
3:R:2948[A]:ASP:H	3:R:2949[A]:LYS:HA	1.23	1.00
3:X:3189[B]:ASN:OD1	3:X:3191[B]:ASN:ND2	1.94	1.00
3:d:2952[A]:ALA:H	3:d:2953[A]:GLY:HA2	1.26	1.00
3:C:2952[A]:ALA:H	3:C:2953[A]:GLY:HA2	1.26	1.00
3:C:3189[A]:ASN:OD1	3:C:3191[A]:ASN:ND2	1.94	1.00
3:F:3307[B]:PHE:HE1	3:F:3309[B]:PRO:HG3	1.23	1.00
3:I:2979[B]:GLN:HE21	3:I:3155[B]:MET:CE	1.74	1.00
3:O:3298[B]:ASN:HB3	3:O:3300[B]:LEU:HD23	1.41	1.00
3:U:2948[B]:ASP:HB3	3:U:2953[B]:GLY:HA3	1.39	1.00
3:U:3141[B]:TYR:CD2	3:U:3142[B]:ASN:N	2.24	1.00
3:C:3120[B]:HIS:NE2	3:L:2969[B]:TYR:CZ	2.27	0.99
3:C:3159[B]:SER:HB3	3:L:2984[B]:THR:CG2	1.83	0.99
3:C:3307[B]:PHE:HE1	3:C:3309[B]:PRO:HG3	1.23	0.99
3:F:3113[A]:ASP:CG	3:F:3114[A]:PRO:HD2	1.87	0.99
3:L:3189[A]:ASN:OD1	3:L:3191[A]:ASN:ND2	1.94	0.99
3:U:3135[B]:LYS:HG2	3:U:3141[B]:TYR:CE1	1.89	0.99
3:X:2960[B]:PHE:CD2	3:X:3157[B]:PRO:HG3	1.97	0.99
3:a:2952[B]:ALA:H	3:a:2953[B]:GLY:HA2	1.26	0.99
3:a:3013[B]:ASP:HA	3:a:3122[B]:ASN:HD21	1.27	0.99
3:a:3189[B]:ASN:OD1	3:a:3191[B]:ASN:ND2	1.94	0.99
3:d:2960[A]:PHE:CD2	3:d:3157[A]:PRO:HG3	1.97	0.99
3:C:2979[B]:GLN:HE21	3:C:3155[B]:MET:CE	1.74	0.99
3:F:3189[A]:ASN:OD1	3:F:3191[A]:ASN:ND2	1.94	0.99
2:H:2868:GLU:CG	3:I:2932[A]:PRO:O	2.09	0.99
3:I:2975[B]:PHE:O	3:R:3253[B]:GLU:CB	2.10	0.99
3:I:3149[B]:ASN:HB3	3:R:3165[B]:ASN:O	1.62	0.99
3:L:2952[B]:ALA:H	3:L:2953[B]:GLY:HA2	1.26	0.99
3:L:3013[A]:ASP:HA	3:L:3122[A]:ASN:HD21	1.27	0.99
3:L:3113[A]:ASP:CG	3:L:3114[A]:PRO:HD2	1.87	0.99
3:O:2952[B]:ALA:H	3:O:2953[B]:GLY:HA2	1.26	0.99
3:O:3169[B]:LYS:HG3	3:X:3148[B]:ILE:HG23	1.01	0.99
1:S:1582:ASN:HB3	1:S:1583:CYS:HB2	1.44	0.99
3:U:3113[A]:ASP:CG	3:U:3114[A]:PRO:HD2	1.87	0.99
3:U:3256[B]:TRP:CD1	3:d:2975[B]:PHE:HE1	1.79	0.99
3:d:2966[B]:SER:HB2	3:d:2977[B]:CYS:HB2	1.39	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3013[A]:ASP:HA	3:d:3122[A]:ASN:HD21	1.27	0.99
3:d:3228[A]:VAL:HG21	3:d:3245[A]:PHE:CZ	1.95	0.99
3:L:3013[B]:ASP:HA	3:L:3122[B]:ASN:HD21	1.27	0.99
3:U:3307[A]:PHE:HE1	3:U:3309[A]:PRO:HG3	1.23	0.99
3:C:2967[B]:CYS:HB3	3:L:2982[B]:MET:N	1.72	0.99
3:C:2972[B]:GLY:HA3	3:L:3090[B]:ASN:ND2	1.74	0.99
3:F:2970[B]:PRO:CD	3:a:2989[B]:HIS:CE1	2.45	0.99
3:F:2972[B]:GLY:CA	3:a:3090[B]:ASN:HB3	1.92	0.99
3:I:2960[B]:PHE:CD2	3:I:3157[B]:PRO:HG3	1.97	0.99
3:I:3149[B]:ASN:ND2	3:R:3163[B]:ASN:CB	2.24	0.99
3:O:2960[A]:PHE:CD2	3:O:3157[A]:PRO:HG3	1.97	0.99
3:O:2966[A]:SER:HB2	3:O:2977[A]:CYS:HB2	1.39	0.99
3:X:2960[A]:PHE:CD2	3:X:3157[A]:PRO:HG3	1.97	0.99
3:X:3113[A]:ASP:CG	3:X:3114[A]:PRO:HD2	1.87	0.99
3:X:3141[A]:TYR:CD2	3:X:3142[A]:ASN:N	2.24	0.99
3:X:3189[A]:ASN:OD1	3:X:3191[A]:ASN:ND2	1.94	0.99
3:d:2979[B]:GLN:HE21	3:d:3155[B]:MET:CE	1.74	0.99
3:d:3013[B]:ASP:HA	3:d:3122[B]:ASN:HD21	1.28	0.99
3:C:2960[A]:PHE:CD2	3:C:3157[A]:PRO:HG3	1.97	0.99
3:F:3135[A]:LYS:HG2	3:F:3141[A]:TYR:CE1	1.89	0.99
3:I:2959[B]:SER:HB2	3:R:3255[B]:PRO:HB2	1.01	0.99
3:I:2972[B]:GLY:HA3	3:R:3090[B]:ASN:HB3	1.01	0.99
3:L:2960[B]:PHE:CD2	3:L:3157[B]:PRO:HG3	1.97	0.99
3:L:3141[B]:TYR:CD2	3:L:3142[B]:ASN:N	2.24	0.99
3:O:3252[B]:TYR:CB	3:X:3156[B]:MET:HB2	1.88	0.99
3:R:3113[B]:ASP:CG	3:R:3114[B]:PRO:HD2	1.87	0.99
3:U:2965[B]:LEU:HD12	3:d:3220[B]:ARG:CB	1.87	0.99
3:U:2975[B]:PHE:CG	3:d:3256[B]:TRP:HD1	1.61	0.99
3:U:3113[B]:ASP:CG	3:U:3114[B]:PRO:HD2	1.87	0.99
3:U:3256[B]:TRP:CD1	3:d:2975[B]:PHE:CE1	2.51	0.99
3:d:3217[B]:PHE:CE1	3:d:3230[B]:PHE:HZ	1.71	0.99
3:C:3013[A]:ASP:HA	3:C:3122[A]:ASN:HD21	1.28	0.99
3:C:3162[B]:ASP:OD1	3:L:3259[B]:ASP:CG	1.96	0.99
3:F:2960[A]:PHE:CD2	3:F:3157[A]:PRO:HG3	1.97	0.99
3:U:2960[A]:PHE:CD2	3:U:3157[A]:PRO:HG3	1.97	0.99
3:U:2979[B]:GLN:HE21	3:U:3155[B]:MET:CE	1.74	0.99
3:U:3013[B]:ASP:HA	3:U:3122[B]:ASN:HD21	1.27	0.99
3:d:3038[B]:ILE:CG2	3:d:3040[B]:VAL:HG22	1.93	0.99
3:d:3113[A]:ASP:CG	3:d:3114[A]:PRO:HD2	1.87	0.99
3:C:3255[B]:PRO:HD2	3:L:2960[B]:PHE:O	1.60	0.99
3:F:2979[A]:GLN:HG2	3:F:3155[A]:MET:HE1	1.01	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3038[A]:ILE:CG2	3:F:3040[A]:VAL:HG22	1.93	0.99
3:F:3153[B]:LYS:HG2	3:a:3155[B]:MET:CB	1.78	0.99
3:I:2982[B]:MET:HG3	3:R:3156[B]:MET:HB2	1.41	0.99
3:L:3038[B]:ILE:CG2	3:L:3040[B]:VAL:HG22	1.93	0.99
3:L:3189[B]:ASN:OD1	3:L:3191[B]:ASN:ND2	1.94	0.99
3:R:2969[B]:TYR:HD2	3:R:2971[B]:ASP:H	1.02	0.99
3:U:2969[B]:TYR:HD2	3:U:2971[B]:ASP:H	1.02	0.99
3:U:2971[B]:ASP:HA	3:d:3090[B]:ASN:HD22	0.83	0.99
3:a:2948[A]:ASP:H	3:a:2949[A]:LYS:HA	1.24	0.99
3:a:2960[B]:PHE:CD2	3:a:3157[B]:PRO:HG3	1.97	0.99
3:a:3189[A]:ASN:OD1	3:a:3191[A]:ASN:ND2	1.94	0.99
3:a:3298[B]:ASN:HB3	3:a:3300[B]:LEU:HD23	1.42	0.99
3:C:3160[B]:SER:HA	3:L:2983[B]:VAL:HG23	1.35	0.99
3:C:3298[A]:ASN:HB3	3:C:3300[A]:LEU:HD23	1.41	0.99
3:F:2975[B]:PHE:HZ	3:a:2961[B]:HIS:HA	1.25	0.99
3:F:2979[A]:GLN:HE21	3:F:3155[A]:MET:CE	1.74	0.99
3:F:3141[A]:TYR:CD2	3:F:3142[A]:ASN:N	2.24	0.99
3:I:2966[A]:SER:HB2	3:I:2977[A]:CYS:HB2	1.39	0.99
3:I:2972[B]:GLY:HA3	3:R:3090[B]:ASN:CB	1.91	0.99
3:I:3298[B]:ASN:HB3	3:I:3300[B]:LEU:HD23	1.41	0.99
3:L:2979[A]:GLN:HE21	3:L:3155[A]:MET:CE	1.74	0.99
3:O:2963[B]:MET:HG2	3:X:2968[B]:GLN:O	1.20	0.99
3:R:2960[B]:PHE:CD2	3:R:3157[B]:PRO:HG3	1.97	0.99
3:R:3038[A]:ILE:CG2	3:R:3040[A]:VAL:HG22	1.93	0.99
3:U:3169[B]:LYS:O	3:d:3148[B]:ILE:HB	1.55	0.99
3:X:3217[A]:PHE:CE1	3:X:3230[A]:PHE:CE1	2.51	0.99
3:a:3038[A]:ILE:CG2	3:a:3040[A]:VAL:HG22	1.93	0.99
3:d:2960[B]:PHE:CD2	3:d:3157[B]:PRO:HG3	1.97	0.99
3:d:2969[A]:TYR:HD2	3:d:2971[A]:ASP:H	1.02	0.99
3:d:3189[A]:ASN:OD1	3:d:3191[A]:ASN:ND2	1.94	0.99
3:F:2960[B]:PHE:CD2	3:F:3157[B]:PRO:HG3	1.97	0.99
3:I:3173[B]:THR:HG1	3:R:3173[B]:THR:CG2	1.62	0.99
3:O:3113[A]:ASP:CG	3:O:3114[A]:PRO:HD2	1.87	0.99
3:O:3189[A]:ASN:OD1	3:O:3191[A]:ASN:ND2	1.94	0.99
3:a:2979[B]:GLN:HG2	3:a:3155[B]:MET:HE1	1.01	0.99
3:C:3038[A]:ILE:CG2	3:C:3040[A]:VAL:HG22	1.93	0.99
3:F:2968[B]:GLN:NE2	3:a:3086[B]:GLU:HG2	1.72	0.99
3:F:2977[B]:CYS:SG	3:a:2982[B]:MET:HE3	2.03	0.99
3:I:2979[A]:GLN:HE21	3:I:3155[A]:MET:CE	1.74	0.99
3:L:3113[B]:ASP:CG	3:L:3114[B]:PRO:HD2	1.87	0.99
3:O:3013[A]:ASP:HA	3:O:3122[A]:ASN:HD21	1.27	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2979[A]:GLN:HE21	3:R:3155[A]:MET:CE	1.74	0.99
3:R:3013[B]:ASP:HA	3:R:3122[B]:ASN:HD21	1.27	0.99
3:X:3298[B]:ASN:HB3	3:X:3300[B]:LEU:HD23	1.42	0.99
3:a:2979[B]:GLN:HE21	3:a:3155[B]:MET:CE	1.75	0.99
3:d:3038[A]:ILE:CG2	3:d:3040[A]:VAL:HG22	1.93	0.99
3:C:2960[B]:PHE:CD2	3:C:3157[B]:PRO:HG3	1.97	0.98
3:C:2965[B]:LEU:HD21	3:L:3253[B]:GLU:OE1	0.81	0.98
3:C:3156[B]:MET:HB2	3:L:2982[B]:MET:CB	1.91	0.98
3:I:2952[A]:ALA:H	3:I:2953[A]:GLY:HA2	1.26	0.98
3:I:2975[B]:PHE:CG	3:R:3107[B]:LEU:HD11	1.97	0.98
3:I:3251[B]:ASP:CB	3:R:3251[B]:ASP:CB	1.86	0.98
3:L:2979[B]:GLN:HE21	3:L:3155[B]:MET:CE	1.74	0.98
3:O:2969[A]:TYR:HD2	3:O:2971[A]:ASP:H	1.02	0.98
3:R:2960[A]:PHE:CD2	3:R:3157[A]:PRO:HG3	1.97	0.98
3:R:3113[A]:ASP:CG	3:R:3114[A]:PRO:HD2	1.87	0.98
3:U:2960[B]:PHE:CD2	3:U:3157[B]:PRO:HG3	1.97	0.98
3:U:3038[A]:ILE:CG2	3:U:3040[A]:VAL:HG22	1.93	0.98
3:U:3153[B]:LYS:CB	3:d:3153[B]:LYS:HD2	1.91	0.98
3:d:2990[B]:ARG:NH2	3:d:3180[B]:TYR:HB3	1.79	0.98
3:d:3298[A]:ASN:HB3	3:d:3300[A]:LEU:HD23	1.42	0.98
3:C:2948[B]:ASP:H	3:C:2949[B]:LYS:HA	1.24	0.98
3:C:2979[A]:GLN:HE21	3:C:3155[A]:MET:CE	1.74	0.98
3:C:3154[B]:PRO:HB2	3:L:3151[B]:LEU:HA	1.44	0.98
3:C:3158[B]:PHE:CD2	3:L:3153[B]:LYS:HE3	1.94	0.98
3:C:3223[B]:GLY:H	3:L:2963[B]:MET:HE1	1.27	0.98
3:F:3038[B]:ILE:CG2	3:F:3040[B]:VAL:HG22	1.93	0.98
3:F:3156[B]:MET:HB2	3:a:2982[B]:MET:CG	1.91	0.98
3:L:2969[A]:TYR:HD2	3:L:2971[A]:ASP:H	1.02	0.98
3:O:3298[A]:ASN:HB3	3:O:3300[A]:LEU:HD23	1.42	0.98
3:U:3155[B]:MET:N	3:d:3150[B]:LYS:CG	2.26	0.98
3:d:3217[A]:PHE:CE1	3:d:3230[A]:PHE:CE1	2.51	0.98
3:C:3258[B]:PHE:HZ	3:L:2968[B]:GLN:CD	1.71	0.98
3:F:2966[B]:SER:CA	3:a:3255[B]:PRO:C	2.36	0.98
3:F:3170[B]:ALA:C	3:a:3152[B]:LYS:CD	2.15	0.98
3:I:2952[B]:ALA:H	3:I:2953[B]:GLY:HA2	1.26	0.98
3:I:2979[B]:GLN:HG2	3:I:3155[B]:MET:HE1	1.01	0.98
3:I:3038[A]:ILE:CG2	3:I:3040[A]:VAL:HG22	1.93	0.98
3:I:3169[B]:LYS:HG3	3:R:3149[B]:ASN:OD1	1.59	0.98
3:O:2960[B]:PHE:CD2	3:O:3157[B]:PRO:HG3	1.97	0.98
3:O:3113[B]:ASP:CG	3:O:3114[B]:PRO:HD2	1.87	0.98
3:U:2990[A]:ARG:NH2	3:U:3180[A]:TYR:HB3	1.79	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3169[B]:LYS:HG3	3:d:3147[B]:GLU:HB3	1.41	0.98
3:X:3013[A]:ASP:HA	3:X:3122[A]:ASN:HD21	1.27	0.98
3:a:2960[A]:PHE:CD2	3:a:3157[A]:PRO:HG3	1.97	0.98
3:a:2979[A]:GLN:HG2	3:a:3155[A]:MET:HE1	1.01	0.98
3:d:3034[B]:HIS:HB3	3:d:3035[B]:HIS:ND1	1.79	0.98
3:C:2965[B]:LEU:HD23	3:L:3253[B]:GLU:CD	1.69	0.98
3:C:2990[A]:ARG:NH2	3:C:3180[A]:TYR:HB3	1.79	0.98
3:C:3159[B]:SER:CA	3:L:3150[B]:LYS:C	2.17	0.98
3:C:3160[B]:SER:CB	3:L:3150[B]:LYS:HZ2	1.55	0.98
3:F:2982[B]:MET:HE2	3:a:2966[B]:SER:CB	1.92	0.98
3:F:3149[B]:ASN:ND2	3:a:3163[B]:ASN:CB	2.26	0.98
3:I:3113[B]:ASP:CG	3:I:3114[B]:PRO:HD2	1.87	0.98
3:I:3174[B]:GLY:HA3	3:R:3154[B]:PRO:HB3	1.44	0.98
3:O:3034[A]:HIS:HB3	3:O:3035[A]:HIS:ND1	1.78	0.98
3:C:3153[B]:LYS:C	3:L:3155[B]:MET:CG	2.36	0.98
3:C:3254[B]:MET:O	3:L:2976[B]:ALA:HA	1.16	0.98
3:F:3066[A]:TYR:OH	3:F:3203[A]:HIS:NE2	1.97	0.98
3:F:3156[B]:MET:HB2	3:a:2982[B]:MET:SD	2.04	0.98
3:I:2990[B]:ARG:NH2	3:I:3180[B]:TYR:HB3	1.79	0.98
3:O:2979[A]:GLN:HE21	3:O:3155[A]:MET:CE	1.74	0.98
3:O:2979[B]:GLN:HG2	3:O:3155[B]:MET:HE1	1.01	0.98
3:O:3038[B]:ILE:HG21	3:X:2969[B]:TYR:CE1	1.97	0.98
3:a:2966[B]:SER:HB2	3:a:2977[B]:CYS:HB2	1.39	0.98
3:C:3159[B]:SER:OG	3:L:3150[B]:LYS:C	2.07	0.98
3:F:3027[A]:GLU:OE1	3:F:3029[A]:LYS:N	1.97	0.98
3:F:3153[B]:LYS:C	3:a:3155[B]:MET:CG	2.16	0.98
3:F:3153[B]:LYS:HB3	3:a:3155[B]:MET:CA	1.94	0.98
3:F:3189[B]:ASN:OD1	3:F:3191[B]:ASN:ND2	1.94	0.98
3:I:3189[B]:ASN:OD1	3:I:3191[B]:ASN:ND2	1.94	0.98
3:I:3298[A]:ASN:HB3	3:I:3300[A]:LEU:HD23	1.42	0.98
3:R:2990[A]:ARG:NH2	3:R:3180[A]:TYR:HB3	1.79	0.98
3:X:2990[B]:ARG:NH2	3:X:3180[B]:TYR:HB3	1.79	0.98
3:a:3034[A]:HIS:HB3	3:a:3035[A]:HIS:ND1	1.78	0.98
3:a:3141[B]:TYR:CD2	3:a:3142[B]:ASN:N	2.23	0.98
3:d:2952[B]:ALA:H	3:d:2953[B]:GLY:HA2	1.26	0.98
3:C:2968[B]:GLN:OE1	3:L:3258[B]:PHE:CZ	2.17	0.98
3:C:3150[B]:LYS:O	3:L:3159[B]:SER:OG	1.82	0.98
3:C:3217[B]:PHE:CE1	3:C:3230[B]:PHE:CE1	2.51	0.98
3:F:2982[B]:MET:HE1	3:a:2966[B]:SER:HB3	1.44	0.98
3:F:3013[A]:ASP:HA	3:F:3122[A]:ASN:HD21	1.28	0.98
3:F:3027[B]:GLU:OE1	3:F:3029[B]:LYS:N	1.97	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3038[B]:ILE:CG2	3:I:3040[B]:VAL:HG22	1.93	0.98
3:I:3161[B]:GLU:HG3	3:R:3079[B]:CYS:SG	1.99	0.98
3:L:3034[B]:HIS:HB3	3:L:3035[B]:HIS:ND1	1.79	0.98
3:O:2990[A]:ARG:NH2	3:O:3180[A]:TYR:HB3	1.79	0.98
3:O:2990[B]:ARG:NH2	3:O:3180[B]:TYR:HB3	1.79	0.98
3:O:3217[B]:PHE:CE1	3:O:3230[B]:PHE:CE1	2.51	0.98
3:C:3155[B]:MET:N	3:L:3153[B]:LYS:O	1.96	0.98
3:F:2982[B]:MET:SD	3:a:3157[B]:PRO:CA	2.50	0.98
3:F:2990[B]:ARG:NH2	3:F:3180[B]:TYR:HB3	1.79	0.98
3:F:3147[B]:GLU:OE1	3:a:3162[B]:ASP:HA	1.63	0.98
3:F:3169[B]:LYS:O	3:a:3152[B]:LYS:CB	2.12	0.98
3:I:2991[A]:LEU:HD23	3:I:3158[A]:PHE:CD1	1.99	0.98
3:O:2979[A]:GLN:HG2	3:O:3155[A]:MET:HE1	1.01	0.98
3:O:3038[B]:ILE:CG2	3:O:3040[B]:VAL:HG22	1.93	0.98
3:O:3255[B]:PRO:HA	3:X:3161[B]:GLU:HA	1.42	0.98
3:R:2952[A]:ALA:H	3:R:2953[A]:GLY:HA2	1.26	0.98
3:U:2973[B]:THR:HG22	3:d:3222[B]:ILE:HG22	1.44	0.98
3:U:3141[A]:TYR:CD2	3:U:3142[A]:ASN:N	2.24	0.98
3:X:2979[B]:GLN:HG2	3:X:3155[B]:MET:HE1	1.01	0.98
1:Y:1620:LEU:HD12	3:d:3189[B]:ASN:HB2	1.45	0.98
3:d:3066[B]:TYR:OH	3:d:3203[B]:HIS:NE2	1.97	0.98
3:C:3173[A]:THR:HB	3:C:3176[A]:LYS:HD2	1.46	0.98
3:F:3173[A]:THR:HB	3:F:3176[A]:LYS:HD2	1.46	0.98
3:I:2968[B]:GLN:HG3	3:R:3086[B]:GLU:CG	1.89	0.98
3:I:3160[B]:SER:HB2	3:R:2982[B]:MET:HB3	1.46	0.98
3:I:3163[B]:ASN:HB3	3:R:3150[B]:LYS:CE	1.83	0.98
3:I:3217[B]:PHE:CE1	3:I:3230[B]:PHE:CE1	2.51	0.98
3:I:3253[B]:GLU:OE1	3:R:2974[B]:ALA:HB1	1.64	0.98
1:J:806:ASN:CG	4:u:1:NAG:H82	1.89	0.98
3:L:2961[B]:HIS:NE2	3:L:2980[B]:HIS:NE2	2.04	0.98
3:L:3298[A]:ASN:HB2	3:L:3300[A]:LEU:N	1.78	0.98
3:O:3160[B]:SER:HA	3:X:3151[B]:LEU:HG	1.44	0.98
3:R:3038[B]:ILE:CG2	3:R:3040[B]:VAL:HG22	1.93	0.98
3:R:3217[A]:PHE:CE1	3:R:3230[A]:PHE:CE1	2.51	0.98
3:U:2979[B]:GLN:HG2	3:U:3155[B]:MET:HE1	1.01	0.98
3:U:3256[B]:TRP:CE3	3:d:2969[B]:TYR:CB	2.45	0.98
1:Y:416:ASN:CG	3:d:3196[A]:THR:HG21	1.88	0.98
3:a:2990[A]:ARG:NH2	3:a:3180[A]:TYR:HB3	1.79	0.98
3:a:3066[A]:TYR:OH	3:a:3203[A]:HIS:NE2	1.97	0.98
3:C:3034[A]:HIS:HB3	3:C:3035[A]:HIS:ND1	1.79	0.98
3:C:3163[B]:ASN:N	3:L:3147[B]:GLU:CD	2.20	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3163[B]:ASN:HD21	3:R:3149[B]:ASN:HB2	0.83	0.98
3:L:2990[A]:ARG:NH2	3:L:3180[A]:TYR:HB3	1.79	0.98
3:R:2991[B]:LEU:HD23	3:R:3158[B]:PHE:CD1	1.99	0.98
3:R:3217[B]:PHE:CE1	3:R:3230[B]:PHE:CE1	2.51	0.98
3:X:2952[B]:ALA:H	3:X:2953[B]:GLY:HA2	1.26	0.98
3:X:3173[A]:THR:HB	3:X:3176[A]:LYS:HD2	1.46	0.98
3:a:2990[B]:ARG:NH2	3:a:3180[B]:TYR:HB3	1.79	0.98
3:d:2991[A]:LEU:HD23	3:d:3158[A]:PHE:CD1	1.99	0.98
3:F:2991[A]:LEU:HD23	3:F:3158[A]:PHE:CD1	1.99	0.97
3:F:3217[A]:PHE:CE1	3:F:3230[A]:PHE:CE1	2.51	0.97
3:F:3217[B]:PHE:CE1	3:F:3230[B]:PHE:CE1	2.51	0.97
3:F:3298[B]:ASN:HB3	3:F:3300[B]:LEU:HD23	1.41	0.97
3:I:3066[B]:TYR:OH	3:I:3203[B]:HIS:NE2	1.97	0.97
3:L:3038[A]:ILE:CG2	3:L:3040[A]:VAL:HG22	1.93	0.97
3:O:2952[A]:ALA:H	3:O:2953[A]:GLY:HA2	1.26	0.97
3:O:3027[A]:GLU:OE1	3:O:3029[A]:LYS:N	1.97	0.97
3:U:3169[B]:LYS:CE	3:d:3146[B]:CYS:HA	1.94	0.97
3:X:2991[B]:LEU:HD23	3:X:3158[B]:PHE:CD1	1.99	0.97
1:Y:1576:THR:HG22	3:d:3196[B]:THR:HG21	1.44	0.97
3:a:2948[B]:ASP:H	3:a:2949[B]:LYS:HA	1.24	0.97
3:C:3034[B]:HIS:HB3	3:C:3035[B]:HIS:ND1	1.79	0.97
3:C:3038[B]:ILE:CG2	3:C:3040[B]:VAL:HG22	1.93	0.97
3:C:3147[B]:GLU:OE1	3:L:3162[B]:ASP:C	2.07	0.97
3:C:3161[B]:GLU:H	3:L:2983[B]:VAL:CG2	1.76	0.97
3:C:3231[B]:ASP:O	3:C:3284[B]:LYS:N	1.98	0.97
3:C:3256[B]:TRP:CE3	3:L:2965[B]:LEU:O	2.17	0.97
3:F:2975[B]:PHE:CZ	3:a:2961[B]:HIS:HA	1.98	0.97
3:F:3154[B]:PRO:CA	3:a:3153[B]:LYS:O	2.11	0.97
3:F:3155[B]:MET:HG3	3:a:3153[B]:LYS:C	1.89	0.97
3:F:3156[B]:MET:HB2	3:a:2982[B]:MET:HG3	1.42	0.97
3:O:3027[B]:GLU:OE1	3:O:3029[B]:LYS:N	1.97	0.97
3:O:3038[A]:ILE:CG2	3:O:3040[A]:VAL:HG22	1.93	0.97
3:U:3156[B]:MET:SD	3:d:2982[B]:MET:SD	2.61	0.97
3:X:3038[B]:ILE:CG2	3:X:3040[B]:VAL:HG22	1.93	0.97
3:C:2968[B]:GLN:OE1	3:L:2981[B]:GLY:HA2	1.64	0.97
3:F:2968[B]:GLN:NE2	3:a:3086[B]:GLU:CG	2.22	0.97
3:F:2970[B]:PRO:N	3:a:2989[B]:HIS:CD2	2.25	0.97
3:F:3254[B]:MET:CG	3:a:2966[B]:SER:HB2	1.94	0.97
3:F:3255[B]:PRO:CG	3:a:2962[B]:GLY:C	2.37	0.97
3:I:3013[A]:ASP:HA	3:I:3122[A]:ASN:HD21	1.28	0.97
3:L:3027[A]:GLU:OE1	3:L:3029[A]:LYS:N	1.97	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2965[B]:LEU:HB2	3:X:3254[B]:MET:CE	1.89	0.97
3:R:2991[A]:LEU:HD23	3:R:3158[A]:PHE:CD1	1.99	0.97
3:U:2979[B]:GLN:HE22	3:d:3153[B]:LYS:NZ	1.55	0.97
3:U:3217[B]:PHE:CE1	3:U:3230[B]:PHE:CE1	2.51	0.97
3:a:3034[B]:HIS:HB3	3:a:3035[B]:HIS:ND1	1.79	0.97
3:a:3196[A]:THR:CG2	1:b:416:ASN:OD1	2.12	0.97
3:d:2979[A]:GLN:HG2	3:d:3155[A]:MET:HE1	1.01	0.97
3:d:3034[A]:HIS:HB3	3:d:3035[A]:HIS:ND1	1.79	0.97
3:C:2964[B]:PRO:O	3:L:3255[B]:PRO:CA	2.10	0.97
3:C:2991[A]:LEU:HD23	3:C:3158[A]:PHE:CD1	1.99	0.97
3:C:3066[A]:TYR:OH	3:C:3203[A]:HIS:NE2	1.97	0.97
3:C:3066[B]:TYR:OH	3:C:3203[B]:HIS:NE2	1.97	0.97
3:F:2990[A]:ARG:NH2	3:F:3180[A]:TYR:HB3	1.78	0.97
3:F:3169[B]:LYS:NZ	3:a:3149[B]:ASN:ND2	2.12	0.97
3:I:2990[A]:ARG:NH2	3:I:3180[A]:TYR:HB3	1.79	0.97
3:I:3034[A]:HIS:HB3	3:I:3035[A]:HIS:ND1	1.79	0.97
3:O:2965[B]:LEU:C	3:X:3153[B]:LYS:NZ	2.22	0.97
3:O:3013[B]:ASP:HA	3:O:3122[B]:ASN:HD21	1.28	0.97
3:O:3109[B]:TYR:HD1	3:X:2970[B]:PRO:HD2	1.24	0.97
3:O:3109[B]:TYR:OH	3:X:2973[B]:THR:N	1.97	0.97
3:U:3027[A]:GLU:OE1	3:U:3029[A]:LYS:N	1.97	0.97
3:a:3027[A]:GLU:OE1	3:a:3029[A]:LYS:N	1.97	0.97
3:I:3223[B]:GLY:CA	3:R:2963[B]:MET:HE1	1.94	0.97
3:O:3154[B]:PRO:HD2	3:X:3176[B]:LYS:NZ	1.77	0.97
3:O:3158[B]:PHE:H	3:X:3152[B]:LYS:HB2	1.26	0.97
3:U:2990[B]:ARG:NH2	3:U:3180[B]:TYR:HB3	1.79	0.97
1:Y:806:ASN:O	1:Y:806:ASN:ND2	1.96	0.97
3:a:2991[A]:LEU:HD23	3:a:3158[A]:PHE:CD1	1.99	0.97
3:d:3066[A]:TYR:OH	3:d:3203[A]:HIS:NE2	1.97	0.97
3:C:2983[B]:VAL:HG23	3:L:3160[B]:SER:HA	0.98	0.97
3:C:2990[B]:ARG:NH2	3:C:3180[B]:TYR:HB3	1.78	0.97
3:C:3027[B]:GLU:OE1	3:C:3029[B]:LYS:N	1.97	0.97
3:F:2966[B]:SER:HA	3:a:3256[B]:TRP:N	1.78	0.97
3:F:2970[B]:PRO:HA	3:a:2985[B]:PHE:HZ	1.15	0.97
3:F:3034[A]:HIS:HB3	3:F:3035[A]:HIS:ND1	1.79	0.97
3:F:3156[B]:MET:CB	3:a:2982[B]:MET:HG3	1.95	0.97
3:I:2968[B]:GLN:HB2	3:I:2972[B]:GLY:HA2	1.47	0.97
3:O:3173[B]:THR:HB	3:O:3176[B]:LYS:HD2	1.46	0.97
3:R:2990[B]:ARG:NH2	3:R:3180[B]:TYR:HB3	1.78	0.97
3:R:3173[A]:THR:HB	3:R:3176[A]:LYS:HD2	1.46	0.97
3:U:2965[B]:LEU:CD1	3:d:3221[B]:ALA:N	2.14	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2968[A]:GLN:HB2	3:X:2972[A]:GLY:HA2	1.47	0.97
3:X:3013[B]:ASP:HA	3:X:3122[B]:ASN:HD21	1.28	0.97
3:X:3298[A]:ASN:HB2	3:X:3300[A]:LEU:N	1.78	0.97
3:a:3027[B]:GLU:OE1	3:a:3029[B]:LYS:N	1.97	0.97
3:a:3038[B]:ILE:CG2	3:a:3040[B]:VAL:HG22	1.93	0.97
3:d:3027[B]:GLU:OE1	3:d:3029[B]:LYS:N	1.97	0.97
3:C:3156[B]:MET:SD	3:L:2982[B]:MET:CG	2.53	0.97
3:C:3162[B]:ASP:CG	3:L:3259[B]:ASP:H	1.70	0.97
3:F:2991[B]:LEU:HD23	3:F:3158[B]:PHE:CD1	1.99	0.97
3:I:3221[B]:ALA:HB3	3:R:2964[B]:PRO:HB3	1.42	0.97
3:L:3066[A]:TYR:OH	3:L:3203[A]:HIS:NE2	1.97	0.97
2:N:2868:GLU:OE2	3:O:2933[A]:SER:N	1.97	0.97
3:O:3066[B]:TYR:OH	3:O:3203[B]:HIS:NE2	1.97	0.97
3:R:3013[A]:ASP:HA	3:R:3122[A]:ASN:HD21	1.27	0.97
3:R:3034[B]:HIS:HB3	3:R:3035[B]:HIS:ND1	1.79	0.97
3:X:3038[A]:ILE:CG2	3:X:3040[A]:VAL:HG22	1.93	0.97
3:a:3173[A]:THR:HB	3:a:3176[A]:LYS:HD2	1.46	0.97
3:C:3168[B]:THR:O	3:L:3149[B]:ASN:O	1.83	0.97
3:C:3172[B]:SER:CA	3:L:3152[B]:LYS:HB2	1.91	0.97
3:C:3173[B]:THR:HB	3:C:3176[B]:LYS:HD2	1.46	0.97
3:C:3217[A]:PHE:CE1	3:C:3230[A]:PHE:CE1	2.51	0.97
3:I:2991[B]:LEU:HD23	3:I:3158[B]:PHE:CD1	1.99	0.97
3:I:3027[B]:GLU:OE1	3:I:3029[B]:LYS:N	1.97	0.97
3:I:3161[B]:GLU:HG2	3:R:3079[B]:CYS:SG	2.05	0.97
3:L:2952[A]:ALA:H	3:L:2953[A]:GLY:HA2	1.26	0.97
3:R:3066[B]:TYR:OH	3:R:3203[B]:HIS:NE2	1.97	0.97
3:U:3231[B]:ASP:O	3:U:3284[B]:LYS:N	1.98	0.97
3:d:2991[B]:LEU:HD23	3:d:3158[B]:PHE:CD1	1.99	0.97
3:C:2984[B]:THR:CG2	3:L:3159[B]:SER:HB3	1.88	0.97
3:F:2981[B]:GLY:N	3:a:2968[B]:GLN:HG2	1.78	0.97
3:F:3066[B]:TYR:OH	3:F:3203[B]:HIS:NE2	1.97	0.97
3:I:3107[B]:LEU:HD11	3:R:2975[B]:PHE:HD1	0.82	0.97
3:I:3173[B]:THR:HB	3:I:3176[B]:LYS:HD2	1.46	0.97
3:I:3217[A]:PHE:CE1	3:I:3230[A]:PHE:CE1	2.51	0.97
3:L:3027[B]:GLU:OE1	3:L:3029[B]:LYS:N	1.97	0.97
3:L:3217[A]:PHE:CE1	3:L:3230[A]:PHE:CE1	2.51	0.97
3:O:2965[B]:LEU:HB3	3:X:3254[B]:MET:HE1	1.46	0.97
3:R:3231[A]:ASP:O	3:R:3284[A]:LYS:N	1.97	0.97
1:S:1636:ASN:HD22	1:S:1639:LYS:HD2	1.29	0.97
3:U:3027[B]:GLU:OE1	3:U:3029[B]:LYS:N	1.97	0.97
3:U:3034[A]:HIS:HB3	3:U:3035[A]:HIS:ND1	1.79	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3034[B]:HIS:HB3	3:U:3035[B]:HIS:ND1	1.79	0.97
3:U:3066[B]:TYR:OH	3:U:3203[B]:HIS:NE2	1.97	0.97
3:X:2990[A]:ARG:NH2	3:X:3180[A]:TYR:HB3	1.79	0.97
3:a:2952[A]:ALA:H	3:a:2953[A]:GLY:HA2	1.26	0.97
3:a:2968[B]:GLN:HB2	3:a:2972[B]:GLY:HA2	1.47	0.97
3:a:3173[B]:THR:HB	3:a:3176[B]:LYS:HD2	1.46	0.97
3:C:2991[B]:LEU:HD23	3:C:3158[B]:PHE:CD1	1.99	0.97
3:F:3153[B]:LYS:CB	3:a:3155[B]:MET:CB	2.34	0.97
2:H:2472:ASN:HD21	4:s:1:NAG:H61	1.25	0.97
3:I:2975[B]:PHE:HA	3:R:3107[B]:LEU:HD21	1.47	0.97
3:I:3013[B]:ASP:HA	3:I:3122[B]:ASN:HD21	1.27	0.97
3:I:3150[B]:LYS:CD	3:R:3160[B]:SER:H	1.73	0.97
3:I:3231[B]:ASP:O	3:I:3284[B]:LYS:N	1.97	0.97
3:O:2991[A]:LEU:HD23	3:O:3158[A]:PHE:CD1	1.99	0.97
3:U:2991[B]:LEU:HD23	3:U:3158[B]:PHE:CD1	1.99	0.97
3:U:3038[B]:ILE:CG2	3:U:3040[B]:VAL:HG22	1.93	0.97
3:U:3152[B]:LYS:CB	3:d:3154[B]:PRO:CA	2.26	0.97
3:X:3231[A]:ASP:O	3:X:3284[A]:LYS:N	1.98	0.97
3:d:3231[B]:ASP:O	3:d:3284[B]:LYS:N	1.98	0.97
3:F:3034[B]:HIS:HB3	3:F:3035[B]:HIS:ND1	1.79	0.96
3:I:3159[B]:SER:CA	3:R:3150[B]:LYS:CB	2.42	0.96
3:I:3169[B]:LYS:HG2	3:R:3151[B]:LEU:H	1.29	0.96
3:L:2990[B]:ARG:NH2	3:L:3180[B]:TYR:HB3	1.79	0.96
3:L:2991[A]:LEU:HD23	3:L:3158[A]:PHE:CD1	1.99	0.96
3:O:3034[B]:HIS:HB3	3:O:3035[B]:HIS:ND1	1.79	0.96
3:O:3231[A]:ASP:O	3:O:3284[A]:LYS:N	1.98	0.96
3:R:2961[B]:HIS:NE2	3:R:2980[B]:HIS:NE2	2.04	0.96
3:R:2968[A]:GLN:HB2	3:R:2972[A]:GLY:HA2	1.47	0.96
3:R:3066[A]:TYR:OH	3:R:3203[A]:HIS:NE2	1.97	0.96
2:T:2800:LYS:O	3:U:3023[A]:ILE:CD1	2.13	0.96
3:C:2969[B]:TYR:OH	3:L:3120[B]:HIS:NE2	1.91	0.96
3:C:2971[B]:ASP:CB	3:L:3093[B]:HIS:CE1	2.46	0.96
3:C:3013[B]:ASP:HA	3:C:3122[B]:ASN:HD21	1.28	0.96
3:C:3159[B]:SER:HA	3:L:3150[B]:LYS:C	1.53	0.96
3:I:3231[A]:ASP:O	3:I:3284[A]:LYS:N	1.97	0.96
3:L:3034[A]:HIS:HB3	3:L:3035[A]:HIS:ND1	1.79	0.96
3:U:3013[A]:ASP:HA	3:U:3122[A]:ASN:HD21	1.27	0.96
3:a:2991[B]:LEU:HD23	3:a:3158[B]:PHE:CD1	1.99	0.96
3:d:3027[A]:GLU:OE1	3:d:3029[A]:LYS:N	1.97	0.96
3:C:3231[A]:ASP:O	3:C:3284[A]:LYS:N	1.97	0.96
3:F:2967[B]:CYS:SG	3:a:2982[B]:MET:CG	2.53	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3120[B]:HIS:CD2	3:R:2969[B]:TYR:HE2	1.83	0.96
3:I:3256[B]:TRP:HE1	3:R:2965[B]:LEU:CD1	1.79	0.96
3:L:2991[B]:LEU:HD23	3:L:3158[B]:PHE:CD1	1.99	0.96
3:R:3034[A]:HIS:HB3	3:R:3035[A]:HIS:ND1	1.79	0.96
2:T:2800:LYS:HB3	3:U:3023[A]:ILE:CD1	1.96	0.96
3:U:2969[A]:TYR:HD2	3:U:2971[A]:ASP:H	1.02	0.96
3:X:2968[B]:GLN:HB2	3:X:2972[B]:GLY:HA2	1.47	0.96
3:X:2991[A]:LEU:HD23	3:X:3158[A]:PHE:CD1	1.99	0.96
3:a:2969[A]:TYR:HD2	3:a:2971[A]:ASP:H	1.02	0.96
6:GA:2:NAG:H62	6:GA:3:BMA:C1	1.95	0.96
3:C:2952[B]:ALA:H	3:C:2953[B]:GLY:HA2	1.26	0.96
3:C:3172[B]:SER:HB3	3:L:3149[B]:ASN:C	1.88	0.96
3:C:3172[B]:SER:HB3	3:L:3149[B]:ASN:O	1.65	0.96
3:I:3172[B]:SER:CB	3:R:3150[B]:LYS:C	2.39	0.96
3:O:3108[B]:HIS:HB3	3:X:2969[B]:TYR:CA	1.95	0.96
2:Q:2868:GLU:CG	3:R:2932[A]:PRO:O	2.14	0.96
3:U:3173[A]:THR:HB	3:U:3176[A]:LYS:HD2	1.46	0.96
3:U:3231[A]:ASP:O	3:U:3284[A]:LYS:N	1.98	0.96
3:X:3027[A]:GLU:OE1	3:X:3029[A]:LYS:N	1.97	0.96
3:X:3231[B]:ASP:O	3:X:3284[B]:LYS:N	1.98	0.96
3:C:2965[B]:LEU:CB	3:L:3256[B]:TRP:CZ2	2.35	0.96
3:F:3013[B]:ASP:HA	3:F:3122[B]:ASN:HD21	1.27	0.96
3:I:3160[B]:SER:HB3	3:R:3150[B]:LYS:NZ	1.80	0.96
3:O:2968[A]:GLN:HB2	3:O:2972[A]:GLY:HA2	1.47	0.96
3:O:2991[B]:LEU:HD23	3:O:3158[B]:PHE:CD1	1.99	0.96
3:R:3027[B]:GLU:OE1	3:R:3029[B]:LYS:N	1.97	0.96
3:X:3034[B]:HIS:HB3	3:X:3035[B]:HIS:ND1	1.79	0.96
3:X:3066[B]:TYR:OH	3:X:3203[B]:HIS:NE2	1.97	0.96
3:X:3293[A]:LYS:HD2	3:X:3294[A]:SER:N	1.81	0.96
7:z:3:BMA:H2	7:z:4:MAN:H3	1.48	0.96
3:I:3034[B]:HIS:HB3	3:I:3035[B]:HIS:ND1	1.79	0.96
3:I:3153[B]:LYS:HD2	3:R:3155[B]:MET:HB2	1.42	0.96
3:L:3173[B]:THR:HB	3:L:3176[B]:LYS:HD2	1.46	0.96
3:L:3231[A]:ASP:O	3:L:3284[A]:LYS:N	1.98	0.96
3:O:3293[B]:LYS:CD	3:O:3294[B]:SER:HB3	1.95	0.96
3:R:3027[A]:GLU:OE1	3:R:3029[A]:LYS:N	1.97	0.96
3:R:3231[B]:ASP:O	3:R:3284[B]:LYS:N	1.98	0.96
3:U:3152[B]:LYS:HB2	3:d:3154[B]:PRO:HA	0.98	0.96
3:U:3156[B]:MET:HE2	3:d:2982[B]:MET:SD	0.43	0.96
3:U:3161[B]:GLU:HA	3:d:3146[B]:CYS:HB2	1.47	0.96
3:X:3066[A]:TYR:OH	3:X:3203[A]:HIS:NE2	1.97	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2988[A]:TRP:HE3	3:d:2989[A]:HIS:HD1	1.14	0.96
3:C:3155[B]:MET:CG	3:L:3154[B]:PRO:N	2.27	0.96
3:I:3154[B]:PRO:CB	3:R:3174[B]:GLY:N	2.28	0.96
3:I:3162[B]:ASP:HB3	3:R:3259[B]:ASP:H	1.28	0.96
3:L:2968[B]:GLN:HB2	3:L:2972[B]:GLY:HA2	1.47	0.96
2:Q:2868:GLU:CD	3:R:2932[A]:PRO:O	2.09	0.96
3:U:3066[A]:TYR:OH	3:U:3203[A]:HIS:NE2	1.97	0.96
3:U:3169[B]:LYS:O	3:d:3148[B]:ILE:CG2	2.13	0.96
3:a:3231[B]:ASP:O	3:a:3284[B]:LYS:N	1.97	0.96
3:C:2979[B]:GLN:HG3	3:L:3156[B]:MET:HE2	0.99	0.96
3:C:3027[A]:GLU:OE1	3:C:3029[A]:LYS:N	1.97	0.96
3:F:3150[B]:LYS:HG3	3:a:3163[B]:ASN:HD22	1.29	0.96
3:L:3066[B]:TYR:OH	3:L:3203[B]:HIS:NE2	1.97	0.96
3:O:2973[B]:THR:OG1	3:X:3158[B]:PHE:CZ	2.17	0.96
3:O:3173[A]:THR:HB	3:O:3176[A]:LYS:HD2	1.46	0.96
3:U:3196[A]:THR:N	3:U:3199[A]:GLN:HB2	1.81	0.96
3:X:3293[A]:LYS:CD	3:X:3294[A]:SER:HB3	1.95	0.96
3:C:3161[B]:GLU:H	3:L:2983[B]:VAL:HG21	0.81	0.96
3:F:3155[B]:MET:HB3	3:a:3153[B]:LYS:CD	1.96	0.96
3:R:3293[A]:LYS:HD2	3:R:3294[A]:SER:N	1.81	0.96
3:U:2970[B]:PRO:HA	3:d:3086[B]:GLU:CG	1.96	0.96
3:U:3293[B]:LYS:CD	3:U:3294[B]:SER:HB3	1.95	0.96
3:X:3293[B]:LYS:CD	3:X:3294[B]:SER:HB3	1.95	0.96
4:j:1:NAG:H61	4:j:2:NAG:N2	1.81	0.96
3:C:3284[B]:LYS:HE2	3:C:3284[B]:LYS:HA	1.48	0.96
3:F:3120[B]:HIS:NE2	3:a:2969[B]:TYR:HE2	1.60	0.96
3:F:3146[B]:CYS:O	3:a:3161[B]:GLU:HG3	1.65	0.96
3:F:3196[A]:THR:N	3:F:3199[A]:GLN:HB2	1.81	0.96
3:F:3231[B]:ASP:O	3:F:3284[B]:LYS:N	1.98	0.96
3:F:3293[B]:LYS:HD2	3:F:3294[B]:SER:N	1.81	0.96
3:I:3293[A]:LYS:HD2	3:I:3294[A]:SER:N	1.81	0.96
3:L:2968[A]:GLN:HB2	3:L:2972[A]:GLY:HA2	1.47	0.96
3:L:3173[A]:THR:HB	3:L:3176[A]:LYS:HD2	1.46	0.96
3:L:3293[A]:LYS:CD	3:L:3294[A]:SER:HB3	1.95	0.96
3:X:2988[A]:TRP:HE3	3:X:2989[A]:HIS:HD1	1.14	0.96
3:X:3027[B]:GLU:OE1	3:X:3029[B]:LYS:N	1.97	0.96
3:X:3034[A]:HIS:HB3	3:X:3035[A]:HIS:ND1	1.79	0.96
3:a:3217[A]:PHE:CE1	3:a:3230[A]:PHE:CE1	2.51	0.96
3:d:3293[A]:LYS:HD2	3:d:3294[A]:SER:N	1.81	0.96
3:F:3160[B]:SER:HB3	3:a:3150[B]:LYS:HZ2	1.24	0.95
3:F:3231[A]:ASP:O	3:F:3284[A]:LYS:N	1.98	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2968[A]:GLN:HB2	3:I:2972[A]:GLY:HA2	1.47	0.95
3:O:3024[B]:LEU:CD1	3:O:3025[B]:VAL:N	2.29	0.95
3:O:3066[A]:TYR:OH	3:O:3203[A]:HIS:NE2	1.97	0.95
3:O:3293[A]:LYS:CD	3:O:3294[A]:SER:HB3	1.95	0.95
3:a:3293[A]:LYS:CD	3:a:3294[A]:SER:HB3	1.95	0.95
3:d:3173[B]:THR:HB	3:d:3176[B]:LYS:HD2	1.46	0.95
3:d:3231[A]:ASP:O	3:d:3284[A]:LYS:N	1.98	0.95
3:C:3149[B]:ASN:CB	3:L:3163[B]:ASN:HD21	1.77	0.95
3:F:3256[B]:TRP:CD1	3:a:2966[B]:SER:C	2.44	0.95
3:I:3149[B]:ASN:OD1	3:R:3169[B]:LYS:CG	2.14	0.95
3:L:3293[B]:LYS:HD2	3:L:3294[B]:SER:N	1.81	0.95
3:O:2976[B]:ALA:CB	3:X:3156[B]:MET:SD	2.53	0.95
3:U:2991[A]:LEU:HD23	3:U:3158[A]:PHE:CD1	1.99	0.95
3:U:3173[B]:THR:HB	3:U:3176[B]:LYS:HD2	1.46	0.95
3:U:3259[B]:ASP:HA	3:d:2968[B]:GLN:NE2	1.80	0.95
3:X:3196[B]:THR:N	3:X:3199[B]:GLN:HB2	1.81	0.95
3:a:3217[B]:PHE:CE1	3:a:3230[B]:PHE:CE1	2.51	0.95
3:a:3293[B]:LYS:HD2	3:a:3294[B]:SER:N	1.81	0.95
3:d:3024[A]:LEU:CD1	3:d:3025[A]:VAL:N	2.29	0.95
3:d:3293[B]:LYS:HD2	3:d:3294[B]:SER:N	1.81	0.95
3:d:3293[B]:LYS:CD	3:d:3294[B]:SER:HB3	1.95	0.95
3:C:3251[B]:ASP:OD1	3:L:3108[B]:HIS:CE1	2.19	0.95
1:D:2:LEU:HD21	1:D:81:VAL:HG21	1.47	0.95
3:F:2968[B]:GLN:HB2	3:F:2972[B]:GLY:HA2	1.47	0.95
3:I:3027[A]:GLU:OE1	3:I:3029[A]:LYS:N	1.97	0.95
3:O:3040[B]:VAL:HG22	3:X:2969[B]:TYR:CE1	2.01	0.95
3:R:3284[A]:LYS:HE2	3:R:3284[A]:LYS:HA	1.48	0.95
3:U:3152[B]:LYS:CB	3:d:3154[B]:PRO:HB3	1.96	0.95
3:X:3024[A]:LEU:CD1	3:X:3025[A]:VAL:N	2.29	0.95
3:X:3217[B]:PHE:CE1	3:X:3230[B]:PHE:CE1	2.51	0.95
3:X:3293[B]:LYS:HD2	3:X:3294[B]:SER:N	1.81	0.95
3:a:3066[B]:TYR:OH	3:a:3203[B]:HIS:NE2	1.97	0.95
3:a:3231[A]:ASP:O	3:a:3284[A]:LYS:N	1.97	0.95
3:a:3293[B]:LYS:CD	3:a:3294[B]:SER:HB3	1.96	0.95
3:d:2987[B]:HIS:NE2	3:d:3178[B]:PHE:CE1	2.35	0.95
3:C:3163[B]:ASN:HD22	3:L:3149[B]:ASN:CB	1.59	0.95
3:C:3293[A]:LYS:HD2	3:C:3294[A]:SER:N	1.81	0.95
3:C:3293[B]:LYS:HD2	3:C:3294[B]:SER:N	1.81	0.95
3:F:2952[A]:ALA:H	3:F:2953[A]:GLY:HA2	1.26	0.95
3:F:3160[B]:SER:HA	3:a:2983[B]:VAL:H	1.30	0.95
3:F:3254[B]:MET:HB2	3:a:2966[B]:SER:OG	1.64	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2965[A]:LEU:HD11	3:I:2975[A]:PHE:H	1.31	0.95
3:I:3173[A]:THR:HB	3:I:3176[A]:LYS:HD2	1.46	0.95
3:I:3293[A]:LYS:CD	3:I:3294[A]:SER:HB3	1.95	0.95
3:L:2988[B]:TRP:HE3	3:L:2989[B]:HIS:HD1	1.14	0.95
3:L:3284[A]:LYS:HE2	3:L:3284[A]:LYS:HA	1.48	0.95
3:O:3153[B]:LYS:HG2	3:X:3176[B]:LYS:NZ	1.80	0.95
3:R:2988[B]:TRP:HE3	3:R:2989[B]:HIS:HD1	1.14	0.95
3:R:3196[B]:THR:N	3:R:3199[B]:GLN:HB2	1.81	0.95
3:R:3293[A]:LYS:CD	3:R:3294[A]:SER:HB3	1.95	0.95
3:U:2968[A]:GLN:HB2	3:U:2972[A]:GLY:HA2	1.47	0.95
3:U:2968[B]:GLN:CG	3:d:3258[B]:PHE:CE1	2.28	0.95
3:a:3024[B]:LEU:CD1	3:a:3025[B]:VAL:N	2.29	0.95
3:d:3293[A]:LYS:CD	3:d:3294[A]:SER:HB3	1.96	0.95
3:C:3024[A]:LEU:CD1	3:C:3025[A]:VAL:N	2.29	0.95
3:C:3196[A]:THR:N	3:C:3199[A]:GLN:HB2	1.81	0.95
3:C:3196[B]:THR:N	3:C:3199[B]:GLN:HB2	1.81	0.95
3:C:3293[A]:LYS:CD	3:C:3294[A]:SER:HB3	1.95	0.95
3:F:2965[B]:LEU:HD11	3:F:2975[B]:PHE:H	1.32	0.95
3:F:2987[A]:HIS:NE2	3:F:3178[A]:PHE:CE1	2.35	0.95
3:I:3024[B]:LEU:CD1	3:I:3025[B]:VAL:N	2.29	0.95
3:I:3284[B]:LYS:HE2	3:I:3284[B]:LYS:HA	1.48	0.95
3:L:2965[B]:LEU:HD11	3:L:2975[B]:PHE:H	1.31	0.95
3:O:3153[B]:LYS:HG2	3:X:3176[B]:LYS:CD	1.90	0.95
3:O:3254[B]:MET:CE	3:X:3172[B]:SER:OG	2.15	0.95
3:U:2948[B]:ASP:OD1	3:U:2950[B]:THR:OG1	1.85	0.95
3:U:2988[B]:TRP:HE3	3:U:2989[B]:HIS:HD1	1.14	0.95
3:C:2968[A]:GLN:HB2	3:C:2972[A]:GLY:HA2	1.47	0.95
3:C:2987[B]:HIS:NE2	3:C:3178[B]:PHE:CE1	2.35	0.95
3:C:3256[B]:TRP:CZ2	3:L:2965[B]:LEU:CB	2.45	0.95
3:C:3293[B]:LYS:CD	3:C:3294[B]:SER:HB3	1.95	0.95
3:F:3255[B]:PRO:HB2	3:a:2959[B]:SER:CB	1.97	0.95
3:I:3155[B]:MET:CG	3:R:3154[B]:PRO:N	2.26	0.95
3:L:2948[A]:ASP:OD1	3:L:2950[A]:THR:OG1	1.85	0.95
3:L:3196[B]:THR:N	3:L:3199[B]:GLN:HB2	1.81	0.95
3:O:3231[B]:ASP:O	3:O:3284[B]:LYS:N	1.98	0.95
3:O:3293[A]:LYS:HD2	3:O:3294[A]:SER:N	1.81	0.95
3:U:3024[B]:LEU:CD1	3:U:3025[B]:VAL:N	2.29	0.95
3:U:3217[A]:PHE:CE1	3:U:3230[A]:PHE:CE1	2.51	0.95
3:a:2946[A]:GLN:O	3:a:3037[A]:TYR:OH	1.85	0.95
3:d:2990[A]:ARG:NH2	3:d:3180[A]:TYR:HB3	1.79	0.95
3:d:3284[A]:LYS:HE2	3:d:3284[A]:LYS:HA	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3163[B]:ASN:HD21	3:L:3149[B]:ASN:CB	1.56	0.95
3:F:3024[B]:LEU:CD1	3:F:3025[B]:VAL:N	2.29	0.95
3:F:3255[B]:PRO:HG3	3:a:2963[B]:MET:C	1.92	0.95
3:I:3024[A]:LEU:CD1	3:I:3025[A]:VAL:N	2.29	0.95
3:I:3066[A]:TYR:OH	3:I:3203[A]:HIS:NE2	1.97	0.95
3:L:3293[B]:LYS:CD	3:L:3294[B]:SER:HB3	1.95	0.95
3:O:2948[B]:ASP:OD1	3:O:2950[B]:THR:OG1	1.85	0.95
3:R:2946[A]:GLN:O	3:R:3037[A]:TYR:OH	1.85	0.95
3:R:3173[B]:THR:HB	3:R:3176[B]:LYS:HD2	1.46	0.95
3:U:3156[B]:MET:CE	3:d:2982[B]:MET:CE	2.45	0.95
3:a:3013[A]:ASP:HA	3:a:3122[A]:ASN:HD21	1.27	0.95
3:a:3196[A]:THR:N	3:a:3199[A]:GLN:HB2	1.81	0.95
3:d:3196[B]:THR:N	3:d:3199[B]:GLN:HB2	1.81	0.95
3:d:3284[B]:LYS:HE2	3:d:3284[B]:LYS:HA	1.48	0.95
3:C:3024[B]:LEU:CD1	3:C:3025[B]:VAL:N	2.29	0.95
3:F:3149[B]:ASN:CG	3:a:3163[B]:ASN:ND2	2.25	0.95
3:F:3160[B]:SER:OG	3:a:2982[B]:MET:HA	1.66	0.95
3:F:3255[B]:PRO:CG	3:a:2962[B]:GLY:O	2.15	0.95
3:L:2987[A]:HIS:NE2	3:L:3178[A]:PHE:CE1	2.35	0.95
3:O:2970[B]:PRO:HG2	3:X:2991[B]:LEU:CB	1.94	0.95
3:O:3196[B]:THR:N	3:O:3199[B]:GLN:HB2	1.81	0.95
3:R:3024[B]:LEU:CD1	3:R:3025[B]:VAL:N	2.29	0.95
3:U:3259[B]:ASP:HA	3:d:2968[B]:GLN:HE21	1.28	0.95
3:X:2987[B]:HIS:NE2	3:X:3178[B]:PHE:CE1	2.35	0.95
3:a:2948[B]:ASP:OD1	3:a:2950[B]:THR:OG1	1.85	0.95
3:a:2987[A]:HIS:NE2	3:a:3178[A]:PHE:CE1	2.35	0.95
3:a:3293[A]:LYS:HD2	3:a:3294[A]:SER:N	1.81	0.95
3:d:2946[A]:GLN:O	3:d:3037[A]:TYR:OH	1.85	0.95
3:C:2988[B]:TRP:HE1	3:L:3153[B]:LYS:HZ3	1.01	0.95
3:F:3293[B]:LYS:CD	3:F:3294[B]:SER:HB3	1.95	0.95
3:L:3196[A]:THR:N	3:L:3199[A]:GLN:HB2	1.81	0.95
3:U:2987[B]:HIS:NE2	3:U:3178[B]:PHE:CE1	2.34	0.95
3:U:3293[A]:LYS:HD2	3:U:3294[A]:SER:N	1.81	0.95
3:a:2987[B]:HIS:NE2	3:a:3178[B]:PHE:CE1	2.35	0.95
3:a:3169[B]:LYS:O	3:a:3172[B]:SER:OG	1.85	0.95
3:C:2987[A]:HIS:NE2	3:C:3178[A]:PHE:CE1	2.34	0.95
3:F:2948[B]:ASP:OD1	3:F:2950[B]:THR:OG1	1.85	0.95
3:F:2989[B]:HIS:HE1	3:a:2969[B]:TYR:HA	1.24	0.95
3:F:3153[B]:LYS:NZ	3:a:3157[B]:PRO:CD	2.27	0.95
3:F:3254[B]:MET:C	3:a:2966[B]:SER:OG	2.09	0.95
3:I:3196[A]:THR:N	3:I:3199[A]:GLN:HB2	1.81	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3196[B]:THR:N	3:I:3199[B]:GLN:HB2	1.81	0.95
3:L:2987[B]:HIS:NE2	3:L:3178[B]:PHE:CE1	2.35	0.95
3:L:3024[B]:LEU:CD1	3:L:3025[B]:VAL:N	2.29	0.95
3:O:2987[A]:HIS:NE2	3:O:3178[A]:PHE:CE1	2.35	0.95
3:O:2988[B]:TRP:HE3	3:O:2989[B]:HIS:HD1	1.14	0.95
3:O:3158[B]:PHE:C	3:X:3148[B]:ILE:O	2.10	0.95
3:U:3149[B]:ASN:C	3:d:3154[B]:PRO:CB	2.40	0.95
3:d:2965[B]:LEU:HD11	3:d:2975[B]:PHE:H	1.31	0.95
3:d:3024[B]:LEU:CD1	3:d:3025[B]:VAL:N	2.29	0.95
3:F:2965[A]:LEU:HD11	3:F:2975[A]:PHE:H	1.31	0.94
3:I:2931[A]:THR:OG1	3:I:2934[A]:GLU:OE2	1.85	0.94
3:I:2965[B]:LEU:H	3:R:3221[B]:ALA:HB1	1.15	0.94
3:I:3174[B]:GLY:H	3:R:3154[B]:PRO:HB3	1.28	0.94
3:L:3231[B]:ASP:O	3:L:3284[B]:LYS:N	1.97	0.94
3:O:2946[A]:GLN:O	3:O:3037[A]:TYR:OH	1.85	0.94
3:O:2968[B]:GLN:HB2	3:O:2972[B]:GLY:HA2	1.47	0.94
3:O:2974[B]:ALA:HB3	3:X:2977[B]:CYS:CB	1.97	0.94
3:R:2948[A]:ASP:OD1	3:R:2950[A]:THR:OG1	1.85	0.94
3:R:3024[A]:LEU:CD1	3:R:3025[A]:VAL:N	2.29	0.94
3:R:3196[A]:THR:N	3:R:3199[A]:GLN:HB2	1.81	0.94
3:R:3298[A]:ASN:HB2	3:R:3300[A]:LEU:N	1.78	0.94
3:d:3173[A]:THR:HB	3:d:3176[A]:LYS:HD2	1.46	0.94
3:F:2931[B]:THR:OG1	3:F:2934[B]:GLU:OE2	1.85	0.94
3:F:2975[B]:PHE:CD1	3:a:3107[B]:LEU:CG	2.47	0.94
3:I:2946[A]:GLN:O	3:I:3037[A]:TYR:OH	1.85	0.94
3:I:2946[B]:GLN:O	3:I:3037[B]:TYR:OH	1.85	0.94
3:L:2931[B]:THR:OG1	3:L:2934[B]:GLU:OE2	1.85	0.94
3:L:2965[A]:LEU:HD11	3:L:2975[A]:PHE:H	1.31	0.94
3:O:2931[A]:THR:OG1	3:O:2934[A]:GLU:OE2	1.85	0.94
3:O:3106[A]:THR:O	3:O:3110[A]:THR:OG1	1.85	0.94
3:O:3169[B]:LYS:O	3:O:3172[B]:SER:OG	1.85	0.94
3:O:3217[A]:PHE:CE1	3:O:3230[A]:PHE:CE1	2.51	0.94
3:U:2946[A]:GLN:O	3:U:3037[A]:TYR:OH	1.85	0.94
3:U:3155[B]:MET:CA	3:d:3150[B]:LYS:CG	2.28	0.94
3:U:3298[B]:ASN:HB2	3:U:3300[B]:LEU:N	1.78	0.94
3:C:2984[B]:THR:HG23	3:L:3159[B]:SER:HB3	0.97	0.94
3:F:3150[B]:LYS:HG2	3:a:3158[B]:PHE:CA	1.54	0.94
3:F:3161[B]:GLU:CA	3:a:3147[B]:GLU:CG	2.45	0.94
3:I:2987[B]:HIS:NE2	3:I:3178[B]:PHE:CE1	2.35	0.94
3:I:3169[A]:LYS:O	3:I:3172[A]:SER:OG	1.85	0.94
3:I:3293[B]:LYS:HD2	3:I:3294[B]:SER:N	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2946[B]:GLN:O	3:O:3037[B]:TYR:OH	1.85	0.94
3:O:2963[B]:MET:CE	3:X:2975[B]:PHE:CD2	2.48	0.94
3:O:3284[B]:LYS:HE2	3:O:3284[B]:LYS:HA	1.48	0.94
3:O:3293[B]:LYS:HD2	3:O:3294[B]:SER:N	1.81	0.94
3:U:3159[B]:SER:HB2	3:d:3150[B]:LYS:CE	1.97	0.94
3:U:3293[A]:LYS:CD	3:U:3294[A]:SER:HB3	1.95	0.94
3:X:2946[A]:GLN:O	3:X:3037[A]:TYR:OH	1.85	0.94
3:X:3024[B]:LEU:CD1	3:X:3025[B]:VAL:N	2.29	0.94
1:Y:1550:ARG:CZ	3:d:3008[B]:GLY:O	2.14	0.94
3:a:2931[A]:THR:OG1	3:a:2934[A]:GLU:OE2	1.85	0.94
3:a:2965[B]:LEU:HD11	3:a:2975[B]:PHE:H	1.31	0.94
3:F:2974[B]:ALA:N	3:a:3248[B]:LEU:C	2.26	0.94
3:F:3163[B]:ASN:ND2	3:a:3149[B]:ASN:CB	2.30	0.94
3:F:3169[B]:LYS:O	3:F:3172[B]:SER:OG	1.85	0.94
3:F:3251[B]:ASP:C	3:a:3252[B]:TYR:HB2	1.91	0.94
3:F:3293[A]:LYS:HD2	3:F:3294[A]:SER:N	1.81	0.94
3:I:3106[A]:THR:O	3:I:3110[A]:THR:OG1	1.86	0.94
3:I:3159[B]:SER:CA	3:R:3150[B]:LYS:C	2.39	0.94
3:L:3024[A]:LEU:CD1	3:L:3025[A]:VAL:N	2.29	0.94
3:O:2965[B]:LEU:HD11	3:O:2975[B]:PHE:H	1.31	0.94
3:O:3024[A]:LEU:CD1	3:O:3025[A]:VAL:N	2.29	0.94
3:R:3106[B]:THR:O	3:R:3110[B]:THR:OG1	1.85	0.94
3:R:3169[B]:LYS:O	3:R:3172[B]:SER:OG	1.85	0.94
3:R:3293[B]:LYS:CD	3:R:3294[B]:SER:HB3	1.95	0.94
3:R:3293[B]:LYS:HD2	3:R:3294[B]:SER:N	1.81	0.94
3:U:2931[A]:THR:OG1	3:U:2934[A]:GLU:OE2	1.85	0.94
3:U:3284[A]:LYS:HA	3:U:3284[A]:LYS:HE2	1.48	0.94
3:X:2987[A]:HIS:NE2	3:X:3178[A]:PHE:CE1	2.35	0.94
3:a:2968[A]:GLN:HB2	3:a:2972[A]:GLY:HA2	1.47	0.94
3:a:3196[B]:THR:N	3:a:3199[B]:GLN:HB2	1.81	0.94
3:a:3298[A]:ASN:HB2	3:a:3300[A]:LEU:N	1.78	0.94
3:d:3217[B]:PHE:CE1	3:d:3230[B]:PHE:CE1	2.51	0.94
1:D:1494:ARG:HH11	1:D:1494:ARG:HG3	1.29	0.94
3:F:2988[B]:TRP:HE3	3:F:2989[B]:HIS:HD1	1.14	0.94
3:F:3149[B]:ASN:HB2	3:a:3163[B]:ASN:HD22	1.22	0.94
3:F:3173[B]:THR:HB	3:F:3176[B]:LYS:HD2	1.46	0.94
3:I:3163[B]:ASN:ND2	3:R:3149[B]:ASN:CG	2.26	0.94
3:L:3217[B]:PHE:CE1	3:L:3230[B]:PHE:CE1	2.51	0.94
2:N:2800:LYS:O	3:O:3023[A]:ILE:CD1	2.14	0.94
3:O:3284[A]:LYS:HE2	3:O:3284[A]:LYS:HA	1.48	0.94
3:U:2931[B]:THR:OG1	3:U:2934[B]:GLU:OE2	1.85	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2965[B]:LEU:H	3:d:3220[B]:ARG:CZ	1.79	0.94
3:U:3196[B]:THR:N	3:U:3199[B]:GLN:HB2	1.81	0.94
3:a:3106[A]:THR:O	3:a:3110[A]:THR:OG1	1.85	0.94
3:F:3024[A]:LEU:CD1	3:F:3025[A]:VAL:N	2.29	0.94
3:F:3106[B]:THR:O	3:F:3110[B]:THR:OG1	1.85	0.94
3:F:3196[B]:THR:N	3:F:3199[B]:GLN:HB2	1.81	0.94
3:I:2987[A]:HIS:NE2	3:I:3178[A]:PHE:CE1	2.35	0.94
3:I:2988[A]:TRP:HE3	3:I:2989[A]:HIS:HD1	1.13	0.94
3:L:2948[B]:ASP:OD1	3:L:2950[B]:THR:OG1	1.85	0.94
3:L:3293[A]:LYS:HD2	3:L:3294[A]:SER:N	1.81	0.94
3:O:2970[B]:PRO:O	3:X:2989[B]:HIS:N	1.99	0.94
3:O:3157[B]:PRO:C	3:X:3149[B]:ASN:C	2.33	0.94
3:U:2975[B]:PHE:HB2	3:d:3256[B]:TRP:CG	2.03	0.94
3:U:3024[A]:LEU:CD1	3:U:3025[A]:VAL:N	2.29	0.94
3:U:3156[B]:MET:CE	3:d:2982[B]:MET:SD	1.04	0.94
3:U:3254[B]:MET:CB	3:d:3254[B]:MET:CB	2.42	0.94
3:U:3293[B]:LYS:HD2	3:U:3294[B]:SER:N	1.81	0.94
3:X:3284[B]:LYS:HE2	3:X:3284[B]:LYS:HA	1.48	0.94
3:a:3024[A]:LEU:CD1	3:a:3025[A]:VAL:N	2.29	0.94
3:d:2946[B]:GLN:O	3:d:3037[B]:TYR:OH	1.85	0.94
3:d:3169[A]:LYS:O	3:d:3172[A]:SER:OG	1.85	0.94
3:d:3196[A]:THR:N	3:d:3199[A]:GLN:HB2	1.81	0.94
3:C:2965[B]:LEU:HD11	3:C:2975[B]:PHE:H	1.31	0.94
3:C:3079[B]:CYS:SG	3:L:3161[B]:GLU:HG3	0.93	0.94
3:F:2979[A]:GLN:CG	3:F:3155[A]:MET:HE1	1.97	0.94
3:I:2969[A]:TYR:HD2	3:I:2971[A]:ASP:H	1.02	0.94
3:I:3251[B]:ASP:OD1	3:R:3108[B]:HIS:CE1	2.20	0.94
3:O:2931[B]:THR:OG1	3:O:2934[B]:GLU:OE2	1.85	0.94
3:O:2987[B]:HIS:NE2	3:O:3178[B]:PHE:CE1	2.35	0.94
3:R:2948[B]:ASP:OD1	3:R:2950[B]:THR:OG1	1.85	0.94
3:U:2974[B]:ALA:HB1	3:d:3220[B]:ARG:HG2	1.47	0.94
3:U:3176[B]:LYS:HD2	3:d:3152[B]:LYS:CD	1.96	0.94
3:U:3284[B]:LYS:HE2	3:U:3284[B]:LYS:HA	1.48	0.94
3:X:2931[A]:THR:OG1	3:X:2934[A]:GLU:OE2	1.85	0.94
3:C:2931[A]:THR:OG1	3:C:2934[A]:GLU:OE2	1.85	0.94
3:C:2968[B]:GLN:HB2	3:C:2972[B]:GLY:HA2	1.47	0.94
3:C:3150[B]:LYS:HA	3:L:3172[B]:SER:CB	1.89	0.94
3:C:3197[B]:ILE:HD12	1:D:1617:LYS:O	1.67	0.94
3:F:2987[B]:HIS:NE2	3:F:3178[B]:PHE:CE1	2.35	0.94
3:F:3120[B]:HIS:CD2	3:a:2969[B]:TYR:HE2	1.86	0.94
3:F:3159[B]:SER:HB3	3:a:2984[B]:THR:HG23	0.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3284[B]:LYS:HE2	3:F:3284[B]:LYS:HA	1.48	0.94
3:I:2948[A]:ASP:OD1	3:I:2950[A]:THR:OG1	1.85	0.94
3:I:2969[B]:TYR:HD2	3:I:2971[B]:ASP:H	1.02	0.94
3:I:2976[B]:ALA:O	3:R:2976[B]:ALA:O	1.84	0.94
3:I:2989[B]:HIS:CG	3:R:2970[B]:PRO:CD	2.31	0.94
3:I:3255[B]:PRO:HB3	3:R:2964[B]:PRO:CB	1.96	0.94
3:I:3293[B]:LYS:CD	3:I:3294[B]:SER:HB3	1.95	0.94
3:L:2931[A]:THR:OG1	3:L:2934[A]:GLU:OE2	1.85	0.94
3:L:2946[B]:GLN:O	3:L:3037[B]:TYR:OH	1.85	0.94
3:L:3298[B]:ASN:HB2	3:L:3300[B]:LEU:N	1.78	0.94
3:O:2965[B]:LEU:C	3:X:3153[B]:LYS:HZ2	1.67	0.94
3:O:2988[A]:TRP:HE3	3:O:2989[A]:HIS:HD1	1.13	0.94
3:O:3160[B]:SER:OG	3:X:3150[B]:LYS:HB2	1.67	0.94
3:O:3163[B]:ASN:HB2	3:X:3149[B]:ASN:HA	0.94	0.94
3:R:2987[B]:HIS:NE2	3:R:3178[B]:PHE:CE1	2.35	0.94
3:U:2975[B]:PHE:CE2	3:d:3254[B]:MET:CG	2.40	0.94
3:U:2980[B]:HIS:HB2	3:d:2969[B]:TYR:CE1	2.03	0.94
3:U:2987[A]:HIS:NE2	3:U:3178[A]:PHE:CE1	2.35	0.94
3:X:2931[B]:THR:OG1	3:X:2934[B]:GLU:OE2	1.85	0.94
3:X:3169[B]:LYS:O	3:X:3172[B]:SER:OG	1.85	0.94
3:a:2948[A]:ASP:OD1	3:a:2950[A]:THR:OG1	1.85	0.94
3:d:2931[B]:THR:OG1	3:d:2934[B]:GLU:OE2	1.85	0.94
3:d:2979[A]:GLN:CG	3:d:3155[A]:MET:HE1	1.97	0.94
3:C:2946[A]:GLN:O	3:C:3037[A]:TYR:OH	1.85	0.94
3:C:3154[B]:PRO:HG3	3:L:3174[B]:GLY:HA2	1.50	0.94
3:C:3174[B]:GLY:HA2	3:L:3154[B]:PRO:CG	1.98	0.94
3:F:2966[B]:SER:CA	3:a:3256[B]:TRP:CG	2.50	0.94
3:F:2969[B]:TYR:HD2	3:F:2971[B]:ASP:H	1.02	0.94
3:F:3158[B]:PHE:H	3:a:3153[B]:LYS:NZ	1.65	0.94
3:O:3196[A]:THR:N	3:O:3199[A]:GLN:HB2	1.81	0.94
3:U:2979[B]:GLN:CG	3:U:3155[B]:MET:HE1	1.97	0.94
3:U:3170[B]:ALA:CA	3:d:3148[B]:ILE:CG2	2.40	0.94
3:U:3253[B]:GLU:HA	3:d:3255[B]:PRO:HG2	0.94	0.94
1:Y:1401:ARG:HD3	3:d:3182[B]:GLN:OE1	1.68	0.94
3:d:3169[B]:LYS:O	3:d:3172[B]:SER:OG	1.85	0.94
3:C:3153[B]:LYS:NZ	3:L:3158[B]:PHE:CE2	2.32	0.94
3:I:3150[B]:LYS:CB	3:R:3159[B]:SER:CA	2.30	0.94
3:I:3169[B]:LYS:O	3:I:3172[B]:SER:OG	1.85	0.94
3:L:3106[A]:THR:O	3:L:3110[A]:THR:OG1	1.85	0.94
3:U:2968[B]:GLN:HB2	3:U:2972[B]:GLY:HA2	1.47	0.94
3:X:2965[A]:LEU:HD11	3:X:2975[A]:PHE:H	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3173[B]:THR:HB	3:X:3176[B]:LYS:HD2	1.46	0.94
3:C:2948[A]:ASP:OD1	3:C:2950[A]:THR:OG1	1.85	0.93
3:C:2979[A]:GLN:CG	3:C:3155[A]:MET:HE1	1.97	0.93
3:C:3106[A]:THR:O	3:C:3110[A]:THR:OG1	1.85	0.93
3:C:3169[B]:LYS:O	3:C:3172[B]:SER:OG	1.85	0.93
3:I:2948[B]:ASP:OD1	3:I:2950[B]:THR:OG1	1.85	0.93
3:R:2946[B]:GLN:O	3:R:3037[B]:TYR:OH	1.85	0.93
3:R:2965[A]:LEU:HD11	3:R:2975[A]:PHE:H	1.31	0.93
3:R:2987[A]:HIS:NE2	3:R:3178[A]:PHE:CE1	2.35	0.93
3:R:3298[B]:ASN:HB2	3:R:3300[B]:LEU:N	1.78	0.93
2:W:2472:ASN:HD21	4:HA:1:NAG:H61	1.31	0.93
3:X:2946[B]:GLN:O	3:X:3037[B]:TYR:OH	1.85	0.93
3:X:3196[A]:THR:N	3:X:3199[A]:GLN:HB2	1.81	0.93
3:X:3284[A]:LYS:HE2	3:X:3284[A]:LYS:HA	1.48	0.93
3:a:2931[B]:THR:OG1	3:a:2934[B]:GLU:OE2	1.85	0.93
3:a:3284[B]:LYS:HE2	3:a:3284[B]:LYS:HA	1.48	0.93
3:C:2948[B]:ASP:OD1	3:C:2950[B]:THR:OG1	1.85	0.93
3:F:2968[A]:GLN:HB2	3:F:2972[A]:GLY:HA2	1.47	0.93
3:F:3293[A]:LYS:CD	3:F:3294[A]:SER:HB3	1.95	0.93
3:L:2946[A]:GLN:O	3:L:3037[A]:TYR:OH	1.85	0.93
3:L:3134[A]:GLN:O	3:L:3137[A]:ARG:N	2.02	0.93
3:O:2969[B]:TYR:HH	3:X:2994[B]:LYS:HB3	1.21	0.93
3:R:2968[B]:GLN:HB2	3:R:2972[B]:GLY:HA2	1.47	0.93
3:d:3106[A]:THR:O	3:d:3110[A]:THR:OG1	1.85	0.93
3:d:3106[B]:THR:O	3:d:3110[B]:THR:OG1	1.85	0.93
3:F:3155[B]:MET:HB2	3:a:3153[B]:LYS:HG2	1.50	0.93
3:F:3169[A]:LYS:O	3:F:3172[A]:SER:OG	1.85	0.93
3:F:3284[A]:LYS:HE2	3:F:3284[A]:LYS:HA	1.48	0.93
3:I:3172[B]:SER:N	3:R:3152[B]:LYS:CB	2.07	0.93
3:L:2960[A]:PHE:HD2	3:L:3157[A]:PRO:CG	1.82	0.93
3:L:2979[A]:GLN:CG	3:L:3155[A]:MET:HE1	1.97	0.93
3:L:3106[B]:THR:O	3:L:3110[B]:THR:OG1	1.85	0.93
3:O:2973[B]:THR:HG1	3:X:3158[B]:PHE:HZ	0.94	0.93
3:U:2965[A]:LEU:HD11	3:U:2975[A]:PHE:H	1.31	0.93
3:U:3255[B]:PRO:HD3	3:d:3253[B]:GLU:O	1.67	0.93
3:U:3298[A]:ASN:HB2	3:U:3300[A]:LEU:N	1.78	0.93
3:X:2963[B]:MET:HG2	3:X:3108[B]:HIS:CD2	2.04	0.93
3:a:3106[B]:THR:O	3:a:3110[B]:THR:OG1	1.85	0.93
3:d:2932[A]:PRO:HA	3:d:2935[A]:ILE:CD1	1.99	0.93
3:d:2932[B]:PRO:HA	3:d:2935[B]:ILE:CD1	1.99	0.93
3:F:3153[B]:LYS:HG2	3:a:3155[B]:MET:CG	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3196[A]:THR:CG2	1:J:416:ASN:ND2	1.75	0.93
3:L:2932[A]:PRO:HA	3:L:2935[A]:ILE:CD1	1.99	0.93
3:O:2963[B]:MET:CG	3:X:2968[B]:GLN:O	2.12	0.93
3:O:2967[B]:CYS:HB2	3:X:3155[B]:MET:CG	1.97	0.93
3:R:2931[B]:THR:OG1	3:R:2934[B]:GLU:OE2	1.85	0.93
3:U:2932[A]:PRO:HA	3:U:2935[A]:ILE:CD1	1.99	0.93
3:U:2948[A]:ASP:OD1	3:U:2950[A]:THR:OG1	1.85	0.93
3:U:3169[B]:LYS:O	3:U:3172[B]:SER:OG	1.85	0.93
3:a:2932[B]:PRO:HA	3:a:2935[B]:ILE:CD1	1.99	0.93
3:a:2963[A]:MET:HG2	3:a:3108[A]:HIS:CD2	2.04	0.93
3:d:2987[A]:HIS:NE2	3:d:3178[A]:PHE:CE1	2.35	0.93
3:C:2969[A]:TYR:HD2	3:C:2971[A]:ASP:H	1.02	0.93
3:C:3161[B]:GLU:HG3	3:L:3146[B]:CYS:O	1.69	0.93
3:C:3172[B]:SER:HB3	3:L:3150[B]:LYS:N	1.82	0.93
3:F:2946[B]:GLN:O	3:F:3037[B]:TYR:OH	1.85	0.93
3:F:2963[B]:MET:HG2	3:F:3108[B]:HIS:CD2	2.04	0.93
3:F:2988[A]:TRP:HE3	3:F:2989[A]:HIS:HD1	1.14	0.93
3:F:3163[B]:ASN:HD21	3:a:3149[B]:ASN:HB2	1.20	0.93
3:I:2932[B]:PRO:HA	3:I:2935[B]:ILE:HD12	1.51	0.93
3:O:2948[A]:ASP:OD1	3:O:2950[A]:THR:OG1	1.85	0.93
3:O:2960[B]:PHE:HD2	3:O:3157[B]:PRO:CG	1.82	0.93
3:O:2965[A]:LEU:HD11	3:O:2975[A]:PHE:H	1.31	0.93
3:O:3040[B]:VAL:HG21	3:X:2969[B]:TYR:HD1	1.21	0.93
3:R:2931[A]:THR:OG1	3:R:2934[A]:GLU:OE2	1.85	0.93
3:U:3106[B]:THR:O	3:U:3110[B]:THR:OG1	1.86	0.93
3:U:3162[B]:ASP:N	3:d:3260[B]:ARG:HH12	1.57	0.93
3:X:2948[B]:ASP:OD1	3:X:2950[B]:THR:OG1	1.85	0.93
2:Z:2867:PRO:HG2	3:a:2932[A]:PRO:CG	1.78	0.93
3:a:2946[B]:GLN:O	3:a:3037[B]:TYR:OH	1.85	0.93
3:d:2963[B]:MET:HG2	3:d:3108[B]:HIS:CD2	2.04	0.93
3:F:2931[A]:THR:OG1	3:F:2934[A]:GLU:OE2	1.85	0.93
3:F:2965[B]:LEU:CD1	3:a:3256[B]:TRP:NE1	2.30	0.93
3:I:2932[A]:PRO:HA	3:I:2935[A]:ILE:HD12	1.51	0.93
3:I:2966[B]:SER:HB3	3:R:2982[B]:MET:HE2	1.46	0.93
3:I:3106[B]:THR:O	3:I:3110[B]:THR:OG1	1.85	0.93
3:I:3254[B]:MET:CB	3:R:2966[B]:SER:OG	2.16	0.93
3:L:3284[B]:LYS:HE2	3:L:3284[B]:LYS:HA	1.48	0.93
3:O:3106[B]:THR:O	3:O:3110[B]:THR:OG1	1.85	0.93
3:R:3106[A]:THR:O	3:R:3110[A]:THR:OG1	1.85	0.93
3:R:3169[A]:LYS:O	3:R:3172[A]:SER:OG	1.85	0.93
3:X:2948[A]:ASP:OD1	3:X:2950[A]:THR:OG1	1.85	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:2932[A]:PRO:HA	3:a:2935[A]:ILE:CD1	1.99	0.93
3:d:2948[A]:ASP:OD1	3:d:2950[A]:THR:OG1	1.85	0.93
3:d:2968[A]:GLN:HB2	3:d:2972[A]:GLY:HA2	1.47	0.93
3:C:2969[B]:TYR:HE2	3:L:3120[B]:HIS:NE2	1.62	0.93
3:C:3158[B]:PHE:CE2	3:L:3153[B]:LYS:CE	2.50	0.93
3:C:3172[B]:SER:HB2	3:L:3150[B]:LYS:C	1.94	0.93
3:C:3283[A]:ILE:HG21	3:C:3305[A]:ILE:HD11	1.51	0.93
3:F:2932[A]:PRO:HA	3:F:2935[A]:ILE:CD1	1.99	0.93
3:F:2948[A]:ASP:OD1	3:F:2950[A]:THR:OG1	1.85	0.93
3:F:2969[A]:TYR:HD2	3:F:2971[A]:ASP:H	1.02	0.93
3:F:3174[B]:GLY:HA3	3:a:3154[B]:PRO:HB3	1.48	0.93
3:I:2967[B]:CYS:HA	3:R:2981[B]:GLY:HA3	1.51	0.93
3:O:2963[B]:MET:HE1	3:X:2975[B]:PHE:CD2	2.03	0.93
3:O:3252[B]:TYR:HB2	3:X:3156[B]:MET:SD	2.09	0.93
3:R:2932[B]:PRO:HA	3:R:2935[B]:ILE:CD1	1.99	0.93
3:U:3152[B]:LYS:CB	3:d:3154[B]:PRO:CB	2.47	0.93
3:a:2979[A]:GLN:CG	3:a:3155[A]:MET:HE1	1.97	0.93
3:a:2988[A]:TRP:HE3	3:a:2989[A]:HIS:HD1	1.14	0.93
3:a:3284[A]:LYS:HE2	3:a:3284[A]:LYS:HA	1.48	0.93
3:d:3298[A]:ASN:HB2	3:d:3300[A]:LEU:HD23	1.50	0.93
3:C:3079[B]:CYS:SG	3:L:3161[B]:GLU:HG2	0.80	0.93
3:C:3258[B]:PHE:CZ	3:L:2968[B]:GLN:NE2	2.37	0.93
2:H:2797:LYS:HZ1	3:I:3028[A]:PRO:HD3	1.14	0.93
3:O:3134[A]:GLN:O	3:O:3137[A]:ARG:N	2.02	0.93
3:O:3253[B]:GLU:HG3	3:X:3161[B]:GLU:OE2	1.69	0.93
3:O:3298[B]:ASN:HB2	3:O:3300[B]:LEU:HD23	1.50	0.93
3:R:3134[A]:GLN:O	3:R:3137[A]:ARG:N	2.02	0.93
3:U:3283[B]:ILE:HG21	3:U:3305[B]:ILE:HD11	1.51	0.93
3:X:2932[B]:PRO:HA	3:X:2935[B]:ILE:CD1	1.99	0.93
3:C:2963[A]:MET:HG2	3:C:3108[A]:HIS:CD2	2.04	0.93
3:C:2967[B]:CYS:N	3:L:3256[B]:TRP:CD1	2.22	0.93
3:C:2979[B]:GLN:HE22	3:L:2979[B]:GLN:HE22	0.97	0.93
3:C:3154[B]:PRO:HD3	3:L:3174[B]:GLY:HA2	1.02	0.93
3:C:3158[B]:PHE:CE2	3:L:3153[B]:LYS:NZ	2.36	0.93
3:C:3298[B]:ASN:HB2	3:C:3300[B]:LEU:HD23	1.50	0.93
3:F:2965[B]:LEU:HD12	3:a:3256[B]:TRP:HE1	1.30	0.93
3:F:3106[A]:THR:O	3:F:3110[A]:THR:OG1	1.85	0.93
3:I:3254[B]:MET:HG3	3:R:2966[B]:SER:HB2	0.93	0.93
3:L:2932[A]:PRO:HA	3:L:2935[A]:ILE:HD12	1.51	0.93
3:O:2932[B]:PRO:HA	3:O:2935[B]:ILE:CD1	1.99	0.93
3:O:3038[B]:ILE:HD13	3:X:2969[B]:TYR:HE2	1.27	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3106[B]:THR:O	3:X:3110[B]:THR:OG1	1.85	0.93
3:a:3298[A]:ASN:HB2	3:a:3300[A]:LEU:HD23	1.51	0.93
3:d:2960[B]:PHE:HD2	3:d:3157[B]:PRO:CG	1.82	0.93
3:C:2932[B]:PRO:HA	3:C:2935[B]:ILE:CD1	1.99	0.93
3:C:2946[B]:GLN:O	3:C:3037[B]:TYR:OH	1.85	0.93
3:C:2965[A]:LEU:HD11	3:C:2975[A]:PHE:H	1.31	0.93
3:C:2967[B]:CYS:H	3:L:3256[B]:TRP:CD1	1.66	0.93
3:C:3106[B]:THR:O	3:C:3110[B]:THR:OG1	1.85	0.93
3:C:3259[B]:ASP:OD2	3:L:3162[B]:ASP:CG	2.11	0.93
3:F:2960[B]:PHE:HD2	3:F:3157[B]:PRO:CG	1.82	0.93
3:F:2963[A]:MET:HG2	3:F:3108[A]:HIS:CD2	2.04	0.93
3:F:3149[B]:ASN:HD22	3:a:3163[B]:ASN:CG	1.78	0.93
3:I:3134[A]:GLN:O	3:I:3137[A]:ARG:N	2.02	0.93
3:I:3149[B]:ASN:OD1	3:R:3169[B]:LYS:HG3	1.69	0.93
3:L:2932[B]:PRO:HA	3:L:2935[B]:ILE:HD12	1.51	0.93
3:L:3096[A]:VAL:HG11	3:L:3115[A]:LEU:CD1	1.99	0.93
3:L:3283[B]:ILE:HG21	3:L:3305[B]:ILE:HD11	1.51	0.93
3:R:2948[A]:ASP:N	3:R:2949[A]:LYS:HA	1.81	0.93
3:U:2980[B]:HIS:HB2	3:d:2969[B]:TYR:HE1	1.34	0.93
3:U:3096[A]:VAL:HG11	3:U:3115[A]:LEU:CD1	1.99	0.93
3:X:2963[A]:MET:HG2	3:X:3108[A]:HIS:CD2	2.04	0.93
2:Z:2472:ASN:CB	4:MA:1:NAG:H82	1.98	0.93
3:d:2931[A]:THR:OG1	3:d:2934[A]:GLU:OE2	1.85	0.93
3:C:2932[B]:PRO:HA	3:C:2935[B]:ILE:HD12	1.51	0.92
3:C:2960[B]:PHE:HD2	3:C:3157[B]:PRO:CG	1.82	0.92
3:F:2976[B]:ALA:HB3	3:a:3252[B]:TYR:O	1.69	0.92
3:F:3221[B]:ALA:HB3	3:a:2964[B]:PRO:CB	1.99	0.92
3:I:2969[A]:TYR:CE2	3:I:2970[A]:PRO:HG2	2.05	0.92
3:I:3160[B]:SER:N	3:R:3150[B]:LYS:HD3	1.76	0.92
3:I:3163[B]:ASN:HB2	3:R:3150[B]:LYS:HE3	0.94	0.92
3:I:3298[A]:ASN:HB2	3:I:3300[A]:LEU:N	1.78	0.92
3:U:3074[A]:GLU:OE1	3:U:3212[A]:ARG:NH2	2.03	0.92
3:X:2932[A]:PRO:HA	3:X:2935[A]:ILE:CD1	1.99	0.92
3:C:3090[B]:ASN:CG	3:L:2972[B]:GLY:CA	2.36	0.92
3:F:2946[A]:GLN:O	3:F:3037[A]:TYR:OH	1.85	0.92
3:I:2982[B]:MET:CE	3:R:2967[B]:CYS:SG	2.58	0.92
3:I:2989[B]:HIS:NE2	3:R:2969[B]:TYR:HA	1.83	0.92
3:O:3102[B]:TYR:CA	3:X:2971[B]:ASP:HA	1.98	0.92
3:R:3134[B]:GLN:O	3:R:3137[B]:ARG:N	2.02	0.92
3:U:2963[A]:MET:HG2	3:U:3108[A]:HIS:CD2	2.04	0.92
3:U:2971[B]:ASP:O	3:d:3247[B]:VAL:CG1	2.16	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3169[B]:LYS:O	3:d:3148[B]:ILE:HG22	1.69	0.92
3:U:3256[B]:TRP:HE3	3:d:2969[B]:TYR:HB3	1.31	0.92
3:d:2979[B]:GLN:CG	3:d:3155[B]:MET:HE1	1.97	0.92
3:C:2956[A]:LYS:O	3:C:2960[A]:PHE:HE1	1.22	0.92
3:C:3252[B]:TYR:CE2	3:L:3223[B]:GLY:O	2.22	0.92
3:F:3298[B]:ASN:HB2	3:F:3300[B]:LEU:HD23	1.50	0.92
3:L:2935[B]:ILE:HD13	3:L:2936[B]:GLU:H	1.35	0.92
3:L:2963[B]:MET:HG2	3:L:3108[B]:HIS:CD2	2.04	0.92
3:L:3169[B]:LYS:O	3:L:3172[B]:SER:OG	1.85	0.92
3:O:2963[A]:MET:HG2	3:O:3108[A]:HIS:CD2	2.04	0.92
3:O:3169[A]:LYS:O	3:O:3172[A]:SER:OG	1.85	0.92
3:R:2931[B]:THR:N	3:R:2934[B]:GLU:OE2	2.02	0.92
3:R:3096[B]:VAL:HG11	3:R:3115[B]:LEU:CD1	1.99	0.92
3:U:3134[A]:GLN:O	3:U:3137[A]:ARG:N	2.02	0.92
3:X:3096[A]:VAL:HG11	3:X:3115[A]:LEU:CD1	1.99	0.92
3:X:3106[A]:THR:O	3:X:3110[A]:THR:OG1	1.85	0.92
3:a:3298[B]:ASN:HB2	3:a:3300[B]:LEU:N	1.78	0.92
3:d:2948[B]:ASP:HB3	3:d:2949[B]:LYS:HA	1.52	0.92
3:d:2948[B]:ASP:OD1	3:d:2950[B]:THR:OG1	1.85	0.92
3:d:3074[B]:GLU:OE1	3:d:3212[B]:ARG:NH2	2.03	0.92
3:C:2969[A]:TYR:CE2	3:C:2970[A]:PRO:HG2	2.05	0.92
3:C:3096[B]:VAL:HG11	3:C:3115[B]:LEU:CD1	1.99	0.92
3:F:2931[A]:THR:N	3:F:2934[A]:GLU:OE2	2.02	0.92
3:F:3074[A]:GLU:OE1	3:F:3212[A]:ARG:NH2	2.03	0.92
3:F:3096[A]:VAL:HG11	3:F:3115[A]:LEU:CD1	2.00	0.92
3:I:2931[B]:THR:OG1	3:I:2934[B]:GLU:OE2	1.85	0.92
3:I:3155[B]:MET:N	3:R:3153[B]:LYS:O	1.99	0.92
3:L:2979[B]:GLN:CG	3:L:3155[B]:MET:HE1	1.97	0.92
3:O:2970[B]:PRO:HD2	3:X:2991[B]:LEU:HB2	1.17	0.92
3:O:3154[B]:PRO:HG3	3:X:3175[B]:TYR:CB	1.95	0.92
3:O:3283[B]:ILE:HG21	3:O:3305[B]:ILE:HD11	1.51	0.92
3:R:2979[A]:GLN:CG	3:R:3155[A]:MET:HE1	1.97	0.92
3:U:3169[A]:LYS:O	3:U:3172[A]:SER:OG	1.85	0.92
3:X:2965[B]:LEU:HD11	3:X:2975[B]:PHE:H	1.32	0.92
3:a:3134[B]:GLN:O	3:a:3137[B]:ARG:N	2.02	0.92
3:d:2931[B]:THR:N	3:d:2934[B]:GLU:OE2	2.02	0.92
3:d:3134[B]:GLN:O	3:d:3137[B]:ARG:N	2.02	0.92
3:C:2931[B]:THR:OG1	3:C:2934[B]:GLU:OE2	1.85	0.92
3:C:3134[B]:GLN:O	3:C:3137[B]:ARG:N	2.02	0.92
3:C:3154[B]:PRO:HB3	3:L:3174[B]:GLY:HA3	0.92	0.92
3:F:3120[B]:HIS:CD2	3:a:2969[B]:TYR:CE2	2.57	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2982[B]:MET:CE	3:R:2977[B]:CYS:HB2	1.99	0.92
3:I:3074[B]:GLU:OE1	3:I:3212[B]:ARG:NH2	2.03	0.92
3:I:3096[A]:VAL:HG11	3:I:3115[A]:LEU:CD1	2.00	0.92
3:I:3148[B]:ILE:O	3:R:3169[B]:LYS:C	2.02	0.92
3:L:2931[A]:THR:N	3:L:2934[A]:GLU:OE2	2.02	0.92
3:O:2948[A]:ASP:HB3	3:O:2949[A]:LYS:HA	1.52	0.92
3:O:2969[A]:TYR:CE2	3:O:2970[A]:PRO:HG2	2.05	0.92
3:O:3161[B]:GLU:CD	3:X:3151[B]:LEU:HD11	1.94	0.92
2:Q:2800:LYS:O	3:R:3023[A]:ILE:HD11	1.69	0.92
3:R:2963[A]:MET:HG2	3:R:3108[A]:HIS:CD2	2.04	0.92
3:R:2963[B]:MET:HG2	3:R:3108[B]:HIS:CD2	2.04	0.92
3:R:3284[B]:LYS:HE2	3:R:3284[B]:LYS:HA	1.48	0.92
3:U:2946[B]:GLN:O	3:U:3037[B]:TYR:OH	1.85	0.92
3:U:3134[B]:GLN:O	3:U:3137[B]:ARG:N	2.02	0.92
3:U:3169[B]:LYS:HG3	3:d:3147[B]:GLU:CB	1.99	0.92
2:W:2800:LYS:O	3:X:3023[A]:ILE:HD13	1.69	0.92
3:X:2935[B]:ILE:HD13	3:X:2936[B]:GLU:H	1.35	0.92
1:Y:1655:SER:HB3	3:d:3007[B]:ILE:HG23	1.49	0.92
3:a:3169[A]:LYS:O	3:a:3172[A]:SER:OG	1.85	0.92
3:d:3283[A]:ILE:HG21	3:d:3305[A]:ILE:HD11	1.51	0.92
3:C:3153[B]:LYS:C	3:L:3155[B]:MET:HG3	1.69	0.92
3:F:3298[A]:ASN:HB2	3:F:3300[A]:LEU:N	1.78	0.92
3:I:2965[B]:LEU:HD11	3:I:2975[B]:PHE:H	1.31	0.92
3:I:2969[B]:TYR:CE2	3:I:2970[B]:PRO:HG2	2.05	0.92
3:I:3096[B]:VAL:HG11	3:I:3115[B]:LEU:CD1	1.99	0.92
3:I:3147[A]:GLU:HB2	3:I:3149[A]:ASN:CG	1.95	0.92
3:I:3155[B]:MET:CB	3:R:3153[B]:LYS:CD	2.34	0.92
3:I:3298[A]:ASN:HB2	3:I:3300[A]:LEU:HD23	1.51	0.92
3:L:2965[A]:LEU:HD11	3:L:2975[A]:PHE:N	1.85	0.92
3:L:3147[A]:GLU:HB2	3:L:3149[A]:ASN:CG	1.95	0.92
3:U:2932[B]:PRO:HA	3:U:2935[B]:ILE:CD1	1.99	0.92
3:U:3106[A]:THR:O	3:U:3110[A]:THR:OG1	1.85	0.92
3:U:3156[B]:MET:HE1	3:d:2982[B]:MET:SD	1.54	0.92
3:X:2935[A]:ILE:HD13	3:X:2936[A]:GLU:H	1.35	0.92
3:X:2948[B]:ASP:HB3	3:X:2949[B]:LYS:HA	1.52	0.92
3:d:2932[B]:PRO:HA	3:d:2935[B]:ILE:HD12	1.51	0.92
3:C:3150[B]:LYS:N	3:L:3172[B]:SER:HB3	1.84	0.92
3:C:3298[A]:ASN:HB2	3:C:3300[A]:LEU:HD23	1.50	0.92
3:F:3283[A]:ILE:HG21	3:F:3305[A]:ILE:HD11	1.51	0.92
3:I:2963[A]:MET:HG2	3:I:3108[A]:HIS:CD2	2.03	0.92
3:I:2963[B]:MET:HG2	3:I:3108[B]:HIS:CD2	2.04	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2979[A]:GLN:CG	3:I:3155[A]:MET:HE1	1.97	0.92
3:I:3074[A]:GLU:OE1	3:I:3212[A]:ARG:NH2	2.03	0.92
3:I:3284[A]:LYS:HA	3:I:3284[A]:LYS:HE2	1.48	0.92
3:L:2932[B]:PRO:HA	3:L:2935[B]:ILE:CD1	1.99	0.92
3:O:2963[B]:MET:HG2	3:O:3108[B]:HIS:CD2	2.04	0.92
3:O:2979[B]:GLN:CG	3:O:3155[B]:MET:HE1	1.97	0.92
3:O:3159[B]:SER:C	3:X:3148[B]:ILE:O	2.11	0.92
3:R:3147[A]:GLU:HB2	3:R:3149[A]:ASN:CG	1.95	0.92
3:U:3074[B]:GLU:OE1	3:U:3212[B]:ARG:NH2	2.03	0.92
3:a:3096[A]:VAL:HG11	3:a:3115[A]:LEU:CD1	1.99	0.92
3:a:3283[B]:ILE:HG21	3:a:3305[B]:ILE:HD11	1.51	0.92
3:d:3096[B]:VAL:HG11	3:d:3115[B]:LEU:CD1	1.99	0.92
3:F:2983[B]:VAL:CB	3:a:3161[B]:GLU:N	2.33	0.92
3:F:3256[B]:TRP:CB	3:a:2966[B]:SER:C	2.43	0.92
3:F:3298[A]:ASN:HB2	3:F:3300[A]:LEU:HD23	1.50	0.92
3:I:2932[A]:PRO:HA	3:I:2935[A]:ILE:CD1	1.99	0.92
3:I:2960[A]:PHE:HD2	3:I:3157[A]:PRO:CG	1.82	0.92
3:I:2960[B]:PHE:HD2	3:I:3157[B]:PRO:CG	1.82	0.92
3:I:3150[B]:LYS:HE3	3:R:3163[B]:ASN:HB3	1.48	0.92
3:I:3220[B]:ARG:HG3	3:I:3220[B]:ARG:HH11	1.35	0.92
3:I:3255[B]:PRO:CG	3:R:2962[B]:GLY:C	2.43	0.92
3:L:2963[A]:MET:HG2	3:L:3108[A]:HIS:CD2	2.04	0.92
3:L:3169[A]:LYS:O	3:L:3172[A]:SER:OG	1.85	0.92
3:O:2960[A]:PHE:HD2	3:O:3157[A]:PRO:CG	1.82	0.92
3:O:3074[A]:GLU:OE1	3:O:3212[A]:ARG:NH2	2.02	0.92
3:R:2931[A]:THR:N	3:R:2934[A]:GLU:OE2	2.02	0.92
3:R:2969[A]:TYR:CE2	3:R:2970[A]:PRO:HG2	2.05	0.92
3:R:3298[A]:ASN:HB2	3:R:3300[A]:LEU:HD23	1.50	0.92
3:U:2960[B]:PHE:HD2	3:U:3157[B]:PRO:CG	1.82	0.92
3:U:2963[B]:MET:HG2	3:U:3108[B]:HIS:CD2	2.04	0.92
3:U:2979[A]:GLN:CG	3:U:3155[A]:MET:HE1	1.97	0.92
3:X:2948[A]:ASP:N	3:X:2949[A]:LYS:HA	1.81	0.92
3:X:3134[A]:GLN:O	3:X:3137[A]:ARG:N	2.02	0.92
3:a:2935[B]:ILE:HD13	3:a:2936[B]:GLU:H	1.35	0.92
3:a:2960[A]:PHE:HD2	3:a:3157[A]:PRO:CG	1.82	0.92
3:a:3134[A]:GLN:O	3:a:3137[A]:ARG:N	2.02	0.92
3:C:3156[B]:MET:HA	3:L:3150[B]:LYS:HD3	1.50	0.92
3:C:3220[A]:ARG:HG3	3:C:3220[A]:ARG:HH11	1.35	0.92
3:F:2966[B]:SER:C	3:a:3256[B]:TRP:CB	2.33	0.92
3:F:3096[B]:VAL:HG11	3:F:3115[B]:LEU:CD1	1.99	0.92
3:F:3134[B]:GLN:O	3:F:3137[B]:ARG:N	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3298[B]:ASN:HB2	3:F:3300[B]:LEU:N	1.78	0.92
3:I:3163[B]:ASN:O	3:R:3149[B]:ASN:ND2	2.02	0.92
3:L:3298[B]:ASN:HB2	3:L:3300[B]:LEU:HD23	1.50	0.92
3:O:2931[B]:THR:N	3:O:2934[B]:GLU:OE2	2.02	0.92
3:O:2971[B]:ASP:N	3:X:2988[B]:TRP:O	2.02	0.92
3:O:3096[A]:VAL:HG11	3:O:3115[A]:LEU:CD1	1.99	0.92
3:O:3108[B]:HIS:HB3	3:X:2969[B]:TYR:O	1.64	0.92
2:Q:2867:PRO:HG3	3:R:2932[A]:PRO:HG2	1.50	0.92
3:R:3074[A]:GLU:OE1	3:R:3212[A]:ARG:NH2	2.03	0.92
3:U:2970[B]:PRO:CB	3:d:2980[B]:HIS:HB3	1.68	0.92
3:U:3162[B]:ASP:OD1	3:d:3260[B]:ARG:NH1	2.02	0.92
3:U:3220[B]:ARG:HA	3:d:2973[B]:THR:N	1.84	0.92
3:X:2960[B]:PHE:HD2	3:X:3157[B]:PRO:CG	1.82	0.92
3:X:2965[A]:LEU:HD11	3:X:2975[A]:PHE:N	1.85	0.92
3:X:2979[B]:GLN:CG	3:X:3155[B]:MET:HE1	1.97	0.92
3:X:3147[A]:GLU:HB2	3:X:3149[A]:ASN:CG	1.95	0.92
3:a:2963[B]:MET:HG2	3:a:3108[B]:HIS:CD2	2.04	0.92
3:a:2969[B]:TYR:CE2	3:a:2970[B]:PRO:HG2	2.05	0.92
3:C:2963[B]:MET:HG2	3:C:3108[B]:HIS:CD2	2.04	0.92
3:C:3169[B]:LYS:O	3:L:3152[B]:LYS:CG	2.18	0.92
3:C:3298[A]:ASN:HB2	3:C:3300[A]:LEU:N	1.78	0.92
3:F:2960[A]:PHE:HD2	3:F:3157[A]:PRO:CG	1.82	0.92
3:F:3169[B]:LYS:O	3:a:3152[B]:LYS:HB2	1.69	0.92
3:F:3251[B]:ASP:CB	3:a:3251[B]:ASP:CG	2.42	0.92
3:I:2932[B]:PRO:HA	3:I:2935[B]:ILE:CD1	1.99	0.92
3:I:2982[B]:MET:CE	3:R:2977[B]:CYS:CB	2.48	0.92
3:L:2965[B]:LEU:HD11	3:L:2975[B]:PHE:N	1.85	0.92
3:O:2931[A]:THR:N	3:O:2934[A]:GLU:OE2	2.02	0.92
3:O:2970[B]:PRO:HD3	3:X:2991[B]:LEU:HD13	1.50	0.92
3:O:2974[B]:ALA:HB3	3:X:2977[B]:CYS:C	1.92	0.92
3:O:3096[B]:VAL:HG11	3:O:3115[B]:LEU:CD1	2.00	0.92
3:O:3220[B]:ARG:HH11	3:O:3220[B]:ARG:HG3	1.35	0.92
3:R:2935[A]:ILE:HD13	3:R:2936[A]:GLU:H	1.35	0.92
3:R:2960[A]:PHE:HD2	3:R:3157[A]:PRO:CG	1.82	0.92
3:R:2960[B]:PHE:HD2	3:R:3157[B]:PRO:CG	1.82	0.92
3:X:2931[A]:THR:N	3:X:2934[A]:GLU:OE2	2.02	0.92
3:X:2969[A]:TYR:CE2	3:X:2970[A]:PRO:HG2	2.05	0.92
3:X:3074[B]:GLU:OE1	3:X:3212[B]:ARG:NH2	2.03	0.92
3:a:3220[B]:ARG:HG3	3:a:3220[B]:ARG:HH11	1.35	0.92
3:d:3298[B]:ASN:HB2	3:d:3300[B]:LEU:HD23	1.50	0.92
3:C:2931[B]:THR:N	3:C:2934[B]:GLU:OE2	2.02	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2960[A]:PHE:HD2	3:C:3157[A]:PRO:CG	1.82	0.91
3:C:3120[B]:HIS:CD2	3:L:2969[B]:TYR:OH	2.22	0.91
3:F:2932[A]:PRO:HA	3:F:2935[A]:ILE:HD12	1.51	0.91
3:F:3074[B]:GLU:OE1	3:F:3212[B]:ARG:NH2	2.03	0.91
3:I:2931[A]:THR:N	3:I:2934[A]:GLU:OE2	2.02	0.91
3:I:2979[B]:GLN:C	3:R:2967[B]:CYS:CB	2.39	0.91
3:L:2960[B]:PHE:HD2	3:L:3157[B]:PRO:CG	1.82	0.91
3:O:2951[B]:ASP:OD2	3:O:2952[B]:ALA:N	2.03	0.91
3:O:2969[B]:TYR:HD2	3:O:2971[B]:ASP:H	1.02	0.91
3:O:3255[B]:PRO:CD	3:X:3169[B]:LYS:HG3	2.00	0.91
3:R:2932[A]:PRO:HA	3:R:2935[A]:ILE:HD12	1.51	0.91
3:R:3074[B]:GLU:OE1	3:R:3212[B]:ARG:NH2	2.03	0.91
3:R:3096[A]:VAL:HG11	3:R:3115[A]:LEU:CD1	1.99	0.91
3:R:3220[A]:ARG:HG3	3:R:3220[A]:ARG:HH11	1.35	0.91
3:U:2965[B]:LEU:HD11	3:U:2975[B]:PHE:H	1.31	0.91
3:U:3254[B]:MET:CE	3:d:3254[B]:MET:HB3	2.00	0.91
3:X:2948[B]:ASP:N	3:X:2949[B]:LYS:HA	1.81	0.91
3:X:2956[B]:LYS:O	3:X:2960[B]:PHE:HE1	1.22	0.91
3:X:3096[B]:VAL:HG11	3:X:3115[B]:LEU:CD1	2.00	0.91
3:X:3283[B]:ILE:HG21	3:X:3305[B]:ILE:HD11	1.51	0.91
1:b:1582:ASN:HB3	1:b:1583:CYS:HB2	1.53	0.91
3:d:3134[A]:GLN:O	3:d:3137[A]:ARG:N	2.01	0.91
3:C:2951[B]:ASP:OD2	3:C:2952[B]:ALA:N	2.03	0.91
3:C:2965[A]:LEU:HD11	3:C:2975[A]:PHE:N	1.85	0.91
3:C:2982[B]:MET:SD	3:L:3156[B]:MET:C	2.53	0.91
3:C:3172[B]:SER:CB	3:L:3150[B]:LYS:CA	2.48	0.91
3:F:2974[B]:ALA:N	3:a:3249[B]:GLY:N	2.10	0.91
3:F:3147[A]:GLU:HB2	3:F:3149[A]:ASN:CG	1.95	0.91
3:F:3153[B]:LYS:HE3	3:a:3158[B]:PHE:N	1.85	0.91
3:F:3173[B]:THR:OG1	3:a:3173[B]:THR:HG23	1.70	0.91
3:I:3220[A]:ARG:HH11	3:I:3220[A]:ARG:HG3	1.35	0.91
3:L:2969[A]:TYR:CE2	3:L:2970[A]:PRO:HG2	2.05	0.91
3:L:3134[B]:GLN:O	3:L:3137[B]:ARG:N	2.02	0.91
3:L:3220[A]:ARG:HH11	3:L:3220[A]:ARG:HG3	1.35	0.91
3:O:3147[A]:GLU:HB2	3:O:3149[A]:ASN:CG	1.95	0.91
3:U:2935[A]:ILE:HD13	3:U:2936[A]:GLU:H	1.35	0.91
3:U:3096[B]:VAL:HG11	3:U:3115[B]:LEU:CD1	1.99	0.91
3:U:3152[B]:LYS:HG3	3:d:3154[B]:PRO:HB3	0.92	0.91
3:U:3256[B]:TRP:CB	3:d:2975[B]:PHE:CE1	2.48	0.91
3:U:3283[A]:ILE:HG21	3:U:3305[A]:ILE:HD11	1.51	0.91
3:U:3298[B]:ASN:HB2	3:U:3300[B]:LEU:HD23	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2956[A]:LYS:O	3:X:2960[A]:PHE:HE1	1.22	0.91
3:X:2960[A]:PHE:HD2	3:X:3157[A]:PRO:CG	1.82	0.91
3:X:3169[A]:LYS:O	3:X:3172[A]:SER:OG	1.85	0.91
3:X:3298[A]:ASN:HB2	3:X:3300[A]:LEU:HD23	1.50	0.91
1:Y:1617:LYS:CE	3:d:3180[B]:TYR:CE2	2.52	0.91
3:a:2931[A]:THR:N	3:a:2934[A]:GLU:OE2	2.02	0.91
3:a:3096[B]:VAL:HG11	3:a:3115[B]:LEU:CD1	1.99	0.91
3:a:3147[A]:GLU:HB2	3:a:3149[A]:ASN:CG	1.95	0.91
3:d:2932[A]:PRO:HA	3:d:2935[A]:ILE:HD12	1.51	0.91
3:d:2935[B]:ILE:HD13	3:d:2936[B]:GLU:H	1.35	0.91
3:d:2960[A]:PHE:HD2	3:d:3157[A]:PRO:CG	1.82	0.91
3:d:3217[A]:PHE:HZ	3:d:3230[A]:PHE:CE1	1.89	0.91
3:C:2988[A]:TRP:HE3	3:C:2989[A]:HIS:HD1	1.14	0.91
3:C:3150[B]:LYS:HZ2	3:L:3160[B]:SER:CB	1.77	0.91
3:C:3169[A]:LYS:O	3:C:3172[A]:SER:OG	1.85	0.91
3:F:2931[B]:THR:N	3:F:2934[B]:GLU:OE2	2.02	0.91
3:F:2932[B]:PRO:HA	3:F:2935[B]:ILE:CD1	1.99	0.91
3:F:3153[B]:LYS:CE	3:a:3158[B]:PHE:H	1.83	0.91
3:L:2948[B]:ASP:N	3:L:2949[B]:LYS:HA	1.81	0.91
3:L:3147[B]:GLU:HB2	3:L:3149[B]:ASN:CG	1.95	0.91
3:L:3298[A]:ASN:HB2	3:L:3300[A]:LEU:HD23	1.51	0.91
3:O:2932[A]:PRO:HA	3:O:2935[A]:ILE:CD1	1.99	0.91
3:R:2932[A]:PRO:HA	3:R:2935[A]:ILE:CD1	1.99	0.91
3:U:3147[A]:GLU:HB2	3:U:3149[A]:ASN:CG	1.95	0.91
3:X:2951[A]:ASP:OD2	3:X:2952[A]:ALA:N	2.03	0.91
3:X:2979[A]:GLN:CG	3:X:3155[A]:MET:HE1	1.97	0.91
3:a:2960[B]:PHE:HD2	3:a:3157[B]:PRO:CG	1.82	0.91
3:a:2969[A]:TYR:CE2	3:a:2970[A]:PRO:HG2	2.05	0.91
3:a:3074[A]:GLU:OE1	3:a:3212[A]:ARG:NH2	2.03	0.91
3:d:2963[A]:MET:HG2	3:d:3108[A]:HIS:CD2	2.04	0.91
3:d:2969[B]:TYR:CE2	3:d:2970[B]:PRO:HG2	2.05	0.91
3:C:2932[A]:PRO:HA	3:C:2935[A]:ILE:HD12	1.51	0.91
3:C:2951[A]:ASP:OD2	3:C:2952[A]:ALA:N	2.03	0.91
3:C:2982[B]:MET:SD	3:L:3157[B]:PRO:N	2.42	0.91
3:F:2951[A]:ASP:OD2	3:F:2952[A]:ALA:N	2.04	0.91
3:F:2965[B]:LEU:HD11	3:F:2975[B]:PHE:N	1.85	0.91
3:F:2969[A]:TYR:CE2	3:F:2970[A]:PRO:HG2	2.05	0.91
3:I:2970[B]:PRO:N	3:R:2989[B]:HIS:NE2	2.18	0.91
3:I:2988[B]:TRP:HE3	3:I:2989[B]:HIS:HD1	1.14	0.91
3:I:3134[B]:GLN:O	3:I:3137[B]:ARG:N	2.02	0.91
3:O:3147[B]:GLU:HB2	3:O:3149[B]:ASN:CG	1.95	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3158[B]:PHE:N	3:X:3152[B]:LYS:CG	2.20	0.91
3:O:3253[B]:GLU:CD	3:X:3161[B]:GLU:OE2	2.13	0.91
3:X:2932[B]:PRO:HA	3:X:2935[B]:ILE:HD12	1.51	0.91
3:a:2951[A]:ASP:OD2	3:a:2952[A]:ALA:N	2.03	0.91
3:a:2951[B]:ASP:OD2	3:a:2952[B]:ALA:N	2.03	0.91
3:a:3283[A]:ILE:HG21	3:a:3305[A]:ILE:HD11	1.51	0.91
3:d:2931[A]:THR:N	3:d:2934[A]:GLU:OE2	2.02	0.91
1:A:1161:ILE:HD11	1:A:1196:ILE:HD11	1.53	0.91
3:C:2968[B]:GLN:O	3:L:2985[B]:PHE:HD2	1.48	0.91
3:C:2988[B]:TRP:CD1	3:L:3153[B]:LYS:NZ	2.35	0.91
3:C:3096[A]:VAL:HG11	3:C:3115[A]:LEU:CD1	1.99	0.91
3:C:3252[B]:TYR:CE1	3:L:3223[B]:GLY:C	2.48	0.91
3:F:2948[A]:ASP:HB3	3:F:2949[A]:LYS:HA	1.52	0.91
3:F:3090[B]:ASN:HA	3:a:2971[B]:ASP:O	1.69	0.91
3:F:3153[B]:LYS:HD2	3:a:3155[B]:MET:C	1.94	0.91
3:I:3147[B]:GLU:HB2	3:I:3149[B]:ASN:CG	1.95	0.91
3:I:3251[B]:ASP:CA	3:R:3251[B]:ASP:HB3	1.99	0.91
3:I:3298[B]:ASN:ND2	3:I:3301[B]:PRO:CA	2.34	0.91
3:L:2931[B]:THR:N	3:L:2934[B]:GLU:OE2	2.02	0.91
3:L:3074[A]:GLU:OE1	3:L:3212[A]:ARG:NH2	2.03	0.91
1:M:1582:ASN:HB3	1:M:1583:CYS:HB2	1.52	0.91
3:U:2931[B]:THR:N	3:U:2934[B]:GLU:OE2	2.02	0.91
3:U:2960[A]:PHE:HD2	3:U:3157[A]:PRO:CG	1.82	0.91
3:U:2968[B]:GLN:OE1	3:d:3258[B]:PHE:N	2.04	0.91
3:X:2931[B]:THR:N	3:X:2934[B]:GLU:OE2	2.02	0.91
3:d:3074[A]:GLU:OE1	3:d:3212[A]:ARG:NH2	2.02	0.91
3:C:2931[A]:THR:N	3:C:2934[A]:GLU:OE2	2.02	0.91
3:C:2969[B]:TYR:O	3:L:2985[B]:PHE:CE2	2.21	0.91
3:C:3074[A]:GLU:OE1	3:C:3212[A]:ARG:NH2	2.02	0.91
3:C:3153[B]:LYS:HB3	3:L:3155[B]:MET:CA	1.78	0.91
3:F:2932[B]:PRO:HA	3:F:2935[B]:ILE:HD12	1.51	0.91
3:F:3134[A]:GLN:O	3:F:3137[A]:ARG:N	2.02	0.91
3:F:3153[B]:LYS:HD2	3:a:3155[B]:MET:HB3	1.46	0.91
3:F:3162[B]:ASP:OD2	3:a:3258[B]:PHE:HA	1.71	0.91
3:F:3252[B]:TYR:N	3:a:3108[B]:HIS:CE1	2.39	0.91
3:F:3255[B]:PRO:HB3	3:a:2964[B]:PRO:CB	1.97	0.91
3:I:3162[B]:ASP:OD2	3:R:3258[B]:PHE:HA	1.70	0.91
3:I:3283[A]:ILE:HG21	3:I:3305[A]:ILE:HD11	1.52	0.91
3:O:2935[A]:ILE:HD13	3:O:2936[A]:GLU:H	1.35	0.91
3:O:2951[A]:ASP:OD2	3:O:2952[A]:ALA:N	2.03	0.91
3:O:2965[B]:LEU:HD11	3:O:2975[B]:PHE:N	1.85	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3134[B]:GLN:O	3:O:3137[B]:ARG:N	2.02	0.91
3:O:3169[B]:LYS:HE3	3:X:3148[B]:ILE:CA	1.57	0.91
2:Q:2867:PRO:HG3	3:R:2932[A]:PRO:CG	2.01	0.91
3:R:2965[B]:LEU:HD11	3:R:2975[B]:PHE:H	1.31	0.91
3:R:3298[B]:ASN:HB2	3:R:3300[B]:LEU:HD23	1.50	0.91
3:U:2969[B]:TYR:CE2	3:U:2970[B]:PRO:HG2	2.05	0.91
3:X:3134[B]:GLN:O	3:X:3137[B]:ARG:N	2.02	0.91
3:a:2931[B]:THR:N	3:a:2934[B]:GLU:OE2	2.02	0.91
3:C:2932[A]:PRO:HA	3:C:2935[A]:ILE:CD1	1.99	0.91
3:C:3284[A]:LYS:HE2	3:C:3284[A]:LYS:HA	1.49	0.91
3:F:3153[B]:LYS:HZ1	3:a:3157[B]:PRO:N	1.67	0.91
3:F:3163[B]:ASN:HB2	3:a:3150[B]:LYS:HE3	1.51	0.91
3:I:2951[A]:ASP:OD2	3:I:2952[A]:ALA:N	2.03	0.91
3:I:3162[B]:ASP:CB	3:R:3259[B]:ASP:HB3	2.00	0.91
3:L:2948[B]:ASP:HB3	3:L:2949[B]:LYS:HA	1.52	0.91
3:L:3074[B]:GLU:OE1	3:L:3212[B]:ARG:NH2	2.02	0.91
3:L:3096[B]:VAL:HG11	3:L:3115[B]:LEU:CD1	1.99	0.91
3:O:2965[A]:LEU:HD11	3:O:2975[A]:PHE:N	1.85	0.91
3:O:3074[B]:GLU:OE1	3:O:3212[B]:ARG:NH2	2.03	0.91
3:O:3283[A]:ILE:HG21	3:O:3305[A]:ILE:HD11	1.51	0.91
3:U:2951[A]:ASP:OD2	3:U:2952[A]:ALA:N	2.04	0.91
3:U:3147[B]:GLU:HB2	3:U:3149[B]:ASN:CG	1.95	0.91
3:U:3170[B]:ALA:HA	3:d:3148[B]:ILE:HG21	0.93	0.91
3:U:3298[A]:ASN:HB2	3:U:3300[A]:LEU:HD23	1.51	0.91
3:X:3074[A]:GLU:OE1	3:X:3212[A]:ARG:NH2	2.03	0.91
3:X:3283[A]:ILE:HG21	3:X:3305[A]:ILE:HD11	1.51	0.91
3:X:3298[B]:ASN:HB2	3:X:3300[B]:LEU:N	1.78	0.91
3:a:2932[A]:PRO:HA	3:a:2935[A]:ILE:HD12	1.51	0.91
3:d:2965[B]:LEU:HD11	3:d:2975[B]:PHE:N	1.85	0.91
3:d:3283[B]:ILE:HG21	3:d:3305[B]:ILE:HD11	1.51	0.91
3:C:2948[B]:ASP:HB3	3:C:2949[B]:LYS:HA	1.52	0.91
3:C:2979[B]:GLN:CG	3:C:3155[B]:MET:HE1	1.97	0.91
3:C:3158[B]:PHE:O	3:L:3149[B]:ASN:CB	2.19	0.91
3:C:3255[B]:PRO:CG	3:L:2959[B]:SER:O	2.17	0.91
3:F:2935[B]:ILE:HD13	3:F:2936[B]:GLU:H	1.35	0.91
3:F:2951[B]:ASP:OD2	3:F:2952[B]:ALA:N	2.03	0.91
3:F:2979[B]:GLN:CG	3:F:3155[B]:MET:HE1	1.97	0.91
3:F:3253[B]:GLU:CA	3:a:2976[B]:ALA:N	2.33	0.91
3:F:3255[B]:PRO:HB3	3:a:2964[B]:PRO:HB2	1.53	0.91
3:I:2961[B]:HIS:CE1	3:I:2980[B]:HIS:HE2	1.77	0.91
3:L:2951[A]:ASP:OD2	3:L:2952[A]:ALA:N	2.03	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2935[B]:ILE:HD13	3:O:2936[B]:GLU:H	1.35	0.91
3:U:2931[A]:THR:N	3:U:2934[A]:GLU:OE2	2.02	0.91
3:U:2972[B]:GLY:C	3:d:3247[B]:VAL:CG1	2.44	0.91
3:d:2948[A]:ASP:HB3	3:d:2949[A]:LYS:HA	1.52	0.91
3:d:2951[B]:ASP:OD2	3:d:2952[B]:ALA:N	2.03	0.91
3:d:2969[A]:TYR:CE2	3:d:2970[A]:PRO:HG2	2.05	0.91
3:d:3147[A]:GLU:HB2	3:d:3149[A]:ASN:CG	1.95	0.91
3:C:3172[B]:SER:HB3	3:L:3150[B]:LYS:HA	1.50	0.91
3:F:3147[B]:GLU:HB2	3:F:3149[B]:ASN:CG	1.95	0.91
3:F:3155[B]:MET:CG	3:a:3154[B]:PRO:N	2.33	0.91
3:I:2965[B]:LEU:HD11	3:I:2975[B]:PHE:N	1.85	0.91
3:O:3220[A]:ARG:HG3	3:O:3220[A]:ARG:HH11	1.35	0.91
3:R:2948[B]:ASP:HB3	3:R:2949[B]:LYS:HA	1.52	0.91
3:X:2951[B]:ASP:OD2	3:X:2952[B]:ALA:N	2.03	0.91
3:a:3298[B]:ASN:HB2	3:a:3300[B]:LEU:HD23	1.50	0.91
3:C:2965[B]:LEU:HD11	3:C:2975[B]:PHE:N	1.85	0.91
3:C:3147[B]:GLU:HB2	3:C:3149[B]:ASN:CG	1.95	0.91
3:F:3169[B]:LYS:HE2	3:a:3147[B]:GLU:N	1.82	0.91
3:F:3217[A]:PHE:HZ	3:F:3230[A]:PHE:CE1	1.89	0.91
3:I:2970[B]:PRO:N	3:R:2989[B]:HIS:CD2	2.38	0.91
3:I:2976[B]:ALA:HB3	3:R:3252[B]:TYR:O	1.71	0.91
3:I:3090[B]:ASN:HB3	3:R:2972[B]:GLY:CA	2.00	0.91
3:L:2948[A]:ASP:HB3	3:L:2949[A]:LYS:HA	1.52	0.91
3:R:3220[B]:ARG:HH11	3:R:3220[B]:ARG:HG3	1.35	0.91
3:U:2948[A]:ASP:HB3	3:U:2949[A]:LYS:HA	1.52	0.91
3:U:3155[B]:MET:H	3:d:3150[B]:LYS:HA	1.14	0.91
3:U:3230[B]:PHE:HB2	3:U:3243[B]:GLY:N	1.86	0.91
3:a:2965[B]:LEU:HD11	3:a:2975[B]:PHE:N	1.85	0.91
3:d:3096[A]:VAL:HG11	3:d:3115[A]:LEU:CD1	1.99	0.91
3:C:3156[B]:MET:CB	3:L:2982[B]:MET:CG	2.46	0.90
3:C:3163[B]:ASN:ND2	3:L:3149[B]:ASN:CG	2.19	0.90
3:C:3298[A]:ASN:ND2	3:C:3301[A]:PRO:CA	2.34	0.90
3:F:2979[A]:GLN:HE21	3:F:3155[A]:MET:HE3	1.37	0.90
3:F:3298[B]:ASN:ND2	3:F:3301[B]:PRO:CA	2.34	0.90
3:I:2935[B]:ILE:HD13	3:I:2936[B]:GLU:H	1.35	0.90
3:I:3149[B]:ASN:OD1	3:R:3169[B]:LYS:CD	2.17	0.90
3:I:3150[B]:LYS:HZ3	3:R:3160[B]:SER:HB3	1.29	0.90
3:I:3173[B]:THR:O	3:R:3154[B]:PRO:CD	2.19	0.90
3:I:3173[B]:THR:C	3:R:3154[B]:PRO:HD3	1.96	0.90
3:O:2974[B]:ALA:HB3	3:X:2977[B]:CYS:CA	2.01	0.90
3:O:3196[A]:THR:HB	3:O:3198[A]:PRO:HD2	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2932[B]:PRO:HA	3:R:2935[B]:ILE:HD12	1.51	0.90
3:R:2951[B]:ASP:OD2	3:R:2952[B]:ALA:N	2.03	0.90
3:R:2965[A]:LEU:HD11	3:R:2975[A]:PHE:N	1.85	0.90
3:R:3283[A]:ILE:HG21	3:R:3305[A]:ILE:HD11	1.51	0.90
3:R:3298[A]:ASN:ND2	3:R:3301[A]:PRO:CA	2.34	0.90
3:U:2935[B]:ILE:HD13	3:U:2936[B]:GLU:H	1.35	0.90
3:U:3220[B]:ARG:HG3	3:U:3220[B]:ARG:HH11	1.35	0.90
3:X:3230[A]:PHE:HB2	3:X:3243[A]:GLY:N	1.86	0.90
3:a:2965[A]:LEU:HD11	3:a:2975[A]:PHE:H	1.31	0.90
3:a:3298[A]:ASN:ND2	3:a:3301[A]:PRO:CA	2.34	0.90
3:a:3298[B]:ASN:ND2	3:a:3301[B]:PRO:CA	2.34	0.90
3:C:3174[B]:GLY:HA3	3:L:3154[B]:PRO:CB	2.00	0.90
3:F:3155[B]:MET:CG	3:a:3153[B]:LYS:HG2	2.00	0.90
3:F:3230[A]:PHE:HB2	3:F:3243[A]:GLY:N	1.87	0.90
3:I:2967[B]:CYS:HA	3:R:2981[B]:GLY:CA	1.94	0.90
3:I:3298[A]:ASN:ND2	3:I:3301[A]:PRO:CA	2.34	0.90
3:L:2951[B]:ASP:OD2	3:L:2952[B]:ALA:N	2.03	0.90
3:O:3157[B]:PRO:O	3:X:3148[B]:ILE:O	1.87	0.90
3:R:2988[A]:TRP:HE3	3:R:2989[A]:HIS:HD1	1.14	0.90
3:U:2969[A]:TYR:CE2	3:U:2970[A]:PRO:HG2	2.05	0.90
3:U:3153[B]:LYS:HB3	3:d:3153[B]:LYS:CG	2.00	0.90
3:U:3160[B]:SER:O	3:d:3147[B]:GLU:OE2	1.55	0.90
3:U:3196[A]:THR:HB	3:U:3198[A]:PRO:HD2	1.54	0.90
3:U:3298[A]:ASN:ND2	3:U:3301[A]:PRO:CA	2.34	0.90
3:a:2948[A]:ASP:HB3	3:a:2949[A]:LYS:HA	1.52	0.90
3:C:2967[B]:CYS:HB3	3:L:2982[B]:MET:H	1.29	0.90
3:C:2974[B]:ALA:CA	3:L:3249[B]:GLY:HA2	2.01	0.90
3:C:3074[B]:GLU:OE1	3:C:3212[B]:ARG:NH2	2.02	0.90
3:C:3134[A]:GLN:O	3:C:3137[A]:ARG:N	2.02	0.90
3:C:3147[A]:GLU:HB2	3:C:3149[A]:ASN:CG	1.95	0.90
1:D:695:TYR:HH	1:D:703:TYR:HD1	1.07	0.90
3:F:2975[B]:PHE:CG	3:a:3107[B]:LEU:HD11	2.04	0.90
3:F:3255[B]:PRO:HB2	3:a:2959[B]:SER:HB2	1.51	0.90
3:F:3283[B]:ILE:HG21	3:F:3305[B]:ILE:HD11	1.51	0.90
3:I:2931[B]:THR:N	3:I:2934[B]:GLU:OE2	2.02	0.90
3:I:3298[B]:ASN:HB2	3:I:3300[B]:LEU:HD23	1.51	0.90
3:L:2979[B]:GLN:HE21	3:L:3155[B]:MET:HE3	1.36	0.90
3:R:2935[B]:ILE:HD13	3:R:2936[B]:GLU:H	1.35	0.90
3:U:2951[B]:ASP:OD2	3:U:2952[B]:ALA:N	2.03	0.90
3:U:3254[B]:MET:CE	3:d:3254[B]:MET:CB	2.45	0.90
3:X:2965[B]:LEU:HD11	3:X:2975[B]:PHE:N	1.85	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3298[B]:ASN:HB2	3:X:3300[B]:LEU:HD23	1.51	0.90
3:d:2951[A]:ASP:OD2	3:d:2952[A]:ALA:N	2.04	0.90
3:d:2988[B]:TRP:HE3	3:d:2989[B]:HIS:HD1	1.14	0.90
3:d:3230[A]:PHE:HB2	3:d:3243[A]:GLY:N	1.87	0.90
3:C:3196[B]:THR:HB	3:C:3198[B]:PRO:HD2	1.54	0.90
3:I:2975[B]:PHE:HZ	3:R:2961[B]:HIS:CB	1.85	0.90
3:I:2978[B]:CYS:O	3:R:2977[B]:CYS:SG	2.28	0.90
3:I:2988[B]:TRP:CH2	3:R:2975[B]:PHE:HE2	1.88	0.90
3:O:2971[B]:ASP:N	3:X:2991[B]:LEU:N	2.19	0.90
3:F:2969[B]:TYR:CE2	3:F:2970[B]:PRO:HG2	2.05	0.90
3:F:3150[B]:LYS:HZ2	3:a:3160[B]:SER:HB3	1.10	0.90
3:I:3172[B]:SER:HB3	3:R:3150[B]:LYS:C	1.96	0.90
3:O:3160[B]:SER:CA	3:X:3151[B]:LEU:HD12	2.01	0.90
3:R:3230[B]:PHE:HB2	3:R:3243[B]:GLY:N	1.87	0.90
3:U:3220[B]:ARG:HA	3:d:2973[B]:THR:HA	0.91	0.90
3:a:2935[A]:ILE:HD13	3:a:2936[A]:GLU:H	1.35	0.90
3:C:3153[B]:LYS:NZ	3:L:2988[B]:TRP:CD1	2.40	0.90
3:F:2948[A]:ASP:N	3:F:2949[A]:LYS:HA	1.81	0.90
3:I:2935[A]:ILE:HD13	3:I:2936[A]:GLU:H	1.35	0.90
3:I:3169[B]:LYS:C	3:R:3148[B]:ILE:O	2.14	0.90
3:I:3196[A]:THR:HB	3:I:3198[A]:PRO:HD2	1.53	0.90
3:I:3230[B]:PHE:HB2	3:I:3243[B]:GLY:N	1.87	0.90
3:L:2988[A]:TRP:HE3	3:L:2989[A]:HIS:HD1	1.14	0.90
3:L:3298[B]:ASN:ND2	3:L:3301[B]:PRO:CA	2.34	0.90
3:O:3160[B]:SER:CB	3:X:3151[B]:LEU:N	2.30	0.90
3:R:3283[B]:ILE:HG21	3:R:3305[B]:ILE:HD11	1.51	0.90
3:U:3162[B]:ASP:CA	3:d:3260[B]:ARG:NH1	2.28	0.90
3:U:3220[A]:ARG:HH11	3:U:3220[A]:ARG:HG3	1.35	0.90
3:X:2948[A]:ASP:HB3	3:X:2949[A]:LYS:HA	1.52	0.90
3:a:2965[A]:LEU:HD11	3:a:2975[A]:PHE:N	1.85	0.90
3:C:3148[B]:ILE:C	3:L:3169[B]:LYS:C	2.37	0.90
3:I:3283[B]:ILE:HG21	3:I:3305[B]:ILE:HD11	1.51	0.90
3:R:2979[B]:GLN:CG	3:R:3155[B]:MET:HE1	1.97	0.90
3:U:2967[B]:CYS:HB2	3:d:3256[B]:TRP:CB	2.00	0.90
3:U:3153[B]:LYS:HE2	3:d:2979[B]:GLN:HE22	0.74	0.90
3:U:3298[B]:ASN:ND2	3:U:3301[B]:PRO:CA	2.34	0.90
3:X:2932[A]:PRO:HA	3:X:2935[A]:ILE:HD12	1.51	0.90
3:X:3220[B]:ARG:HG3	3:X:3220[B]:ARG:HH11	1.35	0.90
3:a:2988[B]:TRP:HE3	3:a:2989[B]:HIS:HD1	1.13	0.90
3:C:3223[B]:GLY:O	3:L:3252[B]:TYR:CE1	2.24	0.90
3:C:3230[B]:PHE:HB2	3:C:3243[B]:GLY:N	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:806:ASN:HD22	6:k:1:NAG:H83	1.36	0.90
3:F:2965[A]:LEU:HD11	3:F:2975[A]:PHE:N	1.85	0.90
3:F:2965[B]:LEU:O	3:a:3221[B]:ALA:HB2	1.72	0.90
3:F:2970[B]:PRO:HD3	3:a:2989[B]:HIS:ND1	1.86	0.90
3:F:2982[B]:MET:CE	3:a:2966[B]:SER:CB	2.49	0.90
3:F:3298[A]:ASN:ND2	3:F:3301[A]:PRO:CA	2.34	0.90
1:G:1582:ASN:HB3	1:G:1583:CYS:HB2	1.53	0.90
2:H:2868:GLU:OE2	3:I:2932[A]:PRO:C	2.14	0.90
3:I:2966[B]:SER:C	3:R:3256[B]:TRP:CG	2.39	0.90
3:I:2967[B]:CYS:SG	3:R:2982[B]:MET:CG	2.60	0.90
3:L:3230[A]:PHE:HB2	3:L:3243[A]:GLY:N	1.86	0.90
3:L:3283[A]:ILE:HG21	3:L:3305[A]:ILE:HD11	1.51	0.90
3:O:2932[A]:PRO:HA	3:O:2935[A]:ILE:HD12	1.51	0.90
3:O:2932[B]:PRO:HA	3:O:2935[B]:ILE:HD12	1.51	0.90
3:O:2973[B]:THR:CB	3:X:3158[B]:PHE:CE2	2.54	0.90
3:O:3230[B]:PHE:HB2	3:O:3243[B]:GLY:N	1.87	0.90
3:U:2948[B]:ASP:HB3	3:U:2949[B]:LYS:HA	1.52	0.90
3:a:3196[A]:THR:HB	3:a:3198[A]:PRO:HD2	1.53	0.90
3:d:3298[B]:ASN:ND2	3:d:3301[B]:PRO:CA	2.34	0.90
3:C:2979[A]:GLN:HE21	3:C:3155[A]:MET:HE3	1.36	0.90
3:C:3220[B]:ARG:HH11	3:C:3220[B]:ARG:HG3	1.35	0.90
3:C:3223[B]:GLY:O	3:L:3252[B]:TYR:CZ	2.24	0.90
3:I:3153[B]:LYS:CD	3:R:3155[B]:MET:CB	2.46	0.90
3:L:3220[B]:ARG:HH11	3:L:3220[B]:ARG:HG3	1.35	0.90
3:O:2964[B]:PRO:HA	3:X:2975[B]:PHE:HE2	1.37	0.90
3:O:2965[B]:LEU:HD11	3:X:2979[B]:GLN:NE2	1.86	0.90
3:O:3298[A]:ASN:HB2	3:O:3300[A]:LEU:N	1.78	0.90
3:R:2951[A]:ASP:OD2	3:R:2952[A]:ALA:N	2.04	0.90
3:R:3196[A]:THR:HB	3:R:3198[A]:PRO:HD2	1.53	0.90
3:U:2932[A]:PRO:HA	3:U:2935[A]:ILE:HD12	1.51	0.90
3:U:2988[A]:TRP:HE3	3:U:2989[A]:HIS:HD1	1.14	0.90
3:U:3252[B]:TYR:HE2	3:d:3222[B]:ILE:HD12	1.37	0.90
3:X:3298[B]:ASN:ND2	3:X:3301[B]:PRO:CA	2.34	0.90
3:d:2965[A]:LEU:HD11	3:d:2975[A]:PHE:H	1.32	0.90
3:d:3298[A]:ASN:HB2	3:d:3300[A]:LEU:N	1.78	0.90
3:C:3252[B]:TYR:HB3	3:L:3253[B]:GLU:HB3	1.52	0.90
3:F:2948[B]:ASP:HB3	3:F:2949[B]:LYS:HA	1.52	0.90
3:F:2967[B]:CYS:SG	3:a:2982[B]:MET:HG2	2.11	0.90
3:F:3024[A]:LEU:CD1	3:F:3025[A]:VAL:H	1.83	0.90
3:F:3196[B]:THR:HB	3:F:3198[B]:PRO:HD2	1.54	0.90
3:F:3220[B]:ARG:HG3	3:F:3220[B]:ARG:HH11	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2968[B]:GLN:HG3	3:R:3086[B]:GLU:HG3	1.53	0.90
3:I:3255[B]:PRO:CG	3:R:2964[B]:PRO:HD2	2.02	0.90
3:L:3217[B]:PHE:HZ	3:L:3230[B]:PHE:CE1	1.89	0.90
3:O:2970[B]:PRO:HG2	3:X:2990[B]:ARG:C	1.97	0.90
3:O:3230[A]:PHE:HB2	3:O:3243[A]:GLY:N	1.87	0.90
3:R:3147[B]:GLU:HB2	3:R:3149[B]:ASN:CG	1.95	0.90
1:Y:1616:LYS:C	3:d:3187[B]:TYR:HB2	1.96	0.90
2:Z:2472:ASN:HB3	4:MA:1:NAG:C8	2.01	0.90
3:a:2979[B]:GLN:HE21	3:a:3155[B]:MET:HE3	1.37	0.90
3:a:3074[B]:GLU:OE1	3:a:3212[B]:ARG:NH2	2.03	0.90
3:a:3217[A]:PHE:HZ	3:a:3230[A]:PHE:CE1	1.89	0.90
3:d:3298[A]:ASN:ND2	3:d:3301[A]:PRO:CA	2.34	0.90
3:C:3248[B]:LEU:HB2	3:L:2972[B]:GLY:C	1.96	0.89
3:F:2935[A]:ILE:HD13	3:F:2936[A]:GLU:H	1.35	0.89
3:F:3155[B]:MET:H	3:a:3153[B]:LYS:C	1.80	0.89
3:I:2965[A]:LEU:HD11	3:I:2975[A]:PHE:N	1.85	0.89
3:I:3173[B]:THR:C	3:R:3154[B]:PRO:CD	2.44	0.89
3:O:2965[B]:LEU:HB3	3:X:3254[B]:MET:SD	2.12	0.89
3:U:3257[B]:ALA:H	3:d:2968[B]:GLN:HA	0.73	0.89
3:a:3196[B]:THR:HB	3:a:3198[B]:PRO:HD2	1.54	0.89
3:d:3217[B]:PHE:HZ	3:d:3230[B]:PHE:CE1	1.89	0.89
3:d:3220[A]:ARG:HH11	3:d:3220[A]:ARG:HG3	1.35	0.89
3:C:2988[A]:TRP:HE3	3:C:2989[A]:HIS:ND1	1.70	0.89
3:I:2948[A]:ASP:HB3	3:I:2949[A]:LYS:HA	1.52	0.89
3:I:2979[B]:GLN:CG	3:I:3155[B]:MET:HE1	1.97	0.89
3:L:3298[A]:ASN:ND2	3:L:3301[A]:PRO:CA	2.34	0.89
3:R:2948[A]:ASP:HB3	3:R:2949[A]:LYS:HA	1.52	0.89
3:R:2988[A]:TRP:HE3	3:R:2989[A]:HIS:ND1	1.70	0.89
3:U:3256[B]:TRP:HB3	3:d:2975[B]:PHE:CE1	2.04	0.89
3:X:3220[A]:ARG:HH11	3:X:3220[A]:ARG:HG3	1.35	0.89
3:d:2965[A]:LEU:HD11	3:d:2975[A]:PHE:N	1.85	0.89
3:d:2988[B]:TRP:HE3	3:d:2989[B]:HIS:ND1	1.70	0.89
3:C:2988[B]:TRP:HE3	3:C:2989[B]:HIS:HD1	1.14	0.89
3:C:3283[B]:ILE:HG21	3:C:3305[B]:ILE:HD11	1.51	0.89
3:F:2969[B]:TYR:C	3:a:2989[B]:HIS:NE2	2.31	0.89
3:I:2951[B]:ASP:OD2	3:I:2952[B]:ALA:N	2.03	0.89
3:L:2988[A]:TRP:HE3	3:L:2989[A]:HIS:ND1	1.70	0.89
3:L:3230[B]:PHE:HB2	3:L:3243[B]:GLY:N	1.87	0.89
3:O:2969[B]:TYR:HD1	3:X:3158[B]:PHE:CD1	1.80	0.89
3:O:2988[A]:TRP:HE3	3:O:2989[A]:HIS:ND1	1.70	0.89
1:P:1582:ASN:HB3	1:P:1583:CYS:HB2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2967[B]:CYS:C	3:d:3256[B]:TRP:HB2	1.97	0.89
3:U:3196[B]:THR:HB	3:U:3198[B]:PRO:HD2	1.53	0.89
2:c:2800:LYS:O	3:d:3023[A]:ILE:CD1	2.19	0.89
3:d:3196[B]:THR:HB	3:d:3198[B]:PRO:HD2	1.54	0.89
3:d:3230[B]:PHE:HB2	3:d:3243[B]:GLY:N	1.87	0.89
3:C:2935[A]:ILE:HD13	3:C:2936[A]:GLU:H	1.35	0.89
3:C:2968[B]:GLN:HE21	3:L:3086[B]:GLU:HB3	1.37	0.89
3:C:2972[B]:GLY:HA3	3:L:3090[B]:ASN:CG	1.96	0.89
3:F:3148[B]:ILE:O	3:a:3169[B]:LYS:C	2.13	0.89
1:M:427:ASP:OD2	1:M:518:LYS:NZ	2.05	0.89
3:O:3298[A]:ASN:ND2	3:O:3301[A]:PRO:CA	2.34	0.89
3:R:3298[B]:ASN:ND2	3:R:3301[B]:PRO:CA	2.34	0.89
3:U:2932[B]:PRO:HA	3:U:2935[B]:ILE:HD12	1.51	0.89
3:U:3230[A]:PHE:HB2	3:U:3243[A]:GLY:N	1.87	0.89
3:a:2948[B]:ASP:HB3	3:a:2949[B]:LYS:HA	1.52	0.89
2:c:2470:ALA:HB2	2:c:2476:LEU:HD21	1.54	0.89
3:C:2969[B]:TYR:HA	3:L:2989[B]:HIS:NE2	1.88	0.89
3:C:3298[B]:ASN:ND2	3:C:3301[B]:PRO:CA	2.34	0.89
3:I:2948[B]:ASP:HB3	3:I:2949[B]:LYS:HA	1.52	0.89
3:I:2956[A]:LYS:O	3:I:2960[A]:PHE:HE1	1.22	0.89
3:I:2988[B]:TRP:HE3	3:I:2989[B]:HIS:ND1	1.70	0.89
3:I:3151[B]:LEU:N	3:R:3159[B]:SER:HA	1.86	0.89
3:R:2988[B]:TRP:HE3	3:R:2989[B]:HIS:ND1	1.70	0.89
3:R:3230[A]:PHE:HB2	3:R:3243[A]:GLY:N	1.87	0.89
3:U:2964[B]:PRO:HA	3:d:3220[B]:ARG:HH22	1.37	0.89
3:U:2965[B]:LEU:HD11	3:U:2975[B]:PHE:N	1.85	0.89
3:U:2975[B]:PHE:HE2	3:d:3254[B]:MET:HG3	0.73	0.89
3:X:2988[B]:TRP:HE3	3:X:2989[B]:HIS:ND1	1.70	0.89
3:a:2979[A]:GLN:HE21	3:a:3155[A]:MET:HE3	1.36	0.89
3:C:2988[B]:TRP:HE3	3:C:2989[B]:HIS:ND1	1.70	0.89
3:C:3108[B]:HIS:HE1	3:L:3251[B]:ASP:OD1	1.56	0.89
3:C:3154[B]:PRO:O	3:L:3155[B]:MET:HG2	1.73	0.89
3:F:2982[B]:MET:SD	3:a:2967[B]:CYS:SG	2.70	0.89
3:I:2976[B]:ALA:CB	3:R:3252[B]:TYR:O	2.19	0.89
3:I:3153[B]:LYS:HB3	3:R:3155[B]:MET:O	1.73	0.89
3:I:3163[B]:ASN:CG	3:R:3149[B]:ASN:ND2	2.31	0.89
3:O:2965[B]:LEU:HD13	3:X:2979[B]:GLN:NE2	1.62	0.89
3:O:3196[B]:THR:H	3:O:3199[B]:GLN:HB2	1.38	0.89
3:O:3298[A]:ASN:HB2	3:O:3300[A]:LEU:HD23	1.50	0.89
3:U:2965[A]:LEU:HD11	3:U:2975[A]:PHE:N	1.85	0.89
3:U:2988[B]:TRP:HE3	3:U:2989[B]:HIS:ND1	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3217[A]:PHE:HZ	3:X:3230[A]:PHE:CE1	1.89	0.89
3:a:3230[B]:PHE:HB2	3:a:3243[B]:GLY:N	1.86	0.89
3:C:3172[B]:SER:H	3:L:3152[B]:LYS:HB2	1.31	0.89
3:F:2948[B]:ASP:N	3:F:2949[B]:LYS:HA	1.81	0.89
3:I:2989[B]:HIS:CD2	3:R:2970[B]:PRO:CA	2.55	0.89
3:U:3169[B]:LYS:CG	3:d:3147[B]:GLU:CA	2.51	0.89
3:X:3298[A]:ASN:ND2	3:X:3301[A]:PRO:CA	2.34	0.89
2:Z:2800:LYS:O	3:a:3023[A]:ILE:HD13	1.72	0.89
3:d:3013[B]:ASP:HA	3:d:3122[B]:ASN:ND2	1.88	0.89
1:A:180:ASN:HD22	1:A:344:LEU:HD22	1.38	0.89
3:C:2948[A]:ASP:HB3	3:C:2949[A]:LYS:HA	1.52	0.89
3:C:2959[B]:SER:O	3:L:3255[B]:PRO:CB	2.20	0.89
3:C:2974[B]:ALA:HB3	3:L:3249[B]:GLY:HA3	0.89	0.89
3:F:2967[B]:CYS:HA	3:a:2981[B]:GLY:CA	1.92	0.89
3:F:3149[B]:ASN:HD22	3:a:3163[B]:ASN:CB	1.81	0.89
3:F:3196[A]:THR:HB	3:F:3198[A]:PRO:HD2	1.54	0.89
3:F:3230[B]:PHE:HB2	3:F:3243[B]:GLY:N	1.87	0.89
3:I:3273[B]:LEU:HB2	3:I:3275[B]:LEU:HD13	1.55	0.89
3:a:3220[A]:ARG:HH11	3:a:3220[A]:ARG:HG3	1.35	0.89
3:a:3273[B]:LEU:HB2	3:a:3275[B]:LEU:HD13	1.55	0.89
8:O:1:NAG:H61	8:O:2:NAG:HN2	1.37	0.89
3:F:2979[B]:GLN:HE21	3:F:3155[B]:MET:HE3	1.36	0.89
3:F:3013[B]:ASP:HA	3:F:3122[B]:ASN:ND2	1.88	0.89
3:I:3273[A]:LEU:HB2	3:I:3275[A]:LEU:HD13	1.55	0.89
3:L:2935[A]:ILE:HD13	3:L:2936[A]:GLU:H	1.35	0.89
3:O:3298[B]:ASN:ND2	3:O:3301[B]:PRO:CA	2.34	0.89
3:R:2965[B]:LEU:HD11	3:R:2975[B]:PHE:N	1.85	0.89
6:GA:1:NAG:H4	6:GA:2:NAG:C7	2.02	0.89
3:C:3153[B]:LYS:HB3	3:L:3155[B]:MET:H	1.38	0.89
3:C:3159[B]:SER:HG	3:L:3150[B]:LYS:C	1.80	0.89
3:C:3273[A]:LEU:HB2	3:C:3275[A]:LEU:HD13	1.55	0.89
2:E:2800:LYS:O	3:F:3023[A]:ILE:HD13	1.73	0.89
3:F:2966[B]:SER:CA	3:a:3256[B]:TRP:CB	2.51	0.89
3:F:3220[A]:ARG:HH11	3:F:3220[A]:ARG:HG3	1.35	0.89
3:F:3273[B]:LEU:HB2	3:F:3275[B]:LEU:HD13	1.55	0.89
3:I:3298[B]:ASN:HB2	3:I:3300[B]:LEU:N	1.78	0.89
3:U:2993[A]:MET:O	3:U:2997[A]:GLU:N	2.07	0.89
3:X:3230[B]:PHE:HB2	3:X:3243[B]:GLY:N	1.87	0.89
1:Y:1612:THR:O	3:d:3186[B]:GLU:HB3	1.73	0.89
3:d:2935[A]:ILE:HD13	3:d:2936[A]:GLU:H	1.35	0.89
6:LA:1:NAG:O4	6:LA:2:NAG:O7	1.89	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3149[B]:ASN:CG	3:L:3163[B]:ASN:HD22	1.80	0.88
3:F:3160[B]:SER:C	3:a:3150[B]:LYS:HZ2	1.80	0.88
3:F:3273[A]:LEU:HB2	3:F:3275[A]:LEU:HD13	1.55	0.88
3:I:2993[A]:MET:O	3:I:2997[A]:GLU:N	2.07	0.88
3:I:2993[B]:MET:O	3:I:2997[B]:GLU:N	2.07	0.88
3:O:2974[B]:ALA:HB2	3:X:2977[B]:CYS:C	1.97	0.88
3:O:3159[B]:SER:C	3:X:3148[B]:ILE:HA	1.98	0.88
3:U:3013[B]:ASP:HA	3:U:3122[B]:ASN:ND2	1.88	0.88
3:d:3196[A]:THR:HB	3:d:3198[A]:PRO:HD2	1.54	0.88
3:C:2971[B]:ASP:HB3	3:L:3089[B]:HIS:CE1	2.06	0.88
3:C:2993[B]:MET:O	3:C:2997[B]:GLU:N	2.07	0.88
3:C:3154[B]:PRO:CB	3:L:3151[B]:LEU:O	2.20	0.88
3:C:3230[A]:PHE:HB2	3:C:3243[A]:GLY:N	1.87	0.88
3:C:3287[B]:ILE:O	3:C:3295[B]:LEU:HA	1.73	0.88
3:F:2966[B]:SER:HA	3:a:3256[B]:TRP:CA	2.03	0.88
3:F:2993[A]:MET:O	3:F:2997[A]:GLU:N	2.07	0.88
3:F:3108[B]:HIS:HE1	3:a:3251[B]:ASP:OD1	1.52	0.88
3:I:2988[A]:TRP:HE3	3:I:2989[A]:HIS:ND1	1.70	0.88
3:I:3153[B]:LYS:HB2	3:R:3158[B]:PHE:CB	2.03	0.88
3:I:3154[B]:PRO:HD3	3:R:3173[B]:THR:O	1.73	0.88
3:O:2948[B]:ASP:N	3:O:2949[B]:LYS:HA	1.81	0.88
3:O:2979[B]:GLN:HE21	3:O:3155[B]:MET:HE3	1.36	0.88
3:a:2988[A]:TRP:HE3	3:a:2989[A]:HIS:ND1	1.70	0.88
3:a:3013[B]:ASP:HA	3:a:3122[B]:ASN:ND2	1.88	0.88
3:C:3162[B]:ASP:CA	3:L:3147[B]:GLU:OE1	1.94	0.88
3:F:3252[B]:TYR:CE2	3:a:3250[B]:GLY:HA2	2.03	0.88
3:I:2975[B]:PHE:CD1	3:R:3107[B]:LEU:CG	2.49	0.88
3:L:3196[B]:THR:HB	3:L:3198[B]:PRO:HD2	1.54	0.88
3:O:2988[B]:TRP:HE3	3:O:2989[B]:HIS:ND1	1.70	0.88
3:a:2932[B]:PRO:HA	3:a:2935[B]:ILE:HD12	1.51	0.88
3:d:3273[B]:LEU:HB2	3:d:3275[B]:LEU:HD13	1.55	0.88
3:C:2979[B]:GLN:HE21	3:C:3155[B]:MET:HE3	1.36	0.88
3:C:2983[B]:VAL:CB	3:L:3160[B]:SER:HA	2.03	0.88
3:F:3252[B]:TYR:CA	3:a:3108[B]:HIS:NE2	2.37	0.88
3:I:3013[A]:ASP:HA	3:I:3122[A]:ASN:ND2	1.88	0.88
3:I:3153[B]:LYS:HE3	3:R:3158[B]:PHE:H	1.37	0.88
3:I:3222[A]:ILE:HD12	3:I:3223[A]:GLY:N	1.89	0.88
3:L:2993[B]:MET:O	3:L:2997[B]:GLU:N	2.07	0.88
3:R:3196[B]:THR:HB	3:R:3198[B]:PRO:HD2	1.54	0.88
3:R:3222[A]:ILE:HD12	3:R:3223[A]:GLY:N	1.89	0.88
3:X:3196[B]:THR:HB	3:X:3198[B]:PRO:HD2	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3273[A]:LEU:HB2	3:X:3275[A]:LEU:HD13	1.55	0.88
3:X:3287[A]:ILE:O	3:X:3295[A]:LEU:HA	1.73	0.88
3:a:3287[A]:ILE:O	3:a:3295[A]:LEU:HA	1.73	0.88
3:d:3298[B]:ASN:HB2	3:d:3300[B]:LEU:N	1.78	0.88
1:A:1582:ASN:HB3	1:A:1583:CYS:HB2	1.55	0.88
3:F:3169[B]:LYS:HE2	3:a:3147[B]:GLU:H	1.36	0.88
1:G:387:ASN:ND2	4:o:1:NAG:O6	2.06	0.88
3:I:3287[B]:ILE:O	3:I:3295[B]:LEU:HA	1.74	0.88
3:L:3013[B]:ASP:HA	3:L:3122[B]:ASN:ND2	1.88	0.88
3:O:2974[B]:ALA:HB3	3:X:2977[B]:CYS:HB3	1.55	0.88
3:O:2993[B]:MET:O	3:O:2997[B]:GLU:N	2.06	0.88
3:O:3255[B]:PRO:HA	3:X:3161[B]:GLU:CA	2.02	0.88
3:O:3273[B]:LEU:HB2	3:O:3275[B]:LEU:HD13	1.55	0.88
3:U:2967[B]:CYS:HB2	3:d:3256[B]:TRP:CA	2.04	0.88
3:U:3013[A]:ASP:HA	3:U:3122[A]:ASN:ND2	1.88	0.88
3:U:3222[A]:ILE:HD12	3:U:3223[A]:GLY:N	1.89	0.88
3:U:3252[B]:TYR:O	3:d:3255[B]:PRO:CG	2.22	0.88
3:a:3230[A]:PHE:HB2	3:a:3243[A]:GLY:N	1.87	0.88
3:d:2988[A]:TRP:HE3	3:d:2989[A]:HIS:ND1	1.70	0.88
3:d:3273[A]:LEU:HB2	3:d:3275[A]:LEU:HD13	1.55	0.88
3:C:3287[A]:ILE:O	3:C:3295[A]:LEU:HA	1.73	0.88
3:F:2943[B]:ALA:O	3:F:2946[B]:GLN:HG3	1.74	0.88
3:F:3155[B]:MET:CB	3:a:3153[B]:LYS:HD3	2.00	0.88
3:F:3256[B]:TRP:NE1	3:a:2965[B]:LEU:HD12	1.87	0.88
3:I:3013[B]:ASP:HA	3:I:3122[B]:ASN:ND2	1.88	0.88
3:O:2948[B]:ASP:HB3	3:O:2949[B]:LYS:HA	1.52	0.88
3:O:3108[B]:HIS:CB	3:X:2970[B]:PRO:N	2.28	0.88
3:O:3173[A]:THR:HB	3:O:3176[A]:LYS:CD	2.04	0.88
3:R:3287[A]:ILE:O	3:R:3295[A]:LEU:HA	1.73	0.88
3:U:2979[B]:GLN:HE21	3:U:3155[B]:MET:HE3	1.36	0.88
3:a:3273[A]:LEU:HB2	3:a:3275[A]:LEU:HD13	1.55	0.88
3:d:2997[A]:GLU:OE2	3:d:3009[A]:ILE:HG13	1.74	0.88
3:C:2948[B]:ASP:OD1	3:C:2950[B]:THR:N	2.07	0.88
3:C:3196[A]:THR:HB	3:C:3198[A]:PRO:HD2	1.54	0.88
3:F:2988[B]:TRP:HE3	3:F:2989[B]:HIS:ND1	1.70	0.88
3:I:3217[A]:PHE:HZ	3:I:3230[A]:PHE:CE1	1.89	0.88
3:I:3250[B]:GLY:HA2	3:R:3252[B]:TYR:CE2	2.06	0.88
3:L:3273[B]:LEU:HB2	3:L:3275[B]:LEU:HD13	1.55	0.88
3:O:2970[B]:PRO:CG	3:X:2990[B]:ARG:C	2.47	0.88
3:O:2979[A]:GLN:HE21	3:O:3155[A]:MET:HE3	1.36	0.88
3:O:3013[A]:ASP:HA	3:O:3122[A]:ASN:ND2	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3254[B]:MET:O	3:d:2975[B]:PHE:CE1	2.27	0.88
3:X:2988[A]:TRP:HE3	3:X:2989[A]:HIS:ND1	1.70	0.88
3:X:3173[A]:THR:HB	3:X:3176[A]:LYS:CD	2.04	0.88
3:a:2948[A]:ASP:OD1	3:a:2950[A]:THR:N	2.07	0.88
1:b:587:PHE:O	1:b:651:ARG:NH2	2.06	0.88
3:d:2979[A]:GLN:HE21	3:d:3155[A]:MET:HE3	1.36	0.88
3:C:2982[B]:MET:CG	3:L:3156[B]:MET:CG	2.41	0.88
3:C:3217[B]:PHE:HZ	3:C:3230[B]:PHE:CE1	1.89	0.88
3:F:2948[A]:ASP:OD1	3:F:2950[A]:THR:N	2.07	0.88
3:F:2993[B]:MET:O	3:F:2997[B]:GLU:N	2.07	0.88
3:F:2997[B]:GLU:OE2	3:F:3009[B]:ILE:HG13	1.74	0.88
3:F:3013[A]:ASP:HA	3:F:3122[A]:ASN:ND2	1.88	0.88
3:F:3163[B]:ASN:N	3:a:3147[B]:GLU:OE1	2.06	0.88
3:F:3173[A]:THR:HB	3:F:3176[A]:LYS:CD	2.04	0.88
3:I:2961[B]:HIS:CB	3:R:2975[B]:PHE:HZ	1.86	0.88
3:I:3230[A]:PHE:HB2	3:I:3243[A]:GLY:N	1.87	0.88
3:L:2997[A]:GLU:OE2	3:L:3009[A]:ILE:HG13	1.74	0.88
3:L:3173[B]:THR:HB	3:L:3176[B]:LYS:CD	2.04	0.88
3:O:2943[A]:ALA:O	3:O:2946[A]:GLN:HG3	1.74	0.88
3:R:2948[A]:ASP:OD1	3:R:2950[A]:THR:N	2.07	0.88
3:U:3253[B]:GLU:CA	3:d:3255[B]:PRO:HG3	2.02	0.88
3:d:2948[B]:ASP:OD1	3:d:2950[B]:THR:N	2.07	0.88
3:C:3013[B]:ASP:HA	3:C:3122[B]:ASN:ND2	1.88	0.88
3:I:2948[B]:ASP:OD1	3:I:2950[B]:THR:N	2.07	0.88
3:I:2967[B]:CYS:SG	3:R:2982[B]:MET:HG2	2.14	0.88
3:O:2997[A]:GLU:OE2	3:O:3009[A]:ILE:HG13	1.74	0.88
3:U:2948[A]:ASP:OD1	3:U:2950[A]:THR:N	2.07	0.88
3:U:2957[A]:ILE:HA	3:U:2960[A]:PHE:CE1	2.09	0.88
3:U:2965[B]:LEU:CD1	3:d:3220[B]:ARG:HA	1.93	0.88
3:U:2988[A]:TRP:HE3	3:U:2989[A]:HIS:ND1	1.70	0.88
3:U:2997[B]:GLU:OE2	3:U:3009[B]:ILE:HG13	1.74	0.88
3:U:3222[B]:ILE:HD12	3:U:3223[B]:GLY:N	1.89	0.88
3:a:2988[B]:TRP:HE3	3:a:2989[B]:HIS:ND1	1.70	0.88
3:a:3013[A]:ASP:HA	3:a:3122[A]:ASN:ND2	1.88	0.88
3:a:3287[B]:ILE:O	3:a:3295[B]:LEU:HA	1.73	0.88
3:C:2943[B]:ALA:O	3:C:2946[B]:GLN:HG3	1.74	0.88
3:C:3174[B]:GLY:CA	3:L:3154[B]:PRO:CB	2.52	0.88
3:F:2966[B]:SER:CA	3:a:3256[B]:TRP:HB3	2.04	0.88
3:F:2971[B]:ASP:O	3:a:3090[B]:ASN:CB	2.22	0.88
3:F:2992[B]:TYR:HE2	3:a:2969[B]:TYR:HE1	1.21	0.88
3:I:2979[B]:GLN:HE21	3:I:3155[B]:MET:HE3	1.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2948[B]:ASP:OD1	3:L:2950[B]:THR:N	2.07	0.88
3:L:3222[A]:ILE:HD12	3:L:3223[A]:GLY:N	1.89	0.88
3:O:3157[B]:PRO:C	3:X:3152[B]:LYS:CG	2.47	0.88
3:U:2948[B]:ASP:OD1	3:U:2950[B]:THR:N	2.07	0.88
3:U:2979[A]:GLN:HE21	3:U:3155[A]:MET:HE3	1.36	0.88
3:U:3254[B]:MET:HB3	3:d:3254[B]:MET:HA	1.28	0.88
3:X:2957[B]:ILE:HA	3:X:2960[B]:PHE:CE1	2.09	0.88
3:X:3287[B]:ILE:O	3:X:3295[B]:LEU:HA	1.73	0.88
3:a:3176[A]:LYS:O	3:a:3177[A]:SER:OG	1.92	0.88
3:d:3222[A]:ILE:HD12	3:d:3223[A]:GLY:N	1.89	0.88
1:A:119:LYS:HB3	1:A:120:LYS:HA	1.54	0.87
3:C:3173[B]:THR:HB	3:C:3176[B]:LYS:CG	2.05	0.87
3:C:3176[A]:LYS:O	3:C:3177[A]:SER:OG	1.92	0.87
3:F:3169[B]:LYS:HZ2	3:a:3149[B]:ASN:HD21	1.22	0.87
3:F:3173[B]:THR:HA	3:a:3153[B]:LYS:C	1.98	0.87
3:F:3287[B]:ILE:O	3:F:3295[B]:LEU:HA	1.74	0.87
3:I:3173[B]:THR:HB	3:I:3176[B]:LYS:CG	2.05	0.87
3:L:2957[A]:ILE:HA	3:L:2960[A]:PHE:CE1	2.09	0.87
3:L:3092[A]:ILE:O	3:L:3096[A]:VAL:HG23	1.75	0.87
3:O:3092[B]:ILE:O	3:O:3096[B]:VAL:HG23	1.74	0.87
3:R:2957[B]:ILE:HA	3:R:2960[B]:PHE:CE1	2.09	0.87
3:R:3173[A]:THR:HB	3:R:3176[A]:LYS:CG	2.04	0.87
3:U:3176[A]:LYS:O	3:U:3177[A]:SER:OG	1.92	0.87
3:U:3287[B]:ILE:O	3:U:3295[B]:LEU:HA	1.73	0.87
3:a:2979[B]:GLN:CG	3:a:3155[B]:MET:HE1	1.97	0.87
3:d:3196[A]:THR:H	3:d:3199[A]:GLN:HB2	1.38	0.87
4:JA:1:NAG:O4	4:JA:2:NAG:O7	1.92	0.87
2:B:2345:ASN:H	2:E:2515:ARG:HD3	1.39	0.87
3:C:2957[B]:ILE:HA	3:C:2960[B]:PHE:CE1	2.09	0.87
3:C:3253[B]:GLU:HB2	3:L:2976[B]:ALA:H	1.34	0.87
3:C:3273[B]:LEU:HB2	3:C:3275[B]:LEU:HD13	1.55	0.87
3:I:2943[A]:ALA:O	3:I:2946[A]:GLN:HG3	1.74	0.87
3:I:3173[A]:THR:HB	3:I:3176[A]:LYS:CD	2.04	0.87
3:I:3173[B]:THR:OG1	3:R:3173[B]:THR:HG21	1.72	0.87
3:L:3217[A]:PHE:HZ	3:L:3230[A]:PHE:CE1	1.89	0.87
3:L:3222[B]:ILE:HD12	3:L:3223[B]:GLY:N	1.89	0.87
2:N:2800:LYS:O	3:O:3023[A]:ILE:HD11	1.72	0.87
3:O:2976[B]:ALA:CA	3:X:3156[B]:MET:HG2	2.04	0.87
3:O:3273[A]:LEU:HB2	3:O:3275[A]:LEU:HD13	1.55	0.87
3:R:2993[B]:MET:O	3:R:2997[B]:GLU:N	2.07	0.87
3:R:3013[A]:ASP:HA	3:R:3122[A]:ASN:ND2	1.88	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3092[B]:ILE:O	3:R:3096[B]:VAL:HG23	1.75	0.87
3:U:2948[B]:ASP:N	3:U:2949[B]:LYS:HA	1.81	0.87
3:U:3092[B]:ILE:O	3:U:3096[B]:VAL:HG23	1.75	0.87
3:U:3273[B]:LEU:HB2	3:U:3275[B]:LEU:HD13	1.55	0.87
3:X:3173[B]:THR:HB	3:X:3176[B]:LYS:CD	2.04	0.87
3:a:2943[A]:ALA:O	3:a:2946[A]:GLN:HG3	1.74	0.87
3:d:2943[B]:ALA:O	3:d:2946[B]:GLN:HG3	1.74	0.87
3:d:2993[A]:MET:O	3:d:2997[A]:GLU:N	2.07	0.87
3:d:2997[B]:GLU:OE2	3:d:3009[B]:ILE:HG13	1.74	0.87
3:C:3225[B]:SER:O	3:C:3290[B]:ILE:HG23	1.75	0.87
3:F:2988[A]:TRP:HE3	3:F:2989[A]:HIS:ND1	1.70	0.87
3:F:3196[B]:THR:H	3:F:3199[B]:GLN:HB2	1.38	0.87
3:F:3223[B]:GLY:HA3	3:a:2963[B]:MET:HE1	1.56	0.87
3:O:2979[A]:GLN:CG	3:O:3155[A]:MET:HE1	1.97	0.87
3:O:3173[B]:THR:HB	3:O:3176[B]:LYS:CG	2.05	0.87
3:U:2975[B]:PHE:CD2	3:d:3256[B]:TRP:CD1	2.55	0.87
3:U:3173[B]:THR:HG23	3:d:3152[B]:LYS:O	1.74	0.87
3:U:3287[A]:ILE:O	3:U:3295[A]:LEU:HA	1.73	0.87
3:X:3013[B]:ASP:HA	3:X:3122[B]:ASN:ND2	1.88	0.87
3:X:3176[A]:LYS:O	3:X:3177[A]:SER:OG	1.92	0.87
3:a:3092[B]:ILE:O	3:a:3096[B]:VAL:HG23	1.75	0.87
3:d:3176[B]:LYS:O	3:d:3177[B]:SER:OG	1.92	0.87
3:C:3090[B]:ASN:HB3	3:L:2972[B]:GLY:CA	1.93	0.87
3:C:3092[A]:ILE:O	3:C:3096[A]:VAL:HG23	1.74	0.87
3:C:3173[A]:THR:HB	3:C:3176[A]:LYS:CG	2.05	0.87
3:C:3217[A]:PHE:HZ	3:C:3230[A]:PHE:CE1	1.89	0.87
3:F:2970[B]:PRO:CA	3:a:2989[B]:HIS:CD2	2.57	0.87
3:F:2997[A]:GLU:OE2	3:F:3009[A]:ILE:HG13	1.74	0.87
3:F:3173[B]:THR:HB	3:F:3176[B]:LYS:CD	2.04	0.87
3:F:3217[B]:PHE:HZ	3:F:3230[B]:PHE:CE1	1.89	0.87
2:H:2797:LYS:NZ	3:I:3028[A]:PRO:CD	2.36	0.87
3:I:3092[B]:ILE:O	3:I:3096[B]:VAL:HG23	1.74	0.87
3:I:3196[B]:THR:HB	3:I:3198[B]:PRO:HD2	1.54	0.87
3:I:3222[B]:ILE:HD12	3:I:3223[B]:GLY:N	1.89	0.87
3:I:3225[A]:SER:O	3:I:3290[A]:ILE:HG23	1.74	0.87
3:I:3256[B]:TRP:HE1	3:R:2965[B]:LEU:CG	1.86	0.87
3:L:3173[A]:THR:HB	3:L:3176[A]:LYS:CD	2.04	0.87
3:O:3038[B]:ILE:CD1	3:X:2969[B]:TYR:CZ	2.57	0.87
3:O:3156[B]:MET:HG2	3:X:3173[B]:THR:CG2	2.04	0.87
3:O:3160[B]:SER:OG	3:X:3150[B]:LYS:CB	2.18	0.87
3:O:3176[A]:LYS:O	3:O:3177[A]:SER:OG	1.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3222[B]:ILE:N	3:X:3161[B]:GLU:HB2	1.89	0.87
3:R:2965[B]:LEU:HD11	3:R:2974[B]:ALA:HA	1.57	0.87
3:R:3176[A]:LYS:O	3:R:3177[A]:SER:OG	1.92	0.87
3:R:3225[B]:SER:O	3:R:3290[B]:ILE:HG23	1.74	0.87
3:U:2975[B]:PHE:CD1	3:d:3255[B]:PRO:HA	1.91	0.87
3:U:3173[B]:THR:HB	3:U:3176[B]:LYS:CG	2.05	0.87
3:X:2948[A]:ASP:OD1	3:X:2950[A]:THR:N	2.07	0.87
3:X:2979[A]:GLN:HE21	3:X:3155[A]:MET:HE3	1.36	0.87
3:X:3013[A]:ASP:HA	3:X:3122[A]:ASN:ND2	1.88	0.87
3:X:3173[A]:THR:HB	3:X:3176[A]:LYS:CG	2.05	0.87
3:X:3222[A]:ILE:HD12	3:X:3223[A]:GLY:N	1.89	0.87
1:Y:497:GLN:HG2	1:Y:683:THR:HG21	1.57	0.87
3:d:2979[B]:GLN:HE21	3:d:3155[B]:MET:HE3	1.36	0.87
3:d:3287[A]:ILE:O	3:d:3295[A]:LEU:HA	1.73	0.87
3:C:2993[A]:MET:O	3:C:2997[A]:GLU:N	2.07	0.87
3:C:3283[A]:ILE:CG2	3:C:3305[A]:ILE:HD11	2.05	0.87
3:F:2968[B]:GLN:OE1	3:a:2981[B]:GLY:HA2	1.72	0.87
3:L:2948[A]:ASP:N	3:L:2949[A]:LYS:HA	1.81	0.87
3:L:2988[B]:TRP:HE3	3:L:2989[B]:HIS:ND1	1.70	0.87
3:O:2957[A]:ILE:HA	3:O:2960[A]:PHE:CE1	2.09	0.87
3:O:2997[B]:GLU:OE2	3:O:3009[B]:ILE:HG13	1.74	0.87
3:O:3108[B]:HIS:HB2	3:X:2969[B]:TYR:O	1.73	0.87
3:O:3287[B]:ILE:O	3:O:3295[B]:LEU:HA	1.73	0.87
3:U:3173[B]:THR:HB	3:U:3176[B]:LYS:CD	2.04	0.87
3:X:2993[A]:MET:O	3:X:2997[A]:GLU:N	2.07	0.87
3:X:3293[B]:LYS:CD	3:X:3294[B]:SER:CB	2.53	0.87
3:d:3173[B]:THR:HB	3:d:3176[B]:LYS:CD	2.04	0.87
3:C:2976[B]:ALA:N	3:L:3253[B]:GLU:CB	2.38	0.87
3:C:3293[B]:LYS:CD	3:C:3294[B]:SER:CB	2.53	0.87
3:F:2948[B]:ASP:OD1	3:F:2950[B]:THR:N	2.07	0.87
3:F:3092[A]:ILE:O	3:F:3096[A]:VAL:HG23	1.74	0.87
3:I:2933[B]:SER:HB3	3:I:2936[B]:GLU:HB3	1.57	0.87
3:I:2957[A]:ILE:HA	3:I:2960[A]:PHE:CE1	2.09	0.87
3:I:3196[A]:THR:HB	1:J:416:ASN:ND2	1.87	0.87
3:L:2943[B]:ALA:O	3:L:2946[B]:GLN:HG3	1.74	0.87
3:L:2997[B]:GLU:OE2	3:L:3009[B]:ILE:HG13	1.74	0.87
3:L:3176[B]:LYS:O	3:L:3177[B]:SER:OG	1.92	0.87
3:L:3225[A]:SER:O	3:L:3290[A]:ILE:HG23	1.75	0.87
3:L:3273[A]:LEU:HB2	3:L:3275[A]:LEU:HD13	1.55	0.87
3:L:3293[A]:LYS:CD	3:L:3294[A]:SER:CB	2.53	0.87
3:O:2948[A]:ASP:OD1	3:O:2950[A]:THR:N	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2977[B]:CYS:N	3:X:3154[B]:PRO:O	2.07	0.87
3:O:3173[B]:THR:HB	3:O:3176[B]:LYS:CD	2.04	0.87
3:O:3176[B]:LYS:O	3:O:3177[B]:SER:OG	1.92	0.87
3:R:2943[B]:ALA:O	3:R:2946[B]:GLN:HG3	1.74	0.87
3:R:2957[A]:ILE:HA	3:R:2960[A]:PHE:CE1	2.09	0.87
3:R:3273[A]:LEU:HB2	3:R:3275[A]:LEU:HD13	1.55	0.87
3:R:3283[B]:ILE:CG2	3:R:3305[B]:ILE:HD11	2.05	0.87
3:R:3287[B]:ILE:O	3:R:3295[B]:LEU:HA	1.73	0.87
3:U:2965[A]:LEU:HD11	3:U:2974[A]:ALA:HA	1.57	0.87
3:U:3173[A]:THR:HB	3:U:3176[A]:LYS:CG	2.05	0.87
3:X:2957[A]:ILE:HA	3:X:2960[A]:PHE:CE1	2.10	0.87
3:X:3196[A]:THR:HB	3:X:3198[A]:PRO:HD2	1.54	0.87
3:X:3225[B]:SER:O	3:X:3290[B]:ILE:HG23	1.75	0.87
3:a:2997[A]:GLU:OE2	3:a:3009[A]:ILE:HG13	1.74	0.87
3:a:3173[A]:THR:HB	3:a:3176[A]:LYS:CG	2.05	0.87
3:d:2943[A]:ALA:O	3:d:2946[A]:GLN:HG3	1.74	0.87
3:d:3173[A]:THR:HB	3:d:3176[A]:LYS:CD	2.04	0.87
3:d:3173[A]:THR:HB	3:d:3176[A]:LYS:CG	2.05	0.87
3:C:3124[A]:ASP:OD2	3:C:3185[A]:TYR:OH	1.93	0.87
3:C:3248[B]:LEU:CD2	3:L:2971[B]:ASP:CG	2.48	0.87
3:F:2957[B]:ILE:HA	3:F:2960[B]:PHE:CE1	2.10	0.87
3:F:3156[B]:MET:CB	3:a:2982[B]:MET:CG	2.52	0.87
3:F:3283[B]:ILE:CG2	3:F:3305[B]:ILE:HD11	2.05	0.87
3:L:2965[B]:LEU:HD11	3:L:2974[B]:ALA:HA	1.57	0.87
3:L:3092[B]:ILE:O	3:L:3096[B]:VAL:HG23	1.75	0.87
3:L:3287[A]:ILE:O	3:L:3295[A]:LEU:HA	1.73	0.87
3:O:2948[B]:ASP:OD1	3:O:2950[B]:THR:N	2.07	0.87
3:O:3284[A]:LYS:HD3	3:O:3285[A]:VAL:H	1.39	0.87
1:P:550:ILE:N	1:P:557:VAL:O	2.07	0.87
3:R:2948[B]:ASP:OD1	3:R:2950[B]:THR:N	2.07	0.87
3:R:2979[B]:GLN:HE21	3:R:3155[B]:MET:HE3	1.36	0.87
3:U:2965[B]:LEU:O	3:d:3257[B]:ALA:CB	2.18	0.87
3:U:3293[A]:LYS:CD	3:U:3294[A]:SER:CB	2.53	0.87
3:X:2993[B]:MET:O	3:X:2997[B]:GLU:N	2.07	0.87
3:X:2997[A]:GLU:OE2	3:X:3009[A]:ILE:HG13	1.74	0.87
3:X:2997[B]:GLU:OE2	3:X:3009[B]:ILE:HG13	1.74	0.87
1:Y:1612:THR:O	3:d:3186[B]:GLU:CB	2.23	0.87
3:a:2943[B]:ALA:O	3:a:2946[B]:GLN:HG3	1.74	0.87
3:d:2993[B]:MET:O	3:d:2997[B]:GLU:N	2.07	0.87
3:d:3222[B]:ILE:HD12	3:d:3223[B]:GLY:N	1.89	0.87
3:C:2935[B]:ILE:HD13	3:C:2936[B]:GLU:H	1.35	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2957[A]:ILE:HA	3:C:2960[A]:PHE:CE1	2.10	0.87
3:C:2971[B]:ASP:OD1	3:L:3248[B]:LEU:HD22	1.74	0.87
3:C:3013[A]:ASP:HA	3:C:3122[A]:ASN:ND2	1.88	0.87
3:F:2956[A]:LYS:O	3:F:2960[A]:PHE:HE1	1.22	0.87
3:F:2965[A]:LEU:HD11	3:F:2974[A]:ALA:HA	1.57	0.87
3:F:3155[B]:MET:HB3	3:a:3153[B]:LYS:HD2	1.54	0.87
3:I:2933[A]:SER:HB3	3:I:2936[A]:GLU:HB3	1.57	0.87
3:I:2979[A]:GLN:HE21	3:I:3155[A]:MET:HE3	1.36	0.87
3:I:2997[A]:GLU:OE2	3:I:3009[A]:ILE:HG13	1.74	0.87
3:L:2993[A]:MET:O	3:L:2997[A]:GLU:N	2.07	0.87
3:L:3283[A]:ILE:CG2	3:L:3305[A]:ILE:HD11	2.05	0.87
3:O:3101[B]:PRO:C	3:X:2971[B]:ASP:CA	2.46	0.87
3:R:2979[A]:GLN:HE21	3:R:3155[A]:MET:HE3	1.37	0.87
3:R:3173[B]:THR:HB	3:R:3176[B]:LYS:CD	2.04	0.87
3:R:3225[A]:SER:O	3:R:3290[A]:ILE:HG23	1.74	0.87
3:U:3254[B]:MET:HA	3:d:3254[B]:MET:CA	2.05	0.87
3:U:3283[B]:ILE:CG2	3:U:3305[B]:ILE:HD11	2.05	0.87
3:X:3196[A]:THR:H	3:X:3199[A]:GLN:HB2	1.38	0.87
3:a:2993[B]:MET:O	3:a:2997[B]:GLU:N	2.06	0.87
3:a:3173[A]:THR:HB	3:a:3176[A]:LYS:CD	2.04	0.87
3:a:3222[A]:ILE:HD12	3:a:3223[A]:GLY:N	1.89	0.87
3:d:3287[B]:ILE:O	3:d:3295[B]:LEU:HA	1.74	0.87
6:CA:1:NAG:H61	6:CA:2:NAG:C7	2.04	0.87
3:C:2948[A]:ASP:N	3:C:2949[A]:LYS:HA	1.81	0.87
3:C:3156[B]:MET:O	3:L:3153[B]:LYS:NZ	2.06	0.87
3:F:2965[B]:LEU:HD11	3:F:2974[B]:ALA:HA	1.57	0.87
3:F:3284[A]:LYS:HD3	3:F:3285[A]:VAL:H	1.39	0.87
3:F:3287[A]:ILE:O	3:F:3295[A]:LEU:HA	1.74	0.87
3:I:2957[B]:ILE:HA	3:I:2960[B]:PHE:CE1	2.10	0.87
3:I:2977[B]:CYS:CB	3:R:2982[B]:MET:HE3	2.05	0.87
3:I:3172[B]:SER:H	3:R:3152[B]:LYS:HB2	0.71	0.87
3:I:3173[B]:THR:HB	3:I:3176[B]:LYS:CD	2.04	0.87
3:I:3176[A]:LYS:O	3:I:3177[A]:SER:OG	1.92	0.87
1:J:566:ARG:HA	1:J:567:LEU:HD22	1.56	0.87
3:L:2933[B]:SER:HB3	3:L:2936[B]:GLU:HB3	1.57	0.87
3:L:3013[A]:ASP:HA	3:L:3122[A]:ASN:ND2	1.88	0.87
3:O:2943[B]:ALA:O	3:O:2946[B]:GLN:HG3	1.74	0.87
3:O:3013[B]:ASP:HA	3:O:3122[B]:ASN:ND2	1.88	0.87
3:O:3092[A]:ILE:O	3:O:3096[A]:VAL:HG23	1.75	0.87
3:R:2956[B]:LYS:O	3:R:2960[B]:PHE:HE1	1.22	0.87
3:R:2993[A]:MET:O	3:R:2997[A]:GLU:N	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3173[B]:THR:HB	3:R:3176[B]:LYS:CG	2.05	0.87
3:X:2948[B]:ASP:OD1	3:X:2950[B]:THR:N	2.07	0.87
3:X:3283[A]:ILE:CG2	3:X:3305[A]:ILE:HD11	2.05	0.87
1:Y:1616:LYS:HD3	3:d:3188[B]:ASP:H	1.39	0.87
3:a:2965[A]:LEU:HD11	3:a:2974[A]:ALA:HA	1.57	0.87
3:a:3124[A]:ASP:OD2	3:a:3185[A]:TYR:OH	1.93	0.87
3:a:3225[A]:SER:O	3:a:3290[A]:ILE:HG23	1.75	0.87
3:d:2933[B]:SER:HB3	3:d:2936[B]:GLU:HB3	1.57	0.87
3:d:2957[B]:ILE:HA	3:d:2960[B]:PHE:CE1	2.09	0.87
3:C:2997[A]:GLU:OE2	3:C:3009[A]:ILE:HG13	1.74	0.86
3:C:3222[A]:ILE:HD12	3:C:3223[A]:GLY:N	1.89	0.86
3:F:3222[A]:ILE:HD12	3:F:3223[A]:GLY:N	1.89	0.86
3:F:3256[B]:TRP:CG	3:a:2966[B]:SER:C	2.53	0.86
3:L:2943[A]:ALA:O	3:L:2946[A]:GLN:HG3	1.74	0.86
3:L:3176[A]:LYS:O	3:L:3177[A]:SER:OG	1.92	0.86
3:O:2933[A]:SER:HB3	3:O:2936[A]:GLU:HB3	1.57	0.86
3:O:2993[A]:MET:O	3:O:2997[A]:GLU:N	2.07	0.86
3:O:3173[A]:THR:HB	3:O:3176[A]:LYS:CG	2.04	0.86
3:O:3283[B]:ILE:CG2	3:O:3305[B]:ILE:HD11	2.05	0.86
3:U:2971[B]:ASP:O	3:d:3248[B]:LEU:N	2.08	0.86
3:U:3153[B]:LYS:HD2	3:d:3153[B]:LYS:CD	2.05	0.86
3:U:3173[A]:THR:HB	3:U:3176[A]:LYS:CD	2.04	0.86
3:X:3092[A]:ILE:O	3:X:3096[A]:VAL:HG23	1.75	0.86
3:a:3124[B]:ASP:OD2	3:a:3185[B]:TYR:OH	1.93	0.86
3:a:3173[B]:THR:HB	3:a:3176[B]:LYS:CD	2.04	0.86
3:d:3013[A]:ASP:HA	3:d:3122[A]:ASN:ND2	1.88	0.86
3:d:3225[A]:SER:O	3:d:3290[A]:ILE:HG23	1.75	0.86
3:d:3225[B]:SER:O	3:d:3290[B]:ILE:HG23	1.75	0.86
3:d:3283[A]:ILE:CG2	3:d:3305[A]:ILE:HD11	2.05	0.86
3:F:2933[A]:SER:HB3	3:F:2936[A]:GLU:HB3	1.57	0.86
3:F:2943[A]:ALA:O	3:F:2946[A]:GLN:HG3	1.74	0.86
3:F:2989[A]:HIS:O	3:F:2992[A]:TYR:N	2.08	0.86
3:F:3255[B]:PRO:O	3:a:2966[B]:SER:OG	1.93	0.86
3:I:2943[B]:ALA:O	3:I:2946[B]:GLN:HG3	1.74	0.86
3:I:2969[B]:TYR:OH	3:R:3116[B]:PHE:HD1	1.33	0.86
3:I:3283[B]:ILE:CG2	3:I:3305[B]:ILE:HD11	2.05	0.86
3:L:3196[A]:THR:HB	3:L:3198[A]:PRO:HD2	1.53	0.86
3:L:3218[A]:LEU:C	3:L:3219[A]:LEU:HD22	2.01	0.86
3:L:3283[B]:ILE:CG2	3:L:3305[B]:ILE:HD11	2.05	0.86
3:O:2948[A]:ASP:N	3:O:2949[A]:LYS:HA	1.81	0.86
3:O:2989[A]:HIS:O	3:O:2992[A]:TYR:N	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3222[B]:ILE:HD12	3:O:3223[B]:GLY:N	1.89	0.86
3:O:3225[B]:SER:O	3:O:3290[B]:ILE:HG23	1.75	0.86
3:O:3287[A]:ILE:O	3:O:3295[A]:LEU:HA	1.73	0.86
3:R:2956[A]:LYS:O	3:R:2960[A]:PHE:HE1	1.22	0.86
3:R:3222[B]:ILE:HD12	3:R:3223[B]:GLY:N	1.89	0.86
3:R:3273[B]:LEU:HB2	3:R:3275[B]:LEU:HD13	1.55	0.86
3:U:2993[B]:MET:O	3:U:2997[B]:GLU:N	2.07	0.86
3:U:3092[A]:ILE:O	3:U:3096[A]:VAL:HG23	1.74	0.86
3:U:3160[B]:SER:OG	3:d:3259[B]:ASP:CG	2.17	0.86
3:U:3225[B]:SER:O	3:U:3290[B]:ILE:HG23	1.74	0.86
3:a:2989[A]:HIS:O	3:a:2992[A]:TYR:N	2.08	0.86
3:d:2965[B]:LEU:HD11	3:d:2974[B]:ALA:HA	1.57	0.86
3:d:3220[B]:ARG:HH11	3:d:3220[B]:ARG:HG3	1.35	0.86
3:C:2948[A]:ASP:OD1	3:C:2950[A]:THR:N	2.07	0.86
3:C:2971[B]:ASP:CG	3:L:3248[B]:LEU:HD22	1.99	0.86
3:F:3147[B]:GLU:HG3	3:a:3160[B]:SER:O	1.72	0.86
3:F:3161[B]:GLU:CA	3:a:3147[B]:GLU:HG2	2.02	0.86
3:F:3173[B]:THR:HB	3:F:3176[B]:LYS:CG	2.04	0.86
3:F:3283[A]:ILE:CG2	3:F:3305[A]:ILE:HD11	2.05	0.86
3:I:2959[B]:SER:CA	3:R:3255[B]:PRO:CB	2.45	0.86
3:I:2965[A]:LEU:HD11	3:I:2974[A]:ALA:HA	1.57	0.86
3:I:3221[B]:ALA:CB	3:R:2964[B]:PRO:CA	2.53	0.86
3:L:2979[A]:GLN:HE21	3:L:3155[A]:MET:HE3	1.36	0.86
3:O:3038[B]:ILE:HG12	3:X:2969[B]:TYR:HH	1.39	0.86
3:O:3153[B]:LYS:CG	3:X:3176[B]:LYS:NZ	2.37	0.86
3:U:3082[B]:GLU:OE1	3:d:2970[B]:PRO:CB	2.20	0.86
3:U:3257[B]:ALA:HB2	3:d:2973[B]:THR:C	1.99	0.86
3:a:2952[A]:ALA:HB3	3:a:2953[A]:GLY:O	1.75	0.86
3:d:2989[B]:HIS:O	3:d:2992[B]:TYR:N	2.08	0.86
3:d:3283[B]:ILE:CG2	3:d:3305[B]:ILE:HD11	2.05	0.86
3:C:2943[A]:ALA:O	3:C:2946[A]:GLN:HG3	1.74	0.86
3:C:2965[B]:LEU:HD11	3:C:2974[B]:ALA:HA	1.57	0.86
3:F:2983[B]:VAL:HG21	3:a:3161[B]:GLU:CB	2.05	0.86
3:F:2983[B]:VAL:HG23	3:a:3160[B]:SER:CB	2.04	0.86
3:F:2989[B]:HIS:O	3:F:2992[B]:TYR:N	2.08	0.86
3:I:3248[B]:LEU:CB	3:R:2972[B]:GLY:C	2.45	0.86
3:I:3283[A]:ILE:CG2	3:I:3305[A]:ILE:HD11	2.05	0.86
3:I:3287[A]:ILE:O	3:I:3295[A]:LEU:HA	1.73	0.86
3:L:2957[B]:ILE:HA	3:L:2960[B]:PHE:CE1	2.10	0.86
3:L:2989[B]:HIS:O	3:L:2992[B]:TYR:N	2.08	0.86
3:L:3173[B]:THR:HB	3:L:3176[B]:LYS:CG	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:126:GLY:HA3	1:M:127:GLU:HB3	1.58	0.86
3:O:3225[A]:SER:O	3:O:3290[A]:ILE:HG23	1.75	0.86
3:R:2989[B]:HIS:O	3:R:2992[B]:TYR:N	2.08	0.86
3:U:2943[A]:ALA:O	3:U:2946[A]:GLN:HG3	1.74	0.86
3:U:2943[B]:ALA:O	3:U:2946[B]:GLN:HG3	1.74	0.86
3:U:3153[B]:LYS:CD	3:d:3153[B]:LYS:HD2	2.05	0.86
3:U:3218[B]:LEU:C	3:U:3219[B]:LEU:HD22	2.01	0.86
2:W:2507:ARG:HA	2:W:2779:ASP:HB2	1.57	0.86
3:X:3092[B]:ILE:O	3:X:3096[B]:VAL:HG23	1.74	0.86
3:X:3273[B]:LEU:HB2	3:X:3275[B]:LEU:HD13	1.55	0.86
3:a:2948[B]:ASP:OD1	3:a:2950[B]:THR:N	2.07	0.86
3:a:2957[A]:ILE:HA	3:a:2960[A]:PHE:CE1	2.10	0.86
3:a:3196[B]:THR:H	3:a:3199[B]:GLN:HB2	1.37	0.86
3:C:2933[A]:SER:HB3	3:C:2936[A]:GLU:HB3	1.57	0.86
3:C:2952[A]:ALA:HB3	3:C:2953[A]:GLY:O	1.76	0.86
3:C:3024[A]:LEU:CD1	3:C:3025[A]:VAL:H	1.83	0.86
3:C:3173[A]:THR:HB	3:C:3176[A]:LYS:CD	2.04	0.86
3:C:3222[B]:ILE:HD12	3:C:3223[B]:GLY:N	1.89	0.86
3:F:2952[A]:ALA:HB3	3:F:2953[A]:GLY:O	1.76	0.86
3:F:3092[B]:ILE:O	3:F:3096[B]:VAL:HG23	1.75	0.86
3:F:3222[B]:ILE:HD12	3:F:3223[B]:GLY:N	1.89	0.86
3:I:2989[A]:HIS:O	3:I:2992[A]:TYR:N	2.08	0.86
3:L:2948[A]:ASP:OD1	3:L:2950[A]:THR:N	2.07	0.86
3:L:3196[A]:THR:H	3:L:3199[A]:GLN:HB2	1.37	0.86
1:M:906:HIS:CD2	9:M:2104:CUO:O1	2.26	0.86
3:O:3293[A]:LYS:CD	3:O:3294[A]:SER:CB	2.53	0.86
3:R:3013[B]:ASP:HA	3:R:3122[B]:ASN:ND2	1.88	0.86
3:R:3176[B]:LYS:O	3:R:3177[B]:SER:OG	1.92	0.86
3:R:3218[A]:LEU:C	3:R:3219[A]:LEU:HD22	2.01	0.86
3:U:2989[A]:HIS:O	3:U:2992[A]:TYR:N	2.08	0.86
3:U:3225[A]:SER:O	3:U:3290[A]:ILE:HG23	1.75	0.86
3:d:3092[B]:ILE:O	3:d:3096[B]:VAL:HG23	1.75	0.86
3:d:3293[B]:LYS:CD	3:d:3294[B]:SER:CB	2.53	0.86
3:C:2967[B]:CYS:CB	3:L:2982[B]:MET:N	2.37	0.86
3:C:3093[B]:HIS:NE2	3:L:2969[B]:TYR:CE2	2.44	0.86
3:C:3150[B]:LYS:N	3:L:3172[B]:SER:CB	2.35	0.86
3:C:3225[A]:SER:O	3:C:3290[A]:ILE:HG23	1.75	0.86
3:C:3253[B]:GLU:CB	3:L:2975[B]:PHE:C	2.43	0.86
3:C:3293[A]:LYS:CD	3:C:3294[A]:SER:CB	2.53	0.86
3:C:3298[B]:ASN:HB2	3:C:3300[B]:LEU:N	1.78	0.86
1:G:456:GLN:NE2	1:G:549:PRO:O	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3160[B]:SER:CA	3:R:3150[B]:LYS:HD2	2.05	0.86
3:I:3173[A]:THR:HB	3:I:3176[A]:LYS:CG	2.04	0.86
3:I:3196[A]:THR:H	3:I:3199[A]:GLN:HB2	1.37	0.86
3:I:3225[B]:SER:O	3:I:3290[B]:ILE:HG23	1.75	0.86
1:J:2:LEU:HD21	1:J:81:VAL:HG21	1.57	0.86
3:L:2989[A]:HIS:O	3:L:2992[A]:TYR:N	2.08	0.86
3:O:3163[B]:ASN:HA	3:X:3149[B]:ASN:HB3	1.55	0.86
3:R:2943[A]:ALA:O	3:R:2946[A]:GLN:HG3	1.74	0.86
3:R:3173[A]:THR:HB	3:R:3176[A]:LYS:CD	2.04	0.86
3:U:3176[B]:LYS:O	3:U:3177[B]:SER:OG	1.92	0.86
3:U:3284[B]:LYS:HD3	3:U:3285[B]:VAL:H	1.39	0.86
3:X:2943[B]:ALA:O	3:X:2946[B]:GLN:HG3	1.74	0.86
3:X:2952[A]:ALA:HB3	3:X:2953[A]:GLY:O	1.76	0.86
3:X:3173[B]:THR:HB	3:X:3176[B]:LYS:CG	2.04	0.86
3:a:2997[B]:GLU:OE2	3:a:3009[B]:ILE:HG13	1.74	0.86
3:a:3092[A]:ILE:O	3:a:3096[A]:VAL:HG23	1.75	0.86
3:a:3225[B]:SER:O	3:a:3290[B]:ILE:HG23	1.75	0.86
3:d:2948[A]:ASP:OD1	3:d:2950[A]:THR:N	2.07	0.86
3:d:2952[A]:ALA:HB3	3:d:2953[A]:GLY:O	1.76	0.86
3:d:2957[A]:ILE:HA	3:d:2960[A]:PHE:CE1	2.09	0.86
3:C:2989[B]:HIS:O	3:C:2992[B]:TYR:N	2.08	0.86
3:C:3196[B]:THR:H	3:C:3199[B]:GLN:HB2	1.38	0.86
3:C:3253[B]:GLU:HA	3:L:3253[B]:GLU:HA	1.57	0.86
3:F:2957[A]:ILE:HA	3:F:2960[A]:PHE:CE1	2.10	0.86
3:F:2965[B]:LEU:HB3	3:a:3256[B]:TRP:NE1	1.89	0.86
3:F:3161[B]:GLU:CB	3:a:3079[B]:CYS:SG	2.63	0.86
3:F:3225[B]:SER:O	3:F:3290[B]:ILE:HG23	1.74	0.86
3:I:3248[B]:LEU:HD11	3:R:2973[B]:THR:HG23	1.57	0.86
3:I:3257[B]:ALA:HB3	3:R:2956[B]:LYS:HD2	1.58	0.86
3:O:2957[B]:ILE:HA	3:O:2960[B]:PHE:CE1	2.10	0.86
3:O:2970[B]:PRO:HB2	3:X:2990[B]:ARG:C	1.81	0.86
3:O:3160[B]:SER:CB	3:X:3149[B]:ASN:OD1	2.20	0.86
3:O:3251[B]:ASP:CB	3:X:2968[B]:GLN:OE1	2.23	0.86
3:U:2957[B]:ILE:HA	3:U:2960[B]:PHE:CE1	2.10	0.86
3:U:3255[B]:PRO:CD	3:d:3252[B]:TYR:C	2.47	0.86
3:a:3173[B]:THR:HB	3:a:3176[B]:LYS:CG	2.05	0.86
3:d:3092[A]:ILE:O	3:d:3096[A]:VAL:HG23	1.75	0.86
2:B:2394:VAL:H	2:B:2448:THR:HG22	1.41	0.86
3:C:3156[B]:MET:HB3	3:L:2982[B]:MET:CB	1.96	0.86
3:C:3252[B]:TYR:CB	3:L:3253[B]:GLU:HB3	1.99	0.86
3:F:3173[A]:THR:HB	3:F:3176[A]:LYS:CG	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3284[B]:LYS:HD3	3:I:3285[B]:VAL:H	1.39	0.86
1:J:329:ARG:HB2	1:M:1583:CYS:H	1.39	0.86
3:L:3287[B]:ILE:O	3:L:3295[B]:LEU:HA	1.73	0.86
1:M:1427:HIS:HD1	1:M:1461:VAL:HG21	1.38	0.86
3:O:3217[A]:PHE:HZ	3:O:3230[A]:PHE:CE1	1.89	0.86
3:R:3124[B]:ASP:OD2	3:R:3185[B]:TYR:OH	1.93	0.86
3:R:3217[A]:PHE:HZ	3:R:3230[A]:PHE:CE1	1.89	0.86
3:R:3218[B]:LEU:C	3:R:3219[B]:LEU:HD22	2.01	0.86
3:U:3124[A]:ASP:OD2	3:U:3185[A]:TYR:OH	1.93	0.86
3:U:3156[B]:MET:HE3	3:d:2982[B]:MET:SD	1.46	0.86
3:X:3196[B]:THR:H	3:X:3199[B]:GLN:HB2	1.38	0.86
1:Y:1546:LYS:HG2	3:d:3001[B]:LYS:HE3	1.52	0.86
3:a:2933[B]:SER:HB3	3:a:2936[B]:GLU:HB3	1.57	0.86
3:a:3222[B]:ILE:HD12	3:a:3223[B]:GLY:N	1.89	0.86
3:d:2933[A]:SER:HB3	3:d:2936[A]:GLU:HB3	1.57	0.86
3:d:2965[A]:LEU:HD11	3:d:2974[A]:ALA:HA	1.57	0.86
3:d:3173[B]:THR:HB	3:d:3176[B]:LYS:CG	2.05	0.86
3:C:2983[B]:VAL:CG2	3:L:3160[B]:SER:OG	2.23	0.86
3:C:3154[B]:PRO:HD3	3:L:3173[B]:THR:C	2.01	0.86
3:C:3218[A]:LEU:C	3:C:3219[A]:LEU:HD22	2.01	0.86
3:C:3218[B]:LEU:C	3:C:3219[B]:LEU:HD22	2.01	0.86
3:F:3176[B]:LYS:O	3:F:3177[B]:SER:OG	1.92	0.86
3:F:3225[A]:SER:O	3:F:3290[A]:ILE:HG23	1.75	0.86
3:I:2948[A]:ASP:OD1	3:I:2950[A]:THR:N	2.07	0.86
3:L:3218[B]:LEU:C	3:L:3219[B]:LEU:HD22	2.01	0.86
3:L:3293[B]:LYS:CD	3:L:3294[B]:SER:CB	2.53	0.86
3:O:2933[B]:SER:HB3	3:O:2936[B]:GLU:HB3	1.57	0.86
3:O:3218[A]:LEU:C	3:O:3219[A]:LEU:HD22	2.01	0.86
3:O:3298[A]:ASN:HA	3:O:3299[A]:LEU:CB	2.06	0.86
3:O:3298[B]:ASN:HB2	3:O:3300[B]:LEU:N	1.78	0.86
1:P:1140:ASN:ND2	1:P:1236:TYR:OH	2.09	0.86
3:R:3298[A]:ASN:HA	3:R:3299[A]:LEU:CB	2.06	0.86
3:X:2952[B]:ALA:HA	3:X:2956[B]:LYS:CB	2.06	0.86
3:X:2989[A]:HIS:O	3:X:2992[A]:TYR:N	2.08	0.86
3:X:3176[B]:LYS:O	3:X:3177[B]:SER:OG	1.92	0.86
3:X:3225[A]:SER:O	3:X:3290[A]:ILE:HG23	1.74	0.86
3:a:2956[A]:LYS:O	3:a:2960[A]:PHE:HE1	1.22	0.86
3:a:2957[B]:ILE:HA	3:a:2960[B]:PHE:CE1	2.10	0.86
3:a:2965[B]:LEU:HD11	3:a:2974[B]:ALA:HA	1.57	0.86
3:a:3283[A]:ILE:CG2	3:a:3305[A]:ILE:HD11	2.05	0.86
3:d:2948[A]:ASP:N	3:d:2949[A]:LYS:HA	1.81	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2933[B]:SER:HB3	3:C:2936[B]:GLU:HB3	1.57	0.86
3:F:2969[B]:TYR:CD1	3:a:2961[B]:HIS:ND1	2.13	0.86
3:F:3176[A]:LYS:O	3:F:3177[A]:SER:OG	1.92	0.86
3:F:3218[B]:LEU:C	3:F:3219[B]:LEU:HD22	2.01	0.86
3:I:2997[B]:GLU:OE2	3:I:3009[B]:ILE:HG13	1.74	0.86
3:I:3153[B]:LYS:HB3	3:R:3155[B]:MET:HB2	1.56	0.86
3:I:3154[B]:PRO:CG	3:R:3174[B]:GLY:HA2	2.05	0.86
3:I:3162[B]:ASP:HA	3:R:3259[B]:ASP:HB3	1.58	0.86
3:I:3284[A]:LYS:HD3	3:I:3285[A]:VAL:H	1.39	0.86
3:L:3225[B]:SER:O	3:L:3290[B]:ILE:HG23	1.74	0.86
3:O:2989[B]:HIS:O	3:O:2992[B]:TYR:N	2.08	0.86
3:O:3172[B]:SER:HB3	3:X:3152[B]:LYS:HE2	1.58	0.86
3:O:3196[B]:THR:HB	3:O:3198[B]:PRO:HD2	1.54	0.86
3:R:2952[B]:ALA:HB3	3:R:2953[B]:GLY:O	1.76	0.86
3:R:3124[A]:ASP:OD2	3:R:3185[A]:TYR:OH	1.93	0.86
3:U:3169[B]:LYS:CE	3:d:3147[B]:GLU:CA	2.52	0.86
3:X:2933[B]:SER:HB3	3:X:2936[B]:GLU:HB3	1.57	0.86
3:X:2965[A]:LEU:HD11	3:X:2974[A]:ALA:HA	1.57	0.86
3:X:3218[A]:LEU:C	3:X:3219[A]:LEU:HD22	2.01	0.86
3:C:2952[B]:ALA:HA	3:C:2956[B]:LYS:CB	2.06	0.85
3:C:2982[B]:MET:SD	3:L:3157[B]:PRO:CA	2.63	0.85
3:C:2997[B]:GLU:OE2	3:C:3009[B]:ILE:HG13	1.74	0.85
3:C:3079[B]:CYS:SG	3:L:3161[B]:GLU:HB3	2.16	0.85
2:E:2800:LYS:O	3:F:3023[A]:ILE:HD11	1.73	0.85
3:F:2983[B]:VAL:HG23	3:a:3161[B]:GLU:N	1.90	0.85
3:F:3153[B]:LYS:NZ	3:a:3156[B]:MET:C	2.33	0.85
3:F:3155[B]:MET:SD	3:a:3154[B]:PRO:HG2	2.16	0.85
3:F:3293[B]:LYS:CD	3:F:3294[B]:SER:CB	2.53	0.85
3:L:2952[B]:ALA:HA	3:L:2956[B]:LYS:CB	2.06	0.85
3:L:2965[A]:LEU:HD11	3:L:2974[A]:ALA:HA	1.57	0.85
3:O:3218[B]:LEU:C	3:O:3219[B]:LEU:HD22	2.01	0.85
3:R:2997[A]:GLU:OE2	3:R:3009[A]:ILE:HG13	1.74	0.85
3:U:2971[B]:ASP:CA	3:d:3090[B]:ASN:ND2	2.22	0.85
3:U:2997[A]:GLU:OE2	3:U:3009[A]:ILE:HG13	1.74	0.85
3:U:3273[A]:LEU:HB2	3:U:3275[A]:LEU:HD13	1.55	0.85
3:X:3222[B]:ILE:HD12	3:X:3223[B]:GLY:N	1.89	0.85
3:X:3298[A]:ASN:HA	3:X:3299[A]:LEU:CB	2.06	0.85
3:d:2989[A]:HIS:O	3:d:2992[A]:TYR:N	2.08	0.85
3:d:3124[A]:ASP:OD2	3:d:3185[A]:TYR:OH	1.93	0.85
3:C:3090[B]:ASN:CB	3:L:2972[B]:GLY:CA	2.52	0.85
1:D:497:GLN:HG2	1:D:683:THR:HG21	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3256[B]:TRP:CB	3:a:2966[B]:SER:CA	2.36	0.85
3:I:2977[B]:CYS:SG	3:R:2979[B]:GLN:HA	2.15	0.85
3:I:3151[B]:LEU:H	3:R:3169[B]:LYS:HG2	1.40	0.85
3:I:3153[B]:LYS:NZ	3:R:3157[B]:PRO:CD	2.38	0.85
3:I:3218[B]:LEU:C	3:I:3219[B]:LEU:HD22	2.01	0.85
3:O:3156[B]:MET:HG3	3:X:3173[B]:THR:HG23	1.58	0.85
3:O:3222[A]:ILE:HD12	3:O:3223[A]:GLY:N	1.89	0.85
1:P:1033:LEU:HA	1:P:1036:SER:HB3	1.55	0.85
3:R:2956[A]:LYS:C	3:R:2960[A]:PHE:CE1	2.47	0.85
3:R:2965[A]:LEU:HD11	3:R:2974[A]:ALA:HA	1.57	0.85
3:R:3298[B]:ASN:HA	3:R:3299[B]:LEU:CB	2.06	0.85
3:U:2933[A]:SER:HB3	3:U:2936[A]:GLU:HB3	1.57	0.85
3:U:2965[B]:LEU:CD2	3:d:3220[B]:ARG:HH11	1.88	0.85
3:U:2989[B]:HIS:O	3:U:2992[B]:TYR:N	2.08	0.85
3:X:2948[B]:ASP:CB	3:X:2953[B]:GLY:HA3	2.07	0.85
3:a:2993[A]:MET:O	3:a:2997[A]:GLU:N	2.07	0.85
3:d:3284[A]:LYS:HD3	3:d:3285[A]:VAL:H	1.39	0.85
3:d:3298[A]:ASN:HA	3:d:3299[A]:LEU:CB	2.06	0.85
3:C:3173[B]:THR:HB	3:C:3176[B]:LYS:CD	2.04	0.85
3:C:3283[B]:ILE:CG2	3:C:3305[B]:ILE:HD11	2.05	0.85
1:D:567:LEU:HB2	1:D:609:TRP:CD1	2.10	0.85
3:F:3256[B]:TRP:CA	3:a:2966[B]:SER:HA	2.06	0.85
3:I:2948[B]:ASP:N	3:I:2949[B]:LYS:HA	1.81	0.85
3:I:3163[B]:ASN:CG	3:R:3149[B]:ASN:HD22	1.82	0.85
3:I:3255[B]:PRO:CB	3:R:2959[B]:SER:CB	2.49	0.85
3:L:2952[A]:ALA:HB3	3:L:2953[A]:GLY:O	1.76	0.85
3:L:3173[A]:THR:HB	3:L:3176[A]:LYS:CG	2.05	0.85
3:O:3283[A]:ILE:CG2	3:O:3305[A]:ILE:HD11	2.05	0.85
3:R:3092[A]:ILE:O	3:R:3096[A]:VAL:HG23	1.75	0.85
3:X:2943[A]:ALA:O	3:X:2946[A]:GLN:HG3	1.74	0.85
3:X:3124[A]:ASP:OD2	3:X:3185[A]:TYR:OH	1.93	0.85
3:X:3217[B]:PHE:HZ	3:X:3230[B]:PHE:CE1	1.89	0.85
3:X:3293[A]:LYS:CD	3:X:3294[A]:SER:CB	2.53	0.85
3:a:2952[B]:ALA:HB3	3:a:2953[B]:GLY:O	1.76	0.85
3:a:3217[B]:PHE:HZ	3:a:3230[B]:PHE:CE1	1.89	0.85
3:a:3298[B]:ASN:HA	3:a:3299[B]:LEU:CB	2.06	0.85
3:d:2948[B]:ASP:CB	3:d:2953[B]:GLY:HA3	2.07	0.85
3:d:3124[B]:ASP:OD2	3:d:3185[B]:TYR:OH	1.93	0.85
3:C:3153[B]:LYS:HE3	3:L:3158[B]:PHE:CD2	2.10	0.85
3:F:3124[B]:ASP:OD2	3:F:3185[B]:TYR:OH	1.93	0.85
3:I:3092[A]:ILE:O	3:I:3096[A]:VAL:HG23	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3124[B]:ASP:OD2	3:L:3185[B]:TYR:OH	1.93	0.85
3:L:3196[B]:THR:H	3:L:3199[B]:GLN:HB2	1.38	0.85
3:R:2989[A]:HIS:O	3:R:2992[A]:TYR:N	2.08	0.85
3:R:2997[B]:GLU:OE2	3:R:3009[B]:ILE:HG13	1.74	0.85
3:U:3283[A]:ILE:CG2	3:U:3305[A]:ILE:HD11	2.05	0.85
3:U:3284[A]:LYS:HD3	3:U:3285[A]:VAL:H	1.39	0.85
3:X:3298[B]:ASN:HA	3:X:3299[B]:LEU:CB	2.06	0.85
3:a:2952[A]:ALA:HA	3:a:2956[A]:LYS:CB	2.06	0.85
3:a:2989[B]:HIS:O	3:a:2992[B]:TYR:N	2.08	0.85
3:a:3176[B]:LYS:O	3:a:3177[B]:SER:OG	1.92	0.85
3:F:2985[B]:PHE:HZ	3:a:2970[B]:PRO:HA	1.37	0.85
3:F:3159[B]:SER:OG	3:a:2984[B]:THR:CG2	2.11	0.85
3:F:3256[B]:TRP:CB	3:a:2966[B]:SER:O	2.24	0.85
3:I:3124[B]:ASP:OD2	3:I:3185[B]:TYR:OH	1.93	0.85
3:I:3176[B]:LYS:O	3:I:3177[B]:SER:OG	1.92	0.85
1:J:1427:HIS:CE1	1:J:1458:HIS:NE2	2.43	0.85
3:L:3089[A]:HIS:ND1	3:L:3119[A]:HIS:NE2	2.25	0.85
3:L:3124[A]:ASP:OD2	3:L:3185[A]:TYR:OH	1.93	0.85
3:L:3298[A]:ASN:HA	3:L:3299[A]:LEU:CB	2.06	0.85
3:R:2952[B]:ALA:HA	3:R:2956[B]:LYS:CB	2.06	0.85
1:V:456:GLN:HG2	1:V:551:GLU:HB2	1.58	0.85
3:d:2952[B]:ALA:HA	3:d:2956[B]:LYS:CB	2.06	0.85
3:d:3089[B]:HIS:ND1	3:d:3119[B]:HIS:NE2	2.25	0.85
3:C:2978[B]:CYS:H	3:L:3254[B]:MET:HB3	1.02	0.85
3:C:2989[A]:HIS:O	3:C:2992[A]:TYR:N	2.08	0.85
3:C:3124[B]:ASP:OD2	3:C:3185[B]:TYR:OH	1.93	0.85
3:C:3176[B]:LYS:O	3:C:3177[B]:SER:OG	1.92	0.85
3:F:3124[A]:ASP:OD2	3:F:3185[A]:TYR:OH	1.93	0.85
3:F:3174[B]:GLY:N	3:a:3154[B]:PRO:CD	2.40	0.85
3:I:2956[B]:LYS:O	3:I:2960[B]:PHE:HE1	1.22	0.85
3:I:3150[B]:LYS:HE3	3:R:3163[B]:ASN:HB2	0.87	0.85
3:I:3218[A]:LEU:C	3:I:3219[A]:LEU:HD22	2.01	0.85
3:L:2948[B]:ASP:CB	3:L:2953[B]:GLY:HA3	2.07	0.85
1:M:497:GLN:HG2	1:M:683:THR:HG21	1.57	0.85
3:O:2965[B]:LEU:N	3:X:3254[B]:MET:HE1	1.92	0.85
3:O:2967[B]:CYS:SG	3:X:3153[B]:LYS:CB	2.53	0.85
3:O:2970[B]:PRO:CB	3:X:2990[B]:ARG:C	2.44	0.85
3:O:3298[B]:ASN:HA	3:O:3299[B]:LEU:CB	2.06	0.85
3:R:2933[A]:SER:HB3	3:R:2936[A]:GLU:HB3	1.57	0.85
3:R:3283[A]:ILE:CG2	3:R:3305[A]:ILE:HD11	2.05	0.85
3:U:3154[B]:PRO:C	3:d:3150[B]:LYS:HG2	2.02	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3298[B]:ASN:HA	3:U:3299[B]:LEU:CB	2.06	0.85
1:Y:1546:LYS:HG3	3:d:3001[B]:LYS:HG3	1.56	0.85
2:Z:2344:LEU:HD13	2:c:2515:ARG:HA	1.57	0.85
3:d:3089[A]:HIS:ND1	3:d:3119[A]:HIS:NE2	2.25	0.85
3:F:2952[A]:ALA:HA	3:F:2956[A]:LYS:CB	2.06	0.85
3:F:3218[A]:LEU:C	3:F:3219[A]:LEU:HD22	2.01	0.85
3:F:3298[B]:ASN:HA	3:F:3299[B]:LEU:CB	2.06	0.85
2:H:2797:LYS:HZ1	3:I:3028[A]:PRO:CD	1.89	0.85
3:I:3150[B]:LYS:HB3	3:R:3160[B]:SER:N	1.90	0.85
3:O:2952[A]:ALA:HA	3:O:2956[A]:LYS:CB	2.06	0.85
3:O:3038[B]:ILE:CD1	3:X:2969[B]:TYR:CE2	2.54	0.85
3:O:3124[B]:ASP:OD2	3:O:3185[B]:TYR:OH	1.93	0.85
3:R:2952[A]:ALA:HA	3:R:2956[A]:LYS:CB	2.06	0.85
3:a:3218[B]:LEU:C	3:a:3219[B]:LEU:HD22	2.01	0.85
3:a:3283[B]:ILE:CG2	3:a:3305[B]:ILE:HD11	2.05	0.85
3:C:2948[B]:ASP:CB	3:C:2953[B]:GLY:HA3	2.07	0.85
3:C:3092[B]:ILE:O	3:C:3096[B]:VAL:HG23	1.75	0.85
3:C:3149[B]:ASN:CG	3:L:3163[B]:ASN:ND2	2.32	0.85
3:C:3172[B]:SER:OG	3:L:3152[B]:LYS:CG	2.24	0.85
3:C:3258[B]:PHE:CZ	3:L:2968[B]:GLN:CD	2.54	0.85
3:I:2952[B]:ALA:HB3	3:I:2953[B]:GLY:O	1.76	0.85
3:I:2989[B]:HIS:O	3:I:2992[B]:TYR:N	2.09	0.85
3:I:3163[B]:ASN:H	3:R:3147[B]:GLU:CD	1.85	0.85
3:I:3251[B]:ASP:C	3:R:3252[B]:TYR:HB2	2.00	0.85
3:L:2952[A]:ALA:HA	3:L:2956[A]:LYS:CB	2.06	0.85
3:O:2933[B]:SER:CB	3:O:2936[B]:GLU:HB3	2.07	0.85
3:O:2948[A]:ASP:CB	3:O:2953[A]:GLY:HA3	2.07	0.85
3:O:3254[B]:MET:HE3	3:X:3172[B]:SER:CB	2.06	0.85
3:R:2948[B]:ASP:N	3:R:2949[B]:LYS:HA	1.81	0.85
3:U:2952[A]:ALA:HB3	3:U:2953[A]:GLY:O	1.76	0.85
3:U:3257[B]:ALA:N	3:d:2969[B]:TYR:N	2.24	0.85
3:U:3293[B]:LYS:CD	3:U:3294[B]:SER:CB	2.53	0.85
3:X:2933[A]:SER:HB3	3:X:2936[A]:GLU:HB3	1.57	0.85
3:X:2933[B]:SER:CB	3:X:2936[B]:GLU:HB3	2.07	0.85
3:a:2948[A]:ASP:CB	3:a:2953[A]:GLY:HA3	2.07	0.85
3:a:3089[A]:HIS:ND1	3:a:3119[A]:HIS:NE2	2.25	0.85
3:a:3185[B]:TYR:CE2	3:a:3187[B]:TYR:CE2	2.65	0.85
3:a:3218[A]:LEU:C	3:a:3219[A]:LEU:HD22	2.01	0.85
3:d:2948[B]:ASP:N	3:d:2949[B]:LYS:HA	1.81	0.85
3:C:2933[B]:SER:CB	3:C:2936[B]:GLU:HB3	2.07	0.85
3:C:3149[B]:ASN:O	3:L:3168[B]:THR:C	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3156[B]:MET:SD	3:L:2979[B]:GLN:HG3	2.17	0.85
3:C:3185[A]:TYR:CE2	3:C:3187[A]:TYR:CE2	2.65	0.85
3:I:3173[B]:THR:C	3:R:3154[B]:PRO:N	2.35	0.85
3:L:2933[A]:SER:HB3	3:L:2936[A]:GLU:HB3	1.57	0.85
2:N:2556:TYR:HE1	2:N:2845:PRO:HD2	1.38	0.85
3:O:2952[A]:ALA:HB3	3:O:2953[A]:GLY:O	1.76	0.85
3:O:2956[B]:LYS:C	3:O:2960[B]:PHE:CE1	2.47	0.85
3:O:2976[B]:ALA:H	3:X:3156[B]:MET:HG2	1.10	0.85
3:O:3169[B]:LYS:HG3	3:X:3148[B]:ILE:HG21	1.04	0.85
3:R:3089[A]:HIS:ND1	3:R:3119[A]:HIS:NE2	2.25	0.85
3:R:3185[B]:TYR:CE2	3:R:3187[B]:TYR:CE2	2.65	0.85
3:U:2952[B]:ALA:HB3	3:U:2953[B]:GLY:O	1.76	0.85
3:U:3185[B]:TYR:CE2	3:U:3187[B]:TYR:CE2	2.65	0.85
3:X:3089[B]:HIS:ND1	3:X:3119[B]:HIS:NE2	2.25	0.85
3:X:3124[B]:ASP:OD2	3:X:3185[B]:TYR:OH	1.93	0.85
3:X:3283[B]:ILE:CG2	3:X:3305[B]:ILE:HD11	2.05	0.85
2:c:2549:PRO:HD2	2:c:2554:PRO:HB3	1.57	0.85
3:d:2952[A]:ALA:HA	3:d:2956[A]:LYS:CB	2.06	0.85
3:d:3218[B]:LEU:C	3:d:3219[B]:LEU:HD22	2.01	0.85
3:F:2952[B]:ALA:HB3	3:F:2953[B]:GLY:O	1.76	0.85
3:F:3162[B]:ASP:HB3	3:a:3259[B]:ASP:CA	2.07	0.85
3:F:3174[B]:GLY:HA3	3:a:3154[B]:PRO:CB	2.03	0.85
3:I:2933[A]:SER:CB	3:I:2936[A]:GLU:HB3	2.07	0.85
3:I:2965[B]:LEU:CD1	3:R:3256[B]:TRP:HE1	1.88	0.85
3:I:2969[B]:TYR:C	3:R:2989[B]:HIS:NE2	2.35	0.85
3:I:3124[A]:ASP:OD2	3:I:3185[A]:TYR:OH	1.93	0.85
3:L:2952[B]:ALA:HB3	3:L:2953[B]:GLY:O	1.76	0.85
3:L:3298[B]:ASN:HA	3:L:3299[B]:LEU:CB	2.06	0.85
3:O:3169[B]:LYS:HB2	3:X:3148[B]:ILE:HG21	1.57	0.85
3:O:3185[B]:TYR:CE2	3:O:3187[B]:TYR:CE2	2.65	0.85
3:O:3293[B]:LYS:CD	3:O:3294[B]:SER:CB	2.53	0.85
3:R:3284[A]:LYS:HD3	3:R:3285[A]:VAL:H	1.40	0.85
3:U:2933[B]:SER:HB3	3:U:2936[B]:GLU:HB3	1.57	0.85
3:U:2965[B]:LEU:HA	3:d:3220[B]:ARG:NH1	1.92	0.85
3:U:3152[B]:LYS:C	3:d:3152[B]:LYS:O	2.19	0.85
3:U:3256[B]:TRP:HD1	3:d:2975[B]:PHE:CE1	1.93	0.85
3:X:2952[A]:ALA:HA	3:X:2956[A]:LYS:CB	2.06	0.85
3:X:3089[A]:HIS:ND1	3:X:3119[A]:HIS:NE2	2.25	0.85
3:X:3218[B]:LEU:C	3:X:3219[B]:LEU:HD22	2.01	0.85
3:d:2952[B]:ALA:HB3	3:d:2953[B]:GLY:O	1.76	0.85
3:d:3176[A]:LYS:O	3:d:3177[A]:SER:OG	1.92	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3218[A]:LEU:C	3:d:3219[A]:LEU:HD22	2.01	0.85
4:MA:1:NAG:H61	4:MA:2:NAG:C1	2.07	0.85
3:C:3149[B]:ASN:C	3:L:3172[B]:SER:HB3	2.02	0.84
3:C:3173[B]:THR:OG1	3:L:3152[B]:LYS:CA	2.24	0.84
3:C:3185[B]:TYR:CE2	3:C:3187[B]:TYR:CE2	2.65	0.84
3:C:3298[B]:ASN:HA	3:C:3299[B]:LEU:CB	2.06	0.84
3:F:2966[B]:SER:HA	3:a:3256[B]:TRP:HB3	1.56	0.84
3:L:3089[B]:HIS:ND1	3:L:3119[B]:HIS:NE2	2.25	0.84
3:L:3284[A]:LYS:HD3	3:L:3285[A]:VAL:H	1.39	0.84
3:O:2952[B]:ALA:HB3	3:O:2953[B]:GLY:O	1.76	0.84
3:O:2965[A]:LEU:HD11	3:O:2974[A]:ALA:HA	1.57	0.84
3:R:2952[A]:ALA:HB3	3:R:2953[A]:GLY:O	1.76	0.84
3:R:2955[A]:GLN:CD	3:R:3037[A]:TYR:CE1	2.55	0.84
3:U:2952[A]:ALA:HA	3:U:2956[A]:LYS:CB	2.06	0.84
3:U:3169[B]:LYS:HE2	3:d:3147[B]:GLU:HA	1.59	0.84
3:U:3185[A]:TYR:CE2	3:U:3187[A]:TYR:CE2	2.65	0.84
3:X:2965[B]:LEU:HD11	3:X:2974[B]:ALA:HA	1.57	0.84
3:a:3089[B]:HIS:ND1	3:a:3119[B]:HIS:NE2	2.25	0.84
3:a:3284[A]:LYS:HD3	3:a:3285[A]:VAL:H	1.39	0.84
1:b:497:GLN:HG2	1:b:683:THR:HG21	1.57	0.84
3:d:3185[B]:TYR:CE2	3:d:3187[B]:TYR:CE2	2.65	0.84
3:C:2933[A]:SER:CB	3:C:2936[A]:GLU:HB3	2.07	0.84
3:C:2952[B]:ALA:HB3	3:C:2953[B]:GLY:O	1.76	0.84
3:C:2982[B]:MET:SD	3:L:3157[B]:PRO:HA	2.17	0.84
3:F:2952[B]:ALA:HA	3:F:2956[B]:LYS:CB	2.06	0.84
3:F:3089[A]:HIS:ND1	3:F:3119[A]:HIS:NE2	2.25	0.84
3:F:3153[B]:LYS:HZ2	3:a:3156[B]:MET:C	1.84	0.84
3:I:3293[B]:LYS:CD	3:I:3294[B]:SER:CB	2.53	0.84
3:I:3298[A]:ASN:HA	3:I:3299[A]:LEU:CB	2.06	0.84
3:O:3038[B]:ILE:CG2	3:X:2969[B]:TYR:OH	2.22	0.84
3:O:3124[A]:ASP:OD2	3:O:3185[A]:TYR:OH	1.93	0.84
3:R:2948[A]:ASP:CB	3:R:2953[A]:GLY:HA3	2.07	0.84
3:R:3293[B]:LYS:CD	3:R:3294[B]:SER:CB	2.53	0.84
1:S:871:GLN:HE22	1:S:964:ILE:HG13	1.40	0.84
3:U:3217[B]:PHE:HZ	3:U:3230[B]:PHE:CE1	1.89	0.84
3:U:3252[B]:TYR:O	3:d:3255[B]:PRO:HB3	1.77	0.84
3:a:2933[A]:SER:CB	3:a:2936[A]:GLU:HB3	2.07	0.84
3:C:2955[B]:GLN:CD	3:C:3037[B]:TYR:CE1	2.55	0.84
3:C:2965[A]:LEU:HD11	3:C:2974[A]:ALA:HA	1.57	0.84
3:C:3284[A]:LYS:HD3	3:C:3285[A]:VAL:H	1.39	0.84
3:F:2933[B]:SER:HB3	3:F:2936[B]:GLU:HB3	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2948[A]:ASP:CB	3:F:2953[A]:GLY:HA3	2.07	0.84
3:I:2952[B]:ALA:HA	3:I:2956[B]:LYS:CB	2.06	0.84
3:I:3089[A]:HIS:ND1	3:I:3119[A]:HIS:NE2	2.25	0.84
3:I:3149[B]:ASN:ND2	3:R:3163[B]:ASN:HB3	1.92	0.84
3:O:2948[B]:ASP:CB	3:O:2953[B]:GLY:HA3	2.07	0.84
3:O:3038[B]:ILE:HG23	3:X:2969[B]:TYR:CE1	2.10	0.84
3:O:3251[B]:ASP:HB3	3:X:2967[B]:CYS:HA	0.90	0.84
3:U:2955[B]:GLN:CD	3:U:3037[B]:TYR:CE1	2.55	0.84
3:U:3169[B]:LYS:HE3	3:d:3147[B]:GLU:HB3	1.59	0.84
3:U:3218[A]:LEU:C	3:U:3219[A]:LEU:HD22	2.01	0.84
3:a:2933[B]:SER:CB	3:a:2936[B]:GLU:HB3	2.07	0.84
3:d:3230[A]:PHE:CB	3:d:3243[A]:GLY:HA2	2.06	0.84
3:F:2933[B]:SER:CB	3:F:2936[B]:GLU:HB3	2.07	0.84
3:F:2971[B]:ASP:O	3:a:3090[B]:ASN:CA	2.24	0.84
3:F:3153[B]:LYS:CB	3:a:3155[B]:MET:O	2.24	0.84
3:F:3185[A]:TYR:CE2	3:F:3187[A]:TYR:CE2	2.65	0.84
3:I:2982[B]:MET:CG	3:R:3156[B]:MET:HB2	2.07	0.84
3:I:3185[A]:TYR:CE2	3:I:3187[A]:TYR:CE2	2.65	0.84
3:L:2955[A]:GLN:CD	3:L:3037[A]:TYR:CE1	2.55	0.84
1:M:401:VAL:HG22	1:M:662:SER:HB3	1.59	0.84
3:O:3196[A]:THR:H	3:O:3199[A]:GLN:HB2	1.37	0.84
3:U:2952[B]:ALA:HA	3:U:2956[B]:LYS:CB	2.06	0.84
3:U:2969[B]:TYR:CE1	3:d:2978[B]:CYS:SG	2.71	0.84
1:Y:883:CYS:N	1:Y:894:CYS:SG	2.51	0.84
3:a:2952[B]:ALA:HA	3:a:2956[B]:LYS:CB	2.06	0.84
3:F:2970[B]:PRO:CB	3:a:2989[B]:HIS:CD2	2.59	0.84
3:F:3089[B]:HIS:ND1	3:F:3119[B]:HIS:NE2	2.25	0.84
3:F:3159[B]:SER:CB	3:a:2984[B]:THR:HG23	1.85	0.84
3:I:2952[A]:ALA:HA	3:I:2956[A]:LYS:CB	2.06	0.84
3:I:2965[B]:LEU:HD11	3:I:2974[B]:ALA:HA	1.57	0.84
3:I:3157[B]:PRO:HD3	3:R:3254[B]:MET:HE2	1.57	0.84
3:I:3185[B]:TYR:CE2	3:I:3187[B]:TYR:CE2	2.65	0.84
3:I:3230[A]:PHE:CB	3:I:3243[A]:GLY:HA2	2.06	0.84
3:L:2948[A]:ASP:CB	3:L:2953[A]:GLY:HA3	2.07	0.84
3:L:3185[A]:TYR:CE2	3:L:3187[A]:TYR:CE2	2.65	0.84
3:U:3196[B]:THR:H	3:U:3199[B]:GLN:HB2	1.37	0.84
3:U:3298[A]:ASN:HA	3:U:3299[A]:LEU:CB	2.06	0.84
3:X:2955[B]:GLN:CD	3:X:3037[B]:TYR:CE1	2.55	0.84
3:a:3298[A]:ASN:HA	3:a:3299[A]:LEU:CB	2.06	0.84
3:d:2956[B]:LYS:O	3:d:2960[B]:PHE:HE1	1.22	0.84
3:C:3222[B]:ILE:CD1	3:L:2963[B]:MET:HE1	2.05	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2933[A]:SER:CB	3:F:2936[A]:GLU:HB3	2.07	0.84
3:F:3185[B]:TYR:CE2	3:F:3187[B]:TYR:CE2	2.65	0.84
3:F:3298[A]:ASN:HA	3:F:3299[A]:LEU:CB	2.06	0.84
3:I:3089[B]:HIS:CD2	3:R:2972[B]:GLY:N	2.46	0.84
3:L:3185[B]:TYR:CE2	3:L:3187[B]:TYR:CE2	2.65	0.84
3:O:2956[B]:LYS:O	3:O:2960[B]:PHE:HE1	1.22	0.84
3:O:3255[B]:PRO:HD3	3:X:3158[B]:PHE:O	1.76	0.84
1:P:392:PRO:HB2	1:P:394:GLN:HG2	1.60	0.84
3:U:2970[B]:PRO:O	3:d:3086[B]:GLU:HG2	1.77	0.84
3:U:3217[A]:PHE:HZ	3:U:3230[A]:PHE:CE1	1.89	0.84
3:X:3185[A]:TYR:CE2	3:X:3187[A]:TYR:CE2	2.65	0.84
3:X:3212[B]:ARG:HG3	3:X:3212[B]:ARG:HH11	1.43	0.84
3:a:2933[A]:SER:HB3	3:a:2936[A]:GLU:HB3	1.57	0.84
3:a:2948[B]:ASP:CB	3:a:2953[B]:GLY:HA3	2.07	0.84
3:a:3196[A]:THR:H	3:a:3199[A]:GLN:HB2	1.37	0.84
3:d:2933[B]:SER:CB	3:d:2936[B]:GLU:HB3	2.07	0.84
3:C:3089[B]:HIS:ND1	3:C:3119[B]:HIS:NE2	2.25	0.84
3:C:3152[B]:LYS:H	3:L:3172[B]:SER:CB	1.90	0.84
3:F:2965[B]:LEU:HD13	3:a:3256[B]:TRP:HE1	1.38	0.84
3:F:2975[B]:PHE:HZ	3:a:2961[B]:HIS:CA	1.88	0.84
3:I:2948[A]:ASP:CB	3:I:2953[A]:GLY:HA3	2.07	0.84
3:I:2948[B]:ASP:CB	3:I:2953[B]:GLY:HA3	2.07	0.84
3:I:2952[A]:ALA:HB3	3:I:2953[A]:GLY:O	1.76	0.84
3:I:3162[B]:ASP:CB	3:R:3259[B]:ASP:H	1.89	0.84
3:I:3170[B]:ALA:N	3:R:3148[B]:ILE:O	2.10	0.84
3:I:3217[B]:PHE:HZ	3:I:3230[B]:PHE:CE1	1.89	0.84
3:L:3089[B]:HIS:HE1	3:L:3119[B]:HIS:CD2	1.96	0.84
3:O:2968[B]:GLN:CD	3:X:2984[B]:THR:OG1	2.20	0.84
3:O:3089[B]:HIS:HE1	3:O:3119[B]:HIS:CD2	1.96	0.84
3:U:2956[A]:LYS:O	3:U:2960[A]:PHE:HE1	1.22	0.84
3:U:2979[A]:GLN:CG	3:U:3155[A]:MET:CE	2.56	0.84
3:U:3124[B]:ASP:OD2	3:U:3185[B]:TYR:OH	1.93	0.84
3:X:2948[A]:ASP:CB	3:X:2953[A]:GLY:HA3	2.07	0.84
3:X:3176[A]:LYS:HE2	3:X:3176[A]:LYS:H	1.43	0.84
3:X:3284[B]:LYS:HD3	3:X:3285[B]:VAL:H	1.40	0.84
3:a:2948[B]:ASP:N	3:a:2949[B]:LYS:HA	1.81	0.84
3:a:2979[A]:GLN:CG	3:a:3155[A]:MET:CE	2.56	0.84
3:L:3212[B]:ARG:HH11	3:L:3212[B]:ARG:HG3	1.43	0.84
1:P:456:GLN:HG2	1:P:551:GLU:HB2	1.57	0.84
3:R:3089[A]:HIS:HE1	3:R:3119[A]:HIS:CD2	1.96	0.84
3:U:2948[B]:ASP:CB	3:U:2953[B]:GLY:HA3	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3089[B]:HIS:HE1	3:X:3119[B]:HIS:CD2	1.96	0.84
3:X:3173[A]:THR:HG22	3:X:3174[A]:GLY:N	1.93	0.84
2:Z:2648:ALA:HA	2:Z:2654:SER:HB2	1.60	0.84
3:a:2948[A]:ASP:N	3:a:2949[A]:LYS:HA	1.81	0.84
3:a:3293[A]:LYS:CD	3:a:3294[A]:SER:CB	2.53	0.84
3:d:3293[A]:LYS:CD	3:d:3294[A]:SER:CB	2.53	0.84
3:C:2985[B]:PHE:CD2	3:L:2968[B]:GLN:O	2.30	0.84
3:C:3154[B]:PRO:N	3:L:3174[B]:GLY:N	2.24	0.84
3:F:2966[B]:SER:O	3:a:3256[B]:TRP:CG	2.23	0.84
3:F:2969[B]:TYR:CE2	3:a:3120[B]:HIS:NE2	2.45	0.84
3:F:3196[A]:THR:H	3:F:3199[A]:GLN:HB2	1.38	0.84
3:I:3160[B]:SER:O	3:R:3150[B]:LYS:HD2	1.76	0.84
3:O:2979[B]:GLN:CG	3:O:3155[B]:MET:CE	2.56	0.84
3:O:3089[B]:HIS:ND1	3:O:3119[B]:HIS:NE2	2.25	0.84
3:O:3176[B]:LYS:HE2	3:O:3176[B]:LYS:H	1.43	0.84
3:R:2933[A]:SER:CB	3:R:2936[A]:GLU:HB3	2.07	0.84
3:U:2948[A]:ASP:CB	3:U:2953[A]:GLY:HA3	2.07	0.84
1:Y:1546:LYS:HG3	3:d:3001[B]:LYS:CE	2.03	0.84
3:d:2933[A]:SER:CB	3:d:2936[A]:GLU:HB3	2.07	0.84
3:d:3185[A]:TYR:CE2	3:d:3187[A]:TYR:CE2	2.65	0.84
3:C:2948[A]:ASP:CB	3:C:2953[A]:GLY:HA3	2.07	0.84
3:C:3158[B]:PHE:O	3:L:3149[B]:ASN:CG	2.21	0.84
3:C:3160[B]:SER:HA	3:L:2983[B]:VAL:CB	2.06	0.84
3:I:3173[B]:THR:HG1	3:R:3173[B]:THR:HG23	0.71	0.84
3:L:2933[B]:SER:CB	3:L:2936[B]:GLU:HB3	2.07	0.84
3:O:3176[A]:LYS:HE2	3:O:3176[A]:LYS:H	1.43	0.84
3:R:2933[B]:SER:HB3	3:R:2936[B]:GLU:HB3	1.57	0.84
3:R:3173[A]:THR:HG22	3:R:3174[A]:GLY:N	1.93	0.84
3:U:3155[B]:MET:HA	3:d:3150[B]:LYS:HG2	1.58	0.84
3:X:2933[A]:SER:CB	3:X:2936[A]:GLU:HB3	2.07	0.84
3:X:3185[B]:TYR:CE2	3:X:3187[B]:TYR:CE2	2.65	0.84
2:c:2267:HIS:HD2	2:c:2297:HIS:HE1	1.26	0.84
3:C:2968[B]:GLN:HE22	3:L:3258[B]:PHE:HZ	1.03	0.83
3:C:3089[A]:HIS:ND1	3:C:3119[A]:HIS:NE2	2.25	0.83
3:C:3093[B]:HIS:NE2	3:L:2969[B]:TYR:CD2	2.46	0.83
3:C:3147[B]:GLU:CD	3:L:3163[B]:ASN:H	1.85	0.83
3:C:3150[B]:LYS:HZ2	3:L:3160[B]:SER:HB3	1.26	0.83
3:F:2959[B]:SER:HB2	3:a:3255[B]:PRO:CB	2.07	0.83
3:F:3256[B]:TRP:N	3:a:2965[B]:LEU:C	2.36	0.83
3:I:2933[B]:SER:CB	3:I:2936[B]:GLU:HB3	2.07	0.83
3:I:3089[B]:HIS:ND1	3:I:3119[B]:HIS:NE2	2.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3212[A]:ARG:HH11	3:I:3212[A]:ARG:HG3	1.43	0.83
3:O:2956[A]:LYS:C	3:O:2960[A]:PHE:CE1	2.47	0.83
3:O:2979[A]:GLN:CG	3:O:3155[A]:MET:CE	2.56	0.83
3:O:3156[B]:MET:CG	3:X:3173[B]:THR:CG2	2.56	0.83
3:O:3284[B]:LYS:HD3	3:O:3285[B]:VAL:H	1.40	0.83
3:U:2933[B]:SER:CB	3:U:2936[B]:GLU:HB3	2.07	0.83
3:U:3212[A]:ARG:HH11	3:U:3212[A]:ARG:HG3	1.42	0.83
3:X:3216[B]:GLY:HA2	3:X:3262[B]:PHE:O	1.78	0.83
3:a:3173[B]:THR:HG22	3:a:3174[B]:GLY:N	1.93	0.83
3:a:3185[A]:TYR:CE2	3:a:3187[A]:TYR:CE2	2.65	0.83
3:d:2979[A]:GLN:CG	3:d:3155[A]:MET:CE	2.55	0.83
3:C:3284[B]:LYS:HD3	3:C:3285[B]:VAL:H	1.40	0.83
3:F:2948[B]:ASP:N	3:F:2949[B]:LYS:CA	2.41	0.83
3:O:2933[A]:SER:CB	3:O:2936[A]:GLU:HB3	2.07	0.83
3:O:2955[B]:GLN:CD	3:O:3037[B]:TYR:CE1	2.55	0.83
3:O:2969[B]:TYR:HB2	3:X:3158[B]:PHE:CE1	2.13	0.83
3:O:2975[B]:PHE:CE2	3:X:3172[B]:SER:CA	2.60	0.83
3:O:3157[B]:PRO:O	3:X:3150[B]:LYS:N	2.11	0.83
3:O:3157[B]:PRO:C	3:X:3152[B]:LYS:CB	2.50	0.83
3:O:3216[B]:GLY:HA2	3:O:3262[B]:PHE:O	1.78	0.83
3:R:3089[B]:HIS:ND1	3:R:3119[B]:HIS:NE2	2.25	0.83
3:R:3196[B]:THR:H	3:R:3199[B]:GLN:HB2	1.37	0.83
3:U:2956[A]:LYS:C	3:U:2960[A]:PHE:CE1	2.47	0.83
3:U:2965[B]:LEU:CD1	3:d:3220[B]:ARG:CB	2.27	0.83
3:U:3156[B]:MET:HE1	3:d:2982[B]:MET:HG2	1.58	0.83
3:U:3171[B]:HIS:HA	3:d:3152[B]:LYS:NZ	1.93	0.83
3:X:3230[A]:PHE:CB	3:X:3243[A]:GLY:HA2	2.06	0.83
1:Y:1543:ILE:HA	3:d:3001[B]:LYS:HE2	1.58	0.83
3:d:2948[A]:ASP:CB	3:d:2953[A]:GLY:HA3	2.07	0.83
3:C:2969[B]:TYR:O	3:L:2985[B]:PHE:CZ	2.26	0.83
3:C:3222[B]:ILE:N	3:L:2965[B]:LEU:HB2	1.94	0.83
3:C:3230[A]:PHE:CB	3:C:3243[A]:GLY:HA2	2.06	0.83
3:F:2948[B]:ASP:CB	3:F:2953[B]:GLY:HA3	2.07	0.83
1:G:1339:SER:HB3	1:G:1340:GLY:HA2	1.60	0.83
3:I:3230[B]:PHE:CB	3:I:3243[B]:GLY:HA2	2.06	0.83
3:L:3176[B]:LYS:HE2	3:L:3176[B]:LYS:H	1.43	0.83
3:O:2973[B]:THR:CB	3:X:3158[B]:PHE:HE2	1.86	0.83
3:O:3185[A]:TYR:CE2	3:O:3187[A]:TYR:CE2	2.65	0.83
3:U:2965[A]:LEU:HG	3:U:2974[A]:ALA:HB1	1.61	0.83
3:U:2965[B]:LEU:HD11	3:d:3256[B]:TRP:O	1.78	0.83
3:U:2979[B]:GLN:CG	3:U:3155[B]:MET:CE	2.56	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3153[B]:LYS:CE	3:d:2979[B]:GLN:NE2	2.27	0.83
3:U:3255[B]:PRO:CG	3:d:3252[B]:TYR:O	2.12	0.83
1:Y:1078:ARG:NH2	2:c:2877:ILE:O	2.11	0.83
3:a:3089[B]:HIS:HE1	3:a:3119[B]:HIS:CD2	1.96	0.83
3:d:3216[B]:GLY:HA2	3:d:3262[B]:PHE:O	1.78	0.83
3:C:2952[A]:ALA:HA	3:C:2956[A]:LYS:CB	2.06	0.83
3:C:3172[B]:SER:CB	3:L:3152[B]:LYS:N	2.41	0.83
2:E:2545:SER:HA	2:E:2546:LEU:HB2	1.59	0.83
3:I:3298[B]:ASN:HA	3:I:3299[B]:LEU:CB	2.06	0.83
3:O:3162[B]:ASP:OD2	3:X:3150[B]:LYS:CD	2.27	0.83
3:O:3212[A]:ARG:HG3	3:O:3212[A]:ARG:HH11	1.43	0.83
3:R:2948[A]:ASP:N	3:R:2949[A]:LYS:CA	2.41	0.83
3:R:2948[B]:ASP:CB	3:R:2953[B]:GLY:HA3	2.07	0.83
3:R:3230[A]:PHE:CB	3:R:3243[A]:GLY:HA2	2.06	0.83
3:U:2967[B]:CYS:C	3:d:3256[B]:TRP:CB	2.52	0.83
3:U:3089[B]:HIS:ND1	3:U:3119[B]:HIS:NE2	2.25	0.83
2:W:2569:TRP:HD1	2:W:2746:MET:HG2	1.42	0.83
3:X:2952[B]:ALA:HB3	3:X:2953[B]:GLY:O	1.76	0.83
3:d:3089[A]:HIS:HE1	3:d:3119[A]:HIS:CD2	1.96	0.83
3:d:3298[B]:ASN:HA	3:d:3299[B]:LEU:CB	2.06	0.83
3:C:3149[B]:ASN:HB3	3:L:3163[B]:ASN:HD21	1.43	0.83
3:F:2965[B]:LEU:HG	3:F:2974[B]:ALA:HB1	1.61	0.83
3:F:3155[B]:MET:HB2	3:a:3153[B]:LYS:CB	2.08	0.83
3:F:3173[B]:THR:HG22	3:F:3174[B]:GLY:N	1.93	0.83
3:I:2955[A]:GLN:CD	3:I:3037[A]:TYR:CE1	2.55	0.83
3:I:2956[A]:LYS:C	3:I:2960[A]:PHE:CE1	2.47	0.83
3:I:3216[B]:GLY:HA2	3:I:3262[B]:PHE:O	1.78	0.83
3:L:2948[B]:ASP:N	3:L:2949[B]:LYS:CA	2.41	0.83
3:L:2965[A]:LEU:CG	3:L:2974[A]:ALA:HB1	2.09	0.83
3:L:2979[A]:GLN:CG	3:L:3155[A]:MET:CE	2.56	0.83
3:O:3173[B]:THR:HG22	3:O:3174[B]:GLY:N	1.93	0.83
3:O:3272[A]:HIS:CD2	1:P:1542:ARG:NH2	2.46	0.83
3:R:2948[B]:ASP:N	3:R:2949[B]:LYS:CA	2.41	0.83
3:U:3259[B]:ASP:CA	3:d:2968[B]:GLN:HE21	1.92	0.83
3:X:3176[B]:LYS:HE2	3:X:3176[B]:LYS:H	1.43	0.83
3:X:3216[A]:GLY:HA2	3:X:3262[A]:PHE:O	1.78	0.83
3:a:3089[A]:HIS:HE1	3:a:3119[A]:HIS:CD2	1.96	0.83
3:a:3284[B]:LYS:HD3	3:a:3285[B]:VAL:H	1.39	0.83
3:d:3173[A]:THR:HG22	3:d:3174[A]:GLY:N	1.93	0.83
3:d:3173[B]:THR:HG22	3:d:3174[B]:GLY:N	1.93	0.83
3:d:3284[B]:LYS:HD3	3:d:3285[B]:VAL:H	1.39	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3153[B]:LYS:NZ	3:L:2988[B]:TRP:NE1	2.27	0.83
3:F:3212[B]:ARG:HH11	3:F:3212[B]:ARG:HG3	1.43	0.83
3:F:3293[A]:LYS:CD	3:F:3294[A]:SER:CB	2.53	0.83
3:L:3216[B]:GLY:HA2	3:L:3262[B]:PHE:O	1.78	0.83
3:O:2965[B]:LEU:H	3:X:3254[B]:MET:HE3	1.41	0.83
3:O:2970[B]:PRO:C	3:X:2988[B]:TRP:C	2.40	0.83
3:O:3157[B]:PRO:C	3:X:3152[B]:LYS:HB2	1.89	0.83
3:O:3253[B]:GLU:CG	3:X:3161[B]:GLU:OE2	2.25	0.83
3:R:2965[B]:LEU:HG	3:R:2974[B]:ALA:HB1	1.61	0.83
3:U:2975[B]:PHE:CE1	3:d:3256[B]:TRP:CD1	2.65	0.83
3:U:3089[A]:HIS:ND1	3:U:3119[A]:HIS:NE2	2.25	0.83
3:U:3155[B]:MET:O	3:d:3149[B]:ASN:HB2	1.76	0.83
3:X:2951[A]:ASP:OD2	3:X:2953[A]:GLY:HA2	1.79	0.83
3:d:2948[A]:ASP:N	3:d:2949[A]:LYS:CA	2.41	0.83
3:d:2955[B]:GLN:CD	3:d:3037[B]:TYR:CE1	2.55	0.83
3:C:2951[A]:ASP:OD2	3:C:2953[A]:GLY:HA2	1.79	0.83
3:C:2965[A]:LEU:CG	3:C:2974[A]:ALA:HB1	2.09	0.83
3:C:3155[B]:MET:SD	3:L:3154[B]:PRO:CD	2.66	0.83
3:F:2965[A]:LEU:CG	3:F:2974[A]:ALA:HB1	2.09	0.83
3:F:3228[A]:VAL:HG21	3:F:3245[A]:PHE:CE2	2.14	0.83
3:F:3253[B]:GLU:HA	3:a:3252[B]:TYR:O	1.78	0.83
3:I:3089[A]:HIS:HE1	3:I:3119[A]:HIS:CD2	1.96	0.83
3:L:2933[A]:SER:CB	3:L:2936[A]:GLU:HB3	2.07	0.83
3:L:3089[A]:HIS:HE1	3:L:3119[A]:HIS:CD2	1.96	0.83
3:R:3284[B]:LYS:HD3	3:R:3285[B]:VAL:H	1.39	0.83
3:a:2965[A]:LEU:CG	3:a:2974[A]:ALA:HB1	2.09	0.83
3:a:3024[A]:LEU:CD1	3:a:3025[A]:VAL:H	1.83	0.83
3:a:3176[A]:LYS:HE2	3:a:3176[A]:LYS:H	1.43	0.83
3:d:2965[A]:LEU:CG	3:d:2974[A]:ALA:HB1	2.09	0.83
3:d:3212[A]:ARG:HH11	3:d:3212[A]:ARG:HG3	1.43	0.83
3:C:3089[B]:HIS:HE1	3:C:3119[B]:HIS:CD2	1.96	0.83
3:C:3156[B]:MET:HE3	3:L:2979[B]:GLN:HG3	1.53	0.83
3:C:3212[B]:ARG:HH11	3:C:3212[B]:ARG:HG3	1.43	0.83
3:C:3298[A]:ASN:HA	3:C:3299[A]:LEU:CB	2.06	0.83
3:F:2971[B]:ASP:O	3:a:3090[B]:ASN:HB3	1.79	0.83
3:F:3089[B]:HIS:HE1	3:F:3119[B]:HIS:CD2	1.96	0.83
3:F:3107[B]:LEU:HD11	3:a:2975[B]:PHE:HD1	0.75	0.83
3:F:3176[B]:LYS:H	3:F:3176[B]:LYS:HE2	1.43	0.83
3:F:3253[B]:GLU:CB	3:a:2975[B]:PHE:C	2.50	0.83
3:I:2979[A]:GLN:CG	3:I:3155[A]:MET:CE	2.56	0.83
3:I:2989[B]:HIS:CE1	3:R:2969[B]:TYR:CA	2.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3089[B]:HIS:HE1	3:I:3119[B]:HIS:CD2	1.96	0.83
3:I:3161[B]:GLU:HG2	3:R:3079[B]:CYS:HA	1.60	0.83
3:O:2952[B]:ALA:HA	3:O:2956[B]:LYS:CB	2.06	0.83
3:O:2965[B]:LEU:HD11	3:O:2974[B]:ALA:HA	1.57	0.83
3:O:2975[B]:PHE:CE2	3:X:3172[B]:SER:HB3	2.14	0.83
3:O:3251[B]:ASP:HB2	3:X:2968[B]:GLN:CD	2.04	0.83
3:R:3185[A]:TYR:CE2	3:R:3187[A]:TYR:CE2	2.65	0.83
1:S:589:GLN:HG2	1:S:594:ASP:HB3	1.60	0.83
3:U:2965[A]:LEU:CG	3:U:2974[A]:ALA:HB1	2.09	0.83
3:U:3176[B]:LYS:HE2	3:U:3176[B]:LYS:H	1.43	0.83
3:U:3216[B]:GLY:HA2	3:U:3262[B]:PHE:O	1.78	0.83
3:U:3259[B]:ASP:CG	3:U:3260[B]:ARG:HG2	2.04	0.83
3:U:3265[A]:ASP:OD1	3:U:3267[A]:SER:OG	1.97	0.83
1:Y:1365:TYR:HD1	1:Y:1372:ILE:HG22	1.44	0.83
1:Y:1546:LYS:CB	3:d:3001[B]:LYS:HZ1	1.83	0.83
3:a:2965[B]:LEU:HG	3:a:2974[B]:ALA:HB1	1.61	0.83
3:d:3176[B]:LYS:HE2	3:d:3176[B]:LYS:H	1.43	0.83
3:d:3265[B]:ASP:OD1	3:d:3267[B]:SER:OG	1.97	0.83
6:GA:2:NAG:C6	6:GA:3:BMA:C1	2.57	0.83
3:C:2964[B]:PRO:C	3:L:3255[B]:PRO:HB3	2.04	0.83
3:C:3149[B]:ASN:HB2	3:L:3163[B]:ASN:ND2	1.93	0.83
3:F:2979[B]:GLN:CG	3:F:3155[B]:MET:CE	2.56	0.83
3:F:3152[B]:LYS:HD2	3:a:3170[B]:ALA:O	0.88	0.83
3:F:3265[B]:ASP:OD1	3:F:3267[B]:SER:OG	1.97	0.83
3:I:2966[B]:SER:HB3	3:R:2982[B]:MET:CE	2.08	0.83
3:I:3259[B]:ASP:CG	3:I:3260[B]:ARG:HG2	2.04	0.83
3:L:2956[A]:LYS:O	3:L:2960[A]:PHE:HE1	1.22	0.83
3:L:2965[A]:LEU:HG	3:L:2974[A]:ALA:HB1	1.61	0.83
3:O:3089[A]:HIS:ND1	3:O:3119[A]:HIS:NE2	2.25	0.83
3:R:3217[B]:PHE:HZ	3:R:3230[B]:PHE:CE1	1.89	0.83
3:R:3259[B]:ASP:CG	3:R:3260[B]:ARG:HG2	2.04	0.83
1:S:423:ARG:NH1	1:S:500:ASN:OD1	2.12	0.83
3:U:2972[B]:GLY:C	3:d:3247[B]:VAL:HG13	2.01	0.83
3:U:2975[B]:PHE:CD1	3:d:3256[B]:TRP:NE1	2.45	0.83
3:U:3120[A]:HIS:HA	3:U:3123[A]:THR:OG1	1.79	0.83
3:X:2965[A]:LEU:CG	3:X:2974[A]:ALA:HB1	2.09	0.83
1:Y:1656:ASP:H	3:d:3006[B]:LYS:HB2	1.43	0.83
2:c:2661:MET:HB3	2:c:2798:GLN:HE22	1.43	0.83
3:d:3298[B]:ASN:HB3	3:d:3300[B]:LEU:CD2	2.09	0.83
3:C:2965[A]:LEU:HG	3:C:2974[A]:ALA:HB1	1.61	0.83
3:C:2965[B]:LEU:HG	3:C:2974[B]:ALA:HB1	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3216[B]:GLY:HA2	3:C:3262[B]:PHE:O	1.78	0.83
3:C:3222[B]:ILE:H	3:L:2965[B]:LEU:HB2	1.44	0.83
3:F:3253[B]:GLU:OE1	3:a:2974[B]:ALA:CB	2.19	0.83
3:I:2965[A]:LEU:HG	3:I:2974[A]:ALA:HB1	1.61	0.83
3:I:3259[A]:ASP:CG	3:I:3260[A]:ARG:HG2	2.04	0.83
3:L:3176[A]:LYS:HE2	3:L:3176[A]:LYS:H	1.43	0.83
3:O:3265[A]:ASP:OD1	3:O:3267[A]:SER:OG	1.97	0.83
2:Q:2867:PRO:HG2	3:R:2932[A]:PRO:HG2	1.58	0.83
3:R:2965[A]:LEU:HG	3:R:2974[A]:ALA:HB1	1.61	0.83
3:R:3120[A]:HIS:HA	3:R:3123[A]:THR:OG1	1.79	0.83
3:U:2933[A]:SER:CB	3:U:2936[A]:GLU:HB3	2.07	0.83
3:U:3176[A]:LYS:HE2	3:U:3176[A]:LYS:H	1.43	0.83
3:X:2965[A]:LEU:HG	3:X:2974[A]:ALA:HB1	1.61	0.83
3:X:3284[A]:LYS:HD3	3:X:3285[A]:VAL:H	1.39	0.83
3:a:2955[B]:GLN:CD	3:a:3037[B]:TYR:CE1	2.55	0.83
3:a:2956[B]:LYS:O	3:a:2960[B]:PHE:HE1	1.22	0.83
3:a:3196[A]:THR:CG2	1:b:416:ASN:CG	2.47	0.83
3:d:2951[B]:ASP:OD2	3:d:2953[B]:GLY:HA2	1.79	0.83
3:d:2965[A]:LEU:HG	3:d:2974[A]:ALA:HB1	1.61	0.83
8:0:1:NAG:C6	8:0:2:NAG:HN2	1.92	0.83
3:C:3120[B]:HIS:HA	3:C:3123[B]:THR:OG1	1.79	0.82
3:C:3172[B]:SER:HB2	3:L:3152[B]:LYS:H	1.42	0.82
2:E:2625:LEU:HG	2:E:2626:ARG:HG2	1.60	0.82
3:F:2966[B]:SER:CB	3:a:3255[B]:PRO:O	2.27	0.82
3:F:3160[B]:SER:HB3	3:a:3150[B]:LYS:HZ3	0.76	0.82
3:F:3183[B]:LEU:H	3:F:3184[B]:ASN:HA	1.44	0.82
3:F:3228[B]:VAL:HG21	3:F:3245[B]:PHE:CE2	2.14	0.82
3:F:3255[B]:PRO:HG3	3:a:2964[B]:PRO:N	1.94	0.82
3:I:2948[A]:ASP:N	3:I:2949[A]:LYS:HA	1.81	0.82
3:I:2965[B]:LEU:HG	3:I:2974[B]:ALA:HB1	1.61	0.82
3:I:3212[B]:ARG:HG3	3:I:3212[B]:ARG:HH11	1.43	0.82
3:I:3293[A]:LYS:CD	3:I:3294[A]:SER:CB	2.53	0.82
3:L:3173[A]:THR:HG22	3:L:3174[A]:GLY:N	1.93	0.82
3:L:3228[A]:VAL:HG21	3:L:3245[A]:PHE:CE2	2.14	0.82
3:O:2965[A]:LEU:HG	3:O:2974[A]:ALA:HB1	1.61	0.82
3:O:3089[A]:HIS:HE1	3:O:3119[A]:HIS:CD2	1.96	0.82
3:R:2965[A]:LEU:CG	3:R:2974[A]:ALA:HB1	2.09	0.82
3:R:2965[B]:LEU:CG	3:R:2974[B]:ALA:HB1	2.09	0.82
3:R:3024[A]:LEU:CD1	3:R:3025[A]:VAL:H	1.84	0.82
3:R:3259[A]:ASP:CG	3:R:3260[A]:ARG:HG2	2.04	0.82
3:R:3293[A]:LYS:CD	3:R:3294[A]:SER:CB	2.53	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3196[A]:THR:H	3:U:3199[A]:GLN:HB2	1.37	0.82
3:U:3228[B]:VAL:HG21	3:U:3245[B]:PHE:CE2	2.14	0.82
2:W:2808:PHE:HZ	2:W:2821:LEU:HD13	1.43	0.82
3:X:2952[A]:ALA:HB3	3:X:2953[A]:GLY:CA	2.09	0.82
3:X:3183[A]:LEU:H	3:X:3184[A]:ASN:HA	1.44	0.82
3:X:3230[B]:PHE:CB	3:X:3243[B]:GLY:HA2	2.06	0.82
3:X:3259[A]:ASP:CG	3:X:3260[A]:ARG:HG2	2.04	0.82
3:a:3173[A]:THR:HG22	3:a:3174[A]:GLY:N	1.93	0.82
2:B:2877:ILE:H	1:D:1078:ARG:HH12	1.21	0.82
3:C:2951[B]:ASP:OD2	3:C:2953[B]:GLY:HA2	1.79	0.82
3:F:3216[B]:GLY:HA2	3:F:3262[B]:PHE:O	1.78	0.82
3:F:3259[A]:ASP:CG	3:F:3260[A]:ARG:HG2	2.04	0.82
1:J:497:GLN:HG2	1:J:683:THR:HG21	1.59	0.82
3:O:2952[B]:ALA:HB3	3:O:2953[B]:GLY:CA	2.10	0.82
3:O:2975[B]:PHE:HE2	3:X:3172[B]:SER:HA	1.44	0.82
3:O:3230[B]:PHE:CB	3:O:3243[B]:GLY:HA2	2.06	0.82
3:O:3259[A]:ASP:CG	3:O:3260[A]:ARG:HG2	2.04	0.82
1:P:497:GLN:HG2	1:P:683:THR:HG21	1.61	0.82
3:R:2933[B]:SER:CB	3:R:2936[B]:GLU:HB3	2.07	0.82
3:R:2955[B]:GLN:CD	3:R:3037[B]:TYR:CE1	2.55	0.82
3:U:3183[A]:LEU:H	3:U:3184[A]:ASN:HA	1.44	0.82
3:U:3183[B]:LEU:H	3:U:3184[B]:ASN:HA	1.44	0.82
3:X:3228[A]:VAL:HG21	3:X:3245[A]:PHE:CE2	2.14	0.82
3:d:2965[B]:LEU:HG	3:d:2974[B]:ALA:HB1	1.61	0.82
3:d:3183[B]:LEU:H	3:d:3184[B]:ASN:HA	1.44	0.82
3:d:3230[B]:PHE:CB	3:d:3243[B]:GLY:HA2	2.06	0.82
3:C:3089[A]:HIS:HE1	3:C:3119[A]:HIS:CD2	1.96	0.82
3:C:3147[B]:GLU:HG2	3:L:3161[B]:GLU:HA	0.83	0.82
3:C:3153[B]:LYS:CE	3:L:3158[B]:PHE:HD2	1.57	0.82
3:C:3183[A]:LEU:H	3:C:3184[A]:ASN:HA	1.44	0.82
3:F:2951[A]:ASP:OD2	3:F:2953[A]:GLY:HA2	1.79	0.82
3:F:2965[B]:LEU:CG	3:F:2974[B]:ALA:HB1	2.09	0.82
3:F:2968[B]:GLN:CG	3:a:2981[B]:GLY:H	1.92	0.82
3:F:3163[B]:ASN:HB3	3:a:3150[B]:LYS:CE	2.09	0.82
3:F:3259[B]:ASP:CG	3:F:3260[B]:ARG:HG2	2.04	0.82
3:I:2951[A]:ASP:OD2	3:I:2953[A]:GLY:HA2	1.79	0.82
3:I:3120[B]:HIS:HA	3:I:3123[B]:THR:OG1	1.79	0.82
3:L:2965[B]:LEU:CG	3:L:2974[B]:ALA:HB1	2.09	0.82
3:L:3023[A]:ILE:O	3:L:3026[A]:THR:N	2.11	0.82
3:L:3259[B]:ASP:CG	3:L:3260[B]:ARG:HG2	2.04	0.82
3:O:2951[A]:ASP:OD2	3:O:2953[A]:GLY:HA2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3120[A]:HIS:HA	3:O:3123[A]:THR:OG1	1.79	0.82
3:O:3216[A]:GLY:HA2	3:O:3262[A]:PHE:O	1.78	0.82
3:O:3217[B]:PHE:HZ	3:O:3230[B]:PHE:CE1	1.89	0.82
1:P:1584:GLY:HA3	1:S:329:ARG:HG2	1.61	0.82
3:R:3228[B]:VAL:HG21	3:R:3245[B]:PHE:CE2	2.14	0.82
3:R:3265[B]:ASP:OD1	3:R:3267[B]:SER:OG	1.97	0.82
3:R:3298[A]:ASN:HB3	3:R:3300[A]:LEU:CD2	2.09	0.82
3:U:2948[A]:ASP:N	3:U:2949[A]:LYS:HA	1.81	0.82
3:U:2956[B]:LYS:O	3:U:2960[B]:PHE:HE1	1.22	0.82
3:U:3089[B]:HIS:HE1	3:U:3119[B]:HIS:CD2	1.96	0.82
3:U:3298[A]:ASN:HB3	3:U:3300[A]:LEU:CD2	2.09	0.82
3:X:2989[B]:HIS:O	3:X:2992[B]:TYR:N	2.08	0.82
3:X:3173[B]:THR:HG22	3:X:3174[B]:GLY:N	1.93	0.82
3:a:2951[B]:ASP:OD2	3:a:2953[B]:GLY:HA2	1.79	0.82
3:a:3259[B]:ASP:CG	3:a:3260[B]:ARG:HG2	2.04	0.82
3:d:2956[A]:LYS:O	3:d:2960[A]:PHE:HE1	1.22	0.82
1:A:497:GLN:HG2	1:A:683:THR:HG21	1.58	0.82
3:C:3153[B]:LYS:C	3:L:3173[B]:THR:HA	1.95	0.82
3:C:3223[B]:GLY:O	3:L:3252[B]:TYR:CD1	2.33	0.82
3:C:3252[B]:TYR:HB2	3:L:3253[B]:GLU:HG2	1.61	0.82
3:F:2965[A]:LEU:HG	3:F:2974[A]:ALA:HB1	1.61	0.82
3:F:3120[A]:HIS:HA	3:F:3123[A]:THR:OG1	1.79	0.82
3:F:3189[A]:ASN:CG	3:F:3191[A]:ASN:HD21	1.87	0.82
3:F:3216[A]:GLY:HA2	3:F:3262[A]:PHE:O	1.78	0.82
3:I:2969[B]:TYR:HA	3:R:2989[B]:HIS:CE1	2.14	0.82
3:I:3189[A]:ASN:CG	3:I:3191[A]:ASN:HD21	1.87	0.82
3:I:3228[B]:VAL:HG21	3:I:3245[B]:PHE:CE2	2.14	0.82
3:L:2965[B]:LEU:HG	3:L:2974[B]:ALA:HB1	1.61	0.82
3:L:3298[B]:ASN:HB3	3:L:3300[B]:LEU:CD2	2.09	0.82
3:O:2965[B]:LEU:CG	3:O:2974[B]:ALA:HB1	2.09	0.82
3:O:2969[B]:TYR:HB2	3:X:3158[B]:PHE:CD1	2.13	0.82
3:O:3298[B]:ASN:HB3	3:O:3300[B]:LEU:CD2	2.09	0.82
3:R:2951[B]:ASP:OD2	3:R:2953[B]:GLY:HA2	1.79	0.82
1:S:1498:ASN:OD1	5:AA:1:NAG:H82	1.79	0.82
3:U:3089[A]:HIS:HE1	3:U:3119[A]:HIS:CD2	1.96	0.82
3:X:3189[B]:ASN:CG	3:X:3191[B]:ASN:HD21	1.87	0.82
3:X:3298[A]:ASN:HB3	3:X:3300[A]:LEU:CD2	2.10	0.82
3:a:3120[B]:HIS:HA	3:a:3123[B]:THR:OG1	1.79	0.82
3:a:3183[B]:LEU:H	3:a:3184[B]:ASN:HA	1.44	0.82
3:d:3189[A]:ASN:CG	3:d:3191[A]:ASN:HD21	1.87	0.82
3:d:3228[A]:VAL:HG21	3:d:3245[A]:PHE:CE2	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:NA:1:NAG:H61	6:NA:2:NAG:HN2	1.44	0.82
3:C:2982[B]:MET:HB2	3:L:3156[B]:MET:HB3	1.59	0.82
3:C:3162[B]:ASP:CG	3:L:3259[B]:ASP:OD2	2.16	0.82
2:E:2161:GLN:OE1	2:E:2345:ASN:ND2	2.13	0.82
3:F:2951[B]:ASP:OD2	3:F:2953[B]:GLY:HA2	1.79	0.82
3:F:2992[B]:TYR:CE2	3:a:2969[B]:TYR:HE1	1.96	0.82
3:F:3284[B]:LYS:HD3	3:F:3285[B]:VAL:H	1.39	0.82
3:I:2965[A]:LEU:CG	3:I:2974[A]:ALA:HB1	2.09	0.82
3:I:2965[B]:LEU:CG	3:I:2974[B]:ALA:HB1	2.09	0.82
3:I:2966[B]:SER:CA	3:R:3256[B]:TRP:HB3	2.08	0.82
3:I:2989[B]:HIS:NE2	3:R:2970[B]:PRO:CD	2.39	0.82
3:I:3093[B]:HIS:HD2	3:R:2973[B]:THR:OG1	1.62	0.82
3:I:3173[A]:THR:HG22	3:I:3174[A]:GLY:N	1.93	0.82
3:L:2951[B]:ASP:OD2	3:L:2953[B]:GLY:HA2	1.79	0.82
3:L:2956[B]:LYS:O	3:L:2960[B]:PHE:HE1	1.22	0.82
3:L:3216[A]:GLY:HA2	3:L:3262[A]:PHE:O	1.78	0.82
3:L:3265[B]:ASP:OD1	3:L:3267[B]:SER:OG	1.97	0.82
3:O:3212[B]:ARG:HH11	3:O:3212[B]:ARG:HG3	1.43	0.82
3:R:3176[A]:LYS:HE2	3:R:3176[A]:LYS:H	1.43	0.82
3:U:2952[B]:ALA:HB3	3:U:2953[B]:GLY:CA	2.10	0.82
3:U:3120[B]:HIS:HA	3:U:3123[B]:THR:OG1	1.79	0.82
3:a:3228[A]:VAL:HG21	3:a:3245[A]:PHE:CE2	2.14	0.82
3:a:3265[A]:ASP:OD1	3:a:3267[A]:SER:OG	1.97	0.82
3:d:3089[B]:HIS:HE1	3:d:3119[B]:HIS:CD2	1.96	0.82
3:d:3228[B]:VAL:HG21	3:d:3245[B]:PHE:CE2	2.14	0.82
3:C:2952[B]:ALA:HB3	3:C:2953[B]:GLY:CA	2.10	0.82
3:F:2965[B]:LEU:HD12	3:a:3256[B]:TRP:NE1	1.94	0.82
3:F:3154[B]:PRO:HD3	3:a:3173[B]:THR:C	2.05	0.82
3:F:3251[B]:ASP:HB2	3:a:3251[B]:ASP:HB3	1.54	0.82
3:I:2965[B]:LEU:CD2	3:I:2974[B]:ALA:HB1	2.10	0.82
3:I:2983[B]:VAL:HG23	3:R:3160[B]:SER:OG	1.78	0.82
3:L:3173[B]:THR:HG22	3:L:3174[B]:GLY:N	1.93	0.82
3:O:2951[B]:ASP:OD2	3:O:2953[B]:GLY:HA2	1.79	0.82
3:O:2965[A]:LEU:CG	3:O:2974[A]:ALA:HB1	2.09	0.82
3:O:3120[B]:HIS:HA	3:O:3123[B]:THR:OG1	1.79	0.82
3:O:3173[A]:THR:HG22	3:O:3174[A]:GLY:N	1.93	0.82
3:O:3253[B]:GLU:HG3	3:X:3160[B]:SER:CA	2.08	0.82
3:U:3173[B]:THR:HG22	3:U:3174[B]:GLY:N	1.93	0.82
3:X:2951[B]:ASP:OD2	3:X:2953[B]:GLY:HA2	1.79	0.82
2:Z:2867:PRO:HG2	3:a:2932[A]:PRO:HG2	0.83	0.82
3:a:2965[B]:LEU:CG	3:a:2974[B]:ALA:HB1	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2951[A]:ASP:OD2	3:d:2953[A]:GLY:HA2	1.79	0.82
3:d:3183[A]:LEU:H	3:d:3184[A]:ASN:HA	1.44	0.82
3:C:2952[A]:ALA:HB3	3:C:2953[A]:GLY:CA	2.10	0.82
3:C:2956[B]:LYS:O	3:C:2960[B]:PHE:CD1	2.33	0.82
3:C:3172[B]:SER:CB	3:L:3149[B]:ASN:O	2.27	0.82
3:C:3173[B]:THR:HG22	3:C:3174[B]:GLY:N	1.93	0.82
3:C:3216[A]:GLY:HA2	3:C:3262[A]:PHE:O	1.78	0.82
3:C:3259[B]:ASP:CG	3:C:3260[B]:ARG:HG2	2.04	0.82
3:C:3265[B]:ASP:OD1	3:C:3267[B]:SER:OG	1.97	0.82
3:F:3089[A]:HIS:HE1	3:F:3119[A]:HIS:CD2	1.96	0.82
3:F:3189[B]:ASN:CG	3:F:3191[B]:ASN:HD21	1.88	0.82
3:I:2979[B]:GLN:C	3:R:2967[B]:CYS:HB3	1.96	0.82
3:I:3153[B]:LYS:CG	3:R:3155[B]:MET:CB	2.55	0.82
3:I:3189[B]:ASN:CG	3:I:3191[B]:ASN:HD21	1.87	0.82
3:I:3248[B]:LEU:CD1	3:R:2973[B]:THR:HG23	2.06	0.82
3:L:3120[B]:HIS:HA	3:L:3123[B]:THR:OG1	1.79	0.82
3:O:2965[B]:LEU:HB3	3:X:3254[B]:MET:CE	2.02	0.82
3:O:2965[B]:LEU:CD2	3:O:2974[B]:ALA:HB1	2.10	0.82
3:O:3023[B]:ILE:O	3:O:3026[B]:THR:N	2.11	0.82
3:O:3228[B]:VAL:HG21	3:O:3245[B]:PHE:CE2	2.14	0.82
3:R:3173[B]:THR:HG22	3:R:3174[B]:GLY:N	1.93	0.82
3:U:2951[B]:ASP:OD2	3:U:2953[B]:GLY:HA2	1.79	0.82
3:U:3259[A]:ASP:CG	3:U:3260[A]:ARG:HG2	2.04	0.82
3:X:2965[B]:LEU:CG	3:X:2974[B]:ALA:HB1	2.09	0.82
1:Y:1576:THR:HG22	3:d:3196[B]:THR:CG2	2.10	0.82
1:Y:1655:SER:O	3:d:3006[B]:LYS:NZ	2.13	0.82
3:a:3120[A]:HIS:HA	3:a:3123[A]:THR:OG1	1.79	0.82
3:a:3216[B]:GLY:HA2	3:a:3262[B]:PHE:O	1.78	0.82
3:d:2955[A]:GLN:CD	3:d:3037[A]:TYR:CE1	2.55	0.82
3:d:3023[B]:ILE:O	3:d:3026[B]:THR:N	2.11	0.82
3:F:2952[A]:ALA:HB3	3:F:2953[A]:GLY:CA	2.10	0.82
3:I:2956[A]:LYS:O	3:I:2960[A]:PHE:CD1	2.33	0.82
3:L:3228[B]:VAL:HG21	3:L:3245[B]:PHE:CE2	2.14	0.82
3:O:2965[B]:LEU:H	3:X:3254[B]:MET:CE	1.92	0.82
3:R:3216[A]:GLY:HA2	3:R:3262[A]:PHE:O	1.78	0.82
1:S:979:LEU:HB3	1:S:980:TYR:HA	1.61	0.82
3:U:2951[A]:ASP:OD2	3:U:2953[A]:GLY:HA2	1.79	0.82
3:d:3216[A]:GLY:HA2	3:d:3262[A]:PHE:O	1.78	0.82
1:A:883:CYS:N	1:A:894:CYS:SG	2.53	0.82
3:C:2965[B]:LEU:CG	3:C:2974[B]:ALA:HB1	2.09	0.82
3:C:3196[A]:THR:H	3:C:3199[A]:GLN:HB2	1.37	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3212[A]:ARG:HG3	3:C:3212[A]:ARG:HH11	1.43	0.82
3:C:3228[B]:VAL:HG21	3:C:3245[B]:PHE:CE2	2.14	0.82
3:C:3265[A]:ASP:OD1	3:C:3267[A]:SER:OG	1.97	0.82
3:C:3298[B]:ASN:HB3	3:C:3300[B]:LEU:CD2	2.09	0.82
3:F:3154[B]:PRO:HG3	3:a:3174[B]:GLY:HA2	1.62	0.82
3:I:2952[B]:ALA:HB3	3:I:2953[B]:GLY:CA	2.10	0.82
3:I:2966[B]:SER:O	3:R:3256[B]:TRP:HB3	1.80	0.82
3:L:3027[A]:GLU:OE2	3:L:3028[A]:PRO:HD2	1.80	0.82
3:O:3027[A]:GLU:OE2	3:O:3028[A]:PRO:HD2	1.80	0.82
3:O:3183[A]:LEU:H	3:O:3184[A]:ASN:HA	1.44	0.82
3:R:2951[A]:ASP:OD2	3:R:2953[A]:GLY:HA2	1.79	0.82
3:R:3298[B]:ASN:HB3	3:R:3300[B]:LEU:CD2	2.09	0.82
3:U:3104[A]:MET:CA	3:U:3110[A]:THR:HG23	2.10	0.82
3:X:3089[A]:HIS:HE1	3:X:3119[A]:HIS:CD2	1.96	0.82
3:a:2956[A]:LYS:O	3:a:2960[A]:PHE:CD1	2.33	0.82
3:d:2952[B]:ALA:HB3	3:d:2953[B]:GLY:CA	2.10	0.82
3:d:3259[A]:ASP:CG	3:d:3260[A]:ARG:HG2	2.04	0.82
3:C:2956[B]:LYS:O	3:C:2960[B]:PHE:HE1	1.22	0.82
3:C:3161[B]:GLU:OE2	3:L:2983[B]:VAL:CB	2.04	0.82
3:C:3173[A]:THR:HG22	3:C:3174[A]:GLY:N	1.93	0.82
3:C:3223[B]:GLY:O	3:L:3252[B]:TYR:CE2	2.33	0.82
3:C:3259[A]:ASP:CG	3:C:3260[A]:ARG:HG2	2.04	0.82
3:F:2972[B]:GLY:HA3	3:a:3090[B]:ASN:CB	2.08	0.82
3:I:2967[B]:CYS:SG	3:R:2982[B]:MET:CE	2.67	0.82
3:I:2968[B]:GLN:NE2	3:R:3086[B]:GLU:CG	1.86	0.82
3:I:2985[B]:PHE:CZ	3:R:2970[B]:PRO:HA	2.15	0.82
3:I:3173[B]:THR:HG22	3:I:3174[B]:GLY:N	1.93	0.82
3:I:3265[A]:ASP:OD1	3:I:3267[A]:SER:OG	1.97	0.82
3:L:3189[A]:ASN:CG	3:L:3191[A]:ASN:HD21	1.87	0.82
2:N:2868:GLU:OE2	3:O:2932[A]:PRO:C	2.15	0.82
3:O:2965[A]:LEU:CD2	3:O:2974[A]:ALA:HB1	2.10	0.82
3:O:3154[B]:PRO:HD2	3:X:3176[B]:LYS:HE3	1.61	0.82
3:O:3183[B]:LEU:H	3:O:3184[B]:ASN:HA	1.44	0.82
3:O:3189[B]:ASN:CG	3:O:3191[B]:ASN:HD21	1.87	0.82
3:U:2956[B]:LYS:O	3:U:2960[B]:PHE:CD1	2.33	0.82
3:U:3150[B]:LYS:O	3:d:3153[B]:LYS:HG2	1.80	0.82
3:U:3189[A]:ASN:CG	3:U:3191[A]:ASN:HD21	1.87	0.82
3:X:2956[B]:LYS:O	3:X:2960[B]:PHE:CD1	2.33	0.82
3:X:3298[B]:ASN:HB3	3:X:3300[B]:LEU:CD2	2.10	0.82
3:d:2948[B]:ASP:N	3:d:2949[B]:LYS:CA	2.41	0.82
3:d:3259[B]:ASP:CG	3:d:3260[B]:ARG:HG2	2.04	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3158[B]:PHE:O	3:L:3149[B]:ASN:HB2	1.80	0.81
3:C:3230[B]:PHE:CB	3:C:3243[B]:GLY:HA2	2.06	0.81
3:I:2965[A]:LEU:CD2	3:I:2974[A]:ALA:HB1	2.10	0.81
3:I:2979[B]:GLN:CG	3:I:3155[B]:MET:CE	2.56	0.81
3:I:3027[B]:GLU:OE2	3:I:3028[B]:PRO:HD2	1.80	0.81
2:K:2409:ALA:HB2	2:K:2468:ILE:HD12	1.59	0.81
3:L:2948[A]:ASP:N	3:L:2949[A]:LYS:CA	2.41	0.81
3:L:2965[B]:LEU:CD2	3:L:2974[B]:ALA:HB1	2.10	0.81
3:O:3255[B]:PRO:HB3	3:X:3161[B]:GLU:O	1.79	0.81
3:O:3298[A]:ASN:HB3	3:O:3300[A]:LEU:CD2	2.09	0.81
3:R:3023[A]:ILE:O	3:R:3026[A]:THR:N	2.11	0.81
3:U:2955[A]:GLN:CD	3:U:3037[A]:TYR:CE1	2.55	0.81
3:U:2956[A]:LYS:O	3:U:2960[A]:PHE:CD1	2.33	0.81
3:U:3254[B]:MET:HE2	3:d:3254[B]:MET:HE3	1.55	0.81
3:U:3298[B]:ASN:HB3	3:U:3300[B]:LEU:CD2	2.09	0.81
2:W:2556:TYR:HE1	2:W:2845:PRO:HD2	1.44	0.81
3:X:3183[B]:LEU:H	3:X:3184[B]:ASN:HA	1.44	0.81
3:X:3228[B]:VAL:HG21	3:X:3245[B]:PHE:CE2	2.14	0.81
3:a:2948[B]:ASP:N	3:a:2949[B]:LYS:CA	2.41	0.81
3:a:2955[A]:GLN:CD	3:a:3037[A]:TYR:CE1	2.55	0.81
3:a:2965[A]:LEU:HG	3:a:2974[A]:ALA:HB1	1.61	0.81
3:a:3216[A]:GLY:HA2	3:a:3262[A]:PHE:O	1.78	0.81
3:a:3293[B]:LYS:CD	3:a:3294[B]:SER:CB	2.53	0.81
3:d:2965[B]:LEU:CG	3:d:2974[B]:ALA:HB1	2.09	0.81
3:C:3104[A]:MET:CA	3:C:3110[A]:THR:HG23	2.10	0.81
3:F:3120[B]:HIS:HA	3:F:3123[B]:THR:OG1	1.79	0.81
3:F:3147[B]:GLU:CD	3:a:3163[B]:ASN:N	2.36	0.81
3:I:3255[B]:PRO:HG3	3:R:2964[B]:PRO:N	1.95	0.81
3:I:3298[B]:ASN:HB3	3:I:3300[B]:LEU:CD2	2.09	0.81
3:R:2956[B]:LYS:O	3:R:2960[B]:PHE:CD1	2.33	0.81
3:R:2979[B]:GLN:CG	3:R:3155[B]:MET:CE	2.56	0.81
3:U:2963[B]:MET:N	3:U:3108[B]:HIS:O	2.13	0.81
3:U:3173[B]:THR:CG2	3:d:3152[B]:LYS:C	2.49	0.81
3:X:2965[B]:LEU:HG	3:X:2974[B]:ALA:HB1	1.61	0.81
3:a:2939[B]:ARG:HB3	3:a:3032[B]:PRO:HG2	1.63	0.81
3:a:2952[B]:ALA:HB3	3:a:2953[B]:GLY:CA	2.10	0.81
3:a:3189[B]:ASN:CG	3:a:3191[B]:ASN:HD21	1.87	0.81
3:a:3259[A]:ASP:CG	3:a:3260[A]:ARG:HG2	2.04	0.81
3:d:3104[B]:MET:CA	3:d:3110[B]:THR:HG23	2.10	0.81
3:d:3189[B]:ASN:CG	3:d:3191[B]:ASN:HD21	1.87	0.81
3:d:3212[B]:ARG:HG3	3:d:3212[B]:ARG:HH11	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2974[B]:ALA:HB3	3:L:3249[B]:GLY:HA2	0.81	0.81
3:C:2979[B]:GLN:CG	3:C:3155[B]:MET:CE	2.56	0.81
3:C:3027[B]:GLU:OE2	3:C:3028[B]:PRO:HD2	1.80	0.81
3:C:3120[A]:HIS:HA	3:C:3123[A]:THR:OG1	1.79	0.81
3:C:3149[B]:ASN:O	3:L:3172[B]:SER:CB	2.29	0.81
3:C:3172[B]:SER:CB	3:L:3150[B]:LYS:C	2.53	0.81
3:C:3176[B]:LYS:HE2	3:C:3176[B]:LYS:H	1.43	0.81
3:C:3228[A]:VAL:HG21	3:C:3245[A]:PHE:CE2	2.14	0.81
3:F:2952[B]:ALA:HB3	3:F:2953[B]:GLY:CA	2.10	0.81
3:F:2955[B]:GLN:CD	3:F:3037[B]:TYR:CE1	2.55	0.81
3:F:2961[B]:HIS:CA	3:a:2975[B]:PHE:HZ	1.89	0.81
3:F:2963[A]:MET:N	3:F:3108[A]:HIS:O	2.14	0.81
3:F:2971[B]:ASP:N	9:F:3401[B]:CUO:O2	2.14	0.81
3:F:3173[A]:THR:HG22	3:F:3174[A]:GLY:N	1.93	0.81
3:F:3176[A]:LYS:HE2	3:F:3176[A]:LYS:H	1.43	0.81
3:F:3298[B]:ASN:HB3	3:F:3300[B]:LEU:CD2	2.09	0.81
3:I:2962[B]:GLY:O	3:R:3255[B]:PRO:HD3	1.79	0.81
3:I:2963[B]:MET:N	3:I:3108[B]:HIS:O	2.14	0.81
3:I:3176[B]:LYS:HE2	3:I:3176[B]:LYS:H	1.43	0.81
3:I:3298[A]:ASN:HB3	3:I:3300[A]:LEU:CD2	2.09	0.81
3:L:3027[B]:GLU:OE2	3:L:3028[B]:PRO:HD2	1.80	0.81
3:L:3120[A]:HIS:HA	3:L:3123[A]:THR:OG1	1.79	0.81
3:L:3183[B]:LEU:H	3:L:3184[B]:ASN:HA	1.44	0.81
3:O:2939[B]:ARG:HB3	3:O:3032[B]:PRO:HG2	1.63	0.81
3:O:2963[A]:MET:N	3:O:3108[A]:HIS:O	2.14	0.81
3:O:2965[B]:LEU:HG	3:O:2974[B]:ALA:HB1	1.61	0.81
3:O:3228[A]:VAL:HG21	3:O:3245[A]:PHE:CE2	2.14	0.81
3:R:2952[A]:ALA:HB3	3:R:2953[A]:GLY:CA	2.09	0.81
3:R:2952[B]:ALA:HB3	3:R:2953[B]:GLY:CA	2.10	0.81
3:R:2965[A]:LEU:CD2	3:R:2974[A]:ALA:HB1	2.10	0.81
3:R:3027[B]:GLU:OE2	3:R:3028[B]:PRO:HD2	1.80	0.81
3:R:3120[B]:HIS:HA	3:R:3123[B]:THR:OG1	1.79	0.81
3:R:3176[B]:LYS:HE2	3:R:3176[B]:LYS:H	1.43	0.81
3:R:3265[A]:ASP:OD1	3:R:3267[A]:SER:OG	1.97	0.81
3:U:2963[A]:MET:N	3:U:3108[A]:HIS:O	2.14	0.81
3:U:2965[B]:LEU:HG	3:U:2974[B]:ALA:HB1	1.61	0.81
3:U:3169[B]:LYS:O	3:d:3148[B]:ILE:CA	2.27	0.81
3:U:3216[A]:GLY:HA2	3:U:3262[A]:PHE:O	1.78	0.81
1:V:589:GLN:HG2	1:V:594:ASP:HB3	1.62	0.81
3:X:2965[B]:LEU:CD2	3:X:2974[B]:ALA:HB1	2.10	0.81
3:X:3176[B]:LYS:HB3	3:X:3176[B]:LYS:HZ2	1.42	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3259[B]:ASP:CG	3:X:3260[B]:ARG:HG2	2.04	0.81
3:a:3023[B]:ILE:O	3:a:3026[B]:THR:N	2.11	0.81
3:a:3189[A]:ASN:CG	3:a:3191[A]:ASN:HD21	1.87	0.81
3:a:3212[A]:ARG:HG3	3:a:3212[A]:ARG:HH11	1.43	0.81
3:a:3228[B]:VAL:HG21	3:a:3245[B]:PHE:CE2	2.14	0.81
3:a:3230[A]:PHE:CB	3:a:3243[A]:GLY:HA2	2.06	0.81
3:d:3120[A]:HIS:HA	3:d:3123[A]:THR:OG1	1.79	0.81
3:d:3298[A]:ASN:HB3	3:d:3300[A]:LEU:CD2	2.09	0.81
3:C:3155[B]:MET:HG2	3:L:3154[B]:PRO:O	1.81	0.81
3:C:3161[B]:GLU:HG3	3:L:3146[B]:CYS:C	2.06	0.81
3:F:2948[A]:ASP:N	3:F:2949[A]:LYS:CA	2.41	0.81
3:F:2965[A]:LEU:CD2	3:F:2974[A]:ALA:HB1	2.10	0.81
3:F:2966[B]:SER:OG	3:a:3255[B]:PRO:O	1.99	0.81
3:F:2977[B]:CYS:O	3:a:3254[B]:MET:HE3	0.92	0.81
3:F:3150[B]:LYS:HZ3	3:a:3160[B]:SER:HB3	1.02	0.81
3:F:3161[B]:GLU:HA	3:a:3147[B]:GLU:HG3	1.61	0.81
3:F:3248[B]:LEU:HB3	3:a:2972[B]:GLY:C	2.05	0.81
3:F:3298[A]:ASN:HB3	3:F:3300[A]:LEU:CD2	2.10	0.81
3:I:2983[B]:VAL:CB	3:R:3160[B]:SER:HA	2.09	0.81
3:L:2952[A]:ALA:HB3	3:L:2953[A]:GLY:CA	2.10	0.81
3:L:2952[B]:ALA:HB3	3:L:2953[B]:GLY:CA	2.09	0.81
3:O:2963[B]:MET:N	3:O:3108[B]:HIS:O	2.13	0.81
3:O:3109[B]:TYR:CE2	3:X:2969[B]:TYR:C	2.58	0.81
3:O:3189[A]:ASN:CG	3:O:3191[A]:ASN:HD21	1.87	0.81
3:R:3089[B]:HIS:HE1	3:R:3119[B]:HIS:CD2	1.96	0.81
3:R:3212[A]:ARG:HG3	3:R:3212[A]:ARG:HH11	1.43	0.81
3:R:3228[A]:VAL:HG21	3:R:3245[A]:PHE:CE2	2.14	0.81
2:T:2545:SER:HA	2:T:2546:LEU:HB2	1.62	0.81
3:U:2975[B]:PHE:CG	3:d:3256[B]:TRP:CG	2.67	0.81
3:U:3162[B]:ASP:HA	3:d:3260[B]:ARG:HH12	1.43	0.81
3:U:3228[A]:VAL:HG21	3:U:3245[A]:PHE:CE2	2.14	0.81
3:X:2948[A]:ASP:N	3:X:2949[A]:LYS:CA	2.41	0.81
3:X:2969[B]:TYR:CE2	3:X:2970[B]:PRO:HG2	2.05	0.81
3:X:3120[A]:HIS:HA	3:X:3123[A]:THR:OG1	1.79	0.81
3:X:3120[B]:HIS:HA	3:X:3123[B]:THR:OG1	1.79	0.81
3:X:3189[A]:ASN:CG	3:X:3191[A]:ASN:HD21	1.87	0.81
3:a:3104[A]:MET:CA	3:a:3110[A]:THR:HG23	2.10	0.81
3:a:3298[B]:ASN:HB3	3:a:3300[B]:LEU:CD2	2.10	0.81
3:C:2939[A]:ARG:HB3	3:C:3032[A]:PRO:HG2	1.63	0.81
3:C:2939[B]:ARG:HB3	3:C:3032[B]:PRO:HG2	1.63	0.81
3:C:2979[B]:GLN:HG3	3:L:3156[B]:MET:SD	2.20	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3023[A]:ILE:O	3:C:3026[A]:THR:N	2.11	0.81
3:C:3189[A]:ASN:CG	3:C:3191[A]:ASN:HD21	1.87	0.81
3:F:3027[B]:GLU:OE2	3:F:3028[B]:PRO:HD2	1.80	0.81
3:I:3027[A]:GLU:OE2	3:I:3028[A]:PRO:HD2	1.80	0.81
3:I:3120[A]:HIS:HA	3:I:3123[A]:THR:OG1	1.79	0.81
3:L:2963[A]:MET:N	3:L:3108[A]:HIS:O	2.14	0.81
3:L:3212[A]:ARG:HH11	3:L:3212[A]:ARG:HG3	1.43	0.81
3:L:3284[B]:LYS:HD3	3:L:3285[B]:VAL:H	1.39	0.81
3:L:3298[A]:ASN:HB3	3:L:3300[A]:LEU:CD2	2.09	0.81
3:O:2955[A]:GLN:CD	3:O:3037[A]:TYR:CE1	2.55	0.81
3:O:3265[B]:ASP:OD1	3:O:3267[B]:SER:OG	1.97	0.81
1:P:387:ASN:ND2	6:3:1:NAG:O7	2.13	0.81
3:R:2963[B]:MET:N	3:R:3108[B]:HIS:O	2.14	0.81
3:R:3183[A]:LEU:H	3:R:3184[A]:ASN:HA	1.44	0.81
3:R:3183[B]:LEU:H	3:R:3184[B]:ASN:HA	1.44	0.81
3:R:3216[B]:GLY:HA2	3:R:3262[B]:PHE:O	1.78	0.81
3:U:2967[B]:CYS:HB2	3:d:3256[B]:TRP:HB2	1.61	0.81
3:a:2963[A]:MET:N	3:a:3108[A]:HIS:O	2.14	0.81
3:a:2963[B]:MET:N	3:a:3108[B]:HIS:O	2.13	0.81
3:d:2952[A]:ALA:HB3	3:d:2953[A]:GLY:CA	2.10	0.81
3:d:3027[A]:GLU:OE2	3:d:3028[A]:PRO:HD2	1.80	0.81
3:C:2955[A]:GLN:CD	3:C:3037[A]:TYR:CE1	2.55	0.81
3:F:3255[B]:PRO:C	3:a:2966[B]:SER:N	2.38	0.81
3:I:3154[B]:PRO:HD2	3:R:3155[B]:MET:SD	2.21	0.81
3:I:3160[B]:SER:CB	3:R:3150[B]:LYS:HZ3	1.91	0.81
3:I:3183[B]:LEU:H	3:I:3184[B]:ASN:HA	1.44	0.81
3:I:3228[A]:VAL:HG21	3:I:3245[A]:PHE:CE2	2.14	0.81
3:I:3265[B]:ASP:OD1	3:I:3267[B]:SER:OG	1.97	0.81
1:J:401:VAL:HG22	1:J:662:SER:HB3	1.62	0.81
3:L:2951[A]:ASP:OD2	3:L:2953[A]:GLY:HA2	1.79	0.81
3:L:3259[A]:ASP:CG	3:L:3260[A]:ARG:HG2	2.04	0.81
3:O:3160[B]:SER:HB2	3:X:3151[B]:LEU:N	1.80	0.81
3:O:3259[B]:ASP:CG	3:O:3260[B]:ARG:HG2	2.04	0.81
3:R:3189[A]:ASN:CG	3:R:3191[A]:ASN:HD21	1.87	0.81
3:R:3212[B]:ARG:HH11	3:R:3212[B]:ARG:HG3	1.43	0.81
1:S:527:LEU:O	1:S:561:ARG:NH1	2.12	0.81
3:X:2963[B]:MET:N	3:X:3108[B]:HIS:O	2.13	0.81
3:a:2952[A]:ALA:HB3	3:a:2953[A]:GLY:CA	2.10	0.81
3:a:3176[B]:LYS:H	3:a:3176[B]:LYS:HE2	1.43	0.81
3:d:2963[A]:MET:N	3:d:3108[A]:HIS:O	2.14	0.81
3:d:3027[B]:GLU:OE2	3:d:3028[B]:PRO:HD2	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3120[B]:HIS:HA	3:d:3123[B]:THR:OG1	1.79	0.81
3:C:2956[A]:LYS:O	3:C:2960[A]:PHE:CD1	2.33	0.81
3:C:2963[A]:MET:N	3:C:3108[A]:HIS:O	2.14	0.81
3:C:3176[A]:LYS:HE2	3:C:3176[A]:LYS:H	1.43	0.81
3:F:3025[A]:VAL:CG2	3:F:3047[A]:ARG:HH12	1.94	0.81
3:F:3025[B]:VAL:CG2	3:F:3047[B]:ARG:HH12	1.94	0.81
3:F:3265[A]:ASP:OD1	3:F:3267[A]:SER:OG	1.97	0.81
3:I:3104[B]:MET:CA	3:I:3110[B]:THR:HG23	2.10	0.81
3:I:3180[A]:TYR:O	3:I:3183[A]:LEU:HD22	1.81	0.81
3:I:3216[A]:GLY:HA2	3:I:3262[A]:PHE:O	1.78	0.81
3:O:2952[A]:ALA:HB3	3:O:2953[A]:GLY:CA	2.09	0.81
3:O:3169[B]:LYS:CA	3:X:3148[B]:ILE:HG21	2.10	0.81
3:O:3180[B]:TYR:O	3:O:3183[B]:LEU:HD22	1.81	0.81
3:R:2939[A]:ARG:HB3	3:R:3032[A]:PRO:HG2	1.63	0.81
3:R:3027[A]:GLU:OE2	3:R:3028[A]:PRO:HD2	1.80	0.81
3:U:3265[B]:ASP:OD1	3:U:3267[B]:SER:OG	1.97	0.81
2:W:2823:ILE:HG13	2:W:2830:GLN:HE22	1.46	0.81
3:X:2952[B]:ALA:HB3	3:X:2953[B]:GLY:CA	2.10	0.81
3:X:2955[A]:GLN:CD	3:X:3037[A]:TYR:CE1	2.55	0.81
3:X:3180[A]:TYR:O	3:X:3183[A]:LEU:HD22	1.81	0.81
3:a:2951[A]:ASP:OD2	3:a:2953[A]:GLY:HA2	1.79	0.81
3:a:3212[B]:ARG:HH11	3:a:3212[B]:ARG:HG3	1.43	0.81
3:C:3149[B]:ASN:HB3	3:L:3163[B]:ASN:ND2	1.95	0.81
3:C:3180[A]:TYR:O	3:C:3183[A]:LEU:HD22	1.81	0.81
1:D:1641:THR:HG21	1:D:1644:ILE:HD11	1.63	0.81
3:F:2956[B]:LYS:O	3:F:2960[B]:PHE:CD1	2.33	0.81
3:F:2963[B]:MET:N	3:F:3108[B]:HIS:O	2.14	0.81
3:F:3101[A]:PRO:O	3:F:3106[A]:THR:HG21	1.81	0.81
3:F:3104[A]:MET:CA	3:F:3110[A]:THR:HG23	2.10	0.81
3:F:3157[B]:PRO:CB	3:a:2982[B]:MET:SD	2.68	0.81
3:I:2963[A]:MET:N	3:I:3108[A]:HIS:O	2.14	0.81
3:I:3172[B]:SER:CB	3:R:3150[B]:LYS:O	2.29	0.81
3:I:3180[B]:TYR:O	3:I:3183[B]:LEU:HD22	1.81	0.81
3:L:2955[B]:GLN:CD	3:L:3037[B]:TYR:CE1	2.55	0.81
3:L:2965[A]:LEU:CD2	3:L:2974[A]:ALA:HB1	2.10	0.81
3:L:3025[A]:VAL:CG2	3:L:3047[A]:ARG:HH12	1.94	0.81
3:L:3180[B]:TYR:O	3:L:3183[B]:LEU:HD22	1.81	0.81
3:L:3265[A]:ASP:OD1	3:L:3267[A]:SER:OG	1.97	0.81
3:O:3104[A]:MET:CA	3:O:3110[A]:THR:HG23	2.10	0.81
3:R:2963[A]:MET:N	3:R:3108[A]:HIS:O	2.14	0.81
3:U:3173[A]:THR:HG22	3:U:3174[A]:GLY:N	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2956[A]:LYS:O	3:X:2960[A]:PHE:CD1	2.33	0.81
3:X:3212[A]:ARG:HH11	3:X:3212[A]:ARG:HG3	1.43	0.81
3:X:3265[B]:ASP:OD1	3:X:3267[B]:SER:OG	1.97	0.81
3:F:2939[B]:ARG:HB3	3:F:3032[B]:PRO:HG2	1.63	0.81
3:F:3231[A]:ASP:N	3:F:3284[A]:LYS:O	2.14	0.81
2:H:2472:ASN:ND2	4:s:1:NAG:H61	1.90	0.81
2:H:2868:GLU:CD	3:I:2933[A]:SER:H	1.88	0.81
3:I:3255[B]:PRO:HG3	3:R:2962[B]:GLY:C	2.05	0.81
3:L:3230[A]:PHE:CB	3:L:3243[A]:GLY:HA2	2.06	0.81
3:L:3231[A]:ASP:N	3:L:3284[A]:LYS:O	2.14	0.81
3:O:3023[A]:ILE:O	3:O:3026[A]:THR:N	2.11	0.81
3:O:3024[B]:LEU:CD1	3:O:3025[B]:VAL:H	1.83	0.81
3:O:3027[B]:GLU:OE2	3:O:3028[B]:PRO:HD2	1.80	0.81
3:R:3180[A]:TYR:O	3:R:3183[A]:LEU:HD22	1.81	0.81
3:R:3231[A]:ASP:N	3:R:3284[A]:LYS:O	2.14	0.81
3:U:2952[A]:ALA:HB3	3:U:2953[A]:GLY:CA	2.10	0.81
3:U:2973[B]:THR:HG22	3:d:3222[B]:ILE:HG23	1.63	0.81
3:U:3152[B]:LYS:NZ	3:d:3172[B]:SER:OG	2.14	0.81
3:U:3176[B]:LYS:HG3	3:d:3152[B]:LYS:HZ2	1.44	0.81
3:X:3025[B]:VAL:CG2	3:X:3047[B]:ARG:HH12	1.94	0.81
3:X:3027[B]:GLU:OE2	3:X:3028[B]:PRO:HD2	1.80	0.81
3:a:3104[B]:MET:CA	3:a:3110[B]:THR:HG23	2.10	0.81
3:a:3231[B]:ASP:N	3:a:3284[B]:LYS:O	2.14	0.81
3:a:3265[B]:ASP:OD1	3:a:3267[B]:SER:OG	1.97	0.81
3:d:2965[B]:LEU:CD2	3:d:2974[B]:ALA:HB1	2.10	0.81
3:d:3231[B]:ASP:N	3:d:3284[B]:LYS:O	2.14	0.81
3:d:3265[A]:ASP:OD1	3:d:3267[A]:SER:OG	1.97	0.81
3:C:3298[A]:ASN:HB3	3:C:3300[A]:LEU:CD2	2.09	0.81
3:F:2977[B]:CYS:CB	3:a:2982[B]:MET:CE	2.59	0.81
3:F:3162[B]:ASP:HB3	3:a:3259[B]:ASP:N	1.96	0.81
3:I:2939[B]:ARG:HB3	3:I:3032[B]:PRO:HG2	1.63	0.81
3:I:3101[B]:PRO:O	3:I:3106[B]:THR:HG21	1.81	0.81
3:I:3108[B]:HIS:HE1	3:R:3251[B]:ASP:OD1	1.59	0.81
3:I:3150[B]:LYS:C	3:R:3172[B]:SER:HB3	2.06	0.81
3:O:3163[B]:ASN:CB	3:X:3149[B]:ASN:N	2.30	0.81
3:O:3180[A]:TYR:O	3:O:3183[A]:LEU:HD22	1.81	0.81
3:R:3101[A]:PRO:O	3:R:3106[A]:THR:HG21	1.81	0.81
1:S:1636:ASN:ND2	1:S:1639:LYS:HD2	1.95	0.81
3:X:3265[A]:ASP:OD1	3:X:3267[A]:SER:OG	1.97	0.81
3:a:2948[A]:ASP:N	3:a:2949[A]:LYS:CA	2.41	0.81
3:a:2965[A]:LEU:CD2	3:a:2974[A]:ALA:HB1	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3298[A]:ASN:HB3	3:a:3300[A]:LEU:CD2	2.09	0.81
3:d:3025[B]:VAL:CG2	3:d:3047[B]:ARG:HH12	1.94	0.81
3:C:2948[B]:ASP:N	3:C:2949[B]:LYS:HA	1.81	0.80
3:C:3025[B]:VAL:CG2	3:C:3047[B]:ARG:HH12	1.94	0.80
3:C:3160[B]:SER:C	3:L:2983[B]:VAL:HG21	2.06	0.80
3:F:3023[B]:ILE:O	3:F:3026[B]:THR:N	2.11	0.80
3:F:3027[A]:GLU:OE2	3:F:3028[A]:PRO:HD2	1.80	0.80
3:F:3183[A]:LEU:H	3:F:3184[A]:ASN:HA	1.44	0.80
3:F:3231[B]:ASP:N	3:F:3284[B]:LYS:O	2.14	0.80
3:I:2939[A]:ARG:HB3	3:I:3032[A]:PRO:HG2	1.63	0.80
3:I:2951[B]:ASP:OD2	3:I:2953[B]:GLY:HA2	1.79	0.80
3:I:2952[A]:ALA:HB3	3:I:2953[A]:GLY:CA	2.10	0.80
3:I:2956[B]:LYS:O	3:I:2960[B]:PHE:CD1	2.33	0.80
3:I:2966[B]:SER:O	3:R:3256[B]:TRP:CB	2.29	0.80
3:I:3180[B]:TYR:HB2	3:I:3183[B]:LEU:HD22	1.63	0.80
1:J:1636:ASN:OD1	6:w:1:NAG:H82	1.81	0.80
3:L:3101[B]:PRO:O	3:L:3106[B]:THR:HG21	1.81	0.80
3:L:3189[B]:ASN:CG	3:L:3191[B]:ASN:HD21	1.87	0.80
3:O:3101[A]:PRO:O	3:O:3106[A]:THR:HG21	1.81	0.80
3:U:3180[A]:TYR:O	3:U:3183[A]:LEU:HD22	1.81	0.80
3:X:2965[A]:LEU:CD2	3:X:2974[A]:ALA:HB1	2.10	0.80
1:b:1442:MET:HE1	1:b:1454:PHE:HA	1.63	0.80
3:C:3023[B]:ILE:O	3:C:3026[B]:THR:N	2.11	0.80
3:C:3027[A]:GLU:OE2	3:C:3028[A]:PRO:HD2	1.80	0.80
3:C:3169[B]:LYS:CE	3:L:3149[B]:ASN:OD1	2.29	0.80
3:C:3174[B]:GLY:CA	3:L:3154[B]:PRO:CD	2.50	0.80
3:C:3183[B]:LEU:H	3:C:3184[B]:ASN:HA	1.44	0.80
3:C:3231[B]:ASP:N	3:C:3284[B]:LYS:O	2.14	0.80
3:F:2965[B]:LEU:CD2	3:F:2974[B]:ALA:HB1	2.10	0.80
3:F:3104[B]:MET:CA	3:F:3110[B]:THR:HG23	2.10	0.80
3:F:3174[B]:GLY:H	3:a:3154[B]:PRO:HB3	0.99	0.80
3:F:3180[A]:TYR:O	3:F:3183[A]:LEU:HD22	1.81	0.80
3:L:2963[B]:MET:N	3:L:3108[B]:HIS:O	2.14	0.80
3:L:3025[B]:VAL:CG2	3:L:3047[B]:ARG:HH12	1.94	0.80
3:R:3025[B]:VAL:CG2	3:R:3047[B]:ARG:HH12	1.94	0.80
3:U:2965[B]:LEU:CD2	3:U:2974[B]:ALA:HB1	2.10	0.80
3:U:3025[B]:VAL:CG2	3:U:3047[B]:ARG:HH12	1.94	0.80
3:U:3231[A]:ASP:N	3:U:3284[A]:LYS:O	2.14	0.80
3:a:2969[B]:TYR:HB3	3:a:2971[B]:ASP:OD1	1.82	0.80
3:a:3027[A]:GLU:OE2	3:a:3028[A]:PRO:HD2	1.80	0.80
3:a:3027[B]:GLU:OE2	3:a:3028[B]:PRO:HD2	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3180[A]:TYR:O	3:a:3183[A]:LEU:HD22	1.81	0.80
3:d:3180[A]:TYR:HB2	3:d:3183[A]:LEU:HD22	1.63	0.80
3:C:2956[B]:LYS:C	3:C:2960[B]:PHE:CE1	2.47	0.80
3:C:2965[B]:LEU:CD2	3:C:2974[B]:ALA:HB1	2.10	0.80
3:C:2969[A]:TYR:HB3	3:C:2971[A]:ASP:OD1	1.82	0.80
3:C:3147[B]:GLU:OE1	3:L:3162[B]:ASP:CA	2.30	0.80
3:C:3172[B]:SER:CB	3:L:3150[B]:LYS:N	2.45	0.80
3:C:3180[B]:TYR:O	3:C:3183[B]:LEU:HD22	1.81	0.80
3:C:3189[B]:ASN:CG	3:C:3191[B]:ASN:HD21	1.87	0.80
1:D:1574:VAL:H	1:G:329:ARG:HH12	1.29	0.80
3:F:2976[B]:ALA:CB	3:a:3252[B]:TYR:O	2.28	0.80
3:I:3155[B]:MET:CE	3:R:3156[B]:MET:HG2	2.12	0.80
3:I:3176[A]:LYS:HE2	3:I:3176[A]:LYS:H	1.43	0.80
3:L:2939[A]:ARG:HB3	3:L:3032[A]:PRO:HG2	1.62	0.80
3:L:3101[A]:PRO:O	3:L:3106[A]:THR:HG21	1.81	0.80
3:O:2939[A]:ARG:HB3	3:O:3032[A]:PRO:HG2	1.63	0.80
3:O:2956[B]:LYS:O	3:O:2960[B]:PHE:CD1	2.33	0.80
3:O:3180[A]:TYR:HB2	3:O:3183[A]:LEU:HD22	1.63	0.80
3:O:3231[A]:ASP:N	3:O:3284[A]:LYS:O	2.14	0.80
3:R:3025[A]:VAL:CG2	3:R:3047[A]:ARG:HH12	1.94	0.80
3:X:2963[A]:MET:N	3:X:3108[A]:HIS:O	2.14	0.80
3:X:2965[B]:LEU:HD11	3:X:2974[B]:ALA:CA	2.11	0.80
3:X:3180[A]:TYR:HB2	3:X:3183[A]:LEU:HD22	1.63	0.80
3:X:3231[A]:ASP:N	3:X:3284[A]:LYS:O	2.14	0.80
1:Y:1617:LYS:HE2	3:d:3180[B]:TYR:CE2	2.15	0.80
3:a:2956[B]:LYS:O	3:a:2960[B]:PHE:CD1	2.33	0.80
3:d:2963[B]:MET:N	3:d:3108[B]:HIS:O	2.14	0.80
3:d:2965[A]:LEU:CD2	3:d:2974[A]:ALA:HB1	2.10	0.80
3:d:3176[A]:LYS:HE2	3:d:3176[A]:LYS:H	1.43	0.80
3:C:2963[B]:MET:N	3:C:3108[B]:HIS:O	2.14	0.80
3:C:2965[A]:LEU:CD2	3:C:2974[A]:ALA:HB1	2.10	0.80
3:C:3231[A]:ASP:N	3:C:3284[A]:LYS:O	2.14	0.80
3:F:3155[B]:MET:HG3	3:a:3154[B]:PRO:CD	2.11	0.80
3:I:2973[B]:THR:HG23	3:R:3248[B]:LEU:HD11	1.63	0.80
3:I:2975[B]:PHE:CZ	3:R:2961[B]:HIS:CD2	2.68	0.80
3:I:3149[B]:ASN:OD1	3:R:3169[B]:LYS:NZ	2.15	0.80
3:I:3223[B]:GLY:HA3	3:R:2963[B]:MET:CE	2.09	0.80
3:I:3231[A]:ASP:N	3:I:3284[A]:LYS:O	2.14	0.80
3:L:2965[A]:LEU:HD11	3:L:2974[A]:ALA:CA	2.12	0.80
3:O:2956[A]:LYS:O	3:O:2960[A]:PHE:CD1	2.33	0.80
3:O:3255[B]:PRO:CA	3:X:3161[B]:GLU:HA	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2952[A]:ALA:CB	3:R:2953[A]:GLY:C	2.48	0.80
3:R:3231[B]:ASP:N	3:R:3284[B]:LYS:O	2.14	0.80
1:S:497:GLN:HG2	1:S:683:THR:HG21	1.63	0.80
3:U:2974[B]:ALA:HB1	3:d:3220[B]:ARG:CG	2.10	0.80
3:U:3152[B]:LYS:HB2	3:d:3154[B]:PRO:CB	2.08	0.80
3:U:3180[A]:TYR:HB2	3:U:3183[A]:LEU:HD22	1.63	0.80
3:d:2956[B]:LYS:O	3:d:2960[B]:PHE:CD1	2.33	0.80
3:d:3101[B]:PRO:O	3:d:3106[B]:THR:HG21	1.81	0.80
3:C:3223[B]:GLY:C	3:L:3252[B]:TYR:CE1	2.60	0.80
3:F:2975[B]:PHE:CD1	3:a:3107[B]:LEU:HD21	2.16	0.80
3:F:2980[B]:HIS:N	3:a:2967[B]:CYS:CB	2.44	0.80
3:F:3180[B]:TYR:O	3:F:3183[B]:LEU:HD22	1.81	0.80
3:F:3251[B]:ASP:OD1	3:a:3108[B]:HIS:CE1	2.35	0.80
3:I:2948[A]:ASP:N	3:I:2949[A]:LYS:CA	2.41	0.80
3:I:2969[A]:TYR:HB3	3:I:2971[A]:ASP:OD1	1.82	0.80
3:I:2969[B]:TYR:HB3	3:I:2971[B]:ASP:OD1	1.82	0.80
3:I:3101[A]:PRO:O	3:I:3106[A]:THR:HG21	1.81	0.80
3:O:2965[B]:LEU:N	3:X:3254[B]:MET:CE	2.43	0.80
3:O:3101[B]:PRO:O	3:O:3106[B]:THR:HG21	1.81	0.80
3:O:3104[B]:MET:CA	3:O:3110[B]:THR:HG23	2.10	0.80
3:R:3180[B]:TYR:O	3:R:3183[B]:LEU:HD22	1.81	0.80
3:U:2965[A]:LEU:CD2	3:U:2974[A]:ALA:HB1	2.10	0.80
3:U:3152[B]:LYS:O	3:d:3153[B]:LYS:N	2.03	0.80
3:X:3025[A]:VAL:CG2	3:X:3047[A]:ARG:HH12	1.94	0.80
3:X:3101[A]:PRO:O	3:X:3106[A]:THR:HG21	1.81	0.80
1:Y:1656:ASP:C	3:d:2937[B]:ASN:ND2	2.38	0.80
3:a:2965[A]:LEU:HD11	3:a:2974[A]:ALA:CA	2.12	0.80
3:a:3101[A]:PRO:O	3:a:3106[A]:THR:HG21	1.81	0.80
3:a:3183[A]:LEU:H	3:a:3184[A]:ASN:HA	1.44	0.80
3:C:3152[B]:LYS:HB2	3:L:3172[B]:SER:H	1.43	0.80
3:C:3163[B]:ASN:CB	3:L:3149[B]:ASN:ND2	2.30	0.80
1:D:115:GLY:HA2	1:D:116:LYS:HB2	1.64	0.80
3:I:3169[B]:LYS:NZ	3:R:3149[B]:ASN:OD1	2.14	0.80
1:P:589:GLN:HG2	1:P:594:ASP:HB3	1.62	0.80
3:R:3101[B]:PRO:O	3:R:3106[B]:THR:HG21	1.81	0.80
3:U:2956[B]:LYS:C	3:U:2960[B]:PHE:CE1	2.47	0.80
3:U:3101[A]:PRO:O	3:U:3106[A]:THR:HG21	1.81	0.80
3:X:3023[A]:ILE:O	3:X:3026[A]:THR:N	2.11	0.80
1:Y:855:ARG:O	1:Y:957:ASN:ND2	2.15	0.80
1:Y:1620:LEU:C	3:d:3189[B]:ASN:HD22	1.89	0.80
3:a:2939[A]:ARG:HB3	3:a:3032[A]:PRO:HG2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3101[B]:PRO:O	3:a:3106[B]:THR:HG21	1.81	0.80
3:d:2969[A]:TYR:HB3	3:d:2971[A]:ASP:OD1	1.82	0.80
3:I:3152[B]:LYS:CB	3:R:3171[B]:HIS:C	2.55	0.80
3:I:3162[B]:ASP:HB3	3:R:3259[B]:ASP:CA	2.11	0.80
2:K:2870:LEU:HD21	2:K:2901:LEU:HD23	1.63	0.80
3:R:3196[A]:THR:H	3:R:3199[A]:GLN:HB2	1.37	0.80
3:U:2939[B]:ARG:HB3	3:U:3032[B]:PRO:HG2	1.63	0.80
3:U:2965[B]:LEU:HD23	3:d:3220[B]:ARG:CD	2.10	0.80
3:U:3189[B]:ASN:CG	3:U:3191[B]:ASN:HD21	1.88	0.80
3:X:2939[B]:ARG:HB3	3:X:3032[B]:PRO:HG2	1.63	0.80
3:X:3231[B]:ASP:N	3:X:3284[B]:LYS:O	2.14	0.80
2:Z:2867:PRO:CD	3:a:2932[A]:PRO:HG2	2.11	0.80
3:C:2979[B]:GLN:HE22	3:L:2979[B]:GLN:NE2	1.79	0.80
3:F:2973[B]:THR:HG23	3:a:3248[B]:LEU:CD1	2.10	0.80
3:F:3153[B]:LYS:CB	3:a:3158[B]:PHE:HB2	2.11	0.80
3:F:3230[A]:PHE:CB	3:F:3243[A]:GLY:HA2	2.06	0.80
3:I:3183[A]:LEU:H	3:I:3184[A]:ASN:HA	1.44	0.80
3:O:2972[B]:GLY:O	3:X:2979[B]:GLN:CB	2.30	0.80
3:R:2939[B]:ARG:HB3	3:R:3032[B]:PRO:HG2	1.63	0.80
3:R:2956[A]:LYS:O	3:R:2960[A]:PHE:CD1	2.33	0.80
3:R:3180[A]:TYR:HB2	3:R:3183[A]:LEU:HD22	1.63	0.80
3:R:3189[B]:ASN:CG	3:R:3191[B]:ASN:HD21	1.87	0.80
3:U:3023[B]:ILE:O	3:U:3026[B]:THR:N	2.11	0.80
3:U:3101[B]:PRO:O	3:U:3106[B]:THR:HG21	1.82	0.80
3:U:3152[B]:LYS:C	3:d:3152[B]:LYS:C	2.41	0.80
3:U:3212[B]:ARG:HG3	3:U:3212[B]:ARG:HH11	1.43	0.80
3:X:3027[A]:GLU:OE2	3:X:3028[A]:PRO:HD2	1.80	0.80
1:Y:1397:LEU:O	1:Y:1400:ASN:ND2	2.15	0.80
3:a:3025[B]:VAL:CG2	3:a:3047[B]:ARG:HH12	1.94	0.80
2:c:2394:VAL:H	2:c:2448:THR:HG22	1.47	0.80
3:d:3180[B]:TYR:O	3:d:3183[B]:LEU:HD22	1.81	0.80
3:C:2965[A]:LEU:HD11	3:C:2974[A]:ALA:CA	2.12	0.80
3:C:2966[B]:SER:O	3:L:2981[B]:GLY:O	2.00	0.80
3:C:2983[B]:VAL:CG2	3:L:3160[B]:SER:C	2.48	0.80
3:F:3153[B]:LYS:HD2	3:a:3155[B]:MET:CA	2.10	0.80
3:I:2965[A]:LEU:HD11	3:I:2974[A]:ALA:CA	2.12	0.80
3:L:2969[B]:TYR:HB3	3:L:2971[B]:ASP:OD1	1.82	0.80
3:L:3183[A]:LEU:H	3:L:3184[A]:ASN:HA	1.44	0.80
3:O:2968[B]:GLN:HB2	3:X:2988[B]:TRP:H	1.47	0.80
3:R:2969[A]:TYR:HB3	3:R:2971[A]:ASP:OD1	1.82	0.80
3:R:3135[A]:LYS:CG	3:R:3141[A]:TYR:CD1	2.65	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1618:LEU:HD22	3:X:3136[B]:TYR:CE2	2.17	0.80
3:U:3025[A]:VAL:CG2	3:U:3047[A]:ARG:HH12	1.94	0.80
3:U:3027[A]:GLU:OE2	3:U:3028[A]:PRO:HD2	1.80	0.80
3:U:3027[B]:GLU:OE2	3:U:3028[B]:PRO:HD2	1.80	0.80
3:U:3104[B]:MET:CA	3:U:3110[B]:THR:HG23	2.10	0.80
1:V:497:GLN:HG2	1:V:683:THR:HG21	1.63	0.80
1:V:961:SER:HB2	1:V:973:ARG:HA	1.64	0.80
3:X:2969[A]:TYR:HB3	3:X:2971[A]:ASP:OD1	1.82	0.80
3:a:2956[A]:LYS:C	3:a:2960[A]:PHE:CE1	2.47	0.80
3:a:3231[A]:ASP:N	3:a:3284[A]:LYS:O	2.14	0.80
3:d:3196[B]:THR:H	3:d:3199[B]:GLN:HB2	1.38	0.80
3:d:3231[A]:ASP:N	3:d:3284[A]:LYS:O	2.14	0.80
3:C:2948[A]:ASP:N	3:C:2949[A]:LYS:CA	2.41	0.80
3:C:2968[B]:GLN:HG2	3:L:2981[B]:GLY:N	1.97	0.80
3:C:2982[B]:MET:CB	3:L:3156[B]:MET:HB2	1.85	0.80
3:C:3154[B]:PRO:HB2	3:L:3151[B]:LEU:CA	2.11	0.80
3:C:3180[B]:TYR:HB2	3:C:3183[B]:LEU:HD22	1.63	0.80
3:F:2939[A]:ARG:HB3	3:F:3032[A]:PRO:HG2	1.63	0.80
3:F:2981[B]:GLY:N	3:a:2968[B]:GLN:OE1	2.15	0.80
3:F:3150[B]:LYS:HE3	3:a:3163[B]:ASN:HB3	1.64	0.80
3:I:2965[B]:LEU:HD11	3:I:2974[B]:ALA:CA	2.12	0.80
3:I:3135[B]:LYS:CG	3:I:3141[B]:TYR:CD1	2.65	0.80
3:I:3158[B]:PHE:HB2	3:R:3153[B]:LYS:HB2	1.64	0.80
3:L:2956[A]:LYS:O	3:L:2960[A]:PHE:CD1	2.33	0.80
3:L:3231[B]:ASP:N	3:L:3284[B]:LYS:O	2.14	0.80
3:R:2965[A]:LEU:HD11	3:R:2974[A]:ALA:CA	2.12	0.80
3:U:2965[A]:LEU:HD11	3:U:2974[A]:ALA:CA	2.12	0.80
3:U:3180[B]:TYR:O	3:U:3183[B]:LEU:HD22	1.81	0.80
1:b:415:VAL:HB	1:b:697:ALA:HB2	1.63	0.80
3:C:2969[B]:TYR:HB3	3:C:2971[B]:ASP:OD1	1.82	0.79
3:C:2988[B]:TRP:CD1	3:L:3153[B]:LYS:HD3	2.10	0.79
3:C:3171[B]:HIS:C	3:L:3152[B]:LYS:HB2	2.06	0.79
3:C:3180[A]:TYR:HB2	3:C:3183[A]:LEU:HD22	1.63	0.79
3:F:2955[A]:GLN:CD	3:F:3037[A]:TYR:CE1	2.55	0.79
3:F:2979[A]:GLN:CG	3:F:3155[A]:MET:CE	2.56	0.79
3:F:2982[B]:MET:SD	3:a:3157[B]:PRO:HB3	2.21	0.79
3:F:3154[B]:PRO:CB	3:a:3174[B]:GLY:CA	2.60	0.79
2:H:2868:GLU:CD	3:I:2933[A]:SER:N	2.40	0.79
3:I:2982[B]:MET:HE1	3:R:2966[B]:SER:HB3	1.63	0.79
3:I:3255[B]:PRO:HG2	3:R:2959[B]:SER:HA	1.64	0.79
3:O:2965[A]:LEU:HD11	3:O:2974[A]:ALA:CA	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2949[A]:LYS:O	3:R:2949[A]:LYS:NZ	2.15	0.79
3:U:2965[B]:LEU:HD23	3:d:3220[B]:ARG:HD3	1.63	0.79
3:U:2969[A]:TYR:HB3	3:U:2971[A]:ASP:OD1	1.82	0.79
3:U:3169[B]:LYS:HE3	3:d:3147[B]:GLU:CB	2.13	0.79
3:U:3231[B]:ASP:N	3:U:3284[B]:LYS:O	2.14	0.79
3:X:2939[A]:ARG:HB3	3:X:3032[A]:PRO:HG2	1.63	0.79
3:X:3101[B]:PRO:O	3:X:3106[B]:THR:HG21	1.81	0.79
3:a:3135[A]:LYS:CG	3:a:3141[A]:TYR:CD1	2.65	0.79
1:b:456:GLN:NE2	1:b:549:PRO:O	2.15	0.79
3:d:2965[B]:LEU:HD11	3:d:2974[B]:ALA:CA	2.12	0.79
3:C:3101[A]:PRO:O	3:C:3106[A]:THR:HG21	1.81	0.79
3:C:3147[B]:GLU:OE1	3:L:3162[B]:ASP:N	1.98	0.79
3:C:3162[B]:ASP:OD1	3:L:3259[B]:ASP:OD2	1.98	0.79
3:F:2956[B]:LYS:O	3:F:2960[B]:PHE:HE1	1.22	0.79
3:F:3135[A]:LYS:CG	3:F:3141[A]:TYR:CD1	2.65	0.79
3:I:2961[B]:HIS:ND1	3:R:2975[B]:PHE:CE1	2.50	0.79
3:I:2965[B]:LEU:HB3	3:R:3256[B]:TRP:CE2	2.14	0.79
3:I:3104[A]:MET:CA	3:I:3110[A]:THR:HG23	2.10	0.79
3:I:3196[B]:THR:H	3:I:3199[B]:GLN:HB2	1.38	0.79
3:L:3180[A]:TYR:O	3:L:3183[A]:LEU:HD22	1.81	0.79
3:O:2949[A]:LYS:O	3:O:2949[A]:LYS:NZ	2.16	0.79
3:O:3135[B]:LYS:CG	3:O:3141[B]:TYR:CD1	2.65	0.79
3:R:2965[B]:LEU:HD11	3:R:2974[B]:ALA:CA	2.12	0.79
3:U:3135[A]:LYS:CG	3:U:3141[A]:TYR:CD1	2.65	0.79
3:U:3135[B]:LYS:CG	3:U:3141[B]:TYR:CD1	2.65	0.79
3:U:3176[B]:LYS:CD	3:d:3152[B]:LYS:CD	2.54	0.79
3:d:2949[B]:LYS:O	3:d:2949[B]:LYS:NZ	2.16	0.79
3:C:2965[B]:LEU:O	3:L:3256[B]:TRP:CA	2.19	0.79
3:C:3090[B]:ASN:HD22	3:L:2972[B]:GLY:CA	1.76	0.79
3:F:2964[B]:PRO:C	3:a:3221[B]:ALA:HB3	2.08	0.79
3:F:2965[B]:LEU:HD11	3:F:2974[B]:ALA:CA	2.12	0.79
3:F:3149[B]:ASN:ND2	3:a:3163[B]:ASN:CG	2.39	0.79
3:F:3180[B]:TYR:HB2	3:F:3183[B]:LEU:HD22	1.63	0.79
3:F:3212[A]:ARG:HG3	3:F:3212[A]:ARG:HH11	1.43	0.79
3:I:3023[B]:ILE:O	3:I:3026[B]:THR:N	2.11	0.79
1:M:915:ASN:ND2	1:M:1095:MET:SD	2.56	0.79
3:O:2948[A]:ASP:N	3:O:2949[A]:LYS:CA	2.41	0.79
3:O:3109[B]:TYR:CD1	3:X:2969[B]:TYR:C	2.56	0.79
3:U:2948[B]:ASP:N	3:U:2949[B]:LYS:CA	2.41	0.79
3:U:3180[B]:TYR:HB2	3:U:3183[B]:LEU:HD22	1.63	0.79
3:X:3180[B]:TYR:O	3:X:3183[B]:LEU:HD22	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:2965[B]:LEU:HD11	3:a:2974[B]:ALA:CA	2.12	0.79
3:d:3101[A]:PRO:O	3:d:3106[A]:THR:HG21	1.81	0.79
1:A:456:GLN:NE2	1:A:549:PRO:O	2.16	0.79
3:C:2963[B]:MET:HE1	3:L:3223[B]:GLY:N	1.97	0.79
3:C:2965[B]:LEU:HD11	3:C:2974[B]:ALA:CA	2.12	0.79
3:C:3101[B]:PRO:O	3:C:3106[B]:THR:HG21	1.81	0.79
3:F:2984[B]:THR:HG23	3:a:3159[B]:SER:HB3	0.80	0.79
3:F:3151[B]:LEU:HB2	3:F:3175[B]:TYR:CD2	2.18	0.79
3:I:2963[B]:MET:CE	3:R:3223[B]:GLY:HA3	2.10	0.79
3:R:3148[A]:ILE:O	3:R:3152[A]:LYS:HE3	1.83	0.79
3:R:3151[B]:LEU:HB2	3:R:3175[B]:TYR:CD2	2.18	0.79
3:a:3025[A]:VAL:HG23	3:a:3033[A]:PHE:O	1.83	0.79
3:a:3180[B]:TYR:O	3:a:3183[B]:LEU:HD22	1.81	0.79
3:d:2939[B]:ARG:HB3	3:d:3032[B]:PRO:HG2	1.63	0.79
3:d:3025[B]:VAL:HG23	3:d:3033[B]:PHE:O	1.83	0.79
3:C:2979[A]:GLN:CG	3:C:3155[A]:MET:CE	2.56	0.79
3:C:3149[B]:ASN:ND2	3:L:3163[B]:ASN:HB3	1.97	0.79
3:C:3151[A]:LEU:HB2	3:C:3175[A]:TYR:CD2	2.18	0.79
3:F:2965[A]:LEU:HD11	3:F:2974[A]:ALA:CA	2.12	0.79
3:F:3101[B]:PRO:O	3:F:3106[B]:THR:HG21	1.81	0.79
3:F:3148[A]:ILE:O	3:F:3152[A]:LYS:HE3	1.83	0.79
3:F:3173[B]:THR:C	3:a:3154[B]:PRO:N	2.41	0.79
2:H:2868:GLU:CD	3:I:2932[A]:PRO:C	2.49	0.79
3:I:3160[B]:SER:CB	3:R:2983[B]:VAL:HG23	2.07	0.79
3:L:2965[B]:LEU:HD11	3:L:2974[B]:ALA:CA	2.12	0.79
3:L:3135[A]:LYS:CG	3:L:3141[A]:TYR:CD1	2.65	0.79
3:O:2969[A]:TYR:HB3	3:O:2971[A]:ASP:OD1	1.82	0.79
3:O:3173[B]:THR:CB	3:O:3176[B]:LYS:HD2	2.13	0.79
3:U:3025[B]:VAL:HG23	3:U:3033[B]:PHE:O	1.83	0.79
3:U:3156[B]:MET:SD	3:d:2982[B]:MET:HB3	2.22	0.79
3:X:2948[B]:ASP:N	3:X:2949[B]:LYS:CA	2.41	0.79
3:X:2979[A]:GLN:CG	3:X:3155[A]:MET:CE	2.56	0.79
3:a:3180[B]:TYR:HB2	3:a:3183[B]:LEU:HD22	1.64	0.79
3:d:2956[A]:LYS:O	3:d:2960[A]:PHE:CD1	2.33	0.79
3:d:2979[B]:GLN:CG	3:d:3155[B]:MET:CE	2.55	0.79
3:d:3180[A]:TYR:O	3:d:3183[A]:LEU:HD22	1.81	0.79
3:C:3150[B]:LYS:HZ3	3:L:3160[B]:SER:HB2	0.62	0.79
3:C:3151[B]:LEU:HB2	3:C:3175[B]:TYR:CD2	2.18	0.79
3:C:3151[B]:LEU:O	3:L:3154[B]:PRO:HB3	1.81	0.79
3:C:3252[B]:TYR:CD1	3:L:3223[B]:GLY:O	2.35	0.79
3:C:3255[B]:PRO:CA	3:L:2964[B]:PRO:O	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2969[B]:TYR:HB3	3:F:2971[B]:ASP:OD1	1.82	0.79
3:F:3153[B]:LYS:HB3	3:a:3155[B]:MET:HB2	1.58	0.79
1:G:1063:ARG:HB3	1:G:1065:LYS:HD2	1.61	0.79
3:I:2976[B]:ALA:N	3:R:3253[B]:GLU:CB	2.38	0.79
3:I:3158[B]:PHE:HB2	3:R:3153[B]:LYS:CB	2.13	0.79
3:I:3180[A]:TYR:HB2	3:I:3183[A]:LEU:HD22	1.63	0.79
3:L:2979[B]:GLN:CG	3:L:3155[B]:MET:CE	2.56	0.79
2:N:2180:TRP:HB2	2:N:2243:LEU:HD13	1.64	0.79
3:O:2969[B]:TYR:HB3	3:O:2971[B]:ASP:OD1	1.82	0.79
1:S:1275:ARG:HH12	1:S:1357:ARG:HH12	1.26	0.79
3:a:2969[A]:TYR:HB3	3:a:2971[A]:ASP:OD1	1.82	0.79
3:d:2939[A]:ARG:HB3	3:d:3032[A]:PRO:HG2	1.63	0.79
3:F:3135[B]:LYS:CG	3:F:3141[B]:TYR:CD1	2.65	0.79
3:F:3151[A]:LEU:HB2	3:F:3175[A]:TYR:CD2	2.18	0.79
3:I:2974[B]:ALA:H	3:R:3249[B]:GLY:N	1.79	0.79
3:I:2982[B]:MET:CE	3:R:2966[B]:SER:CB	2.55	0.79
3:I:3148[B]:ILE:O	3:I:3152[B]:LYS:HE3	1.83	0.79
3:I:3156[B]:MET:H	3:R:2979[B]:GLN:NE2	1.79	0.79
3:L:2952[A]:ALA:CB	3:L:2953[A]:GLY:C	2.48	0.79
3:L:3151[B]:LEU:HB2	3:L:3175[B]:TYR:CD2	2.18	0.79
3:O:2956[A]:LYS:O	3:O:2960[A]:PHE:HE1	1.22	0.79
3:O:3231[B]:ASP:N	3:O:3284[B]:LYS:O	2.14	0.79
3:O:3255[B]:PRO:HG3	3:X:3163[B]:ASN:HB3	1.62	0.79
3:R:3180[B]:TYR:HB2	3:R:3183[B]:LEU:HD22	1.64	0.79
1:V:1137:LYS:HA	1:V:1141:ARG:HH12	1.47	0.79
1:V:1140:ASN:ND2	1:V:1236:TYR:OH	2.16	0.79
3:a:3025[A]:VAL:CG2	3:a:3047[A]:ARG:HH12	1.94	0.79
1:b:550:ILE:N	1:b:557:VAL:O	2.16	0.79
3:d:2965[A]:LEU:HD11	3:d:2974[A]:ALA:CA	2.12	0.79
3:d:3023[A]:ILE:O	3:d:3026[A]:THR:N	2.11	0.79
3:d:3025[A]:VAL:CG2	3:d:3047[A]:ARG:HH12	1.94	0.79
3:C:3255[B]:PRO:HB2	3:L:2959[B]:SER:C	2.07	0.79
3:C:3256[B]:TRP:CZ2	3:L:2965[B]:LEU:CG	2.47	0.79
3:F:2977[B]:CYS:CB	3:a:2982[B]:MET:HE3	2.12	0.79
3:F:3230[B]:PHE:CB	3:F:3243[B]:GLY:HA2	2.06	0.79
1:G:724:LYS:HA	1:G:728:ARG:HH12	1.47	0.79
2:H:2797:LYS:HZ3	3:I:3028[A]:PRO:HD3	1.48	0.79
3:I:2949[B]:LYS:O	3:I:2949[B]:LYS:NZ	2.16	0.79
3:I:3025[B]:VAL:CG2	3:I:3047[B]:ARG:HH12	1.94	0.79
3:I:3162[B]:ASP:CA	3:R:3259[B]:ASP:HB3	2.13	0.79
3:I:3231[B]:ASP:N	3:I:3284[B]:LYS:O	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2625:LEU:HD13	2:K:2626:ARG:HG2	1.64	0.79
3:L:2956[B]:LYS:O	3:L:2960[B]:PHE:CD1	2.33	0.79
3:L:2956[B]:LYS:C	3:L:2960[B]:PHE:CE1	2.47	0.79
3:O:3025[B]:VAL:HG23	3:O:3033[B]:PHE:O	1.83	0.79
3:O:3173[A]:THR:CB	3:O:3176[A]:LYS:HD2	2.13	0.79
3:R:2949[B]:LYS:O	3:R:2949[B]:LYS:NZ	2.16	0.79
3:R:3135[B]:LYS:CG	3:R:3141[B]:TYR:CD1	2.65	0.79
3:R:3151[A]:LEU:HB2	3:R:3175[A]:TYR:CD2	2.18	0.79
3:U:3148[B]:ILE:O	3:U:3152[B]:LYS:HE3	1.83	0.79
3:U:3256[B]:TRP:HB2	3:d:2969[B]:TYR:H	1.44	0.79
3:X:3151[A]:LEU:HB2	3:X:3175[A]:TYR:CD2	2.18	0.79
3:d:3148[B]:ILE:O	3:d:3152[B]:LYS:HE3	1.83	0.79
3:C:2965[B]:LEU:HB3	3:L:3256[B]:TRP:CZ2	1.72	0.79
3:F:2969[A]:TYR:HB3	3:F:2971[A]:ASP:OD1	1.82	0.79
3:F:3161[B]:GLU:CA	3:a:3147[B]:GLU:HG3	2.12	0.79
3:I:2955[B]:GLN:CD	3:I:3037[B]:TYR:CE1	2.55	0.79
3:I:2956[B]:LYS:HD2	3:R:3257[B]:ALA:CB	2.13	0.79
3:I:2975[B]:PHE:CE2	3:R:2961[B]:HIS:HA	2.18	0.79
1:J:589:GLN:HG2	1:J:594:ASP:HB3	1.65	0.79
3:L:2939[B]:ARG:HB3	3:L:3032[B]:PRO:HG2	1.63	0.79
3:L:3025[B]:VAL:HG23	3:L:3033[B]:PHE:O	1.83	0.79
3:L:3148[A]:ILE:O	3:L:3152[A]:LYS:HE3	1.83	0.79
3:O:2965[B]:LEU:HD11	3:O:2974[B]:ALA:CA	2.12	0.79
3:O:3153[B]:LYS:NZ	3:X:3170[B]:ALA:O	2.13	0.79
2:Q:2114:ARG:HH12	2:Q:2120:GLU:HG3	1.47	0.79
3:U:2980[B]:HIS:HB3	3:d:2969[B]:TYR:OH	1.83	0.79
3:U:3256[B]:TRP:C	3:d:2969[B]:TYR:H	1.90	0.79
3:X:3135[B]:LYS:CG	3:X:3141[B]:TYR:CD1	2.65	0.79
3:a:2979[B]:GLN:CG	3:a:3155[B]:MET:CE	2.56	0.79
3:a:3135[B]:LYS:CG	3:a:3141[B]:TYR:CD1	2.65	0.79
3:a:3173[A]:THR:CB	3:a:3176[A]:LYS:HD2	2.13	0.79
3:d:3180[B]:TYR:HB2	3:d:3183[B]:LEU:HD22	1.63	0.79
3:C:2952[A]:ALA:CB	3:C:2953[A]:GLY:C	2.48	0.79
3:C:2988[B]:TRP:HD1	3:L:3153[B]:LYS:CD	1.95	0.79
3:C:3025[A]:VAL:CG2	3:C:3047[A]:ARG:HH12	1.94	0.79
3:C:3025[A]:VAL:HG23	3:C:3033[A]:PHE:O	1.83	0.79
3:C:3104[B]:MET:CA	3:C:3110[B]:THR:HG23	2.10	0.79
3:C:3148[B]:ILE:O	3:C:3152[B]:LYS:HE3	1.83	0.79
3:F:3150[B]:LYS:O	3:a:3159[B]:SER:OG	1.82	0.79
3:F:3170[B]:ALA:O	3:a:3152[B]:LYS:HB3	1.82	0.79
3:I:3173[B]:THR:CB	3:I:3176[B]:LYS:HD2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:210:HIS:HA	1:J:213:VAL:HG22	1.64	0.79
3:L:3180[A]:TYR:HB2	3:L:3183[A]:LEU:HD22	1.63	0.79
3:O:3135[A]:LYS:CG	3:O:3141[A]:TYR:CD1	2.65	0.79
3:O:3148[B]:ILE:O	3:O:3152[B]:LYS:HE3	1.83	0.79
3:O:3180[B]:TYR:HB2	3:O:3183[B]:LEU:HD22	1.64	0.79
3:O:3196[A]:THR:HG21	1:P:416:ASN:CG	2.06	0.79
3:R:2969[B]:TYR:HB3	3:R:2971[B]:ASP:OD1	1.82	0.79
3:U:2971[B]:ASP:O	3:d:3247[B]:VAL:HG13	1.82	0.79
3:a:3151[A]:LEU:HB2	3:a:3175[A]:TYR:CD2	2.18	0.79
3:a:3185[B]:TYR:HE2	3:a:3187[B]:TYR:CE2	2.01	0.79
3:d:3024[B]:LEU:CD1	3:d:3025[B]:VAL:H	1.83	0.79
3:d:3135[B]:LYS:CG	3:d:3141[B]:TYR:CD1	2.65	0.79
3:d:3173[A]:THR:CB	3:d:3176[A]:LYS:HD2	2.13	0.79
3:C:3135[B]:LYS:CG	3:C:3141[B]:TYR:CD1	2.65	0.78
3:C:3150[B]:LYS:H	3:L:3169[B]:LYS:HG2	1.46	0.78
3:F:3173[A]:THR:CB	3:F:3176[A]:LYS:HD2	2.13	0.78
3:I:2949[A]:LYS:O	3:I:2949[A]:LYS:NZ	2.16	0.78
3:I:2982[B]:MET:HB3	3:R:3160[B]:SER:HB2	1.65	0.78
3:I:2989[B]:HIS:HD2	3:R:2970[B]:PRO:CA	1.96	0.78
3:I:3153[B]:LYS:C	3:R:3155[B]:MET:H	1.90	0.78
3:I:3155[B]:MET:HB2	3:R:3153[B]:LYS:CB	2.13	0.78
3:L:3230[B]:PHE:CB	3:L:3243[B]:GLY:HA2	2.06	0.78
3:O:3148[A]:ILE:O	3:O:3152[A]:LYS:HE3	1.83	0.78
3:U:3151[A]:LEU:HB2	3:U:3175[A]:TYR:CD2	2.18	0.78
3:U:3173[B]:THR:CB	3:U:3176[B]:LYS:HD2	2.13	0.78
3:X:2949[A]:LYS:NZ	3:X:2949[A]:LYS:O	2.16	0.78
3:X:2965[A]:LEU:HD11	3:X:2974[A]:ALA:CA	2.12	0.78
3:X:3025[B]:VAL:HG23	3:X:3033[B]:PHE:O	1.83	0.78
3:X:3180[B]:TYR:HB2	3:X:3183[B]:LEU:HD22	1.63	0.78
1:Y:1551:ASP:OD1	3:d:3007[B]:ILE:HD13	1.82	0.78
3:d:3135[A]:LYS:CG	3:d:3141[A]:TYR:CD1	2.65	0.78
3:C:2949[B]:LYS:NZ	3:C:2949[B]:LYS:O	2.16	0.78
3:C:3159[B]:SER:CB	3:L:2984[B]:THR:HG21	1.96	0.78
3:C:3258[B]:PHE:CZ	3:L:2968[B]:GLN:OE1	2.36	0.78
3:F:2985[B]:PHE:HE2	3:a:2969[B]:TYR:O	1.66	0.78
3:F:3180[A]:TYR:HB2	3:F:3183[A]:LEU:HD22	1.64	0.78
3:F:3254[B]:MET:HG3	3:a:2966[B]:SER:CB	2.08	0.78
3:I:2948[B]:ASP:N	3:I:2949[B]:LYS:CA	2.41	0.78
3:I:2961[A]:HIS:HD2	3:I:2988[A]:TRP:HZ3	1.32	0.78
3:I:2964[B]:PRO:HB2	3:R:3255[B]:PRO:HB3	1.63	0.78
3:I:2982[B]:MET:HE3	3:R:2977[B]:CYS:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3024[A]:LEU:CD1	3:I:3025[A]:VAL:H	1.84	0.78
3:L:2949[A]:LYS:O	3:L:2949[A]:LYS:NZ	2.16	0.78
3:L:3185[A]:TYR:HE2	3:L:3187[A]:TYR:CE2	2.01	0.78
3:O:2970[B]:PRO:CG	3:X:2991[B]:LEU:HB2	2.03	0.78
3:U:3153[B]:LYS:CD	3:d:2979[B]:GLN:NE2	2.47	0.78
3:U:3256[B]:TRP:CB	3:d:2969[B]:TYR:N	2.46	0.78
1:V:527:LEU:HD22	1:V:629:MET:HG3	1.66	0.78
1:V:1046:HIS:HA	1:V:1049:VAL:HB	1.64	0.78
1:Y:1616:LYS:HD3	3:d:3188[B]:ASP:CA	2.11	0.78
2:Z:2545:SER:HA	2:Z:2546:LEU:HB2	1.65	0.78
3:a:3025[B]:VAL:HG23	3:a:3033[B]:PHE:O	1.83	0.78
2:c:2166:LEU:HA	2:c:2169:HIS:HB2	1.65	0.78
3:C:3135[A]:LYS:CG	3:C:3141[A]:TYR:CD1	2.65	0.78
1:D:567:LEU:HB2	1:D:609:TRP:HD1	1.45	0.78
3:F:2952[B]:ALA:CB	3:F:2953[B]:GLY:C	2.48	0.78
3:F:2965[B]:LEU:CA	3:a:3221[B]:ALA:CB	2.49	0.78
3:F:2985[B]:PHE:HE2	3:a:2969[B]:TYR:C	1.90	0.78
3:I:2961[B]:HIS:HD2	3:I:2988[B]:TRP:HZ3	1.31	0.78
3:L:3104[B]:MET:CA	3:L:3110[B]:THR:HG23	2.10	0.78
3:O:2952[A]:ALA:CB	3:O:2953[A]:GLY:C	2.48	0.78
3:O:2975[B]:PHE:C	3:X:3156[B]:MET:HG3	2.06	0.78
3:O:3025[A]:VAL:HG23	3:O:3033[A]:PHE:O	1.83	0.78
3:O:3025[B]:VAL:CG2	3:O:3047[B]:ARG:HH12	1.94	0.78
1:P:979:LEU:HB2	1:P:980:TYR:HA	1.65	0.78
3:R:3025[A]:VAL:HG23	3:R:3033[A]:PHE:O	1.83	0.78
3:R:3173[A]:THR:CB	3:R:3176[A]:LYS:HD2	2.13	0.78
3:U:2949[B]:LYS:NZ	3:U:2949[B]:LYS:O	2.16	0.78
3:U:3148[A]:ILE:O	3:U:3152[A]:LYS:HE3	1.83	0.78
3:U:3151[B]:LEU:HB2	3:U:3175[B]:TYR:CD2	2.18	0.78
3:U:3160[B]:SER:CB	3:d:3259[B]:ASP:HB3	2.12	0.78
3:U:3185[A]:TYR:HE2	3:U:3187[A]:TYR:CE2	2.01	0.78
3:X:3135[A]:LYS:CG	3:X:3141[A]:TYR:CD1	2.65	0.78
3:X:3173[B]:THR:CB	3:X:3176[B]:LYS:HD2	2.13	0.78
2:Z:2898:LYS:HE2	2:Z:2898:LYS:H	1.48	0.78
3:C:3141[A]:TYR:HD2	3:C:3142[A]:ASN:H	0.78	0.78
3:C:3159[B]:SER:CB	3:L:3150[B]:LYS:C	2.57	0.78
3:F:2961[B]:HIS:HD2	3:F:2988[B]:TRP:HZ3	1.31	0.78
3:F:3025[B]:VAL:HG23	3:F:3033[B]:PHE:O	1.83	0.78
3:F:3185[A]:TYR:HE2	3:F:3187[A]:TYR:CE2	2.01	0.78
3:I:2966[B]:SER:HB2	3:R:3254[B]:MET:HG3	0.85	0.78
3:I:3135[A]:LYS:CG	3:I:3141[A]:TYR:CD1	2.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2952[B]:ALA:CB	3:L:2953[B]:GLY:C	2.48	0.78
3:L:2979[B]:GLN:NE2	3:L:3155[B]:MET:CE	2.47	0.78
3:O:3141[A]:TYR:HD2	3:O:3142[A]:ASN:H	0.78	0.78
1:P:161:ASN:OD1	1:P:174:GLN:NE2	2.16	0.78
3:R:2979[A]:GLN:CG	3:R:3155[A]:MET:CE	2.56	0.78
3:R:3185[A]:TYR:HE2	3:R:3187[A]:TYR:CE2	2.02	0.78
3:R:3259[B]:ASP:OD2	3:R:3260[B]:ARG:HG2	1.84	0.78
3:U:2949[A]:LYS:O	3:U:2949[A]:LYS:NZ	2.16	0.78
3:U:2965[B]:LEU:CA	3:d:3220[B]:ARG:HH11	1.70	0.78
3:X:3185[B]:TYR:HE2	3:X:3187[B]:TYR:CE2	2.02	0.78
3:a:2949[B]:LYS:O	3:a:2949[B]:LYS:NZ	2.16	0.78
3:F:2956[A]:LYS:O	3:F:2960[A]:PHE:CD1	2.33	0.78
3:F:3185[B]:TYR:HE2	3:F:3187[B]:TYR:CE2	2.01	0.78
3:I:3141[A]:TYR:HD2	3:I:3142[A]:ASN:H	0.78	0.78
3:I:3148[A]:ILE:O	3:I:3152[A]:LYS:HE3	1.83	0.78
3:I:3150[B]:LYS:HB2	3:R:3169[B]:LYS:HG3	1.64	0.78
3:L:2969[A]:TYR:HB3	3:L:2971[A]:ASP:OD1	1.82	0.78
3:L:3185[B]:TYR:HE2	3:L:3187[B]:TYR:CE2	2.01	0.78
3:O:3151[B]:LEU:HB2	3:O:3175[B]:TYR:CD2	2.18	0.78
3:O:3159[B]:SER:C	3:X:3148[B]:ILE:C	2.51	0.78
1:S:573:LYS:HB3	1:S:574:GLY:HA2	1.66	0.78
1:S:1618:LEU:HD22	3:X:3136[B]:TYR:HE2	1.49	0.78
2:T:2184:MET:HE3	2:T:2231:LEU:HG	1.65	0.78
3:U:3169[B]:LYS:HE3	3:d:3147[B]:GLU:HA	1.61	0.78
3:U:3255[B]:PRO:HG2	3:d:3252[B]:TYR:CB	2.13	0.78
3:U:3259[A]:ASP:OD2	3:U:3260[A]:ARG:HG2	1.84	0.78
1:Y:1546:LYS:HB2	3:d:3001[B]:LYS:HZ1	0.95	0.78
3:a:3023[A]:ILE:O	3:a:3026[A]:THR:N	2.11	0.78
3:a:3151[B]:LEU:HB2	3:a:3175[B]:TYR:CD2	2.18	0.78
3:d:3259[A]:ASP:OD2	3:d:3260[A]:ARG:HG2	1.84	0.78
3:C:2981[B]:GLY:N	3:L:2968[B]:GLN:HG2	1.97	0.78
3:C:3173[B]:THR:CB	3:C:3176[B]:LYS:HD2	2.13	0.78
3:I:3025[A]:VAL:HG23	3:I:3033[A]:PHE:O	1.83	0.78
3:I:3151[A]:LEU:HB2	3:I:3175[A]:TYR:CD2	2.18	0.78
3:I:3185[B]:TYR:HE2	3:I:3187[B]:TYR:CE2	2.01	0.78
1:J:1137:LYS:HA	1:J:1141:ARG:HH12	1.48	0.78
3:L:3173[A]:THR:CB	3:L:3176[A]:LYS:HD2	2.13	0.78
3:L:3259[B]:ASP:OD2	3:L:3260[B]:ARG:HG2	1.84	0.78
3:O:2979[A]:GLN:NE2	3:O:3155[A]:MET:CE	2.47	0.78
3:R:2961[A]:HIS:HD2	3:R:2988[A]:TRP:HZ3	1.31	0.78
3:U:2948[A]:ASP:N	3:U:2949[A]:LYS:CA	2.41	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2975[B]:PHE:N	3:d:3256[B]:TRP:O	2.16	0.78
3:U:2982[B]:MET:C	3:d:2970[B]:PRO:HD3	2.00	0.78
3:U:3169[B]:LYS:CD	3:d:3147[B]:GLU:CA	2.61	0.78
3:U:3259[B]:ASP:OD2	3:U:3260[B]:ARG:HG2	1.84	0.78
3:X:3141[A]:TYR:HD2	3:X:3142[A]:ASN:H	0.78	0.78
3:d:2949[A]:LYS:O	3:d:2949[A]:LYS:NZ	2.16	0.78
3:d:3173[B]:THR:CB	3:d:3176[B]:LYS:HD2	2.13	0.78
2:B:2867:PRO:HG2	3:C:2932[A]:PRO:CG	2.14	0.78
3:C:3155[B]:MET:CE	3:L:3154[B]:PRO:O	2.31	0.78
3:C:3256[B]:TRP:CE2	3:L:2965[B]:LEU:C	2.52	0.78
3:F:3160[B]:SER:OG	3:a:2982[B]:MET:CA	2.30	0.78
3:I:3141[B]:TYR:HD2	3:I:3142[B]:ASN:H	0.78	0.78
3:L:3104[A]:MET:CA	3:L:3110[A]:THR:HG23	2.10	0.78
3:L:3173[B]:THR:CB	3:L:3176[B]:LYS:HD2	2.13	0.78
3:O:3185[B]:TYR:HE2	3:O:3187[B]:TYR:CE2	2.01	0.78
3:O:3259[B]:ASP:OD2	3:O:3260[B]:ARG:HG2	1.84	0.78
3:R:3023[B]:ILE:O	3:R:3026[B]:THR:N	2.11	0.78
3:R:3173[B]:THR:CB	3:R:3176[B]:LYS:HD2	2.13	0.78
3:U:2939[A]:ARG:HB3	3:U:3032[A]:PRO:HG2	1.63	0.78
3:U:3025[A]:VAL:HG23	3:U:3033[A]:PHE:O	1.83	0.78
3:a:2979[A]:GLN:NE2	3:a:3155[A]:MET:CE	2.47	0.78
3:a:3259[B]:ASP:OD2	3:a:3260[B]:ARG:HG2	1.84	0.78
4:q:2:NAG:H83	4:q:2:NAG:H3	1.66	0.78
3:C:2961[B]:HIS:HD2	3:C:2988[B]:TRP:HZ3	1.31	0.78
3:C:2965[B]:LEU:O	3:L:3256[B]:TRP:CE3	2.13	0.78
1:D:1296:VAL:HB	1:D:1446:ASP:HB3	1.65	0.78
3:F:2949[A]:LYS:O	3:F:2949[A]:LYS:NZ	2.16	0.78
3:I:2979[B]:GLN:NE2	3:I:3155[B]:MET:CE	2.47	0.78
3:L:3148[B]:ILE:O	3:L:3152[B]:LYS:HE3	1.83	0.78
1:P:142:ARG:NH1	1:P:340:GLN:OE1	2.16	0.78
3:R:3259[A]:ASP:OD2	3:R:3260[A]:ARG:HG2	1.84	0.78
2:T:2711:HIS:HA	2:T:2714:VAL:HG22	1.66	0.78
3:U:3173[A]:THR:CB	3:U:3176[A]:LYS:HD2	2.13	0.78
3:U:3256[B]:TRP:HB3	3:d:2975[B]:PHE:CZ	2.18	0.78
3:U:3284[A]:LYS:CD	3:U:3285[A]:VAL:N	2.47	0.78
3:X:2949[B]:LYS:O	3:X:2949[B]:LYS:NZ	2.16	0.78
3:X:3151[B]:LEU:HB2	3:X:3175[B]:TYR:CD2	2.18	0.78
1:Y:898:GLY:HA2	1:Y:1186:TRP:HB2	1.64	0.78
2:c:2638:ARG:NH1	2:c:2704:ASP:OD1	2.16	0.78
3:d:3151[A]:LEU:HB2	3:d:3175[A]:TYR:CD2	2.18	0.78
1:A:401:VAL:HG22	1:A:662:SER:HB3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3093[B]:HIS:ND1	3:L:2971[B]:ASP:HB3	1.72	0.78
3:C:3150[B]:LYS:HD3	3:L:3156[B]:MET:HA	1.66	0.78
3:C:3185[A]:TYR:HE2	3:C:3187[A]:TYR:CE2	2.01	0.78
3:F:3173[B]:THR:CB	3:F:3176[B]:LYS:HD2	2.13	0.78
3:I:3153[B]:LYS:HD3	3:R:2988[B]:TRP:CD1	2.18	0.78
3:I:3259[B]:ASP:OD2	3:I:3260[B]:ARG:HG2	1.84	0.78
3:L:2949[B]:LYS:O	3:L:2949[B]:LYS:NZ	2.16	0.78
3:O:2963[B]:MET:HE1	3:X:2975[B]:PHE:HB2	1.65	0.78
3:R:3025[B]:VAL:HG23	3:R:3033[B]:PHE:O	1.83	0.78
3:U:2969[B]:TYR:HB3	3:U:2971[B]:ASP:OD1	1.82	0.78
3:U:3252[B]:TYR:O	3:d:3255[B]:PRO:CB	2.32	0.78
1:V:401:VAL:HG22	1:V:662:SER:HB3	1.65	0.78
3:X:3104[A]:MET:CA	3:X:3110[A]:THR:HG23	2.10	0.78
3:X:3259[B]:ASP:OD2	3:X:3260[B]:ARG:HG2	1.84	0.78
3:a:2961[A]:HIS:HD2	3:a:2988[A]:TRP:HZ3	1.31	0.78
3:C:2974[B]:ALA:HB2	3:L:3249[B]:GLY:HA3	1.66	0.78
3:C:2979[A]:GLN:NE2	3:C:3155[A]:MET:CE	2.47	0.78
3:C:3154[B]:PRO:CB	3:L:3151[B]:LEU:C	2.57	0.78
3:C:3173[A]:THR:CB	3:C:3176[A]:LYS:HD2	2.13	0.78
3:C:3259[A]:ASP:OD2	3:C:3260[A]:ARG:HG2	1.84	0.78
3:F:2949[B]:LYS:O	3:F:2949[B]:LYS:NZ	2.16	0.78
3:I:2979[A]:GLN:NE2	3:I:3155[A]:MET:CE	2.47	0.78
3:I:2988[B]:TRP:CH2	3:R:2975[B]:PHE:CE2	2.71	0.78
3:L:3180[B]:TYR:HB2	3:L:3183[B]:LEU:HD22	1.63	0.78
3:O:2976[B]:ALA:C	3:X:3154[B]:PRO:O	2.27	0.78
3:O:3151[A]:LEU:HB2	3:O:3175[A]:TYR:CD2	2.18	0.78
3:R:3104[A]:MET:CA	3:R:3110[A]:THR:HG23	2.10	0.78
3:R:3148[B]:ILE:O	3:R:3152[B]:LYS:HE3	1.83	0.78
1:S:19:GLN:NE2	1:S:121:ASN:OD1	2.17	0.78
3:U:2965[B]:LEU:CD1	3:d:3220[B]:ARG:C	2.57	0.78
3:U:3141[A]:TYR:HD2	3:U:3142[A]:ASN:H	0.78	0.78
3:U:3154[B]:PRO:HG3	3:d:2984[B]:THR:HG23	1.64	0.78
3:X:3025[A]:VAL:HG23	3:X:3033[A]:PHE:O	1.83	0.78
3:a:3148[B]:ILE:O	3:a:3152[B]:LYS:HE3	1.83	0.78
3:a:3173[B]:THR:CB	3:a:3176[B]:LYS:HD2	2.13	0.78
3:a:3259[A]:ASP:OD2	3:a:3260[A]:ARG:HG2	1.84	0.78
3:d:3148[A]:ILE:O	3:d:3152[A]:LYS:HE3	1.83	0.78
3:d:3185[B]:TYR:HE2	3:d:3187[B]:TYR:CE2	2.01	0.78
2:B:2107:LEU:HD23	2:B:2208:PRO:HB2	1.64	0.77
3:C:2982[B]:MET:N	3:L:2967[B]:CYS:HB3	1.99	0.77
3:C:3149[B]:ASN:O	3:L:3172[B]:SER:HB3	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3172[B]:SER:OG	3:L:3152[B]:LYS:N	2.15	0.77
3:F:3259[A]:ASP:OD2	3:F:3260[A]:ARG:HG2	1.84	0.77
3:I:3023[A]:ILE:O	3:I:3026[A]:THR:N	2.11	0.77
3:I:3148[B]:ILE:O	3:R:3170[B]:ALA:N	2.17	0.77
3:I:3149[B]:ASN:CB	3:R:3163[B]:ASN:CG	2.55	0.77
3:L:2948[A]:ASP:H	3:L:2949[A]:LYS:CA	1.98	0.77
3:L:3135[B]:LYS:CG	3:L:3141[B]:TYR:CD1	2.65	0.77
3:L:3284[B]:LYS:CD	3:L:3285[B]:VAL:N	2.47	0.77
3:O:3230[A]:PHE:CB	3:O:3243[A]:GLY:HA2	2.06	0.77
3:U:2979[B]:GLN:NE2	3:U:3155[B]:MET:CE	2.47	0.77
3:U:3284[B]:LYS:CD	3:U:3285[B]:VAL:N	2.47	0.77
3:U:3306[B]:LEU:HD12	3:U:3307[B]:PHE:N	2.00	0.77
3:C:3255[B]:PRO:HD2	3:L:2960[B]:PHE:C	2.10	0.77
3:C:3284[B]:LYS:CD	3:C:3285[B]:VAL:N	2.47	0.77
3:F:3023[A]:ILE:O	3:F:3026[A]:THR:N	2.11	0.77
3:F:3147[B]:GLU:H	3:a:3161[B]:GLU:HA	1.48	0.77
3:I:3151[B]:LEU:HB2	3:I:3175[B]:TYR:CD2	2.18	0.77
1:J:325:THR:OG1	1:J:332:ASP:N	2.17	0.77
3:L:3025[A]:VAL:HG23	3:L:3033[A]:PHE:O	1.83	0.77
3:L:3141[A]:TYR:HD2	3:L:3142[A]:ASN:H	0.78	0.77
3:L:3151[A]:LEU:HB2	3:L:3175[A]:TYR:CD2	2.18	0.77
1:M:456:GLN:NE2	1:M:549:PRO:O	2.17	0.77
1:M:1280:GLN:HE22	1:M:1337:ARG:HB3	1.47	0.77
2:N:2528:LYS:NZ	2:N:2626:ARG:O	2.16	0.77
3:R:2956[B]:LYS:C	3:R:2960[B]:PHE:CE1	2.47	0.77
1:V:1442:MET:HE1	1:V:1454:PHE:HA	1.66	0.77
3:a:2949[A]:LYS:O	3:a:2949[A]:LYS:NZ	2.16	0.77
3:a:3180[A]:TYR:HB2	3:a:3183[A]:LEU:HD22	1.64	0.77
3:F:2955[A]:GLN:CD	3:F:3037[A]:TYR:HE1	1.92	0.77
3:F:2985[B]:PHE:CE2	3:a:2969[B]:TYR:O	2.37	0.77
3:F:3153[B]:LYS:HB3	3:a:3155[B]:MET:CB	2.06	0.77
3:I:3160[B]:SER:HA	3:R:2983[B]:VAL:CA	2.14	0.77
3:I:3173[A]:THR:CB	3:I:3176[A]:LYS:HD2	2.13	0.77
3:L:2961[B]:HIS:HD2	3:L:2988[B]:TRP:HZ3	1.32	0.77
3:O:2968[B]:GLN:HA	3:X:2988[B]:TRP:CD1	2.20	0.77
3:O:2969[B]:TYR:HA	3:X:2991[B]:LEU:HD22	1.67	0.77
3:O:3185[A]:TYR:HE2	3:O:3187[A]:TYR:CE2	2.01	0.77
3:R:3284[A]:LYS:CD	3:R:3285[A]:VAL:N	2.47	0.77
3:R:3284[B]:LYS:CD	3:R:3285[B]:VAL:N	2.47	0.77
1:S:161:ASN:ND2	1:S:174:GLN:OE1	2.17	0.77
3:U:2955[B]:GLN:CD	3:U:3037[B]:TYR:HE1	1.92	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2952[A]:ALA:CB	3:X:2953[A]:GLY:C	2.48	0.77
3:X:3284[B]:LYS:CD	3:X:3285[B]:VAL:N	2.47	0.77
3:d:3259[B]:ASP:OD2	3:d:3260[B]:ARG:HG2	1.84	0.77
3:C:3148[A]:ILE:O	3:C:3152[A]:LYS:HE3	1.83	0.77
3:C:3155[B]:MET:HG3	3:L:3154[B]:PRO:N	1.92	0.77
3:C:3252[B]:TYR:OH	3:L:3224[B]:GLN:HA	1.85	0.77
3:F:2965[B]:LEU:C	3:a:3255[B]:PRO:HA	2.08	0.77
3:F:3148[B]:ILE:O	3:F:3152[B]:LYS:HE3	1.83	0.77
3:I:2963[B]:MET:HE1	3:R:3223[B]:GLY:CA	2.10	0.77
3:I:2975[B]:PHE:CE1	3:R:2961[B]:HIS:O	2.37	0.77
3:I:2983[B]:VAL:HB	3:R:3160[B]:SER:HA	1.65	0.77
3:I:3120[B]:HIS:NE2	3:R:2969[B]:TYR:CD2	2.53	0.77
3:I:3150[B]:LYS:C	3:R:3172[B]:SER:CB	2.57	0.77
3:L:3113[B]:ASP:CG	3:L:3114[B]:PRO:CD	2.56	0.77
3:L:3306[B]:LEU:HD12	3:L:3307[B]:PHE:N	2.00	0.77
3:O:2948[A]:ASP:H	3:O:2949[A]:LYS:CA	1.98	0.77
3:O:2948[B]:ASP:N	3:O:2949[B]:LYS:CA	2.41	0.77
3:O:2949[B]:LYS:NZ	3:O:2949[B]:LYS:O	2.16	0.77
3:O:2975[B]:PHE:CE2	3:X:3172[B]:SER:HA	2.17	0.77
3:R:3185[B]:TYR:HE2	3:R:3187[B]:TYR:CE2	2.01	0.77
1:S:724:LYS:HA	1:S:728:ARG:HH12	1.49	0.77
3:U:3220[B]:ARG:CG	3:d:2973[B]:THR:HG22	2.15	0.77
3:X:3259[A]:ASP:OD2	3:X:3260[A]:ARG:HG2	1.84	0.77
3:a:2979[B]:GLN:NE2	3:a:3155[B]:MET:CE	2.47	0.77
3:a:3306[A]:LEU:HD12	3:a:3307[A]:PHE:N	2.00	0.77
3:d:3211[A]:ASP:HB3	3:d:3309[A]:PRO:HA	1.67	0.77
3:C:2955[A]:GLN:CD	3:C:3037[A]:TYR:HE1	1.92	0.77
3:C:3152[B]:LYS:HB2	3:L:3171[B]:HIS:C	2.09	0.77
3:C:3306[A]:LEU:HD12	3:C:3307[A]:PHE:N	2.00	0.77
3:F:2961[B]:HIS:HB3	3:F:3111[B]:SER:OG	1.85	0.77
3:F:2966[B]:SER:N	3:a:3255[B]:PRO:C	2.43	0.77
3:F:3141[A]:TYR:HD2	3:F:3142[A]:ASN:H	0.78	0.77
3:F:3159[B]:SER:OG	3:a:3150[B]:LYS:O	2.02	0.77
3:F:3284[B]:LYS:CD	3:F:3285[B]:VAL:N	2.47	0.77
3:I:2937[A]:ASN:HB2	3:I:3006[A]:LYS:CE	2.14	0.77
3:I:2975[B]:PHE:CE1	3:R:2961[B]:HIS:ND1	2.53	0.77
3:L:2961[A]:HIS:HD2	3:L:2988[A]:TRP:HZ3	1.31	0.77
3:O:2937[B]:ASN:CB	3:O:3006[B]:LYS:HE2	2.14	0.77
3:O:2952[B]:ALA:CB	3:O:2953[B]:GLY:C	2.48	0.77
1:P:2:LEU:HD21	1:P:81:VAL:HG21	1.66	0.77
3:X:3173[A]:THR:CB	3:X:3176[A]:LYS:HD2	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3306[B]:LEU:HD12	3:X:3307[B]:PHE:N	2.00	0.77
3:a:3148[A]:ILE:O	3:a:3152[A]:LYS:HE3	1.83	0.77
2:c:2554:PRO:HA	2:c:2555:GLU:HB3	1.67	0.77
1:A:1583:CYS:H	1:b:329:ARG:HB3	1.49	0.77
3:C:2981[B]:GLY:HA2	3:L:2968[B]:GLN:OE1	1.83	0.77
3:C:3185[B]:TYR:HE2	3:C:3187[B]:TYR:CE2	2.01	0.77
3:F:3025[A]:VAL:HG23	3:F:3033[A]:PHE:O	1.83	0.77
3:F:3158[B]:PHE:H	3:a:3153[B]:LYS:CE	1.96	0.77
3:I:3025[B]:VAL:HG23	3:I:3033[B]:PHE:O	1.83	0.77
3:I:3154[B]:PRO:HB3	3:R:3174[B]:GLY:HA3	1.64	0.77
2:N:2549:PRO:HD3	2:N:2556:TYR:HD2	1.50	0.77
3:U:3185[B]:TYR:HE2	3:U:3187[B]:TYR:CE2	2.01	0.77
3:U:3254[B]:MET:HE1	3:d:3254[B]:MET:HE1	1.59	0.77
3:U:3306[A]:LEU:HD12	3:U:3307[A]:PHE:N	2.00	0.77
1:Y:401:VAL:HG22	1:Y:662:SER:HB3	1.65	0.77
3:d:3025[A]:VAL:HG23	3:d:3033[A]:PHE:O	1.83	0.77
3:d:3104[A]:MET:CA	3:d:3110[A]:THR:HG23	2.10	0.77
3:d:3151[B]:LEU:HB2	3:d:3175[B]:TYR:CD2	2.18	0.77
3:C:2937[A]:ASN:HB2	3:C:3006[A]:LYS:CE	2.14	0.77
3:F:2979[B]:GLN:NE2	3:F:3155[B]:MET:CE	2.47	0.77
3:I:3090[B]:ASN:CA	3:R:2971[B]:ASP:O	2.31	0.77
3:I:3306[B]:LEU:HD12	3:I:3307[B]:PHE:N	2.00	0.77
2:K:2236:ALA:HB3	2:K:2239:LYS:HB2	1.66	0.77
3:L:3211[B]:ASP:HB3	3:L:3309[B]:PRO:HA	1.67	0.77
3:O:3259[A]:ASP:OD2	3:O:3260[A]:ARG:HG2	1.84	0.77
3:R:2961[B]:HIS:HB3	3:R:3111[B]:SER:OG	1.85	0.77
3:R:2979[B]:GLN:NE2	3:R:3155[B]:MET:CE	2.47	0.77
1:S:1617:LYS:CE	3:X:3135[B]:LYS:NZ	2.43	0.77
3:U:2948[B]:ASP:HB3	3:U:2949[B]:LYS:CA	2.15	0.77
3:U:2964[B]:PRO:C	3:d:3220[B]:ARG:HH12	1.92	0.77
3:X:2961[B]:HIS:HD2	3:X:2988[B]:TRP:HZ3	1.31	0.77
1:Y:567:LEU:N	1:Y:568:PHE:HA	2.00	0.77
3:a:2961[B]:HIS:HB3	3:a:3111[B]:SER:OG	1.85	0.77
3:C:2961[A]:HIS:HB3	3:C:3111[A]:SER:OG	1.85	0.77
3:C:3089[B]:HIS:ND1	3:L:2971[B]:ASP:HA	1.95	0.77
3:C:3211[A]:ASP:HB3	3:C:3309[A]:PRO:HA	1.67	0.77
3:F:2961[A]:HIS:HD2	3:F:2988[A]:TRP:HZ3	1.32	0.77
3:F:3161[B]:GLU:HB3	3:a:3079[B]:CYS:SG	2.25	0.77
3:F:3259[B]:ASP:OD2	3:F:3260[B]:ARG:HG2	1.84	0.77
3:I:2962[B]:GLY:C	3:R:3255[B]:PRO:HG3	2.09	0.77
3:I:2964[B]:PRO:HB3	3:R:3221[B]:ALA:HB3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2973[B]:THR:HG21	3:R:3106[B]:THR:C	2.09	0.77
1:J:164:GLU:O	1:J:297:ARG:NH2	2.17	0.77
3:L:2961[B]:HIS:HB3	3:L:3111[B]:SER:OG	1.85	0.77
3:L:3306[A]:LEU:HD12	3:L:3307[A]:PHE:N	2.00	0.77
3:O:3025[A]:VAL:CG2	3:O:3047[A]:ARG:HH12	1.94	0.77
3:R:2979[A]:GLN:NE2	3:R:3155[A]:MET:CE	2.47	0.77
3:R:3211[B]:ASP:HB3	3:R:3309[B]:PRO:HA	1.67	0.77
3:U:2969[B]:TYR:HH	3:d:3107[B]:LEU:HD12	1.49	0.77
3:U:3211[B]:ASP:HB3	3:U:3309[B]:PRO:HA	1.67	0.77
3:X:2948[A]:ASP:HB3	3:X:2949[A]:LYS:CA	2.15	0.77
3:X:2961[A]:HIS:HD2	3:X:2988[A]:TRP:HZ3	1.31	0.77
3:X:3141[B]:TYR:HD2	3:X:3142[B]:ASN:H	0.78	0.77
3:X:3148[A]:ILE:O	3:X:3152[A]:LYS:HE3	1.83	0.77
3:X:3288[B]:MET:HG2	3:X:3295[B]:LEU:HD21	1.67	0.77
3:X:3306[A]:LEU:HD12	3:X:3307[A]:PHE:N	2.00	0.77
3:a:2961[A]:HIS:HB3	3:a:3111[A]:SER:OG	1.85	0.77
3:a:3211[B]:ASP:HB3	3:a:3309[B]:PRO:HA	1.67	0.77
3:a:3284[A]:LYS:CD	3:a:3285[A]:VAL:N	2.47	0.77
3:d:2948[A]:ASP:HB3	3:d:2949[A]:LYS:CA	2.15	0.77
3:d:2956[A]:LYS:C	3:d:2960[A]:PHE:CE1	2.47	0.77
4:HA:1:NAG:O7	4:HA:1:NAG:O3	2.02	0.77
3:C:3156[B]:MET:CG	3:L:2982[B]:MET:HG3	2.14	0.77
3:C:3172[B]:SER:HB2	3:L:3152[B]:LYS:N	1.99	0.77
3:F:2961[B]:HIS:CG	3:a:2975[B]:PHE:CZ	2.73	0.77
3:F:2966[B]:SER:N	3:a:3255[B]:PRO:CA	2.48	0.77
3:F:3169[B]:LYS:HZ2	3:a:3149[B]:ASN:ND2	1.80	0.77
3:F:3306[A]:LEU:HD12	3:F:3307[A]:PHE:N	2.00	0.77
3:I:2961[A]:HIS:HB3	3:I:3111[A]:SER:OG	1.85	0.77
3:I:2969[B]:TYR:CE2	3:R:3120[B]:HIS:CD2	2.72	0.77
2:K:2394:VAL:H	2:K:2448:THR:HG22	1.50	0.77
3:O:3284[A]:LYS:CD	3:O:3285[A]:VAL:N	2.47	0.77
3:O:3288[A]:MET:HG2	3:O:3295[A]:LEU:HD21	1.67	0.77
3:U:2969[B]:TYR:N	3:d:3256[B]:TRP:NE1	2.32	0.77
3:U:3288[A]:MET:HG2	3:U:3295[A]:LEU:HD21	1.67	0.77
3:X:3113[B]:ASP:CG	3:X:3114[B]:PRO:CD	2.56	0.77
1:Y:105:VAL:HG12	1:Y:123:PHE:HB3	1.67	0.77
3:a:3288[B]:MET:HG2	3:a:3295[B]:LEU:HD21	1.67	0.77
3:a:3306[B]:LEU:HD12	3:a:3307[B]:PHE:N	2.00	0.77
3:d:2952[B]:ALA:HA	3:d:2956[B]:LYS:HB3	1.67	0.77
3:d:2979[B]:GLN:NE2	3:d:3155[B]:MET:CE	2.47	0.77
3:C:3151[B]:LEU:HA	3:L:3154[B]:PRO:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3212[B]:ARG:HG3	3:C:3212[B]:ARG:NH1	2.00	0.77
1:D:1170:MET:HB3	1:D:1203:MET:HE2	1.65	0.77
3:F:2965[B]:LEU:H	3:a:3221[B]:ALA:HB1	0.96	0.77
3:F:2980[B]:HIS:N	3:a:2967[B]:CYS:HB2	1.99	0.77
3:F:3211[A]:ASP:HB3	3:F:3309[A]:PRO:HA	1.67	0.77
3:F:3220[A]:ARG:HG3	3:F:3220[A]:ARG:NH1	1.98	0.77
3:I:3025[A]:VAL:CG2	3:I:3047[A]:ARG:HH12	1.94	0.77
3:I:3204[A]:LEU:O	3:I:3208[A]:GLN:HG3	1.85	0.77
3:I:3284[A]:LYS:CD	3:I:3285[A]:VAL:N	2.47	0.77
3:L:2948[A]:ASP:HB3	3:L:2949[A]:LYS:CA	2.15	0.77
3:L:3023[B]:ILE:O	3:L:3026[B]:THR:N	2.11	0.77
3:O:2967[B]:CYS:C	3:X:2979[B]:GLN:HG2	1.91	0.77
3:U:3086[B]:GLU:CD	3:d:2970[B]:PRO:CG	2.57	0.77
3:U:3254[B]:MET:CE	3:d:3254[B]:MET:HB2	2.09	0.77
3:X:2955[A]:GLN:CD	3:X:3037[A]:TYR:HE1	1.93	0.77
3:a:2948[B]:ASP:HB3	3:a:2949[B]:LYS:CA	2.15	0.77
3:d:3306[B]:LEU:HD12	3:d:3307[B]:PHE:N	2.00	0.77
3:C:2979[B]:GLN:NE2	3:C:3155[B]:MET:CE	2.47	0.76
3:C:3152[B]:LYS:N	3:L:3172[B]:SER:OG	2.16	0.76
3:F:3248[B]:LEU:CB	3:a:2972[B]:GLY:C	2.58	0.76
3:I:2961[B]:HIS:HB3	3:I:3111[B]:SER:OG	1.85	0.76
3:I:3211[A]:ASP:HB3	3:I:3309[A]:PRO:HA	1.67	0.76
3:I:3211[B]:ASP:HB3	3:I:3309[B]:PRO:HA	1.67	0.76
3:L:3259[A]:ASP:OD2	3:L:3260[A]:ARG:HG2	1.84	0.76
3:L:3307[B]:PHE:CE1	3:L:3309[B]:PRO:HG3	2.16	0.76
1:M:1301:PRO:O	1:M:1494:ARG:NH2	2.18	0.76
3:O:2961[B]:HIS:HD2	3:O:2988[B]:TRP:HZ3	1.31	0.76
3:O:3160[B]:SER:CA	3:X:3151[B]:LEU:H	1.97	0.76
3:R:2948[B]:ASP:H	3:R:2949[B]:LYS:CA	1.98	0.76
2:T:2800:LYS:HB3	3:U:3023[A]:ILE:HD11	1.67	0.76
3:U:3162[B]:ASP:CB	3:d:3260[B]:ARG:NH1	2.48	0.76
1:V:1636:ASN:HB3	1:V:1639:LYS:HD3	1.67	0.76
3:X:2979[A]:GLN:NE2	3:X:3155[A]:MET:CE	2.47	0.76
3:X:3104[B]:MET:CA	3:X:3110[B]:THR:HG23	2.10	0.76
3:X:3185[A]:TYR:HE2	3:X:3187[A]:TYR:CE2	2.01	0.76
3:a:2961[B]:HIS:HD2	3:a:2988[B]:TRP:HZ3	1.31	0.76
3:a:3220[B]:ARG:HG3	3:a:3220[B]:ARG:NH1	1.98	0.76
1:b:456:GLN:HG2	1:b:551:GLU:HB2	1.67	0.76
3:d:2952[A]:ALA:HA	3:d:2956[A]:LYS:HB3	1.67	0.76
3:C:3025[B]:VAL:HG23	3:C:3033[B]:PHE:O	1.83	0.76
3:C:3156[B]:MET:CB	3:L:2982[B]:MET:SD	2.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2948[B]:ASP:HB3	3:F:2949[B]:LYS:CA	2.15	0.76
3:F:2979[A]:GLN:NE2	3:F:3155[A]:MET:CE	2.47	0.76
3:F:3152[B]:LYS:HB2	3:a:3172[B]:SER:CA	2.14	0.76
3:F:3251[B]:ASP:C	3:a:3251[B]:ASP:HB3	2.10	0.76
1:G:417:MET:SD	3:L:3199[A]:GLN:NE2	2.58	0.76
3:I:2961[B]:HIS:CG	3:R:2975[B]:PHE:CE1	2.74	0.76
3:I:2970[B]:PRO:CD	3:R:2989[B]:HIS:NE2	2.47	0.76
3:I:3155[B]:MET:SD	3:R:3154[B]:PRO:CG	2.71	0.76
3:O:2967[B]:CYS:CB	3:X:3155[B]:MET:HG2	2.04	0.76
3:O:3163[B]:ASN:CB	3:X:3149[B]:ASN:CB	2.62	0.76
3:O:3306[A]:LEU:HD12	3:O:3307[A]:PHE:N	2.00	0.76
3:R:3141[A]:TYR:HD2	3:R:3142[A]:ASN:H	0.78	0.76
3:R:3288[B]:MET:HG2	3:R:3295[B]:LEU:HD21	1.67	0.76
2:T:2546:LEU:H	2:T:2557:ALA:HA	1.49	0.76
3:U:3219[B]:LEU:C	3:d:2971[B]:ASP:O	2.27	0.76
3:U:3254[B]:MET:HB3	3:d:3254[B]:MET:HB2	1.65	0.76
3:X:2956[A]:LYS:C	3:X:2960[A]:PHE:CE1	2.47	0.76
3:X:3023[B]:ILE:O	3:X:3026[B]:THR:N	2.11	0.76
3:a:2937[A]:ASN:HB2	3:a:3006[A]:LYS:CE	2.14	0.76
3:a:3204[A]:LEU:O	3:a:3208[A]:GLN:HG3	1.86	0.76
1:A:324:PRO:HG2	1:A:376:ASN:HD21	1.50	0.76
3:C:2955[B]:GLN:CD	3:C:3037[B]:TYR:HE1	1.92	0.76
3:C:3149[B]:ASN:C	3:L:3172[B]:SER:CB	2.57	0.76
3:C:3159[B]:SER:HA	3:L:3151[B]:LEU:N	2.01	0.76
3:F:2955[B]:GLN:CD	3:F:3037[B]:TYR:HE1	1.92	0.76
3:F:2961[A]:HIS:HB3	3:F:3111[A]:SER:OG	1.85	0.76
3:F:3288[B]:MET:HG2	3:F:3295[B]:LEU:HD21	1.67	0.76
3:I:2988[B]:TRP:CE3	3:I:2989[B]:HIS:ND1	2.53	0.76
3:L:2988[A]:TRP:CE3	3:L:2989[A]:HIS:ND1	2.53	0.76
3:L:3024[A]:LEU:CD1	3:L:3025[A]:VAL:H	1.84	0.76
3:L:3204[A]:LEU:O	3:L:3208[A]:GLN:HG3	1.86	0.76
3:L:3212[B]:ARG:HG3	3:L:3212[B]:ARG:NH1	2.00	0.76
3:O:2952[B]:ALA:HA	3:O:2956[B]:LYS:HB3	1.67	0.76
3:O:2961[A]:HIS:HD2	3:O:2988[A]:TRP:HZ3	1.31	0.76
3:O:2979[B]:GLN:NE2	3:O:3155[B]:MET:CE	2.47	0.76
3:O:3108[B]:HIS:CB	3:X:2970[B]:PRO:CA	2.63	0.76
3:O:3211[A]:ASP:HB3	3:O:3309[A]:PRO:HA	1.67	0.76
3:R:3230[B]:PHE:CB	3:R:3243[B]:GLY:HA2	2.06	0.76
3:U:2961[B]:HIS:HB3	3:U:3111[B]:SER:OG	1.85	0.76
3:U:3256[B]:TRP:HE3	3:d:2973[B]:THR:H	1.34	0.76
3:X:3148[B]:ILE:O	3:X:3152[B]:LYS:HE3	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:2135:PRO:O	2:Z:2140:ARG:NH2	2.18	0.76
3:d:2948[B]:ASP:HB3	3:d:2949[B]:LYS:CA	2.15	0.76
3:d:2961[A]:HIS:HB3	3:d:3111[A]:SER:OG	1.85	0.76
3:d:3211[B]:ASP:HB3	3:d:3309[B]:PRO:HA	1.67	0.76
3:d:3306[A]:LEU:HD12	3:d:3307[A]:PHE:N	2.00	0.76
1:A:1442:MET:HE1	1:A:1454:PHE:HA	1.67	0.76
3:C:2937[A]:ASN:CB	3:C:3006[A]:LYS:HE2	2.14	0.76
3:C:3113[B]:ASP:CG	3:C:3114[B]:PRO:CD	2.56	0.76
3:F:3147[A]:GLU:HB2	3:F:3149[A]:ASN:OD1	1.86	0.76
3:F:3180[B]:TYR:HB2	3:F:3183[B]:LEU:CD2	2.16	0.76
2:H:2168:ARG:NH1	2:K:2587:SER:OG	2.18	0.76
3:I:2948[A]:ASP:HB3	3:I:2949[A]:LYS:CA	2.15	0.76
3:I:3147[A]:GLU:HB2	3:I:3149[A]:ASN:OD1	1.86	0.76
3:I:3185[A]:TYR:HE2	3:I:3187[A]:TYR:CE2	2.01	0.76
3:I:3253[B]:GLU:CB	3:R:2975[B]:PHE:C	2.58	0.76
1:J:456:GLN:NE2	1:J:549:PRO:O	2.17	0.76
2:K:2545:SER:HA	2:K:2546:LEU:HG	1.68	0.76
3:L:3288[A]:MET:HG2	3:L:3295[A]:LEU:HD21	1.67	0.76
3:O:3284[B]:LYS:CD	3:O:3285[B]:VAL:N	2.47	0.76
3:R:3147[A]:GLU:HB2	3:R:3149[A]:ASN:OD1	1.86	0.76
3:R:3204[A]:LEU:O	3:R:3208[A]:GLN:HG3	1.86	0.76
3:R:3211[A]:ASP:HB3	3:R:3309[A]:PRO:HA	1.67	0.76
3:R:3307[B]:PHE:CE1	3:R:3309[B]:PRO:HG3	2.16	0.76
3:U:2948[A]:ASP:H	3:U:2949[A]:LYS:CA	1.98	0.76
3:U:2973[B]:THR:CG2	3:d:3222[B]:ILE:HG23	2.15	0.76
3:U:2979[A]:GLN:NE2	3:U:3155[A]:MET:CE	2.47	0.76
3:U:3147[A]:GLU:HB2	3:U:3149[A]:ASN:OD1	1.86	0.76
1:V:1372:ILE:HD11	1:Y:1392:ASP:HB2	1.66	0.76
3:X:3204[B]:LEU:O	3:X:3208[B]:GLN:HG3	1.86	0.76
3:X:3211[B]:ASP:HB3	3:X:3309[B]:PRO:HA	1.67	0.76
3:a:3113[A]:ASP:CG	3:a:3114[A]:PRO:CD	2.56	0.76
3:d:3204[B]:LEU:O	3:d:3208[B]:GLN:HG3	1.86	0.76
1:A:22:LEU:HG	1:A:122:VAL:HG11	1.68	0.76
3:C:2949[A]:LYS:O	3:C:2949[A]:LYS:NZ	2.16	0.76
3:C:2952[B]:ALA:HA	3:C:2956[B]:LYS:HB3	1.67	0.76
3:C:2961[A]:HIS:HD2	3:C:2988[A]:TRP:HZ3	1.32	0.76
3:C:3306[B]:LEU:HD12	3:C:3307[B]:PHE:N	2.00	0.76
3:F:2965[B]:LEU:CB	3:a:3256[B]:TRP:NE1	2.49	0.76
3:F:2979[B]:GLN:C	3:a:2967[B]:CYS:CB	2.59	0.76
3:F:3180[A]:TYR:HB2	3:F:3183[A]:LEU:CD2	2.16	0.76
3:I:2974[B]:ALA:N	3:R:3249[B]:GLY:N	2.30	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3180[A]:TYR:HB2	3:I:3183[A]:LEU:CD2	2.16	0.76
3:I:3256[B]:TRP:HB3	3:R:2966[B]:SER:C	2.10	0.76
3:I:3256[B]:TRP:CZ2	3:R:2965[B]:LEU:HB3	2.19	0.76
3:L:3212[A]:ARG:HG3	3:L:3212[A]:ARG:NH1	2.00	0.76
3:O:2961[A]:HIS:HB3	3:O:3111[A]:SER:OG	1.85	0.76
3:O:3163[B]:ASN:HD22	3:X:3148[B]:ILE:HG22	1.50	0.76
3:O:3204[A]:LEU:O	3:O:3208[A]:GLN:HG3	1.85	0.76
3:O:3307[A]:PHE:CE1	3:O:3309[A]:PRO:HG3	2.16	0.76
3:R:2988[B]:TRP:CE3	3:R:2989[B]:HIS:ND1	2.53	0.76
3:R:3306[A]:LEU:HD12	3:R:3307[A]:PHE:N	2.00	0.76
3:U:2961[B]:HIS:HD2	3:U:2988[B]:TRP:HZ3	1.31	0.76
3:U:3204[B]:LEU:O	3:U:3208[B]:GLN:HG3	1.86	0.76
3:U:3230[B]:PHE:CB	3:U:3243[B]:GLY:HA2	2.06	0.76
3:X:3288[A]:MET:HG2	3:X:3295[A]:LEU:HD21	1.67	0.76
3:a:2952[A]:ALA:HA	3:a:2956[A]:LYS:HB3	1.67	0.76
3:a:3180[A]:TYR:HB2	3:a:3183[A]:LEU:CD2	2.16	0.76
3:d:3185[A]:TYR:HE2	3:d:3187[A]:TYR:CE2	2.01	0.76
3:C:2948[A]:ASP:HB3	3:C:2949[A]:LYS:CA	2.15	0.76
3:C:2988[A]:TRP:CE3	3:C:2989[A]:HIS:ND1	2.53	0.76
3:C:3156[B]:MET:HG2	3:L:2984[B]:THR:OG1	1.86	0.76
3:F:2965[B]:LEU:C	3:a:3221[B]:ALA:HB2	2.10	0.76
3:F:3306[B]:LEU:HD12	3:F:3307[B]:PHE:N	2.00	0.76
3:I:2952[A]:ALA:CB	3:I:2953[A]:GLY:C	2.48	0.76
3:I:3107[B]:LEU:HD21	3:R:2975[B]:PHE:HA	1.67	0.76
3:L:2952[A]:ALA:HA	3:L:2956[A]:LYS:HB3	1.67	0.76
3:O:2971[B]:ASP:H	3:X:2991[B]:LEU:N	1.82	0.76
3:O:2971[B]:ASP:O	3:X:2988[B]:TRP:HE3	1.68	0.76
3:R:3114[A]:PRO:HD2	3:R:3115[A]:LEU:H	1.51	0.76
3:R:3180[B]:TYR:HB2	3:R:3183[B]:LEU:CD2	2.16	0.76
3:U:3150[B]:LYS:HG2	3:d:3156[B]:MET:HG2	1.66	0.76
3:U:3204[A]:LEU:O	3:U:3208[A]:GLN:HG3	1.86	0.76
3:U:3230[A]:PHE:CB	3:U:3243[A]:GLY:HA2	2.06	0.76
3:X:3220[B]:ARG:HG3	3:X:3220[B]:ARG:NH1	1.98	0.76
3:a:2952[B]:ALA:CB	3:a:2953[B]:GLY:C	2.48	0.76
3:a:3147[A]:GLU:HB2	3:a:3149[A]:ASN:OD1	1.86	0.76
3:d:2937[A]:ASN:HB2	3:d:3006[A]:LYS:CE	2.14	0.76
3:d:3180[B]:TYR:HB2	3:d:3183[B]:LEU:CD2	2.16	0.76
1:A:550:ILE:N	1:A:557:VAL:O	2.15	0.76
3:C:2985[B]:PHE:CZ	3:L:2969[B]:TYR:C	2.58	0.76
3:C:2988[B]:TRP:CE3	3:C:2989[B]:HIS:ND1	2.53	0.76
3:C:3158[B]:PHE:O	3:L:3150[B]:LYS:N	2.05	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3253[B]:GLU:CG	3:L:2976[B]:ALA:HB2	2.14	0.76
3:F:2952[B]:ALA:HA	3:F:2956[B]:LYS:HB3	1.67	0.76
3:F:2956[B]:LYS:C	3:F:2960[B]:PHE:CE1	2.47	0.76
3:F:3220[B]:ARG:HG3	3:F:3220[B]:ARG:NH1	1.98	0.76
3:I:2956[B]:LYS:C	3:I:2960[B]:PHE:CE1	2.47	0.76
3:I:2974[B]:ALA:HB1	3:R:3253[B]:GLU:OE1	1.84	0.76
1:J:723:ALA:O	1:J:728:ARG:NH1	2.19	0.76
3:L:2948[B]:ASP:H	3:L:2949[B]:LYS:CA	1.98	0.76
3:L:2955[B]:GLN:CD	3:L:3037[B]:TYR:HE1	1.92	0.76
1:M:1210:LYS:HA	1:M:1211:TYR:CB	2.15	0.76
3:O:3141[B]:TYR:HD2	3:O:3142[B]:ASN:H	0.78	0.76
3:R:2948[A]:ASP:HB3	3:R:2949[A]:LYS:CA	2.15	0.76
3:R:2948[B]:ASP:HB3	3:R:2949[B]:LYS:CA	2.15	0.76
1:S:898:GLY:HA2	1:S:1186:TRP:HB2	1.66	0.76
3:U:3180[B]:TYR:HB2	3:U:3183[B]:LEU:CD2	2.16	0.76
3:X:2937[B]:ASN:CB	3:X:3006[B]:LYS:HE2	2.14	0.76
3:X:2952[A]:ALA:HA	3:X:2956[A]:LYS:HB3	1.67	0.76
3:X:2952[B]:ALA:HA	3:X:2956[B]:LYS:HB3	1.67	0.76
3:X:2961[A]:HIS:HB3	3:X:3111[A]:SER:OG	1.85	0.76
3:X:2961[B]:HIS:HB3	3:X:3111[B]:SER:OG	1.85	0.76
3:X:3089[B]:HIS:HD1	3:X:3119[B]:HIS:CE1	2.04	0.76
3:a:3147[B]:GLU:HB2	3:a:3149[B]:ASN:CG	1.95	0.76
3:a:3180[B]:TYR:HB2	3:a:3183[B]:LEU:CD2	2.16	0.76
3:d:3196[B]:THR:H	3:d:3199[B]:GLN:CD	1.94	0.76
3:C:3114[B]:PRO:HD2	3:C:3115[B]:LEU:H	1.51	0.76
3:C:3172[B]:SER:CB	3:L:3149[B]:ASN:C	2.58	0.76
3:F:2952[A]:ALA:HA	3:F:2956[A]:LYS:HB3	1.67	0.76
3:F:2975[B]:PHE:HA	3:a:3107[B]:LEU:CD2	2.15	0.76
3:F:3120[A]:HIS:O	3:F:3121[A]:SER:C	2.29	0.76
3:F:3154[B]:PRO:HD3	3:a:3173[B]:THR:O	1.86	0.76
3:F:3255[B]:PRO:HG3	3:a:2962[B]:GLY:C	2.10	0.76
3:I:2971[B]:ASP:OD1	3:I:2973[B]:THR:OG1	2.04	0.76
3:I:3153[B]:LYS:CE	3:R:3158[B]:PHE:H	1.98	0.76
3:I:3196[B]:THR:H	3:I:3199[B]:GLN:CD	1.94	0.76
3:I:3221[B]:ALA:HB3	3:R:2964[B]:PRO:CA	2.12	0.76
3:I:3259[A]:ASP:OD2	3:I:3260[A]:ARG:HG2	1.84	0.76
3:I:3306[A]:LEU:HD12	3:I:3307[A]:PHE:N	2.00	0.76
3:L:2961[A]:HIS:HB3	3:L:3111[A]:SER:OG	1.85	0.76
3:O:3089[A]:HIS:HD1	3:O:3119[A]:HIS:CE1	2.04	0.76
3:O:3114[B]:PRO:HD2	3:O:3115[B]:LEU:H	1.51	0.76
3:O:3204[B]:LEU:O	3:O:3208[B]:GLN:HG3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3196[B]:THR:H	3:R:3199[B]:GLN:CD	1.94	0.76
3:U:2965[B]:LEU:HD13	3:d:3256[B]:TRP:O	1.85	0.76
3:U:2970[B]:PRO:CA	3:d:3086[B]:GLU:CD	2.43	0.76
3:X:3114[B]:PRO:HD2	3:X:3115[B]:LEU:H	1.51	0.76
3:d:2971[A]:ASP:OD1	3:d:2973[A]:THR:OG1	2.04	0.76
3:C:2952[A]:ALA:HA	3:C:2956[A]:LYS:HB3	1.67	0.76
3:C:3252[B]:TYR:CE2	3:L:3249[B]:GLY:O	2.35	0.76
2:E:2394:VAL:H	2:E:2448:THR:HG22	1.50	0.76
3:F:2948[A]:ASP:HB3	3:F:2949[A]:LYS:CA	2.15	0.76
3:F:3150[B]:LYS:HG2	3:a:3158[B]:PHE:HA	1.63	0.76
3:I:2969[B]:TYR:CE2	3:R:3120[B]:HIS:NE2	2.48	0.76
3:I:3255[B]:PRO:CB	3:R:2959[B]:SER:CA	2.64	0.76
3:L:2988[B]:TRP:CE3	3:L:2989[B]:HIS:ND1	2.53	0.76
3:L:3089[A]:HIS:HD1	3:L:3119[A]:HIS:CE1	2.04	0.76
3:L:3220[A]:ARG:HG3	3:L:3220[A]:ARG:NH1	1.98	0.76
3:O:2971[B]:ASP:OD1	3:O:2973[B]:THR:OG1	2.04	0.76
1:P:1296:VAL:HB	1:P:1446:ASP:HB3	1.66	0.76
3:R:2930[B]:LEU:H	3:R:2930[B]:LEU:CD2	1.98	0.76
3:R:2952[A]:ALA:HA	3:R:2956[A]:LYS:HB3	1.67	0.76
3:a:3212[A]:ARG:HG3	3:a:3212[A]:ARG:NH1	2.00	0.76
3:a:3288[A]:MET:HG2	3:a:3295[A]:LEU:HD21	1.67	0.76
1:b:1358:LEU:HD23	1:b:1456:LEU:HD21	1.68	0.76
3:d:3180[A]:TYR:HB2	3:d:3183[A]:LEU:CD2	2.16	0.76
4:q:2:NAG:H83	4:q:2:NAG:C3	2.16	0.76
3:C:3089[B]:HIS:HD1	3:C:3119[B]:HIS:CE1	2.04	0.76
3:F:2971[A]:ASP:OD1	3:F:2973[A]:THR:OG1	2.04	0.76
3:F:2971[B]:ASP:OD1	3:a:3248[B]:LEU:CD2	2.34	0.76
3:F:3089[A]:HIS:HD1	3:F:3119[A]:HIS:CE1	2.04	0.76
3:F:3114[B]:PRO:HD2	3:F:3115[B]:LEU:H	1.51	0.76
3:I:2948[A]:ASP:H	3:I:2949[A]:LYS:CA	1.98	0.76
3:I:3114[B]:PRO:HD2	3:I:3115[B]:LEU:H	1.51	0.76
3:I:3180[B]:TYR:HB2	3:I:3183[B]:LEU:CD2	2.16	0.76
3:I:3204[B]:LEU:O	3:I:3208[B]:GLN:HG3	1.86	0.76
3:I:3255[B]:PRO:HD3	3:R:2962[B]:GLY:C	2.11	0.76
3:I:3288[A]:MET:HG2	3:I:3295[A]:LEU:HD21	1.67	0.76
3:L:3089[B]:HIS:HD1	3:L:3119[B]:HIS:CE1	2.04	0.76
3:L:3114[B]:PRO:HD2	3:L:3115[B]:LEU:H	1.51	0.76
3:L:3220[B]:ARG:HG3	3:L:3220[B]:ARG:NH1	1.98	0.76
3:O:2948[B]:ASP:H	3:O:2949[B]:LYS:CA	1.98	0.76
3:O:2952[A]:ALA:HA	3:O:2956[A]:LYS:HB3	1.67	0.76
3:O:2955[A]:GLN:CD	3:O:3037[A]:TYR:HE1	1.92	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2961[B]:HIS:HB3	3:O:3111[B]:SER:OG	1.85	0.76
3:R:2952[B]:ALA:CB	3:R:2953[B]:GLY:C	2.48	0.76
3:R:2988[A]:TRP:CE3	3:R:2989[A]:HIS:ND1	2.53	0.76
3:U:2930[B]:LEU:H	3:U:2930[B]:LEU:CD2	1.97	0.76
3:U:2952[A]:ALA:HA	3:U:2956[A]:LYS:HB3	1.67	0.76
3:U:2961[A]:HIS:HB3	3:U:3111[A]:SER:OG	1.85	0.76
3:U:3023[A]:ILE:O	3:U:3026[A]:THR:N	2.11	0.76
3:X:2948[A]:ASP:H	3:X:2949[A]:LYS:CA	1.98	0.76
3:X:2988[B]:TRP:CE3	3:X:2989[B]:HIS:ND1	2.53	0.76
3:X:3114[A]:PRO:HD2	3:X:3115[A]:LEU:H	1.51	0.76
1:Y:14:GLU:O	1:Y:17:ASN:ND2	2.18	0.76
3:a:2955[A]:GLN:CD	3:a:3037[A]:TYR:HE1	1.92	0.76
3:a:3220[A]:ARG:HG3	3:a:3220[A]:ARG:NH1	1.98	0.76
1:b:439:LEU:HD23	1:b:509:ILE:HD12	1.68	0.76
3:d:2961[B]:HIS:HD2	3:d:2988[B]:TRP:HZ3	1.31	0.76
3:d:3089[A]:HIS:HD1	3:d:3119[A]:HIS:CE1	2.04	0.76
3:d:3113[A]:ASP:CG	3:d:3114[A]:PRO:CD	2.56	0.76
3:C:3089[A]:HIS:HD1	3:C:3119[A]:HIS:CE1	2.04	0.75
3:C:3259[B]:ASP:OD2	3:C:3260[B]:ARG:HG2	1.84	0.75
3:F:2937[A]:ASN:CB	3:F:3006[A]:LYS:HE2	2.14	0.75
3:F:3174[B]:GLY:N	3:a:3154[B]:PRO:CG	2.47	0.75
3:I:2967[B]:CYS:SG	3:R:2982[B]:MET:HE2	2.26	0.75
3:L:3120[B]:HIS:O	3:L:3121[B]:SER:C	2.29	0.75
3:O:2968[B]:GLN:HG2	3:X:2984[B]:THR:CB	2.16	0.75
3:O:2969[B]:TYR:CD1	3:X:3158[B]:PHE:HD1	1.97	0.75
3:O:2969[B]:TYR:HB2	3:X:3158[B]:PHE:CZ	2.19	0.75
3:O:3156[B]:MET:HE2	3:X:3173[B]:THR:CG2	1.94	0.75
3:O:3180[B]:TYR:HB2	3:O:3183[B]:LEU:CD2	2.16	0.75
3:R:2937[B]:ASN:HB2	3:R:3006[B]:LYS:CE	2.14	0.75
3:R:2965[B]:LEU:CD2	3:R:2974[B]:ALA:HB1	2.10	0.75
1:S:1046:HIS:HA	1:S:1049:VAL:HB	1.67	0.75
3:a:2955[B]:GLN:CD	3:a:3037[B]:TYR:HE1	1.92	0.75
3:a:3185[A]:TYR:HE2	3:a:3187[A]:TYR:CE2	2.01	0.75
3:d:2979[A]:GLN:NE2	3:d:3155[A]:MET:CE	2.47	0.75
3:d:3288[A]:MET:HG2	3:d:3295[A]:LEU:HD21	1.67	0.75
3:C:3024[B]:LEU:CD1	3:C:3025[B]:VAL:H	1.84	0.75
3:C:3180[B]:TYR:HB2	3:C:3183[B]:LEU:CD2	2.16	0.75
3:C:3204[B]:LEU:O	3:C:3208[B]:GLN:HG3	1.86	0.75
3:C:3288[A]:MET:HG2	3:C:3295[A]:LEU:HD21	1.67	0.75
3:F:2971[B]:ASP:OD1	3:F:2973[B]:THR:OG1	2.04	0.75
3:F:2981[B]:GLY:H	3:a:2968[B]:GLN:CD	1.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3170[B]:ALA:O	3:a:3152[B]:LYS:CB	2.33	0.75
1:G:92:TRP:O	1:G:212:ASN:ND2	2.20	0.75
3:I:3288[B]:MET:HG2	3:I:3295[B]:LEU:HD21	1.67	0.75
1:J:975:PRO:HG2	1:J:1024:GLY:HA3	1.67	0.75
3:L:3288[B]:MET:HG2	3:L:3295[B]:LEU:HD21	1.67	0.75
3:O:2948[A]:ASP:HB3	3:O:2949[A]:LYS:CA	2.15	0.75
3:O:2948[B]:ASP:HB3	3:O:2949[B]:LYS:CA	2.15	0.75
3:O:2988[B]:TRP:CE3	3:O:2989[B]:HIS:ND1	2.53	0.75
3:R:3180[A]:TYR:HB2	3:R:3183[A]:LEU:CD2	2.16	0.75
3:U:3156[B]:MET:SD	3:d:2982[B]:MET:HA	2.26	0.75
3:U:3288[B]:MET:HG2	3:U:3295[B]:LEU:HD21	1.67	0.75
1:V:456:GLN:NE2	1:V:549:PRO:O	2.19	0.75
1:Y:1612:THR:O	3:d:3186[B]:GLU:CG	2.32	0.75
1:b:718:ARG:NH1	1:b:830:ASN:OD1	2.17	0.75
3:d:2961[A]:HIS:HD2	3:d:2988[A]:TRP:HZ3	1.32	0.75
3:d:2961[B]:HIS:HB3	3:d:3111[B]:SER:OG	1.85	0.75
3:d:3114[B]:PRO:HD2	3:d:3115[B]:LEU:H	1.51	0.75
3:C:2930[A]:LEU:H	3:C:2930[A]:LEU:CD2	1.98	0.75
3:C:2961[B]:HIS:HB3	3:C:3111[B]:SER:OG	1.85	0.75
3:C:3090[B]:ASN:HB3	3:L:2972[B]:GLY:C	2.10	0.75
3:C:3150[B]:LYS:N	3:L:3172[B]:SER:OG	2.19	0.75
3:C:3172[B]:SER:HG	3:L:3152[B]:LYS:HG3	1.49	0.75
3:C:3174[B]:GLY:CA	3:L:3154[B]:PRO:CG	2.63	0.75
1:D:1046:HIS:HA	1:D:1049:VAL:HB	1.69	0.75
1:D:1240:ILE:HG23	1:D:1247:ARG:HG3	1.66	0.75
3:F:3149[B]:ASN:HB3	3:a:3163[B]:ASN:ND2	1.98	0.75
3:F:3162[B]:ASP:CA	3:a:3259[B]:ASP:HB3	2.15	0.75
3:F:3173[B]:THR:CA	3:a:3153[B]:LYS:C	2.58	0.75
3:F:3196[B]:THR:H	3:F:3199[B]:GLN:CD	1.94	0.75
3:I:2971[A]:ASP:OD1	3:I:2973[A]:THR:OG1	2.04	0.75
3:I:3113[A]:ASP:CG	3:I:3114[A]:PRO:CD	2.56	0.75
3:L:3141[B]:TYR:HD2	3:L:3142[B]:ASN:H	0.78	0.75
3:L:3180[A]:TYR:HB2	3:L:3183[A]:LEU:CD2	2.16	0.75
3:L:3211[A]:ASP:HB3	3:L:3309[A]:PRO:HA	1.67	0.75
1:M:999:LEU:O	1:M:1063:ARG:NH2	2.20	0.75
3:O:2954[B]:TYR:O	3:O:2957[B]:ILE:HG22	1.87	0.75
3:O:3120[B]:HIS:O	3:O:3121[B]:SER:C	2.29	0.75
3:O:3180[A]:TYR:HB2	3:O:3183[A]:LEU:CD2	2.16	0.75
3:R:2952[B]:ALA:HA	3:R:2956[B]:LYS:HB3	1.67	0.75
3:R:2961[A]:HIS:HB3	3:R:3111[A]:SER:OG	1.85	0.75
3:R:3114[B]:PRO:HD2	3:R:3115[B]:LEU:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3204[B]:LEU:O	3:R:3208[B]:GLN:HG3	1.86	0.75
3:U:2969[B]:TYR:H	3:d:3256[B]:TRP:NE1	1.81	0.75
3:U:2988[B]:TRP:CE3	3:U:2989[B]:HIS:ND1	2.53	0.75
3:U:3038[B]:ILE:HG22	3:U:3040[B]:VAL:HG22	1.68	0.75
3:U:3089[B]:HIS:HD1	3:U:3119[B]:HIS:CE1	2.04	0.75
3:U:3180[A]:TYR:HB2	3:U:3183[A]:LEU:CD2	2.16	0.75
3:U:3212[A]:ARG:HG3	3:U:3212[A]:ARG:NH1	2.00	0.75
3:X:3180[A]:TYR:HB2	3:X:3183[A]:LEU:CD2	2.16	0.75
3:a:2948[A]:ASP:HB3	3:a:2949[A]:LYS:CA	2.15	0.75
3:a:3038[A]:ILE:HG22	3:a:3040[A]:VAL:HG22	1.68	0.75
3:d:2954[B]:TYR:O	3:d:2957[B]:ILE:HG22	1.87	0.75
3:d:3204[A]:LEU:O	3:d:3208[A]:GLN:HG3	1.86	0.75
1:A:979:LEU:HB3	1:A:980:TYR:HA	1.69	0.75
3:C:3079[B]:CYS:CA	3:L:3161[B]:GLU:HG2	2.16	0.75
3:F:3204[A]:LEU:O	3:F:3208[A]:GLN:HG3	1.86	0.75
3:F:3293[A]:LYS:HB2	3:F:3294[A]:SER:HB2	0.82	0.75
1:G:527:LEU:HD21	1:G:632:LEU:HD12	1.68	0.75
3:I:3114[A]:PRO:HD2	3:I:3115[A]:LEU:H	1.51	0.75
3:L:3114[A]:PRO:HD2	3:L:3115[A]:LEU:H	1.51	0.75
3:O:3147[B]:GLU:HB2	3:O:3149[B]:ASN:OD1	1.86	0.75
3:O:3255[B]:PRO:CA	3:X:3160[B]:SER:C	2.50	0.75
3:R:2955[A]:GLN:CD	3:R:3037[A]:TYR:HE1	1.92	0.75
3:R:3141[B]:TYR:HD2	3:R:3142[B]:ASN:H	0.78	0.75
3:U:2975[B]:PHE:CD2	3:d:3255[B]:PRO:O	2.32	0.75
3:U:3114[B]:PRO:HD2	3:U:3115[B]:LEU:H	1.51	0.75
3:X:2948[B]:ASP:HB3	3:X:2949[B]:LYS:CA	2.15	0.75
3:X:3089[A]:HIS:HD1	3:X:3119[A]:HIS:CE1	2.04	0.75
3:a:3089[A]:HIS:HD1	3:a:3119[A]:HIS:CE1	2.04	0.75
3:a:3089[B]:HIS:HD1	3:a:3119[B]:HIS:CE1	2.04	0.75
3:a:3204[B]:LEU:O	3:a:3208[B]:GLN:HG3	1.86	0.75
3:a:3230[B]:PHE:CB	3:a:3243[B]:GLY:HA2	2.06	0.75
3:d:3196[A]:THR:H	3:d:3199[A]:GLN:CD	1.94	0.75
3:d:3220[A]:ARG:HG3	3:d:3220[A]:ARG:NH1	1.98	0.75
3:C:2954[B]:TYR:O	3:C:2957[B]:ILE:HG22	1.87	0.75
3:C:3204[A]:LEU:O	3:C:3208[A]:GLN:HG3	1.86	0.75
3:C:3288[B]:MET:HG2	3:C:3295[B]:LEU:HD21	1.67	0.75
3:F:2984[B]:THR:HG23	3:a:3159[B]:SER:CB	1.75	0.75
3:F:3038[B]:ILE:HG22	3:F:3040[B]:VAL:HG22	1.68	0.75
3:F:3120[B]:HIS:O	3:F:3121[B]:SER:C	2.29	0.75
3:I:2948[B]:ASP:HB3	3:I:2949[B]:LYS:CA	2.15	0.75
3:I:2954[A]:TYR:O	3:I:2957[A]:ILE:HG22	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2965[B]:LEU:HA	3:R:3253[B]:GLU:HG3	1.69	0.75
3:I:2968[B]:GLN:CG	3:R:3086[B]:GLU:CG	2.53	0.75
3:I:2982[B]:MET:HE3	3:R:2977[B]:CYS:SG	2.26	0.75
3:I:3137[B]:ARG:HB3	3:I:3139[B]:LEU:CD2	2.17	0.75
3:L:2937[A]:ASN:HB2	3:L:3006[A]:LYS:CE	2.14	0.75
3:L:3180[B]:TYR:HB2	3:L:3183[B]:LEU:CD2	2.16	0.75
3:O:2969[B]:TYR:OH	3:X:2991[B]:LEU:O	1.94	0.75
3:O:2969[B]:TYR:HB2	3:X:3158[B]:PHE:CG	2.22	0.75
3:O:2974[B]:ALA:CB	3:X:2977[B]:CYS:CA	2.62	0.75
3:O:3162[B]:ASP:N	3:X:3149[B]:ASN:OD1	2.15	0.75
3:O:3255[B]:PRO:HA	3:X:3160[B]:SER:C	2.12	0.75
3:O:3288[B]:MET:HG2	3:O:3295[B]:LEU:HD21	1.67	0.75
3:O:3306[B]:LEU:HD12	3:O:3307[B]:PHE:N	2.00	0.75
2:Q:2124:SER:HB2	2:Q:2129:PRO:HG2	1.67	0.75
3:R:3113[A]:ASP:CG	3:R:3114[A]:PRO:CD	2.56	0.75
3:R:3220[A]:ARG:HG3	3:R:3220[A]:ARG:NH1	1.98	0.75
3:R:3306[B]:LEU:HD12	3:R:3307[B]:PHE:N	2.00	0.75
3:U:2948[A]:ASP:HB3	3:U:2949[A]:LYS:CA	2.15	0.75
3:U:3169[B]:LYS:CG	3:d:3147[B]:GLU:HA	2.14	0.75
3:U:3219[B]:LEU:HD22	3:U:3219[B]:LEU:N	2.02	0.75
3:X:2956[B]:LYS:C	3:X:2960[B]:PHE:CE1	2.47	0.75
3:a:2952[B]:ALA:HA	3:a:2956[B]:LYS:HB3	1.67	0.75
3:a:3038[B]:ILE:HG22	3:a:3040[B]:VAL:HG22	1.68	0.75
3:a:3284[B]:LYS:CD	3:a:3285[B]:VAL:N	2.47	0.75
3:C:2948[B]:ASP:HB3	3:C:2949[B]:LYS:CA	2.15	0.75
3:C:2979[B]:GLN:HG3	3:L:3156[B]:MET:CG	2.17	0.75
3:C:2982[B]:MET:CB	3:L:3156[B]:MET:CG	2.64	0.75
3:F:3204[B]:LEU:O	3:F:3208[B]:GLN:HG3	1.86	0.75
3:F:3254[B]:MET:CB	3:a:2966[B]:SER:OG	2.35	0.75
3:F:3288[A]:MET:HG2	3:F:3295[A]:LEU:HD21	1.67	0.75
2:H:2400:LEU:HB2	2:H:2439:PHE:HD2	1.50	0.75
3:I:2954[B]:TYR:O	3:I:2957[B]:ILE:HG22	1.87	0.75
3:I:3089[A]:HIS:HD1	3:I:3119[A]:HIS:CE1	2.04	0.75
3:I:3219[B]:LEU:HD22	3:I:3219[B]:LEU:N	2.02	0.75
3:L:2954[B]:TYR:O	3:L:2957[B]:ILE:HG22	1.87	0.75
3:L:2955[A]:GLN:CD	3:L:3037[A]:TYR:HE1	1.92	0.75
3:O:2971[A]:ASP:OD1	3:O:2973[A]:THR:OG1	2.04	0.75
3:O:2976[B]:ALA:HB2	3:X:3156[B]:MET:CE	2.15	0.75
3:O:3089[B]:HIS:HD1	3:O:3119[B]:HIS:CE1	2.04	0.75
3:O:3147[A]:GLU:HB2	3:O:3149[A]:ASN:OD1	1.86	0.75
3:O:3219[A]:LEU:HD22	3:O:3219[A]:LEU:N	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2961[A]:HIS:HD2	3:U:2988[A]:TRP:HZ3	1.32	0.75
3:U:3219[A]:LEU:HD22	3:U:3219[A]:LEU:N	2.02	0.75
1:V:907:ARG:NH2	1:V:1106:PHE:O	2.20	0.75
2:W:2472:ASN:ND2	4:HA:1:NAG:H61	1.99	0.75
2:W:2823:ILE:O	2:W:2830:GLN:NE2	2.20	0.75
3:X:3147[A]:GLU:HB2	3:X:3149[A]:ASN:OD1	1.86	0.75
3:a:3212[B]:ARG:HG3	3:a:3212[B]:ARG:NH1	2.00	0.75
1:b:392:PRO:HB2	1:b:394:GLN:HG2	1.68	0.75
3:d:3114[A]:PRO:HD2	3:d:3115[A]:LEU:H	1.51	0.75
3:d:3288[B]:MET:HG2	3:d:3295[B]:LEU:HD21	1.67	0.75
3:C:2948[A]:ASP:H	3:C:2949[A]:LYS:CA	1.98	0.75
3:C:3211[B]:ASP:HB3	3:C:3309[B]:PRO:HA	1.67	0.75
3:F:2965[B]:LEU:HB3	3:a:3256[B]:TRP:CE2	2.20	0.75
3:F:2968[B]:GLN:OE1	3:a:2981[B]:GLY:CA	2.34	0.75
3:F:3212[B]:ARG:HG3	3:F:3212[B]:ARG:NH1	2.00	0.75
3:I:2937[B]:ASN:HB2	3:I:3006[B]:LYS:CE	2.14	0.75
3:I:2952[A]:ALA:HA	3:I:2956[A]:LYS:HB3	1.67	0.75
3:I:2955[A]:GLN:CD	3:I:3037[A]:TYR:HE1	1.92	0.75
3:I:3159[B]:SER:C	3:R:3150[B]:LYS:CD	2.60	0.75
3:I:3250[B]:GLY:CA	3:R:3252[B]:TYR:CE2	2.40	0.75
3:L:3147[A]:GLU:CG	3:L:3149[A]:ASN:HD21	2.00	0.75
3:L:3196[B]:THR:H	3:L:3199[B]:GLN:CD	1.94	0.75
1:M:1046:HIS:HA	1:M:1049:VAL:HB	1.69	0.75
3:O:3012[B]:TRP:O	3:O:3122[B]:ASN:ND2	2.20	0.75
3:O:3196[A]:THR:H	3:O:3199[A]:GLN:CD	1.94	0.75
3:R:2937[A]:ASN:CB	3:R:3006[A]:LYS:HE2	2.14	0.75
3:R:3038[B]:ILE:HG22	3:R:3040[B]:VAL:HG22	1.68	0.75
3:U:2937[B]:ASN:HB2	3:U:3006[B]:LYS:CE	2.14	0.75
3:X:3176[B]:LYS:HE2	3:X:3176[B]:LYS:N	2.02	0.75
3:X:3196[B]:THR:H	3:X:3199[B]:GLN:CD	1.94	0.75
3:C:2954[A]:TYR:O	3:C:2957[A]:ILE:HG22	1.87	0.75
3:C:3196[B]:THR:H	3:C:3199[B]:GLN:CD	1.94	0.75
3:F:2952[B]:ALA:HA	3:F:2956[B]:LYS:HB2	1.69	0.75
3:F:2966[B]:SER:C	3:a:3256[B]:TRP:HD1	1.54	0.75
3:F:2969[B]:TYR:HA	3:a:2989[B]:HIS:CE1	2.20	0.75
3:F:2982[B]:MET:SD	3:a:3157[B]:PRO:CB	2.75	0.75
3:F:2983[B]:VAL:CG2	3:a:3160[B]:SER:C	2.59	0.75
3:F:3153[B]:LYS:CA	3:a:3155[B]:MET:HG3	2.16	0.75
3:I:2962[B]:GLY:C	3:R:3255[B]:PRO:CG	2.60	0.75
3:I:3120[A]:HIS:O	3:I:3121[A]:SER:C	2.29	0.75
3:I:3137[A]:ARG:HB3	3:I:3139[A]:LEU:CD2	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3153[B]:LYS:HZ2	3:R:3157[B]:PRO:HD2	1.51	0.75
3:L:2979[A]:GLN:NE2	3:L:3155[A]:MET:CE	2.47	0.75
1:P:499:GLU:HG3	1:P:511:VAL:HG12	1.67	0.75
3:R:2930[A]:LEU:H	3:R:2930[A]:LEU:CD2	1.98	0.75
3:U:2969[B]:TYR:HE1	3:d:3107[B]:LEU:HD11	0.90	0.75
3:U:2973[B]:THR:N	3:d:3247[B]:VAL:CG1	2.50	0.75
3:X:3137[A]:ARG:HB3	3:X:3139[A]:LEU:CD2	2.17	0.75
3:X:3180[B]:TYR:HB2	3:X:3183[B]:LEU:CD2	2.16	0.75
3:a:2971[A]:ASP:OD1	3:a:2973[A]:THR:OG1	2.04	0.75
3:a:3141[A]:TYR:HD2	3:a:3142[A]:ASN:H	0.78	0.75
3:a:3147[A]:GLU:CG	3:a:3149[A]:ASN:HD21	2.00	0.75
3:a:3211[A]:ASP:HB3	3:a:3309[A]:PRO:HA	1.67	0.75
3:d:2937[B]:ASN:HB2	3:d:3006[B]:LYS:CE	2.13	0.75
3:d:2954[A]:TYR:O	3:d:2957[A]:ILE:HG22	1.87	0.75
3:d:3120[A]:HIS:O	3:d:3121[A]:SER:C	2.29	0.75
3:d:3137[A]:ARG:HB3	3:d:3139[A]:LEU:CD2	2.17	0.75
3:d:3137[A]:ARG:HB3	3:d:3139[A]:LEU:HD23	1.69	0.75
3:d:3147[A]:GLU:HB2	3:d:3149[A]:ASN:OD1	1.86	0.75
3:d:3284[B]:LYS:CD	3:d:3285[B]:VAL:N	2.47	0.75
2:B:2867:PRO:HG2	3:C:2932[A]:PRO:HG2	1.69	0.75
3:C:3137[A]:ARG:HB3	3:C:3139[A]:LEU:HD23	1.69	0.75
3:C:3137[B]:ARG:HB3	3:C:3139[B]:LEU:CD2	2.17	0.75
3:F:2988[B]:TRP:CE3	3:F:2989[B]:HIS:ND1	2.53	0.75
3:F:2992[B]:TYR:HE2	3:a:2969[B]:TYR:CE1	2.03	0.75
3:F:3176[A]:LYS:HE2	3:F:3176[A]:LYS:N	2.02	0.75
3:I:2952[A]:ALA:HA	3:I:2956[A]:LYS:HB2	1.69	0.75
3:I:3107[B]:LEU:CD1	3:R:2975[B]:PHE:CD1	2.41	0.75
3:I:3147[B]:GLU:HB2	3:I:3149[B]:ASN:OD1	1.86	0.75
3:I:3154[B]:PRO:HG3	3:R:3174[B]:GLY:HA2	1.67	0.75
3:L:3137[A]:ARG:HB3	3:L:3139[A]:LEU:CD2	2.17	0.75
3:L:3176[B]:LYS:HE2	3:L:3176[B]:LYS:N	2.02	0.75
3:O:3137[B]:ARG:HB3	3:O:3139[B]:LEU:CD2	2.17	0.75
3:R:3104[B]:MET:CA	3:R:3110[B]:THR:HG23	2.10	0.75
3:U:3141[B]:TYR:HD2	3:U:3142[B]:ASN:H	0.78	0.75
3:U:3255[B]:PRO:CD	3:d:3253[B]:GLU:C	2.59	0.75
3:X:2971[A]:ASP:OD1	3:X:2973[A]:THR:OG1	2.04	0.75
3:X:3196[A]:THR:H	3:X:3199[A]:GLN:CD	1.94	0.75
3:X:3204[A]:LEU:O	3:X:3208[A]:GLN:HG3	1.86	0.75
3:X:3307[A]:PHE:CE1	3:X:3309[A]:PRO:HG3	2.16	0.75
2:c:2625:LEU:HA	2:c:2638:ARG:HH12	1.51	0.75
3:d:2955[A]:GLN:CD	3:d:3037[A]:TYR:HE1	1.92	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3038[A]:ILE:HG22	3:d:3040[A]:VAL:HG22	1.68	0.75
3:d:3089[B]:HIS:HD1	3:d:3119[B]:HIS:CE1	2.04	0.75
3:d:3137[B]:ARG:HB3	3:d:3139[B]:LEU:CD2	2.17	0.75
3:C:3180[A]:TYR:HB2	3:C:3183[A]:LEU:CD2	2.16	0.74
3:C:3219[A]:LEU:HD22	3:C:3219[A]:LEU:N	2.02	0.74
3:C:3219[B]:LEU:HD22	3:C:3219[B]:LEU:N	2.02	0.74
3:F:2983[B]:VAL:HG23	3:a:3160[B]:SER:CA	2.17	0.74
3:F:3149[B]:ASN:CB	3:a:3163[B]:ASN:CG	2.60	0.74
3:F:3153[B]:LYS:HD3	3:a:2988[B]:TRP:CD1	2.22	0.74
3:F:3223[B]:GLY:CA	3:a:2963[B]:MET:HE1	2.17	0.74
3:I:3174[B]:GLY:N	3:R:3154[B]:PRO:CA	2.49	0.74
3:I:3176[B]:LYS:HE2	3:I:3176[B]:LYS:N	2.02	0.74
3:I:3220[A]:ARG:HG3	3:I:3220[A]:ARG:NH1	1.98	0.74
3:I:3293[B]:LYS:HB2	3:I:3294[B]:SER:HB2	0.82	0.74
1:J:1627:ARG:NH2	1:J:1629:GLU:OE1	2.19	0.74
3:L:2954[A]:TYR:O	3:L:2957[A]:ILE:HG22	1.87	0.74
3:L:3204[B]:LEU:O	3:L:3208[B]:GLN:HG3	1.86	0.74
3:O:2952[A]:ALA:HA	3:O:2956[A]:LYS:HB2	1.69	0.74
3:O:3211[B]:ASP:HB3	3:O:3309[B]:PRO:HA	1.67	0.74
3:R:2971[B]:ASP:N	9:R:3401[B]:CUO:O2	2.19	0.74
3:R:3137[A]:ARG:HB3	3:R:3139[A]:LEU:HD23	1.69	0.74
3:R:3288[A]:MET:HG2	3:R:3295[A]:LEU:HD21	1.67	0.74
3:X:2952[A]:ALA:HA	3:X:2956[A]:LYS:HB2	1.69	0.74
3:X:3211[A]:ASP:HB3	3:X:3309[A]:PRO:HA	1.67	0.74
3:a:3114[B]:PRO:HD2	3:a:3115[B]:LEU:H	1.51	0.74
3:d:2969[B]:TYR:HD2	3:d:2971[B]:ASP:N	1.84	0.74
3:d:3120[B]:HIS:O	3:d:3121[B]:SER:C	2.29	0.74
3:d:3212[B]:ARG:HG3	3:d:3212[B]:ARG:NH1	2.00	0.74
3:C:3114[A]:PRO:HD2	3:C:3115[A]:LEU:H	1.51	0.74
1:D:806:ASN:ND2	6:k:1:NAG:H83	2.02	0.74
3:F:2979[B]:GLN:C	3:a:2967[B]:CYS:HB3	2.12	0.74
3:F:3012[A]:TRP:O	3:F:3122[A]:ASN:ND2	2.20	0.74
3:F:3137[A]:ARG:HB3	3:F:3139[A]:LEU:HD23	1.69	0.74
3:I:2971[B]:ASP:N	9:I:3401[B]:CUO:O2	2.20	0.74
3:I:3150[B]:LYS:NZ	3:R:3162[B]:ASP:O	2.19	0.74
3:I:3155[B]:MET:O	3:I:3159[B]:SER:N	2.20	0.74
3:I:3219[A]:LEU:HD22	3:I:3219[A]:LEU:N	2.02	0.74
3:L:2952[B]:ALA:HA	3:L:2956[B]:LYS:HB3	1.67	0.74
3:L:3012[B]:TRP:O	3:L:3122[B]:ASN:ND2	2.20	0.74
3:O:2965[A]:LEU:HD21	3:O:2974[A]:ALA:HB1	1.70	0.74
3:O:2968[B]:GLN:HB3	3:X:2979[B]:GLN:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3219[B]:LEU:HD22	3:O:3219[B]:LEU:N	2.02	0.74
3:R:2971[A]:ASP:OD1	3:R:2973[A]:THR:OG1	2.04	0.74
3:U:2952[A]:ALA:HA	3:U:2956[A]:LYS:HB2	1.69	0.74
3:U:2965[B]:LEU:CG	3:U:2974[B]:ALA:HB1	2.09	0.74
3:U:3082[B]:GLU:CD	3:d:2970[B]:PRO:HB3	2.12	0.74
3:U:3114[A]:PRO:HD2	3:U:3115[A]:LEU:H	1.51	0.74
3:X:2954[A]:TYR:O	3:X:2957[A]:ILE:HG22	1.87	0.74
3:X:3012[A]:TRP:O	3:X:3122[A]:ASN:ND2	2.20	0.74
3:X:3307[B]:PHE:CE1	3:X:3309[B]:PRO:HG3	2.16	0.74
3:a:3196[A]:THR:H	3:a:3199[A]:GLN:CD	1.94	0.74
3:d:3012[B]:TRP:O	3:d:3122[B]:ASN:ND2	2.20	0.74
3:d:3176[B]:LYS:HE2	3:d:3176[B]:LYS:N	2.02	0.74
1:A:527:LEU:O	1:A:561:ARG:NH1	2.19	0.74
1:A:1063:ARG:HB3	1:A:1065:LYS:HD2	1.68	0.74
3:C:2969[B]:TYR:HD2	3:C:2971[B]:ASP:N	1.84	0.74
3:C:3137[B]:ARG:HB3	3:C:3139[B]:LEU:HD23	1.69	0.74
3:C:3147[B]:GLU:CG	3:C:3149[B]:ASN:HD21	2.00	0.74
3:C:3284[A]:LYS:CD	3:C:3285[A]:VAL:N	2.47	0.74
3:F:3038[A]:ILE:HG22	3:F:3040[A]:VAL:HG22	1.68	0.74
3:F:3089[B]:HIS:HD1	3:F:3119[B]:HIS:CE1	2.04	0.74
3:F:3113[A]:ASP:CG	3:F:3114[A]:PRO:CD	2.56	0.74
3:F:3113[B]:ASP:CG	3:F:3114[B]:PRO:CD	2.56	0.74
3:F:3147[A]:GLU:CG	3:F:3149[A]:ASN:HD21	2.00	0.74
3:F:3176[B]:LYS:HE2	3:F:3176[B]:LYS:N	2.02	0.74
3:F:3219[B]:LEU:HD22	3:F:3219[B]:LEU:N	2.02	0.74
2:H:2142:ALA:HB2	2:H:2433:THR:HG23	1.68	0.74
3:I:3024[B]:LEU:CD1	3:I:3025[B]:VAL:H	1.83	0.74
3:I:3038[A]:ILE:HG22	3:I:3040[A]:VAL:HG22	1.68	0.74
3:I:3089[B]:HIS:HD1	3:I:3119[B]:HIS:CE1	2.04	0.74
3:I:3137[A]:ARG:HB3	3:I:3139[A]:LEU:HD23	1.69	0.74
3:I:3137[B]:ARG:HB3	3:I:3139[B]:LEU:HD23	1.69	0.74
3:I:3157[B]:PRO:HD3	3:R:3254[B]:MET:CE	2.16	0.74
3:L:2948[B]:ASP:HB3	3:L:2949[B]:LYS:CA	2.15	0.74
3:L:3196[A]:THR:H	3:L:3199[A]:GLN:CD	1.94	0.74
3:O:2969[B]:TYR:HB3	3:X:2988[B]:TRP:O	1.88	0.74
3:O:3137[A]:ARG:HB3	3:O:3139[A]:LEU:HD23	1.69	0.74
3:O:3222[B]:ILE:N	3:X:3161[B]:GLU:CB	2.40	0.74
3:U:3170[B]:ALA:N	3:d:3148[B]:ILE:HB	2.03	0.74
3:X:2952[B]:ALA:CB	3:X:2953[B]:GLY:C	2.48	0.74
3:X:2969[A]:TYR:O	3:X:2972[A]:GLY:N	2.21	0.74
3:X:2969[B]:TYR:O	3:X:2972[B]:GLY:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3155[B]:MET:O	3:X:3159[B]:SER:N	2.20	0.74
3:a:3114[A]:PRO:HD2	3:a:3115[A]:LEU:H	1.51	0.74
3:a:3137[A]:ARG:HB3	3:a:3139[A]:LEU:HD23	1.69	0.74
3:a:3155[A]:MET:O	3:a:3159[A]:SER:N	2.20	0.74
3:C:3153[B]:LYS:O	3:L:3154[B]:PRO:C	2.29	0.74
3:F:2954[B]:TYR:O	3:F:2957[B]:ILE:HG22	1.87	0.74
3:F:2988[A]:TRP:CE3	3:F:2989[A]:HIS:ND1	2.53	0.74
3:F:3137[A]:ARG:HB3	3:F:3139[A]:LEU:CD2	2.17	0.74
3:F:3211[B]:ASP:HB3	3:F:3309[B]:PRO:HA	1.67	0.74
1:G:1145:THR:HG1	1:G:1233:SER:HG	1.33	0.74
3:I:2952[B]:ALA:HA	3:I:2956[B]:LYS:HB3	1.67	0.74
3:I:2977[B]:CYS:CB	3:R:2982[B]:MET:CE	2.65	0.74
3:I:3012[A]:TRP:O	3:I:3122[A]:ASN:ND2	2.20	0.74
3:I:3012[B]:TRP:O	3:I:3122[B]:ASN:ND2	2.20	0.74
3:L:3219[B]:LEU:HD22	3:L:3219[B]:LEU:N	2.02	0.74
3:R:2954[B]:TYR:O	3:R:2957[B]:ILE:HG22	1.87	0.74
3:R:2963[A]:MET:HG2	3:R:3108[A]:HIS:CG	2.23	0.74
3:R:3012[A]:TRP:O	3:R:3122[A]:ASN:ND2	2.20	0.74
3:R:3089[B]:HIS:HD1	3:R:3119[B]:HIS:CE1	2.04	0.74
3:R:3134[A]:GLN:HG3	3:R:3139[A]:LEU:HB2	1.70	0.74
3:R:3147[A]:GLU:CG	3:R:3149[A]:ASN:HD21	2.00	0.74
3:R:3219[B]:LEU:HD22	3:R:3219[B]:LEU:N	2.02	0.74
3:U:2988[A]:TRP:CE3	3:U:2989[A]:HIS:ND1	2.53	0.74
3:U:3137[A]:ARG:HB3	3:U:3139[A]:LEU:CD2	2.17	0.74
3:U:3147[A]:GLU:CG	3:U:3149[A]:ASN:HD21	2.00	0.74
3:X:3176[A]:LYS:HE2	3:X:3176[A]:LYS:N	2.02	0.74
1:Y:133:LYS:HE3	1:Y:134:VAL:H	1.53	0.74
3:a:2952[B]:ALA:HA	3:a:2956[B]:LYS:HB2	1.69	0.74
3:a:3137[A]:ARG:HB3	3:a:3139[A]:LEU:CD2	2.17	0.74
3:a:3147[B]:GLU:CG	3:a:3149[B]:ASN:HD21	2.00	0.74
3:a:3219[B]:LEU:HD22	3:a:3219[B]:LEU:N	2.02	0.74
1:b:1228:LEU:HB3	1:b:1229:LYS:HB2	1.69	0.74
3:d:2952[B]:ALA:HA	3:d:2956[B]:LYS:HB2	1.69	0.74
3:d:2988[A]:TRP:CE3	3:d:2989[A]:HIS:ND1	2.53	0.74
3:d:3038[B]:ILE:HG22	3:d:3040[B]:VAL:HG22	1.68	0.74
3:d:3141[A]:TYR:HD2	3:d:3142[A]:ASN:H	0.78	0.74
3:d:3155[A]:MET:O	3:d:3159[A]:SER:N	2.21	0.74
3:C:3012[A]:TRP:O	3:C:3122[A]:ASN:ND2	2.20	0.74
3:C:3137[A]:ARG:HB3	3:C:3139[A]:LEU:CD2	2.17	0.74
3:C:3147[A]:GLU:HB2	3:C:3149[A]:ASN:OD1	1.86	0.74
3:C:3152[B]:LYS:CB	3:L:3173[B]:THR:N	2.30	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3196[A]:THR:H	3:C:3199[A]:GLN:CD	1.94	0.74
3:F:2937[B]:ASN:HB2	3:F:3006[B]:LYS:CE	2.14	0.74
3:F:2963[B]:MET:HG2	3:F:3108[B]:HIS:CG	2.23	0.74
3:F:3137[B]:ARG:HB3	3:F:3139[B]:LEU:CD2	2.17	0.74
3:I:2963[A]:MET:HG2	3:I:3108[A]:HIS:CG	2.23	0.74
3:I:2974[B]:ALA:N	3:R:3248[B]:LEU:C	2.45	0.74
3:I:2988[A]:TRP:CE3	3:I:2989[A]:HIS:ND1	2.53	0.74
3:I:3155[B]:MET:HE1	3:R:3156[B]:MET:HG2	1.67	0.74
3:I:3196[A]:THR:HG21	1:J:416:ASN:HD22	0.68	0.74
3:I:3307[A]:PHE:CE1	3:I:3309[A]:PRO:HG3	2.16	0.74
1:J:1392:ASP:HB2	1:M:1372:ILE:HD11	1.70	0.74
3:O:3038[B]:ILE:CB	3:X:2969[B]:TYR:OH	2.35	0.74
3:O:3159[B]:SER:C	3:X:3148[B]:ILE:CA	2.60	0.74
1:P:240:PHE:HA	1:P:263:ALA:HB3	1.69	0.74
1:P:1357:ARG:HH11	1:P:1357:ARG:HB3	1.53	0.74
3:R:2952[A]:ALA:HA	3:R:2956[A]:LYS:HB2	1.70	0.74
3:R:2961[B]:HIS:HD2	3:R:2988[B]:TRP:HZ3	1.31	0.74
3:R:2969[B]:TYR:O	3:R:2972[B]:GLY:N	2.20	0.74
3:R:2971[B]:ASP:OD1	3:R:2973[B]:THR:OG1	2.04	0.74
3:R:3113[B]:ASP:CG	3:R:3114[B]:PRO:CD	2.56	0.74
3:U:2954[B]:TYR:O	3:U:2957[B]:ILE:HG22	1.87	0.74
3:U:2971[A]:ASP:OD1	3:U:2973[A]:THR:OG1	2.04	0.74
3:U:3147[B]:GLU:HB2	3:U:3149[B]:ASN:OD1	1.86	0.74
3:U:3155[B]:MET:O	3:U:3159[B]:SER:N	2.20	0.74
3:U:3156[B]:MET:CE	3:d:2982[B]:MET:CB	2.66	0.74
3:U:3256[B]:TRP:CG	3:d:2975[B]:PHE:CE1	2.75	0.74
3:X:2937[A]:ASN:CB	3:X:3006[A]:LYS:HE2	2.14	0.74
3:X:2952[B]:ALA:HA	3:X:2956[B]:LYS:HB2	1.70	0.74
3:X:2963[B]:MET:HG2	3:X:3108[B]:HIS:CG	2.23	0.74
3:X:2965[A]:LEU:HD21	3:X:2974[A]:ALA:HB1	1.69	0.74
3:X:3038[A]:ILE:HG22	3:X:3040[A]:VAL:HG22	1.68	0.74
3:X:3212[B]:ARG:HG3	3:X:3212[B]:ARG:NH1	2.00	0.74
1:Y:136:ALA:O	1:Y:193:SER:OG	2.04	0.74
3:a:2954[A]:TYR:O	3:a:2957[A]:ILE:HG22	1.87	0.74
3:a:2954[B]:TYR:O	3:a:2957[B]:ILE:HG22	1.87	0.74
3:a:2971[B]:ASP:OD1	3:a:2973[B]:THR:OG1	2.04	0.74
3:d:2937[B]:ASN:CB	3:d:3006[B]:LYS:HE2	2.14	0.74
3:d:2952[A]:ALA:HA	3:d:2956[A]:LYS:HB2	1.69	0.74
3:d:2955[B]:GLN:CD	3:d:3037[B]:TYR:HE1	1.92	0.74
3:d:2965[B]:LEU:HD21	3:d:2974[B]:ALA:HB1	1.70	0.74
8:0:2:NAG:O3	8:0:3:BMA:H2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2963[A]:MET:HG2	3:C:3108[A]:HIS:CG	2.23	0.74
3:C:3012[B]:TRP:O	3:C:3122[B]:ASN:ND2	2.20	0.74
3:C:3113[A]:ASP:CG	3:C:3114[A]:PRO:CD	2.56	0.74
3:F:3147[B]:GLU:CG	3:F:3149[B]:ASN:HD21	2.00	0.74
3:F:3155[A]:MET:O	3:F:3159[A]:SER:N	2.20	0.74
2:H:2869:ALA:O	2:H:2875:SER:OG	2.05	0.74
3:I:2971[B]:ASP:O	3:R:3093[B]:HIS:CG	2.40	0.74
3:I:3120[B]:HIS:O	3:I:3121[B]:SER:C	2.29	0.74
3:I:3196[A]:THR:H	3:I:3199[A]:GLN:CD	1.94	0.74
3:I:3256[B]:TRP:NE1	3:R:2965[B]:LEU:CD1	2.50	0.74
1:J:187:GLY:HA3	1:J:195:SER:HB3	1.70	0.74
3:O:2954[A]:TYR:O	3:O:2957[A]:ILE:HG22	1.87	0.74
3:O:3147[A]:GLU:CG	3:O:3149[A]:ASN:HD21	2.00	0.74
3:O:3159[B]:SER:O	3:X:3148[B]:ILE:CA	2.30	0.74
3:O:3163[B]:ASN:HB2	3:X:3149[B]:ASN:CB	2.17	0.74
3:O:3196[B]:THR:H	3:O:3199[B]:GLN:CD	1.94	0.74
3:R:3089[A]:HIS:HD1	3:R:3119[A]:HIS:CE1	2.04	0.74
3:U:2963[A]:MET:HG2	3:U:3108[A]:HIS:CG	2.23	0.74
3:U:3157[B]:PRO:O	3:d:3147[B]:GLU:OE1	2.06	0.74
3:U:3211[A]:ASP:HB3	3:U:3309[A]:PRO:HA	1.67	0.74
3:X:2955[B]:GLN:CD	3:X:3037[B]:TYR:HE1	1.92	0.74
3:a:2988[B]:TRP:CE3	3:a:2989[B]:HIS:ND1	2.53	0.74
2:c:2570:HIS:HD2	2:c:2711:HIS:CE1	2.05	0.74
3:d:2948[A]:ASP:H	3:d:2949[A]:LYS:CA	1.98	0.74
3:d:2969[A]:TYR:O	3:d:2972[A]:GLY:N	2.20	0.74
3:d:3307[B]:PHE:CE1	3:d:3309[B]:PRO:HG3	2.16	0.74
1:A:1187:LYS:HD3	2:E:2897:PRO:HG3	1.70	0.74
3:C:2965[A]:LEU:HD21	3:C:2974[A]:ALA:HB1	1.70	0.74
3:C:3155[B]:MET:O	3:C:3159[B]:SER:N	2.20	0.74
3:F:2937[B]:ASN:CB	3:F:3006[B]:LYS:HE2	2.14	0.74
3:F:3134[A]:GLN:HG3	3:F:3139[A]:LEU:HB2	1.70	0.74
3:L:2971[A]:ASP:OD1	3:L:2973[A]:THR:OG1	2.04	0.74
3:L:3137[A]:ARG:HB3	3:L:3139[A]:LEU:HD23	1.69	0.74
3:L:3219[A]:LEU:HD22	3:L:3219[A]:LEU:N	2.02	0.74
3:O:2955[B]:GLN:CD	3:O:3037[B]:TYR:HE1	1.92	0.74
3:O:3134[A]:GLN:HG3	3:O:3139[A]:LEU:HB2	1.70	0.74
3:O:3147[B]:GLU:CG	3:O:3149[B]:ASN:HD21	2.00	0.74
3:O:3155[A]:MET:O	3:O:3159[A]:SER:N	2.20	0.74
3:O:3176[A]:LYS:HE2	3:O:3176[A]:LYS:N	2.02	0.74
3:O:3252[B]:TYR:HB3	3:X:3156[B]:MET:CB	2.13	0.74
3:R:2965[B]:LEU:HD21	3:R:2974[B]:ALA:HB1	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3137[B]:ARG:HB3	3:R:3139[B]:LEU:HD23	1.69	0.74
3:R:3176[A]:LYS:HE2	3:R:3176[A]:LYS:N	2.02	0.74
3:U:2952[B]:ALA:HA	3:U:2956[B]:LYS:HB3	1.67	0.74
3:U:2954[A]:TYR:O	3:U:2957[A]:ILE:HG22	1.87	0.74
3:U:2967[B]:CYS:CB	3:d:3256[B]:TRP:HB2	2.18	0.74
3:U:2982[B]:MET:O	3:d:2970[B]:PRO:HD3	1.87	0.74
3:U:3137[B]:ARG:HB3	3:U:3139[B]:LEU:CD2	2.17	0.74
3:U:3137[B]:ARG:HB3	3:U:3139[B]:LEU:HD23	1.69	0.74
3:U:3155[A]:MET:O	3:U:3159[A]:SER:N	2.20	0.74
3:U:3220[B]:ARG:HG3	3:U:3220[B]:ARG:NH1	1.98	0.74
3:U:3254[B]:MET:HB2	3:d:3254[B]:MET:HA	1.66	0.74
3:U:3255[B]:PRO:CB	3:d:2974[B]:ALA:O	2.36	0.74
3:X:3012[B]:TRP:O	3:X:3122[B]:ASN:ND2	2.20	0.74
3:X:3038[B]:ILE:HG22	3:X:3040[B]:VAL:HG22	1.68	0.74
3:X:3137[B]:ARG:HB3	3:X:3139[B]:LEU:CD2	2.17	0.74
3:X:3220[A]:ARG:HG3	3:X:3220[A]:ARG:NH1	1.98	0.74
3:a:2965[B]:LEU:HD21	3:a:2974[B]:ALA:HB1	1.70	0.74
3:d:2937[A]:ASN:CB	3:d:3006[A]:LYS:HE2	2.14	0.74
3:C:2963[B]:MET:HG2	3:C:3108[B]:HIS:CG	2.23	0.74
3:C:3147[A]:GLU:CG	3:C:3149[A]:ASN:HD21	2.00	0.74
3:C:3158[B]:PHE:O	3:L:3149[B]:ASN:C	2.31	0.74
3:C:3307[B]:PHE:CE1	3:C:3309[B]:PRO:HG3	2.16	0.74
1:D:1631:GLU:OE1	1:G:328:LYS:NZ	2.21	0.74
3:F:2954[A]:TYR:O	3:F:2957[A]:ILE:HG22	1.87	0.74
3:F:3012[B]:TRP:O	3:F:3122[B]:ASN:ND2	2.20	0.74
3:F:3155[B]:MET:O	3:F:3159[B]:SER:N	2.20	0.74
3:F:3173[B]:THR:CA	3:a:3154[B]:PRO:N	2.51	0.74
3:F:3284[A]:LYS:CD	3:F:3285[A]:VAL:N	2.47	0.74
2:K:2124:SER:HB2	2:K:2129:PRO:HG2	1.70	0.74
3:L:3038[A]:ILE:HG22	3:L:3040[A]:VAL:HG22	1.68	0.74
3:L:3038[B]:ILE:HG22	3:L:3040[B]:VAL:HG22	1.68	0.74
3:U:3212[B]:ARG:HG3	3:U:3212[B]:ARG:NH1	2.00	0.74
3:X:2954[B]:TYR:O	3:X:2957[B]:ILE:HG22	1.87	0.74
3:X:2963[A]:MET:HG2	3:X:3108[A]:HIS:CG	2.23	0.74
3:X:3120[A]:HIS:O	3:X:3121[A]:SER:C	2.29	0.74
3:X:3155[A]:MET:O	3:X:3159[A]:SER:N	2.20	0.74
3:a:3113[B]:ASP:CG	3:a:3114[B]:PRO:CD	2.56	0.74
1:b:460:GLU:OE2	1:b:1368:ARG:NH2	2.21	0.74
2:c:2806:ALA:HB2	2:c:2856:ILE:HD11	1.69	0.74
1:A:1302:SER:HB3	1:A:1303:GLU:HA	1.68	0.74
3:C:2968[B]:GLN:HE21	3:L:3086[B]:GLU:CB	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2426:PHE:HB3	2:E:2445:MET:HE1	1.69	0.74
3:F:3114[A]:PRO:HD2	3:F:3115[A]:LEU:H	1.51	0.74
3:F:3221[B]:ALA:HB3	3:a:2964[B]:PRO:HB3	1.68	0.74
3:I:2965[A]:LEU:HD21	3:I:2974[A]:ALA:HB1	1.70	0.74
3:L:3012[A]:TRP:O	3:L:3122[A]:ASN:ND2	2.20	0.74
3:L:3093[B]:HIS:HE1	3:L:3119[B]:HIS:CD2	2.06	0.74
3:O:2930[B]:LEU:H	3:O:2930[B]:LEU:CD2	1.97	0.74
3:O:3113[A]:ASP:CG	3:O:3114[A]:PRO:CD	2.56	0.74
3:O:3160[B]:SER:CA	3:X:3151[B]:LEU:HG	2.18	0.74
3:R:2955[B]:GLN:CD	3:R:3037[B]:TYR:HE1	1.92	0.74
3:R:3012[B]:TRP:O	3:R:3122[B]:ASN:ND2	2.20	0.74
3:R:3137[B]:ARG:HB3	3:R:3139[B]:LEU:CD2	2.17	0.74
3:U:2965[A]:LEU:HD21	3:U:2974[A]:ALA:HB1	1.69	0.74
3:U:3012[B]:TRP:O	3:U:3122[B]:ASN:ND2	2.20	0.74
3:U:3089[A]:HIS:HD1	3:U:3119[A]:HIS:CE1	2.04	0.74
3:U:3093[A]:HIS:HE1	3:U:3119[A]:HIS:CD2	2.06	0.74
3:U:3113[A]:ASP:CG	3:U:3114[A]:PRO:CD	2.56	0.74
3:U:3176[A]:LYS:HE2	3:U:3176[A]:LYS:N	2.02	0.74
3:U:3196[A]:THR:H	3:U:3199[A]:GLN:CD	1.94	0.74
3:U:3254[B]:MET:HB2	3:d:3254[B]:MET:HB3	1.70	0.74
3:U:3257[B]:ALA:H	3:d:2968[B]:GLN:C	1.95	0.74
3:X:2971[B]:ASP:OD1	3:X:2973[B]:THR:OG1	2.04	0.74
3:a:2988[A]:TRP:CE3	3:a:2989[A]:HIS:ND1	2.53	0.74
3:a:3012[A]:TRP:O	3:a:3122[A]:ASN:ND2	2.20	0.74
3:a:3219[A]:LEU:HD22	3:a:3219[A]:LEU:N	2.02	0.74
3:d:3093[A]:HIS:HE1	3:d:3119[A]:HIS:CD2	2.06	0.74
3:d:3293[A]:LYS:HB2	3:d:3294[A]:SER:HB2	0.82	0.74
4:t:1:NAG:H83	4:t:1:NAG:O3	1.88	0.74
1:A:105:VAL:HG12	1:A:123:PHE:HB3	1.70	0.74
1:A:589:GLN:HG2	1:A:594:ASP:HB3	1.68	0.74
1:A:1036:SER:OG	1:A:1037:ALA:N	2.20	0.74
3:C:2952[A]:ALA:HA	3:C:2956[A]:LYS:HB2	1.70	0.74
3:C:2971[A]:ASP:OD1	3:C:2973[A]:THR:OG1	2.04	0.74
3:F:2956[A]:LYS:C	3:F:2960[A]:PHE:CE1	2.47	0.74
3:F:2963[A]:MET:HG2	3:F:3108[A]:HIS:CG	2.23	0.74
3:F:3163[B]:ASN:CB	3:a:3150[B]:LYS:CE	2.60	0.74
3:I:3147[B]:GLU:CG	3:I:3149[B]:ASN:HD21	2.00	0.74
3:L:2952[B]:ALA:HA	3:L:2956[B]:LYS:HB2	1.69	0.74
3:L:2963[A]:MET:HG2	3:L:3108[A]:HIS:CG	2.23	0.74
3:L:3137[B]:ARG:HB3	3:L:3139[B]:LEU:CD2	2.17	0.74
3:L:3147[A]:GLU:HB2	3:L:3149[A]:ASN:OD1	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3147[B]:GLU:HB2	3:L:3149[B]:ASN:OD1	1.86	0.74
1:M:898:GLY:N	1:M:899:MET:SD	2.56	0.74
3:O:3025[A]:VAL:HG22	3:O:3047[A]:ARG:NH1	2.02	0.74
3:O:3137[A]:ARG:HB3	3:O:3139[A]:LEU:CD2	2.17	0.74
1:P:1301:PRO:HB3	1:P:1308:VAL:HG12	1.69	0.74
3:R:3137[A]:ARG:HB3	3:R:3139[A]:LEU:CD2	2.17	0.74
3:U:2937[B]:ASN:CB	3:U:3006[B]:LYS:HE2	2.14	0.74
3:U:2975[B]:PHE:CE1	3:d:3253[B]:GLU:HG3	2.23	0.74
3:U:3134[B]:GLN:HG3	3:U:3139[B]:LEU:HB2	1.70	0.74
3:X:3212[A]:ARG:HG3	3:X:3212[A]:ARG:NH1	2.00	0.74
1:Y:1617:LYS:HE3	3:d:3180[B]:TYR:CE2	2.22	0.74
3:a:2963[A]:MET:HG2	3:a:3108[A]:HIS:CG	2.23	0.74
3:d:3012[A]:TRP:O	3:d:3122[A]:ASN:ND2	2.20	0.74
3:d:3137[B]:ARG:HB3	3:d:3139[B]:LEU:HD23	1.69	0.74
3:d:3141[B]:TYR:HD2	3:d:3142[B]:ASN:H	0.78	0.74
3:C:2969[A]:TYR:HD2	3:C:2971[A]:ASP:N	1.85	0.73
3:C:3038[B]:ILE:HG22	3:C:3040[B]:VAL:HG22	1.68	0.73
3:C:3212[A]:ARG:HG3	3:C:3212[A]:ARG:NH1	2.00	0.73
3:C:3223[B]:GLY:O	3:L:3252[B]:TYR:CD2	2.40	0.73
3:C:3293[B]:LYS:HB2	3:C:3294[B]:SER:HB2	0.82	0.73
1:D:1161:ILE:HD11	1:D:1196:ILE:HD11	1.69	0.73
3:F:2937[A]:ASN:HB2	3:F:3006[A]:LYS:CE	2.14	0.73
3:F:3089[B]:HIS:CD2	3:a:2972[B]:GLY:N	2.55	0.73
3:F:3141[B]:TYR:HD2	3:F:3142[B]:ASN:H	0.78	0.73
3:F:3153[B]:LYS:HZ3	3:a:3157[B]:PRO:HD2	1.49	0.73
3:F:3154[B]:PRO:CG	3:a:3174[B]:GLY:HA2	2.16	0.73
3:F:3154[B]:PRO:C	3:a:3153[B]:LYS:O	2.31	0.73
3:F:3158[B]:PHE:N	3:a:3153[B]:LYS:HE3	2.03	0.73
1:J:142:ARG:NH1	1:J:340:GLN:OE1	2.21	0.73
3:L:3155[A]:MET:O	3:L:3159[A]:SER:N	2.20	0.73
3:L:3176[A]:LYS:HE2	3:L:3176[A]:LYS:N	2.02	0.73
3:L:3307[A]:PHE:CE1	3:L:3309[A]:PRO:HG3	2.16	0.73
3:O:3134[B]:GLN:HG3	3:O:3139[B]:LEU:HB2	1.70	0.73
1:S:573:LYS:HB3	1:S:574:GLY:CA	2.18	0.73
3:U:2955[A]:GLN:CD	3:U:3037[A]:TYR:HE1	1.92	0.73
3:X:2937[A]:ASN:HB2	3:X:3006[A]:LYS:CE	2.14	0.73
3:X:3284[A]:LYS:CD	3:X:3285[A]:VAL:N	2.47	0.73
3:a:3120[B]:HIS:O	3:a:3121[B]:SER:C	2.29	0.73
3:a:3155[B]:MET:O	3:a:3159[B]:SER:N	2.20	0.73
3:a:3196[B]:THR:H	3:a:3199[B]:GLN:CD	1.94	0.73
3:C:2937[B]:ASN:HB2	3:C:3006[B]:LYS:CE	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3038[A]:ILE:HG22	3:C:3040[A]:VAL:HG22	1.68	0.73
3:C:3172[B]:SER:OG	3:L:3152[B]:LYS:CB	2.36	0.73
1:D:1144:VAL:HB	1:D:1196:ILE:HD12	1.70	0.73
3:F:3093[B]:HIS:HE1	3:F:3119[B]:HIS:CD2	2.06	0.73
3:F:3196[A]:THR:H	3:F:3199[A]:GLN:CD	1.94	0.73
3:I:3093[A]:HIS:HE1	3:I:3119[A]:HIS:CD2	2.06	0.73
3:I:3147[A]:GLU:CG	3:I:3149[A]:ASN:HD21	2.00	0.73
3:I:3155[A]:MET:O	3:I:3159[A]:SER:N	2.20	0.73
3:I:3221[B]:ALA:HB1	3:R:2964[B]:PRO:CA	2.13	0.73
3:I:3255[B]:PRO:CG	3:R:2964[B]:PRO:CD	2.66	0.73
3:I:3293[A]:LYS:HB2	3:I:3294[A]:SER:HB2	0.82	0.73
1:J:639:ARG:NH2	1:J:707:PHE:O	2.21	0.73
2:K:2722:GLN:NE2	2:K:2769:PHE:O	2.20	0.73
3:R:3093[A]:HIS:HE1	3:R:3119[A]:HIS:CD2	2.06	0.73
3:U:3012[A]:TRP:O	3:U:3122[A]:ASN:ND2	2.20	0.73
3:U:3147[B]:GLU:CG	3:U:3149[B]:ASN:HD21	2.00	0.73
3:U:3275[A]:LEU:N	3:U:3275[A]:LEU:HD12	2.04	0.73
3:X:3134[A]:GLN:HG3	3:X:3139[A]:LEU:HB2	1.70	0.73
1:Y:1546:LYS:HG3	3:d:3001[B]:LYS:CG	2.17	0.73
3:a:2948[B]:ASP:H	3:a:2949[B]:LYS:CA	1.98	0.73
3:a:2952[A]:ALA:HA	3:a:2956[A]:LYS:HB2	1.70	0.73
3:a:3176[A]:LYS:HE2	3:a:3176[A]:LYS:N	2.02	0.73
3:a:3176[B]:LYS:HE2	3:a:3176[B]:LYS:N	2.02	0.73
3:d:2969[B]:TYR:O	3:d:2972[B]:GLY:N	2.21	0.73
3:d:3025[A]:VAL:HG22	3:d:3047[A]:ARG:NH1	2.01	0.73
3:d:3219[B]:LEU:HD22	3:d:3219[B]:LEU:N	2.02	0.73
3:d:3307[A]:PHE:CE1	3:d:3309[A]:PRO:HG3	2.16	0.73
3:C:2937[B]:ASN:CB	3:C:3006[B]:LYS:HE2	2.14	0.73
3:C:3176[B]:LYS:HE2	3:C:3176[B]:LYS:N	2.02	0.73
3:F:2971[B]:ASP:OD2	3:a:3110[B]:THR:HG21	1.88	0.73
3:F:2975[B]:PHE:CZ	3:a:2961[B]:HIS:CG	2.75	0.73
3:F:3159[B]:SER:HG	3:a:2984[B]:THR:HG21	1.52	0.73
3:I:2985[B]:PHE:HZ	3:R:2970[B]:PRO:HA	1.52	0.73
1:J:164:GLU:OE1	1:J:296:ARG:NH1	2.21	0.73
3:L:2968[A]:GLN:CB	3:L:2972[A]:GLY:HA2	2.18	0.73
3:L:3137[B]:ARG:HB3	3:L:3139[B]:LEU:HD23	1.69	0.73
3:L:3155[B]:MET:O	3:L:3159[B]:SER:N	2.20	0.73
3:O:3089[B]:HIS:NE2	9:O:3401[B]:CUO:CU1	1.54	0.73
3:O:3093[B]:HIS:HE1	3:O:3119[B]:HIS:CD2	2.06	0.73
3:R:2937[A]:ASN:HB2	3:R:3006[A]:LYS:CE	2.14	0.73
3:R:2968[B]:GLN:CB	3:R:2972[B]:GLY:HA2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3120[A]:HIS:O	3:R:3121[A]:SER:C	2.29	0.73
3:R:3155[A]:MET:O	3:R:3159[A]:SER:N	2.20	0.73
3:R:3275[A]:LEU:HD12	3:R:3275[A]:LEU:N	2.04	0.73
3:U:2952[B]:ALA:HA	3:U:2956[B]:LYS:HB2	1.69	0.73
3:U:3025[A]:VAL:HG22	3:U:3047[A]:ARG:NH1	2.02	0.73
3:U:3038[A]:ILE:HG22	3:U:3040[A]:VAL:HG22	1.68	0.73
3:U:3093[B]:HIS:HE1	3:U:3119[B]:HIS:CD2	2.06	0.73
3:X:3025[B]:VAL:HG22	3:X:3047[B]:ARG:NH1	2.02	0.73
3:X:3093[B]:HIS:HE1	3:X:3119[B]:HIS:CD2	2.06	0.73
3:X:3134[B]:GLN:HG3	3:X:3139[B]:LEU:HB2	1.70	0.73
3:a:3012[B]:TRP:O	3:a:3122[B]:ASN:ND2	2.20	0.73
3:d:2963[B]:MET:HG2	3:d:3108[B]:HIS:CG	2.23	0.73
3:d:3176[A]:LYS:HE2	3:d:3176[A]:LYS:N	2.02	0.73
1:A:898:GLY:HA2	1:A:1186:TRP:HB2	1.68	0.73
3:C:3158[B]:PHE:HD2	3:L:3153[B]:LYS:NZ	1.72	0.73
3:F:3275[B]:LEU:HD12	3:F:3275[B]:LEU:N	2.04	0.73
3:I:2968[B]:GLN:CB	3:I:2972[B]:GLY:HA2	2.18	0.73
1:J:572:SER:HB2	1:J:578:PHE:HB2	1.68	0.73
3:L:2965[B]:LEU:HD21	3:L:2974[B]:ALA:HB1	1.70	0.73
3:O:3038[B]:ILE:HD13	3:X:2969[B]:TYR:OH	1.75	0.73
3:O:3114[A]:PRO:HD2	3:O:3115[A]:LEU:H	1.51	0.73
3:O:3154[B]:PRO:CD	3:X:3176[B]:LYS:CE	2.64	0.73
3:O:3176[B]:LYS:HE2	3:O:3176[B]:LYS:N	2.02	0.73
3:O:3196[A]:THR:HG21	1:P:416:ASN:HD21	1.50	0.73
3:R:3147[B]:GLU:CG	3:R:3149[B]:ASN:HD21	2.00	0.73
1:S:1636:ASN:HD22	1:S:1639:LYS:CD	2.01	0.73
3:U:3293[B]:LYS:HB2	3:U:3294[B]:SER:HB2	0.82	0.73
3:d:2965[A]:LEU:HD21	3:d:2974[A]:ALA:HB1	1.70	0.73
3:d:3155[B]:MET:O	3:d:3159[B]:SER:N	2.20	0.73
3:C:2966[B]:SER:HB2	3:L:2982[B]:MET:HE2	1.70	0.73
3:F:2974[B]:ALA:CB	3:a:3253[B]:GLU:OE1	2.34	0.73
3:F:3156[B]:MET:C	3:a:3153[B]:LYS:NZ	2.45	0.73
3:I:2948[B]:ASP:H	3:I:2949[B]:LYS:CA	1.98	0.73
3:I:2955[B]:GLN:CD	3:I:3037[B]:TYR:HE1	1.92	0.73
3:I:2983[B]:VAL:CG2	3:R:3162[B]:ASP:H	2.01	0.73
3:I:3149[B]:ASN:CG	3:R:3163[B]:ASN:HD22	1.96	0.73
3:I:3149[B]:ASN:ND2	3:R:3163[B]:ASN:ND2	2.34	0.73
3:I:3155[B]:MET:CG	3:R:3153[B]:LYS:C	2.56	0.73
3:L:3293[A]:LYS:HB2	3:L:3294[A]:SER:HB2	0.82	0.73
1:M:557:VAL:HG23	1:M:558:HIS:HA	1.69	0.73
1:M:838:ARG:NH2	1:M:1112:PHE:O	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3012[A]:TRP:O	3:O:3122[A]:ASN:ND2	2.20	0.73
3:O:3113[B]:ASP:CG	3:O:3114[B]:PRO:CD	2.56	0.73
1:P:984:ASP:OD1	1:P:984:ASP:N	2.22	0.73
3:R:3275[B]:LEU:HD12	3:R:3275[B]:LEU:N	2.04	0.73
1:S:1617:LYS:CE	3:X:3135[B]:LYS:HZ1	1.99	0.73
3:U:2963[B]:MET:HG2	3:U:3108[B]:HIS:CG	2.23	0.73
3:U:2965[B]:LEU:CD2	3:d:3220[B]:ARG:HD3	2.17	0.73
2:W:2806:ALA:HB2	2:W:2856:ILE:HD11	1.70	0.73
3:X:3219[A]:LEU:HD22	3:X:3219[A]:LEU:N	2.02	0.73
3:a:3134[B]:GLN:HG3	3:a:3139[B]:LEU:HB2	1.70	0.73
3:a:3137[B]:ARG:HB3	3:a:3139[B]:LEU:CD2	2.17	0.73
3:d:2968[A]:GLN:CB	3:d:2972[A]:GLY:HA2	2.18	0.73
3:d:3275[B]:LEU:HD12	3:d:3275[B]:LEU:N	2.04	0.73
3:C:3307[A]:PHE:CE1	3:C:3309[A]:PRO:HG3	2.16	0.73
1:D:1195:ASP:O	1:D:1197:THR:N	2.22	0.73
3:F:3134[B]:GLN:HG3	3:F:3139[B]:LEU:HB2	1.70	0.73
3:F:3137[B]:ARG:HB3	3:F:3139[B]:LEU:HD23	1.69	0.73
3:F:3155[B]:MET:CB	3:a:3153[B]:LYS:HG2	2.06	0.73
3:I:2952[B]:ALA:CB	3:I:2953[B]:GLY:C	2.48	0.73
3:I:2963[B]:MET:HG2	3:I:3108[B]:HIS:CG	2.23	0.73
3:I:2975[B]:PHE:CD1	3:R:3107[B]:LEU:HG	2.22	0.73
3:I:2981[B]:GLY:H	3:R:2968[B]:GLN:HG2	1.53	0.73
3:I:3093[B]:HIS:HE1	3:I:3119[B]:HIS:CD2	2.06	0.73
3:I:3150[B]:LYS:HZ2	3:R:3160[B]:SER:HB3	1.52	0.73
3:I:3159[B]:SER:O	3:R:3150[B]:LYS:HB3	1.88	0.73
3:I:3171[B]:HIS:N	3:R:3152[B]:LYS:HB2	1.88	0.73
3:I:3212[A]:ARG:HG3	3:I:3212[A]:ARG:NH1	2.00	0.73
3:I:3248[B]:LEU:HB3	3:R:2972[B]:GLY:C	2.07	0.73
3:L:3025[A]:VAL:HG22	3:L:3047[A]:ARG:NH1	2.02	0.73
3:L:3134[A]:GLN:HG3	3:L:3139[A]:LEU:HB2	1.70	0.73
3:O:2963[A]:MET:HG2	3:O:3108[A]:HIS:CG	2.23	0.73
3:O:3038[A]:ILE:HG22	3:O:3040[A]:VAL:HG22	1.68	0.73
3:O:3089[A]:HIS:NE2	9:O:3401[A]:CUO:CU1	1.54	0.73
3:R:2948[A]:ASP:H	3:R:2949[A]:LYS:CA	1.98	0.73
3:R:2963[B]:MET:HG2	3:R:3108[B]:HIS:CG	2.23	0.73
3:R:3196[A]:THR:H	3:R:3199[A]:GLN:CD	1.94	0.73
3:U:3113[B]:ASP:CG	3:U:3114[B]:PRO:CD	2.56	0.73
3:U:3149[B]:ASN:O	3:d:3154[B]:PRO:CB	2.36	0.73
2:W:2252:GLU:OE2	2:W:2393:ARG:NH1	2.21	0.73
3:X:3275[B]:LEU:HD12	3:X:3275[B]:LEU:N	2.04	0.73
3:d:2948[B]:ASP:H	3:d:2949[B]:LYS:CA	1.98	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2952[A]:ALA:CB	3:d:2953[A]:GLY:C	2.48	0.73
3:d:3284[A]:LYS:CD	3:d:3285[A]:VAL:N	2.47	0.73
6:GA:1:NAG:C4	6:GA:2:NAG:O7	2.33	0.73
3:C:2965[B]:LEU:HD21	3:C:2974[B]:ALA:HB1	1.70	0.73
3:C:3093[B]:HIS:HE1	3:C:3119[B]:HIS:CD2	2.06	0.73
3:C:3223[B]:GLY:O	3:L:3252[B]:TYR:CG	2.42	0.73
1:D:1209:ASP:OD1	1:D:1210:LYS:N	2.21	0.73
3:F:2948[A]:ASP:H	3:F:2949[A]:LYS:CA	1.98	0.73
3:F:3172[B]:SER:N	3:a:3152[B]:LYS:CB	2.51	0.73
3:I:3134[B]:GLN:HG3	3:I:3139[B]:LEU:HB2	1.70	0.73
3:L:2937[A]:ASN:CB	3:L:3006[A]:LYS:HE2	2.14	0.73
3:O:3212[A]:ARG:HG3	3:O:3212[A]:ARG:NH1	2.00	0.73
3:R:2954[A]:TYR:O	3:R:2957[A]:ILE:HG22	1.87	0.73
1:S:456:GLN:NE2	1:S:549:PRO:O	2.22	0.73
3:U:3154[B]:PRO:HA	3:d:3153[B]:LYS:H	1.53	0.73
3:X:3147[A]:GLU:CG	3:X:3149[A]:ASN:HD21	2.00	0.73
3:d:3219[A]:LEU:HD22	3:d:3219[A]:LEU:N	2.02	0.73
3:C:3154[B]:PRO:CB	3:L:3151[B]:LEU:HA	2.18	0.73
3:C:3154[B]:PRO:HG3	3:L:3174[B]:GLY:CA	2.13	0.73
3:C:3174[B]:GLY:N	3:L:3154[B]:PRO:HD3	2.03	0.73
3:C:3176[A]:LYS:HE2	3:C:3176[A]:LYS:N	2.02	0.73
3:C:3256[B]:TRP:C	3:L:2965[B]:LEU:O	2.30	0.73
1:D:1152:LYS:HB3	1:D:1181:GLU:HA	1.71	0.73
3:F:2968[B]:GLN:CB	3:F:2972[B]:GLY:HA2	2.19	0.73
3:F:3219[A]:LEU:HD22	3:F:3219[A]:LEU:N	2.02	0.73
1:J:1442:MET:HE1	1:J:1454:PHE:HA	1.70	0.73
3:L:3275[A]:LEU:HD12	3:L:3275[A]:LEU:N	2.04	0.73
3:L:3293[B]:LYS:HB2	3:L:3294[B]:SER:HB2	0.82	0.73
3:O:2969[A]:TYR:O	3:O:2972[A]:GLY:N	2.20	0.73
3:O:3293[A]:LYS:HB2	3:O:3294[A]:SER:HB2	0.82	0.73
3:U:3176[A]:LYS:HB3	3:U:3176[A]:LYS:HZ2	1.53	0.73
3:U:3196[B]:THR:H	3:U:3199[B]:GLN:CD	1.94	0.73
3:U:3220[B]:ARG:CG	3:d:2974[B]:ALA:H	2.01	0.73
3:X:2968[B]:GLN:CB	3:X:2972[B]:GLY:HA2	2.19	0.73
3:X:3024[B]:LEU:CD1	3:X:3025[B]:VAL:H	1.83	0.73
3:X:3093[A]:HIS:HE1	3:X:3119[A]:HIS:CD2	2.06	0.73
3:X:3113[A]:ASP:CG	3:X:3114[A]:PRO:CD	2.56	0.73
3:a:3025[A]:VAL:HG22	3:a:3047[A]:ARG:NH1	2.01	0.73
3:a:3275[A]:LEU:HD12	3:a:3275[A]:LEU:N	2.04	0.73
3:d:2963[A]:MET:HG2	3:d:3108[A]:HIS:CG	2.23	0.73
3:d:2988[B]:TRP:CE3	3:d:2989[B]:HIS:ND1	2.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2971[B]:ASP:OD1	3:C:2973[B]:THR:OG1	2.04	0.73
3:C:3093[A]:HIS:HE1	3:C:3119[A]:HIS:CD2	2.06	0.73
3:C:3150[B]:LYS:N	3:L:3169[B]:LYS:CG	2.52	0.73
3:C:3285[A]:VAL:HG22	3:C:3286[A]:THR:N	2.04	0.73
2:E:2889:ALA:N	2:E:2890:VAL:HA	2.03	0.73
3:F:2969[B]:TYR:HD2	3:F:2971[B]:ASP:N	1.84	0.73
3:F:2970[B]:PRO:CD	3:a:2989[B]:HIS:CG	2.42	0.73
3:F:3093[A]:HIS:HE1	3:F:3119[A]:HIS:CD2	2.06	0.73
3:F:3162[B]:ASP:C	3:a:3150[B]:LYS:HZ1	1.97	0.73
3:F:3170[B]:ALA:C	3:a:3152[B]:LYS:CB	2.62	0.73
2:H:2340:ALA:HB1	2:H:2341:PRO:HD2	1.70	0.73
3:I:2968[A]:GLN:CB	3:I:2972[A]:GLY:HA2	2.18	0.73
3:I:3169[B]:LYS:O	3:R:3152[B]:LYS:HB2	1.86	0.73
3:I:3174[B]:GLY:HA3	3:R:3154[B]:PRO:CB	2.04	0.73
1:P:1358:LEU:HD23	1:P:1456:LEU:HD21	1.71	0.73
2:Q:2868:GLU:HG2	3:R:2932[A]:PRO:O	1.89	0.73
3:R:3155[B]:MET:O	3:R:3159[B]:SER:N	2.20	0.73
3:R:3176[B]:LYS:HE2	3:R:3176[B]:LYS:N	2.02	0.73
3:R:3220[B]:ARG:HG3	3:R:3220[B]:ARG:NH1	1.98	0.73
3:U:2952[B]:ALA:CB	3:U:2953[B]:GLY:C	2.48	0.73
1:V:1604:ASP:OD1	1:V:1605:ARG:NH1	2.22	0.73
3:X:3137[A]:ARG:HB3	3:X:3139[A]:LEU:HD23	1.69	0.73
2:Z:2515:ARG:HB3	2:c:2344:LEU:HB3	1.71	0.73
3:a:3134[A]:GLN:HG3	3:a:3139[A]:LEU:HB2	1.70	0.73
2:c:2180:TRP:HA	2:c:2184:MET:HE3	1.70	0.73
3:d:2949[A]:LYS:O	3:d:2953[A]:GLY:N	2.22	0.73
3:d:3089[B]:HIS:NE2	9:d:3401[B]:CUO:CU1	1.54	0.73
3:C:2949[A]:LYS:O	3:C:2953[A]:GLY:N	2.22	0.73
3:C:3149[B]:ASN:CG	3:L:3158[B]:PHE:O	2.32	0.73
1:D:17:ASN:HD21	1:D:86:THR:H	1.37	0.73
3:F:2965[A]:LEU:HD21	3:F:2974[A]:ALA:HB1	1.70	0.73
3:F:2982[B]:MET:HG3	3:a:3156[B]:MET:HB2	1.71	0.73
1:G:838:ARG:HD3	1:G:918:ARG:HD3	1.71	0.73
3:I:3157[B]:PRO:HD2	3:R:3153[B]:LYS:NZ	2.04	0.73
3:I:3172[B]:SER:HB2	3:R:3150[B]:LYS:O	1.89	0.73
3:I:3176[A]:LYS:HE2	3:I:3176[A]:LYS:N	2.02	0.73
3:I:3220[B]:ARG:HG3	3:I:3220[B]:ARG:NH1	1.98	0.73
3:I:3256[B]:TRP:HB3	3:R:2966[B]:SER:O	1.89	0.73
9:I:3401[A]:CUO:CU1	3:R:3089[A]:HIS:NE2	1.54	0.73
3:O:3038[B]:ILE:HG22	3:O:3040[B]:VAL:HG22	1.68	0.73
3:O:3093[A]:HIS:HE1	3:O:3119[A]:HIS:CD2	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3163[B]:ASN:HB3	3:X:3148[B]:ILE:C	2.14	0.73
3:O:3212[B]:ARG:HG3	3:O:3212[B]:ARG:NH1	2.00	0.73
1:P:557:VAL:HG23	1:P:558:HIS:HA	1.71	0.73
3:R:2952[B]:ALA:HA	3:R:2956[B]:LYS:HB2	1.69	0.73
3:U:2937[A]:ASN:HB2	3:U:3006[A]:LYS:CE	2.14	0.73
3:U:2965[B]:LEU:HD21	3:U:2974[B]:ALA:HB1	1.70	0.73
3:U:3176[B]:LYS:HE2	3:U:3176[B]:LYS:N	2.02	0.73
1:V:949:ASP:HB3	1:V:953:GLU:HB2	1.71	0.73
2:c:2524:LEU:HA	2:c:2581:MET:HE1	1.70	0.73
3:d:3113[B]:ASP:CG	3:d:3114[B]:PRO:CD	2.56	0.73
3:d:3147[A]:GLU:CG	3:d:3149[A]:ASN:HD21	2.01	0.73
3:d:3212[A]:ARG:HG3	3:d:3212[A]:ARG:NH1	2.00	0.73
3:C:2972[B]:GLY:HA2	3:L:3086[B]:GLU:HG2	1.71	0.72
9:C:3401[A]:CUO:CU1	3:L:3089[A]:HIS:NE2	1.54	0.72
1:D:1140:ASN:ND2	1:D:1236:TYR:OH	2.22	0.72
3:F:2949[A]:LYS:O	3:F:2953[A]:GLY:N	2.22	0.72
3:F:2965[B]:LEU:HD21	3:F:2974[B]:ALA:HB1	1.69	0.72
3:F:3212[A]:ARG:HG3	3:F:3212[A]:ARG:NH1	2.00	0.72
3:L:3147[B]:GLU:CG	3:L:3149[B]:ASN:HD21	2.00	0.72
3:L:3196[A]:THR:H	3:L:3199[A]:GLN:CB	2.02	0.72
3:L:3284[A]:LYS:CD	3:L:3285[A]:VAL:N	2.47	0.72
3:O:2952[B]:ALA:HA	3:O:2956[B]:LYS:HB2	1.69	0.72
3:O:3137[B]:ARG:HB3	3:O:3139[B]:LEU:HD23	1.69	0.72
3:O:3255[B]:PRO:HD2	3:X:3169[B]:LYS:CG	2.17	0.72
3:R:3038[A]:ILE:HG22	3:R:3040[A]:VAL:HG22	1.68	0.72
3:R:3133[A]:LEU:O	3:R:3134[A]:GLN:C	2.32	0.72
3:R:3133[B]:LEU:O	3:R:3134[B]:GLN:C	2.32	0.72
3:R:3219[A]:LEU:HD22	3:R:3219[A]:LEU:N	2.02	0.72
3:U:3120[A]:HIS:O	3:U:3121[A]:SER:C	2.29	0.72
3:U:3159[B]:SER:HB2	3:d:3150[B]:LYS:HD2	1.50	0.72
3:X:2965[B]:LEU:HD21	3:X:2974[B]:ALA:HB1	1.69	0.72
3:X:3293[A]:LYS:HB2	3:X:3294[A]:SER:HB2	0.82	0.72
3:a:3093[A]:HIS:HE1	3:a:3119[A]:HIS:CD2	2.06	0.72
3:a:3093[B]:HIS:HE1	3:a:3119[B]:HIS:CD2	2.06	0.72
3:d:3134[A]:GLN:HG3	3:d:3139[A]:LEU:HB2	1.70	0.72
3:C:2952[B]:ALA:HA	3:C:2956[B]:LYS:HB2	1.70	0.72
3:C:2972[B]:GLY:CA	3:L:3090[B]:ASN:CG	2.60	0.72
3:C:3133[A]:LEU:O	3:C:3134[A]:GLN:C	2.32	0.72
3:C:3141[B]:TYR:HD2	3:C:3142[B]:ASN:H	0.78	0.72
3:C:3149[B]:ASN:HD22	3:L:3163[B]:ASN:CB	2.01	0.72
3:C:3155[A]:MET:O	3:C:3159[A]:SER:N	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3196[A]:THR:H	3:C:3199[A]:GLN:CB	2.02	0.72
3:C:3196[B]:THR:H	3:C:3199[B]:GLN:CB	2.02	0.72
3:F:2975[B]:PHE:HZ	3:a:2961[B]:HIS:CG	2.06	0.72
3:F:2982[B]:MET:CG	3:a:3156[B]:MET:HB2	2.18	0.72
3:F:2992[B]:TYR:CE2	3:a:2969[B]:TYR:CE1	2.77	0.72
3:F:3147[B]:GLU:N	3:a:3161[B]:GLU:HA	2.05	0.72
2:H:2650:GLY:HA3	2:H:2653:GLU:O	1.89	0.72
3:I:3038[B]:ILE:HG22	3:I:3040[B]:VAL:HG22	1.68	0.72
3:I:3134[A]:GLN:HG3	3:I:3139[A]:LEU:HB2	1.70	0.72
3:I:3171[B]:HIS:C	3:R:3152[B]:LYS:HB2	2.14	0.72
3:L:2969[A]:TYR:O	3:L:2972[A]:GLY:N	2.20	0.72
3:O:2969[B]:TYR:H	3:X:2988[B]:TRP:CD1	2.08	0.72
3:O:2979[B]:GLN:HE21	3:O:3155[B]:MET:HE2	1.54	0.72
3:O:3285[B]:VAL:HG22	3:O:3286[B]:THR:N	2.04	0.72
3:R:3134[B]:GLN:HG3	3:R:3139[B]:LEU:HB2	1.70	0.72
3:R:3196[B]:THR:H	3:R:3199[B]:GLN:CB	2.02	0.72
3:U:2930[A]:LEU:H	3:U:2930[A]:LEU:CD2	1.98	0.72
3:U:2949[A]:LYS:O	3:U:2953[A]:GLY:N	2.22	0.72
3:U:3152[B]:LYS:CG	3:d:3154[B]:PRO:CB	2.48	0.72
3:U:3196[B]:THR:H	3:U:3199[B]:GLN:CB	2.02	0.72
2:W:2340:ALA:HB1	2:W:2341:PRO:HD2	1.71	0.72
3:a:2949[B]:LYS:O	3:a:2953[B]:GLY:N	2.22	0.72
3:a:2963[B]:MET:HG2	3:a:3108[B]:HIS:CG	2.23	0.72
3:a:3285[B]:VAL:HG22	3:a:3286[B]:THR:N	2.04	0.72
3:a:3307[A]:PHE:CE1	3:a:3309[A]:PRO:HG3	2.16	0.72
1:b:118:ALA:HB1	1:b:119:LYS:HA	1.69	0.72
3:d:3093[B]:HIS:HE1	3:d:3119[B]:HIS:CD2	2.06	0.72
3:C:2984[B]:THR:HB	3:L:3154[B]:PRO:HG2	1.70	0.72
3:C:3120[B]:HIS:O	3:C:3121[B]:SER:C	2.29	0.72
3:F:3196[B]:THR:H	3:F:3199[B]:GLN:CB	2.02	0.72
9:F:3401[A]:CUO:CU1	3:a:3089[A]:HIS:NE2	1.54	0.72
3:I:2981[B]:GLY:HA2	3:R:2968[B]:GLN:OE1	1.89	0.72
3:I:3113[B]:ASP:CG	3:I:3114[B]:PRO:CD	2.56	0.72
3:I:3163[B]:ASN:ND2	3:R:3149[B]:ASN:ND2	2.37	0.72
3:L:2949[B]:LYS:O	3:L:2953[B]:GLY:N	2.22	0.72
3:L:3093[A]:HIS:HE1	3:L:3119[A]:HIS:CD2	2.06	0.72
3:L:3285[B]:VAL:HG22	3:L:3286[B]:THR:N	2.04	0.72
3:O:2963[B]:MET:HE3	3:X:2975[B]:PHE:CE1	2.24	0.72
3:U:2949[B]:LYS:O	3:U:2953[B]:GLY:N	2.22	0.72
3:X:3219[B]:LEU:HD22	3:X:3219[B]:LEU:N	2.02	0.72
1:Y:1046:HIS:HA	1:Y:1049:VAL:HB	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:2965[A]:LEU:HD21	3:a:2974[A]:ALA:HB1	1.70	0.72
3:a:3196[B]:THR:H	3:a:3199[B]:GLN:CB	2.02	0.72
3:a:3293[A]:LYS:HD2	3:a:3293[A]:LYS:C	2.15	0.72
3:d:2956[B]:LYS:C	3:d:2960[B]:PHE:CE1	2.47	0.72
3:d:3089[A]:HIS:NE2	9:d:3401[A]:CUO:CU1	1.54	0.72
3:C:2968[B]:GLN:CB	3:C:2972[B]:GLY:HA2	2.18	0.72
3:C:3153[B]:LYS:HE2	3:L:3158[B]:PHE:CE2	2.25	0.72
3:C:3220[B]:ARG:HG3	3:C:3220[B]:ARG:NH1	1.98	0.72
3:F:2969[A]:TYR:O	3:F:2972[A]:GLY:N	2.21	0.72
3:I:3196[A]:THR:HG21	1:J:416:ASN:CB	2.19	0.72
3:I:3285[A]:VAL:HG22	3:I:3286[A]:THR:N	2.04	0.72
3:O:2968[B]:GLN:OE1	3:X:2979[B]:GLN:HG3	1.90	0.72
3:O:2979[A]:GLN:HE21	3:O:3155[A]:MET:HE2	1.54	0.72
3:R:3120[B]:HIS:O	3:R:3121[B]:SER:C	2.29	0.72
1:S:755:PHE:HB2	1:S:788:LEU:HD21	1.69	0.72
3:U:3256[B]:TRP:HD1	3:d:2975[B]:PHE:HE1	1.25	0.72
1:V:142:ARG:NH1	1:V:340:GLN:OE1	2.23	0.72
2:W:2711:HIS:HA	2:W:2714:VAL:HG22	1.71	0.72
3:X:2937[B]:ASN:HB2	3:X:3006[B]:LYS:CE	2.14	0.72
3:X:2949[B]:LYS:O	3:X:2953[B]:GLY:N	2.22	0.72
3:X:3120[B]:HIS:O	3:X:3121[B]:SER:C	2.29	0.72
3:X:3137[B]:ARG:HB3	3:X:3139[B]:LEU:HD23	1.69	0.72
3:a:3293[B]:LYS:HB2	3:a:3294[B]:SER:HB2	0.82	0.72
1:b:444:GLU:HG3	1:b:544:PRO:HG3	1.70	0.72
3:C:3285[B]:VAL:HG22	3:C:3286[B]:THR:N	2.04	0.72
3:F:3155[B]:MET:O	3:a:3153[B]:LYS:HB3	1.90	0.72
3:I:2982[B]:MET:HE3	3:R:2967[B]:CYS:SG	2.27	0.72
3:I:3156[B]:MET:CB	3:R:2982[B]:MET:CG	2.57	0.72
3:I:3293[A]:LYS:HD2	3:I:3293[A]:LYS:C	2.15	0.72
3:I:3293[B]:LYS:HD2	3:I:3293[B]:LYS:C	2.15	0.72
3:L:2968[B]:GLN:CB	3:L:2972[B]:GLY:HA2	2.19	0.72
3:L:2969[B]:TYR:O	3:L:2972[B]:GLY:N	2.20	0.72
3:L:3133[B]:LEU:O	3:L:3134[B]:GLN:C	2.32	0.72
3:O:2963[B]:MET:HB2	3:X:2970[B]:PRO:CD	2.19	0.72
3:O:3158[B]:PHE:O	3:X:3148[B]:ILE:HG23	1.86	0.72
3:U:2968[A]:GLN:CB	3:U:2972[A]:GLY:HA2	2.18	0.72
3:U:2969[A]:TYR:O	3:U:2972[A]:GLY:N	2.20	0.72
3:U:3171[B]:HIS:CA	3:d:3152[B]:LYS:NZ	2.52	0.72
3:X:3217[A]:PHE:HE1	3:X:3230[A]:PHE:HZ	0.81	0.72
3:a:2979[A]:GLN:HE21	3:a:3155[A]:MET:HE2	1.54	0.72
3:a:3141[B]:TYR:HD2	3:a:3142[B]:ASN:H	0.78	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3134[B]:GLN:HG3	3:d:3139[B]:LEU:HB2	1.70	0.72
1:A:1153:LYS:HB2	1:A:1155:LEU:HD23	1.72	0.72
1:A:1639:LYS:HB2	1:b:472:ASP:HB3	1.71	0.72
3:C:2935[B]:ILE:HD13	3:C:2936[B]:GLU:N	2.05	0.72
3:C:2969[B]:TYR:CD2	3:L:3089[B]:HIS:NE2	2.58	0.72
3:C:3089[A]:HIS:NE2	9:L:3401[A]:CUO:CU1	1.54	0.72
3:C:3168[B]:THR:C	3:L:3149[B]:ASN:O	2.25	0.72
3:F:2977[B]:CYS:SG	3:a:2978[B]:CYS:O	2.48	0.72
3:F:3025[B]:VAL:HG22	3:F:3047[B]:ARG:NH1	2.01	0.72
1:G:589:GLN:HG2	1:G:594:ASP:HB3	1.71	0.72
3:I:2969[A]:TYR:O	3:I:2972[A]:GLY:N	2.21	0.72
3:I:3108[B]:HIS:CE1	3:R:3251[B]:ASP:CG	2.67	0.72
3:I:3149[B]:ASN:HD22	3:R:3163[B]:ASN:CB	1.97	0.72
3:I:3150[B]:LYS:CA	3:R:3159[B]:SER:CA	2.61	0.72
3:I:3275[A]:LEU:HD12	3:I:3275[A]:LEU:N	2.04	0.72
1:J:417:MET:HG2	1:J:419:THR:HG23	1.71	0.72
1:J:836:GLN:HG3	1:J:838:ARG:HH21	1.53	0.72
3:O:2968[A]:GLN:CB	3:O:2972[A]:GLY:HA2	2.18	0.72
3:O:3153[B]:LYS:HD3	3:X:3176[B]:LYS:HD3	0.92	0.72
3:O:3196[A]:THR:H	3:O:3199[A]:GLN:CB	2.02	0.72
3:R:2949[B]:LYS:O	3:R:2953[B]:GLY:N	2.22	0.72
2:T:2900:SER:HA	1:V:1075:GLU:HG2	1.72	0.72
3:U:2968[B]:GLN:CB	3:U:2972[B]:GLY:HA2	2.19	0.72
3:U:3293[A]:LYS:HD2	3:U:3293[A]:LYS:C	2.15	0.72
2:Z:2900:SER:HA	1:b:1075:GLU:HG2	1.71	0.72
3:a:2935[A]:ILE:HD13	3:a:2936[A]:GLU:N	2.05	0.72
2:c:2149:ALA:HA	2:c:2260:GLU:HG2	1.71	0.72
2:B:2851:ASN:ND2	1:D:1189:ASP:HB2	2.04	0.72
3:C:3134[B]:GLN:HG3	3:C:3139[B]:LEU:HB2	1.70	0.72
3:C:3169[B]:LYS:O	3:L:3152[B]:LYS:CE	2.37	0.72
3:F:2966[B]:SER:HA	3:a:3256[B]:TRP:CG	2.17	0.72
3:F:3283[A]:ILE:HD13	3:F:3283[A]:ILE:C	2.15	0.72
3:I:2961[A]:HIS:HD2	3:I:2988[A]:TRP:CZ3	2.08	0.72
3:I:3285[B]:VAL:HG22	3:I:3286[B]:THR:N	2.04	0.72
3:I:3307[B]:PHE:CE1	3:I:3309[B]:PRO:HG3	2.16	0.72
3:L:2956[A]:LYS:C	3:L:2960[A]:PHE:CE1	2.47	0.72
3:L:2963[B]:MET:HG2	3:L:3108[B]:HIS:CG	2.23	0.72
3:L:3134[B]:GLN:HG3	3:L:3139[B]:LEU:HB2	1.70	0.72
3:L:3228[A]:VAL:HG22	3:L:3245[A]:PHE:O	1.90	0.72
3:L:3283[B]:ILE:HD13	3:L:3283[B]:ILE:C	2.15	0.72
3:L:3293[B]:LYS:HD2	3:L:3293[B]:LYS:C	2.15	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:965:ASP:OD2	1:M:968:GLY:N	2.22	0.72
3:O:2949[A]:LYS:O	3:O:2953[A]:GLY:N	2.22	0.72
3:O:2969[B]:TYR:HB2	3:X:3158[B]:PHE:CE2	2.25	0.72
3:O:3157[B]:PRO:O	3:X:3152[B]:LYS:HG3	1.89	0.72
3:O:3283[A]:ILE:C	3:O:3283[A]:ILE:HD13	2.15	0.72
1:P:456:GLN:NE2	1:P:549:PRO:O	2.21	0.72
3:R:2937[B]:ASN:CB	3:R:3006[B]:LYS:HE2	2.14	0.72
3:R:3293[A]:LYS:HB2	3:R:3294[A]:SER:HB2	0.82	0.72
3:U:2969[B]:TYR:O	3:U:2972[B]:GLY:N	2.20	0.72
3:U:3024[A]:LEU:CD1	3:U:3025[A]:VAL:H	1.84	0.72
3:U:3256[B]:TRP:CD2	3:d:2969[B]:TYR:CG	2.76	0.72
3:d:3283[A]:ILE:HD13	3:d:3283[A]:ILE:C	2.15	0.72
3:C:2948[B]:ASP:N	3:C:2949[B]:LYS:CA	2.41	0.72
3:F:2935[B]:ILE:HD13	3:F:2936[B]:GLU:N	2.05	0.72
3:F:3173[B]:THR:OG1	3:a:3173[B]:THR:CG2	2.38	0.72
1:G:1485:ALA:HB3	1:G:1489:MET:HE2	1.72	0.72
3:I:3283[B]:ILE:C	3:I:3283[B]:ILE:HD13	2.15	0.72
3:I:3284[B]:LYS:CD	3:I:3285[B]:VAL:N	2.47	0.72
3:O:2949[B]:LYS:O	3:O:2953[B]:GLY:N	2.22	0.72
3:O:2977[B]:CYS:CA	3:X:3154[B]:PRO:O	2.38	0.72
3:O:2988[A]:TRP:CE3	3:O:2989[A]:HIS:ND1	2.53	0.72
3:R:2965[A]:LEU:HD21	3:R:2974[A]:ALA:HB1	1.69	0.72
3:R:2979[A]:GLN:HE21	3:R:3155[A]:MET:HE2	1.54	0.72
3:R:3093[B]:HIS:HE1	3:R:3119[B]:HIS:CD2	2.06	0.72
3:R:3212[B]:ARG:HG3	3:R:3212[B]:ARG:NH1	2.00	0.72
1:S:1618:LEU:CD2	3:X:3136[B]:TYR:CE2	2.72	0.72
3:U:3134[A]:GLN:HG3	3:U:3139[A]:LEU:HB2	1.70	0.72
3:U:3149[B]:ASN:O	3:d:3155[B]:MET:N	2.22	0.72
3:U:3156[B]:MET:SD	3:d:2982[B]:MET:CB	2.77	0.72
3:U:3162[B]:ASP:N	3:d:3260[B]:ARG:HH11	1.84	0.72
1:V:1520:GLN:HE21	1:V:1526:LYS:HG3	1.55	0.72
3:X:2949[A]:LYS:O	3:X:2953[A]:GLY:N	2.22	0.72
3:X:2988[A]:TRP:CE3	3:X:2989[A]:HIS:ND1	2.53	0.72
3:X:3196[A]:THR:H	3:X:3199[A]:GLN:CB	2.03	0.72
2:Z:2743:ALA:HB1	1:b:1210:LYS:HG2	1.72	0.72
2:Z:2867:PRO:HD2	3:a:2932[A]:PRO:HB2	1.71	0.72
3:a:2937[B]:ASN:HB2	3:a:3006[B]:LYS:CE	2.14	0.72
3:a:3196[A]:THR:H	3:a:3199[A]:GLN:CB	2.02	0.72
3:a:3285[A]:VAL:HG22	3:a:3286[A]:THR:N	2.04	0.72
3:d:2961[B]:HIS:HD2	3:d:2988[B]:TRP:CZ3	2.08	0.72
3:d:3133[B]:LEU:O	3:d:3134[B]:GLN:C	2.32	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3293[B]:LYS:HD2	3:d:3293[B]:LYS:C	2.15	0.72
1:A:830:ASN:HA	1:A:831:VAL:HB	1.71	0.72
3:C:3134[A]:GLN:HG3	3:C:3139[A]:LEU:HB2	1.70	0.72
3:C:3275[A]:LEU:HD12	3:C:3275[A]:LEU:N	2.04	0.72
3:C:3275[B]:LEU:HD12	3:C:3275[B]:LEU:N	2.04	0.72
3:F:2961[B]:HIS:HD2	3:F:2988[B]:TRP:CZ3	2.08	0.72
3:F:3228[A]:VAL:HG22	3:F:3245[A]:PHE:O	1.90	0.72
3:F:3275[A]:LEU:HD12	3:F:3275[A]:LEU:N	2.04	0.72
3:I:2969[B]:TYR:O	3:I:2972[B]:GLY:N	2.21	0.72
3:I:3160[B]:SER:CB	3:R:2983[B]:VAL:N	2.40	0.72
3:I:3196[B]:THR:H	3:I:3199[B]:GLN:CB	2.02	0.72
3:L:2979[B]:GLN:HE21	3:L:3155[B]:MET:HE2	1.54	0.72
3:O:2968[B]:GLN:HE22	3:X:2985[B]:PHE:CA	1.94	0.72
3:O:3133[B]:LEU:O	3:O:3134[B]:GLN:C	2.32	0.72
3:O:3228[A]:VAL:HG22	3:O:3245[A]:PHE:O	1.90	0.72
3:O:3306[A]:LEU:HD12	3:O:3306[A]:LEU:C	2.15	0.72
1:S:157:GLU:OE2	1:S:296:ARG:NH2	2.22	0.72
1:S:1019:HIS:NE2	1:S:1046:HIS:CE1	2.57	0.72
3:U:2965[B]:LEU:HD11	3:U:2974[B]:ALA:HA	1.57	0.72
3:U:3228[A]:VAL:HG22	3:U:3245[A]:PHE:O	1.90	0.72
3:X:3089[A]:HIS:NE2	9:X:3401[A]:CUO:CU1	1.54	0.72
3:d:3285[A]:VAL:HG22	3:d:3286[A]:THR:N	2.04	0.72
3:C:3090[B]:ASN:CB	3:L:2972[B]:GLY:C	2.63	0.72
3:C:3120[A]:HIS:O	3:C:3121[A]:SER:C	2.29	0.72
3:F:2980[B]:HIS:CA	3:a:2968[B]:GLN:HG2	2.19	0.72
3:F:3172[B]:SER:HB3	3:a:3150[B]:LYS:HA	1.72	0.72
3:F:3307[B]:PHE:CE1	3:F:3309[B]:PRO:HG3	2.16	0.72
2:H:2727:HIS:HB2	2:H:2788:ILE:HD11	1.70	0.72
3:I:2933[B]:SER:O	3:I:2936[B]:GLU:N	2.23	0.72
3:I:2965[A]:LEU:HG	3:I:2974[A]:ALA:CB	2.20	0.72
3:I:2979[A]:GLN:HE21	3:I:3155[A]:MET:HE2	1.54	0.72
3:I:2982[B]:MET:HE2	3:R:2967[B]:CYS:SG	2.30	0.72
3:I:3160[B]:SER:C	3:R:3150[B]:LYS:HD2	2.13	0.72
3:L:2935[B]:ILE:HD13	3:L:2936[B]:GLU:N	2.04	0.72
3:L:2965[A]:LEU:HD21	3:L:2974[A]:ALA:HB1	1.70	0.72
3:L:3228[B]:VAL:HG22	3:L:3245[B]:PHE:O	1.90	0.72
1:M:804:ASP:OD1	1:M:805:VAL:N	2.23	0.72
3:O:2933[B]:SER:O	3:O:2936[B]:GLU:N	2.23	0.72
3:O:3255[B]:PRO:CD	3:X:3158[B]:PHE:O	2.37	0.72
3:O:3285[A]:VAL:HG22	3:O:3286[A]:THR:N	2.04	0.72
1:P:926:LEU:HD11	1:P:1043:MET:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:2340:ALA:HB1	2:Q:2341:PRO:HD2	1.72	0.72
3:R:2961[B]:HIS:HD2	3:R:2988[B]:TRP:CZ3	2.08	0.72
3:R:3025[A]:VAL:HG22	3:R:3047[A]:ARG:NH1	2.02	0.72
3:U:3137[A]:ARG:HB3	3:U:3139[A]:LEU:HD23	1.69	0.72
3:U:3155[B]:MET:H	3:d:3150[B]:LYS:CA	1.93	0.72
3:U:3285[A]:VAL:HG22	3:U:3286[A]:THR:N	2.04	0.72
3:U:3306[A]:LEU:HD12	3:U:3306[A]:LEU:C	2.15	0.72
1:V:121:ASN:HD21	1:V:124:TYR:HB2	1.54	0.72
3:X:3306[B]:LEU:HD12	3:X:3306[B]:LEU:C	2.15	0.72
3:a:2948[A]:ASP:H	3:a:2949[A]:LYS:CA	1.98	0.72
3:a:2968[B]:GLN:CB	3:a:2972[B]:GLY:HA2	2.19	0.72
3:a:2969[A]:TYR:O	3:a:2972[A]:GLY:N	2.20	0.72
3:a:3306[A]:LEU:HD12	3:a:3306[A]:LEU:C	2.15	0.72
3:a:3307[B]:PHE:CE1	3:a:3309[B]:PRO:HG3	2.16	0.72
1:b:1394:GLN:HG2	1:b:1395:PRO:HD2	1.72	0.72
3:d:2933[B]:SER:O	3:d:2936[B]:GLU:N	2.23	0.72
3:d:2952[B]:ALA:CB	3:d:2953[B]:GLY:C	2.48	0.72
3:d:3306[B]:LEU:HD12	3:d:3306[B]:LEU:C	2.15	0.72
2:B:2547:MET:HB3	2:B:2558:CYS:HB2	1.72	0.71
3:C:2933[B]:SER:O	3:C:2936[B]:GLU:N	2.23	0.71
3:C:2949[B]:LYS:O	3:C:2953[B]:GLY:N	2.22	0.71
3:C:2974[B]:ALA:HB1	3:L:3253[B]:GLU:OE1	1.89	0.71
3:C:3283[A]:ILE:C	3:C:3283[A]:ILE:HD13	2.15	0.71
3:C:3293[A]:LYS:HB2	3:C:3294[A]:SER:HB2	0.82	0.71
3:C:3293[A]:LYS:HD2	3:C:3293[A]:LYS:C	2.15	0.71
3:C:3293[B]:LYS:HD2	3:C:3293[B]:LYS:C	2.15	0.71
3:F:2930[A]:LEU:H	3:F:2930[A]:LEU:CD2	1.98	0.71
3:F:2935[A]:ILE:HD13	3:F:2936[A]:GLU:N	2.05	0.71
3:F:3133[B]:LEU:O	3:F:3134[B]:GLN:C	2.32	0.71
3:F:3173[B]:THR:HA	3:a:3154[B]:PRO:N	2.04	0.71
3:F:3293[B]:LYS:HD2	3:F:3293[B]:LYS:C	2.15	0.71
1:G:965:ASP:OD1	1:G:965:ASP:N	2.22	0.71
3:I:2949[B]:LYS:O	3:I:2953[B]:GLY:N	2.22	0.71
3:I:3152[B]:LYS:HB2	3:R:3171[B]:HIS:C	2.09	0.71
3:I:3160[B]:SER:HA	3:R:2983[B]:VAL:CB	2.19	0.71
3:I:3306[B]:LEU:HD12	3:I:3306[B]:LEU:C	2.15	0.71
1:J:1296:VAL:HB	1:J:1446:ASP:HB3	1.72	0.71
3:L:3283[A]:ILE:C	3:L:3283[A]:ILE:HD13	2.15	0.71
1:M:17:ASN:HD21	1:M:86:THR:H	1.37	0.71
3:O:2969[A]:TYR:HD2	3:O:2971[A]:ASP:N	1.84	0.71
3:O:2971[B]:ASP:OD1	3:X:3158[B]:PHE:CZ	2.42	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2949[A]:LYS:O	3:R:2953[A]:GLY:N	2.22	0.71
3:R:2968[A]:GLN:CB	3:R:2972[A]:GLY:HA2	2.19	0.71
3:U:2933[B]:SER:O	3:U:2936[B]:GLU:N	2.23	0.71
3:U:2935[B]:ILE:HD13	3:U:2936[B]:GLU:N	2.05	0.71
3:U:2965[B]:LEU:HG	3:U:2974[B]:ALA:CB	2.20	0.71
3:U:2969[B]:TYR:CZ	3:d:2980[B]:HIS:CE1	2.77	0.71
3:U:2975[B]:PHE:CE2	3:d:3256[B]:TRP:HD1	2.08	0.71
3:U:3161[B]:GLU:C	3:d:3260[B]:ARG:NH1	2.48	0.71
3:U:3220[A]:ARG:HG3	3:U:3220[A]:ARG:NH1	1.98	0.71
3:X:3228[B]:VAL:HG22	3:X:3245[B]:PHE:O	1.90	0.71
2:Z:2344:LEU:HB3	2:c:2515:ARG:HB3	1.72	0.71
3:a:2968[A]:GLN:CB	3:a:2972[A]:GLY:HA2	2.18	0.71
3:a:3137[B]:ARG:HB3	3:a:3139[B]:LEU:HD23	1.69	0.71
3:a:3293[B]:LYS:HD2	3:a:3293[B]:LYS:C	2.15	0.71
1:b:979:LEU:HB2	1:b:980:TYR:HB3	1.71	0.71
3:d:2961[A]:HIS:HD2	3:d:2988[A]:TRP:CZ3	2.08	0.71
3:d:3025[B]:VAL:HG22	3:d:3047[B]:ARG:NH1	2.02	0.71
3:d:3133[A]:LEU:O	3:d:3134[A]:GLN:C	2.32	0.71
3:d:3285[B]:VAL:HG22	3:d:3286[B]:THR:N	2.04	0.71
3:d:3306[A]:LEU:HD12	3:d:3306[A]:LEU:C	2.15	0.71
3:F:2952[A]:ALA:HA	3:F:2956[A]:LYS:HB2	1.69	0.71
3:F:2961[A]:HIS:HD2	3:F:2988[A]:TRP:CZ3	2.08	0.71
3:F:2965[B]:LEU:HG	3:F:2974[B]:ALA:CB	2.21	0.71
3:F:3155[B]:MET:HG3	3:a:3153[B]:LYS:HG2	1.71	0.71
3:F:3285[A]:VAL:HG22	3:F:3286[A]:THR:N	2.04	0.71
2:H:2541:GLY:O	2:H:2545:SER:OG	2.07	0.71
3:I:2935[B]:ILE:HD13	3:I:2936[B]:GLU:N	2.05	0.71
3:I:2965[B]:LEU:HD21	3:I:2974[B]:ALA:HB1	1.69	0.71
3:I:2979[B]:GLN:HE21	3:I:3155[B]:MET:HE2	1.54	0.71
3:I:3159[B]:SER:C	3:R:3150[B]:LYS:HD2	2.14	0.71
3:I:3196[A]:THR:HB	1:J:416:ASN:HD21	1.53	0.71
3:L:3226[B]:ALA:HB1	3:L:3288[B]:MET:O	1.91	0.71
3:O:2961[B]:HIS:HD2	3:O:2988[B]:TRP:CZ3	2.08	0.71
3:O:2965[B]:LEU:HD21	3:O:2974[B]:ALA:HB1	1.69	0.71
3:O:3251[B]:ASP:OD2	3:X:2968[B]:GLN:OE1	2.08	0.71
3:R:3169[A]:LYS:C	3:R:3172[A]:SER:HG	1.98	0.71
3:R:3283[B]:ILE:C	3:R:3283[B]:ILE:HD13	2.15	0.71
3:R:3285[B]:VAL:HG22	3:R:3286[B]:THR:N	2.04	0.71
3:R:3293[A]:LYS:HD2	3:R:3293[A]:LYS:C	2.15	0.71
3:R:3293[B]:LYS:HD2	3:R:3293[B]:LYS:C	2.15	0.71
3:U:2961[B]:HIS:HD2	3:U:2988[B]:TRP:CZ3	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3275[B]:LEU:HD12	3:a:3275[B]:LEU:N	2.04	0.71
1:b:110:PHE:N	1:b:119:LYS:O	2.23	0.71
1:b:401:VAL:HG22	1:b:662:SER:HB3	1.72	0.71
3:d:2949[B]:LYS:O	3:d:2953[B]:GLY:N	2.22	0.71
3:d:3226[B]:ALA:HB1	3:d:3288[B]:MET:O	1.90	0.71
3:C:2933[A]:SER:O	3:C:2936[A]:GLU:N	2.23	0.71
3:C:2935[A]:ILE:HD13	3:C:2936[A]:GLU:N	2.05	0.71
3:C:2961[A]:HIS:HD2	3:C:2988[A]:TRP:CZ3	2.08	0.71
3:C:2969[A]:TYR:O	3:C:2972[A]:GLY:N	2.20	0.71
3:C:3133[B]:LEU:O	3:C:3134[B]:GLN:C	2.32	0.71
3:C:3160[B]:SER:HG	3:L:2983[B]:VAL:CG2	2.04	0.71
3:C:3228[A]:VAL:HG22	3:C:3245[A]:PHE:O	1.90	0.71
3:C:3306[B]:LEU:HD12	3:C:3306[B]:LEU:C	2.15	0.71
3:F:2949[B]:LYS:O	3:F:2953[B]:GLY:N	2.22	0.71
3:F:2975[B]:PHE:CD1	3:a:3107[B]:LEU:CD2	2.72	0.71
3:F:3090[B]:ASN:HB3	3:a:2972[B]:GLY:HA3	1.72	0.71
3:I:2933[A]:SER:O	3:I:2936[A]:GLU:N	2.23	0.71
3:I:3275[B]:LEU:HD12	3:I:3275[B]:LEU:N	2.04	0.71
3:I:3306[A]:LEU:HD12	3:I:3306[A]:LEU:C	2.15	0.71
1:J:163:LEU:HD21	1:J:219:LEU:HD13	1.72	0.71
3:L:2933[A]:SER:O	3:L:2936[A]:GLU:N	2.23	0.71
3:L:2949[A]:LYS:O	3:L:2953[A]:GLY:N	2.22	0.71
3:L:2952[A]:ALA:HA	3:L:2956[A]:LYS:HB2	1.69	0.71
3:L:2961[B]:HIS:HD2	3:L:2988[B]:TRP:CZ3	2.08	0.71
3:L:3120[A]:HIS:O	3:L:3121[A]:SER:C	2.29	0.71
1:M:1618:LEU:O	3:R:3198[B]:PRO:HD3	1.90	0.71
3:O:2968[B]:GLN:CA	3:X:2979[B]:GLN:HG2	2.19	0.71
3:O:3226[A]:ALA:HB1	3:O:3288[A]:MET:O	1.91	0.71
3:O:3293[A]:LYS:HD2	3:O:3293[A]:LYS:C	2.15	0.71
3:O:3307[B]:PHE:CE1	3:O:3309[B]:PRO:HG3	2.16	0.71
1:P:428:ILE:HD12	1:P:514:TRP:HB3	1.72	0.71
3:R:2933[A]:SER:O	3:R:2936[A]:GLU:N	2.23	0.71
3:R:3226[B]:ALA:HB1	3:R:3288[B]:MET:O	1.90	0.71
3:R:3228[B]:VAL:HG22	3:R:3245[B]:PHE:O	1.90	0.71
3:R:3283[A]:ILE:C	3:R:3283[A]:ILE:HD13	2.15	0.71
3:R:3285[A]:VAL:HG22	3:R:3286[A]:THR:N	2.04	0.71
3:U:2961[A]:HIS:HD2	3:U:2988[A]:TRP:CZ3	2.08	0.71
3:U:3089[B]:HIS:NE2	9:U:3401[B]:CUO:CU1	1.54	0.71
3:U:3196[A]:THR:H	3:U:3199[A]:GLN:CB	2.02	0.71
3:U:3256[B]:TRP:N	3:d:2974[B]:ALA:O	2.24	0.71
3:U:3275[B]:LEU:HD12	3:U:3275[B]:LEU:N	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1655:SER:C	3:d:3006[B]:LYS:NZ	2.48	0.71
3:a:3133[B]:LEU:O	3:a:3134[B]:GLN:C	2.32	0.71
3:a:3283[B]:ILE:C	3:a:3283[B]:ILE:HD13	2.15	0.71
3:d:3196[A]:THR:H	3:d:3199[A]:GLN:CB	2.02	0.71
1:A:806:ASN:ND2	4:f:1:NAG:O7	2.23	0.71
2:B:2598:PRO:HG3	2:B:2651:GLN:HB3	1.71	0.71
3:C:2965[B]:LEU:HG	3:C:2974[B]:ALA:CB	2.21	0.71
3:C:3226[B]:ALA:HB1	3:C:3288[B]:MET:O	1.91	0.71
3:F:3089[A]:HIS:NE2	9:a:3401[A]:CUO:CU1	1.54	0.71
3:F:3283[B]:ILE:C	3:F:3283[B]:ILE:HD13	2.15	0.71
3:F:3306[A]:LEU:HD12	3:F:3306[A]:LEU:C	2.15	0.71
3:F:3306[B]:LEU:HD12	3:F:3306[B]:LEU:C	2.15	0.71
3:I:2961[B]:HIS:CE1	3:R:2975[B]:PHE:CE1	2.78	0.71
3:L:2933[B]:SER:O	3:L:2936[B]:GLU:N	2.23	0.71
3:L:3226[A]:ALA:HB1	3:L:3288[A]:MET:O	1.91	0.71
3:L:3285[A]:VAL:HG22	3:L:3286[A]:THR:N	2.04	0.71
2:N:2090:LYS:NZ	2:N:2099:GLU:OE2	2.23	0.71
3:O:2933[A]:SER:O	3:O:2936[A]:GLU:N	2.23	0.71
3:O:3163[B]:ASN:CB	3:X:3149[B]:ASN:HB3	2.20	0.71
3:O:3275[A]:LEU:HD12	3:O:3275[A]:LEU:N	2.04	0.71
3:R:3161[B]:GLU:OE2	3:R:3161[B]:GLU:N	1.88	0.71
1:S:164:GLU:OE2	1:S:301:ARG:NH2	2.22	0.71
3:U:2935[A]:ILE:HD13	3:U:2936[A]:GLU:N	2.05	0.71
3:U:3285[B]:VAL:HG22	3:U:3286[B]:THR:N	2.04	0.71
3:X:3196[B]:THR:H	3:X:3199[B]:GLN:CB	2.02	0.71
3:X:3228[A]:VAL:HG22	3:X:3245[A]:PHE:O	1.90	0.71
3:X:3285[B]:VAL:HG22	3:X:3286[B]:THR:N	2.04	0.71
3:X:3293[B]:LYS:HD2	3:X:3293[B]:LYS:C	2.15	0.71
1:Y:2:LEU:HD21	1:Y:81:VAL:HG21	1.72	0.71
1:Y:1421:VAL:HG23	1:Y:1422:HIS:HD1	1.55	0.71
3:a:3133[A]:LEU:O	3:a:3134[A]:GLN:C	2.32	0.71
3:a:3283[A]:ILE:HD13	3:a:3283[A]:ILE:C	2.15	0.71
1:b:884:PRO:HG2	1:b:888:ALA:HB2	1.73	0.71
3:C:3163[B]:ASN:HB3	3:L:3149[B]:ASN:HD21	1.56	0.71
3:F:2965[A]:LEU:HG	3:F:2974[A]:ALA:CB	2.20	0.71
3:F:2979[B]:GLN:HE21	3:F:3155[B]:MET:HE2	1.55	0.71
3:F:3025[A]:VAL:HG22	3:F:3047[A]:ARG:NH1	2.01	0.71
3:F:3133[A]:LEU:O	3:F:3134[A]:GLN:C	2.32	0.71
3:I:2937[B]:ASN:CB	3:I:3006[B]:LYS:HE2	2.14	0.71
3:I:2952[B]:ALA:HA	3:I:2956[B]:LYS:HB2	1.70	0.71
3:I:2964[B]:PRO:HB2	3:R:3221[B]:ALA:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2982[A]:MET:HE1	3:I:3254[A]:MET:HE2	1.73	0.71
3:I:3089[A]:HIS:NE2	9:R:3401[A]:CUO:CU1	1.54	0.71
3:I:3107[B]:LEU:CD2	3:R:2975[B]:PHE:HA	2.21	0.71
3:I:3212[B]:ARG:HG3	3:I:3212[B]:ARG:NH1	2.00	0.71
3:L:3275[B]:LEU:HD12	3:L:3275[B]:LEU:N	2.04	0.71
3:O:3041[B]:ALA:HB2	3:X:2971[B]:ASP:OD2	1.89	0.71
3:O:3163[B]:ASN:CA	3:X:3149[B]:ASN:CB	2.66	0.71
1:P:1636:ASN:HB3	1:P:1638:SER:O	1.91	0.71
3:R:2965[A]:LEU:HG	3:R:2974[A]:ALA:CB	2.21	0.71
3:R:3147[B]:GLU:HB2	3:R:3149[B]:ASN:OD1	1.86	0.71
3:U:3133[A]:LEU:O	3:U:3134[A]:GLN:C	2.32	0.71
3:U:3228[B]:VAL:HG22	3:U:3245[B]:PHE:O	1.90	0.71
3:U:3252[B]:TYR:C	3:d:3255[B]:PRO:HG3	2.15	0.71
3:X:2933[B]:SER:O	3:X:2936[B]:GLU:N	2.23	0.71
3:X:2982[A]:MET:HE1	3:X:3254[A]:MET:HE2	1.73	0.71
3:X:3275[A]:LEU:HD12	3:X:3275[A]:LEU:N	2.04	0.71
3:a:2952[A]:ALA:CB	3:a:2953[A]:GLY:C	2.48	0.71
3:a:2965[A]:LEU:HG	3:a:2974[A]:ALA:CB	2.21	0.71
3:a:2969[B]:TYR:O	3:a:2972[B]:GLY:N	2.20	0.71
2:B:2373:MET:HE3	2:B:2374:ASN:HB2	1.73	0.71
3:C:2968[B]:GLN:O	3:L:2985[B]:PHE:CE2	2.44	0.71
3:C:3025[B]:VAL:HG22	3:C:3047[B]:ARG:NH1	2.01	0.71
3:C:3226[A]:ALA:HB1	3:C:3288[A]:MET:O	1.91	0.71
3:C:3252[B]:TYR:CB	3:L:3253[B]:GLU:CB	2.68	0.71
3:C:3283[B]:ILE:HD13	3:C:3283[B]:ILE:C	2.15	0.71
3:C:3306[A]:LEU:HD12	3:C:3306[A]:LEU:C	2.15	0.71
3:F:2933[A]:SER:O	3:F:2936[A]:GLU:N	2.23	0.71
3:I:2935[A]:ILE:HD13	3:I:2936[A]:GLU:N	2.05	0.71
3:I:2949[A]:LYS:O	3:I:2953[A]:GLY:N	2.22	0.71
3:I:3172[B]:SER:HB3	3:R:3150[B]:LYS:CA	2.21	0.71
1:J:1140:ASN:ND2	1:J:1236:TYR:OH	2.22	0.71
3:L:2930[A]:LEU:HD22	3:L:2930[A]:LEU:N	2.02	0.71
3:L:3306[A]:LEU:HD12	3:L:3306[A]:LEU:C	2.15	0.71
1:M:975:PRO:HG2	1:M:1024:GLY:HA3	1.73	0.71
3:O:3108[B]:HIS:CB	3:X:2970[B]:PRO:HA	2.20	0.71
3:O:3228[B]:VAL:HG22	3:O:3245[B]:PHE:O	1.90	0.71
3:U:2965[A]:LEU:HG	3:U:2974[A]:ALA:CB	2.20	0.71
3:U:3169[B]:LYS:HE2	3:d:3146[B]:CYS:CB	2.20	0.71
3:U:3293[B]:LYS:HD2	3:U:3293[B]:LYS:C	2.15	0.71
3:X:2961[A]:HIS:HD2	3:X:2988[A]:TRP:CZ3	2.08	0.71
3:X:3283[B]:ILE:HD13	3:X:3283[B]:ILE:C	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1284:GLU:HG3	1:Y:1337:ARG:HH12	1.55	0.71
3:a:2949[A]:LYS:O	3:a:2953[A]:GLY:N	2.22	0.71
3:a:2961[A]:HIS:HD2	3:a:2988[A]:TRP:CZ3	2.08	0.71
1:b:972:SER:HA	1:b:1028:VAL:HG22	1.70	0.71
3:d:3196[B]:THR:H	3:d:3199[B]:GLN:CB	2.02	0.71
3:d:3228[B]:VAL:HG22	3:d:3245[B]:PHE:O	1.90	0.71
3:d:3283[B]:ILE:C	3:d:3283[B]:ILE:HD13	2.15	0.71
3:C:2969[B]:TYR:HD2	3:L:3089[B]:HIS:NE2	1.87	0.71
3:F:3153[B]:LYS:NZ	3:a:3157[B]:PRO:N	2.31	0.71
3:F:3293[B]:LYS:HB2	3:F:3294[B]:SER:HB2	0.82	0.71
2:H:2180:TRP:HB2	2:H:2243:LEU:HD13	1.73	0.71
3:I:3226[A]:ALA:HB1	3:I:3288[A]:MET:O	1.91	0.71
3:I:3228[A]:VAL:HG22	3:I:3245[A]:PHE:O	1.90	0.71
3:I:3255[B]:PRO:HB2	3:R:2959[B]:SER:C	2.13	0.71
3:O:3158[B]:PHE:H	3:X:3152[B]:LYS:CB	1.92	0.71
3:O:3160[B]:SER:OG	3:X:3151[B]:LEU:HG	1.89	0.71
3:R:3228[A]:VAL:HG22	3:R:3245[A]:PHE:O	1.90	0.71
2:T:2133:PRO:HG2	2:T:2140:ARG:HA	1.71	0.71
3:U:2970[B]:PRO:CA	3:d:3086[B]:GLU:CG	2.68	0.71
3:U:3283[A]:ILE:HD13	3:U:3283[A]:ILE:C	2.15	0.71
3:X:3306[A]:LEU:HD12	3:X:3306[A]:LEU:C	2.15	0.71
3:a:3120[A]:HIS:O	3:a:3121[A]:SER:C	2.29	0.71
3:a:3228[A]:VAL:HG22	3:a:3245[A]:PHE:O	1.90	0.71
3:d:2935[B]:ILE:HD13	3:d:2936[B]:GLU:N	2.05	0.71
3:d:2982[B]:MET:HE1	3:d:3254[B]:MET:HE2	1.73	0.71
3:C:3156[B]:MET:HE3	3:L:2979[B]:GLN:CG	2.04	0.71
3:F:2933[B]:SER:O	3:F:2936[B]:GLU:N	2.23	0.71
3:F:3255[B]:PRO:CG	3:a:2964[B]:PRO:N	2.54	0.71
3:I:2960[B]:PHE:C	3:R:3255[B]:PRO:HD2	2.16	0.71
3:I:2962[B]:GLY:O	3:R:3255[B]:PRO:CD	2.38	0.71
3:I:3228[B]:VAL:HG22	3:I:3245[B]:PHE:O	1.90	0.71
3:I:3283[A]:ILE:HD13	3:I:3283[A]:ILE:C	2.15	0.71
1:J:1152:LYS:NZ	1:J:1180:SER:O	2.21	0.71
3:L:2965[B]:LEU:HG	3:L:2974[B]:ALA:CB	2.20	0.71
3:O:2969[B]:TYR:HD2	3:O:2971[B]:ASP:N	1.84	0.71
3:O:3275[B]:LEU:HD12	3:O:3275[B]:LEU:N	2.04	0.71
3:O:3283[B]:ILE:HD13	3:O:3283[B]:ILE:C	2.15	0.71
3:O:3306[B]:LEU:HD12	3:O:3306[B]:LEU:C	2.15	0.71
1:P:975:PRO:HG2	1:P:1024:GLY:HA3	1.72	0.71
3:R:2935[A]:ILE:HD13	3:R:2936[A]:GLU:N	2.05	0.71
1:S:1170:MET:HB3	1:S:1203:MET:HE2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2970[B]:PRO:CA	3:d:2980[B]:HIS:HB3	2.08	0.71
3:U:3283[B]:ILE:C	3:U:3283[B]:ILE:HD13	2.15	0.71
3:X:2965[A]:LEU:HG	3:X:2974[A]:ALA:CB	2.20	0.71
3:X:3089[B]:HIS:NE2	9:X:3401[B]:CUO:CU1	1.54	0.71
3:a:2933[B]:SER:O	3:a:2936[B]:GLU:N	2.23	0.71
3:a:3306[B]:LEU:HD12	3:a:3306[B]:LEU:C	2.15	0.71
2:B:2671:ASP:OD1	2:B:2850:ARG:NH1	2.23	0.71
3:C:2961[B]:HIS:HD2	3:C:2988[B]:TRP:CZ3	2.08	0.71
3:C:2964[B]:PRO:O	3:L:3256[B]:TRP:N	2.24	0.71
3:C:2969[B]:TYR:CA	3:L:2989[B]:HIS:NE2	2.52	0.71
3:C:2979[B]:GLN:NE2	3:L:2979[B]:GLN:HE22	1.82	0.71
3:C:3228[B]:VAL:HG22	3:C:3245[B]:PHE:O	1.90	0.71
3:C:3252[B]:TYR:HB2	3:L:3253[B]:GLU:CG	2.20	0.71
2:E:2806:ALA:HB2	2:E:2856:ILE:HD11	1.73	0.71
3:F:2952[A]:ALA:CB	3:F:2953[A]:GLY:C	2.48	0.71
3:F:2968[A]:GLN:CB	3:F:2972[A]:GLY:HA2	2.19	0.71
3:F:3160[B]:SER:OG	3:a:2983[B]:VAL:N	2.24	0.71
3:F:3248[B]:LEU:HB2	3:a:2972[B]:GLY:O	1.88	0.71
3:L:3024[B]:LEU:CD1	3:L:3025[B]:VAL:H	1.83	0.71
3:O:2935[A]:ILE:HD13	3:O:2936[A]:GLU:N	2.05	0.71
3:O:2935[B]:ILE:HD13	3:O:2936[B]:GLU:N	2.04	0.71
3:O:2969[B]:TYR:HE1	3:X:3168[B]:THR:HG22	1.55	0.71
3:O:3169[B]:LYS:C	3:O:3172[B]:SER:HG	1.98	0.71
3:R:3226[A]:ALA:HB1	3:R:3288[A]:MET:O	1.91	0.71
3:X:2933[A]:SER:O	3:X:2936[A]:GLU:N	2.23	0.71
1:Y:439:LEU:HD23	1:Y:509:ILE:HD12	1.71	0.71
1:Y:1470:GLU:HG3	1:Y:1530:LEU:HD12	1.73	0.71
3:a:2933[A]:SER:O	3:a:2936[A]:GLU:N	2.23	0.71
1:b:127:GLU:N	1:b:127:GLU:OE1	2.23	0.71
3:d:2933[A]:SER:O	3:d:2936[A]:GLU:N	2.23	0.71
3:d:2935[A]:ILE:HD13	3:d:2936[A]:GLU:N	2.05	0.71
3:F:2973[B]:THR:HG21	3:a:3106[B]:THR:C	2.15	0.71
3:F:3154[B]:PRO:HB3	3:a:3174[B]:GLY:HA3	1.72	0.71
3:F:3154[B]:PRO:CB	3:a:3174[B]:GLY:N	2.50	0.71
3:F:3226[B]:ALA:HB1	3:F:3288[B]:MET:O	1.91	0.71
1:J:622:HIS:CE1	1:J:767:LYS:H	2.09	0.71
3:L:2937[B]:ASN:CB	3:L:3006[B]:LYS:HE2	2.14	0.71
3:L:2982[A]:MET:HE1	3:L:3254[A]:MET:HE2	1.73	0.71
3:O:3133[A]:LEU:O	3:O:3134[A]:GLN:C	2.32	0.71
3:R:2969[A]:TYR:O	3:R:2972[A]:GLY:N	2.20	0.71
3:R:2982[A]:MET:HE1	3:R:3254[A]:MET:HE2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3066[B]:TYR:CD1	3:R:3193[B]:HIS:CE1	2.79	0.71
3:R:3306[A]:LEU:HD12	3:R:3306[A]:LEU:C	2.15	0.71
3:R:3307[A]:PHE:CE1	3:R:3309[A]:PRO:HG3	2.16	0.71
3:X:2968[A]:GLN:CB	3:X:2972[A]:GLY:HA2	2.18	0.71
3:X:3226[A]:ALA:HB1	3:X:3288[A]:MET:O	1.90	0.71
3:X:3226[B]:ALA:HB1	3:X:3288[B]:MET:O	1.90	0.71
2:Z:2867:PRO:CD	3:a:2932[A]:PRO:CG	2.69	0.71
3:a:2961[B]:HIS:HD2	3:a:2988[B]:TRP:CZ3	2.08	0.71
3:a:3066[B]:TYR:CD1	3:a:3193[B]:HIS:CE1	2.79	0.71
3:C:2974[B]:ALA:O	3:L:3107[B]:LEU:CD1	2.33	0.70
1:D:1258:ARG:NH2	1:D:1332:ASP:OD1	2.23	0.70
3:F:2971[B]:ASP:C	3:a:3248[B]:LEU:HD22	2.15	0.70
3:F:3162[B]:ASP:HA	3:a:3259[B]:ASP:HB3	1.73	0.70
3:F:3293[A]:LYS:HD2	3:F:3293[A]:LYS:C	2.15	0.70
3:I:3066[A]:TYR:CD1	3:I:3193[A]:HIS:CE1	2.79	0.70
3:I:3150[B]:LYS:HD2	3:R:3160[B]:SER:C	2.16	0.70
3:I:3162[B]:ASP:CB	3:R:3259[B]:ASP:N	2.49	0.70
3:I:3166[B]:GLU:O	3:R:3149[B]:ASN:HA	1.90	0.70
3:I:3179[A]:ASP:OD1	3:I:3181[A]:GLN:HB2	1.91	0.70
3:I:3196[A]:THR:H	3:I:3199[A]:GLN:CB	2.02	0.70
3:I:3252[B]:TYR:CE2	3:R:3250[B]:GLY:HA2	2.26	0.70
3:L:3066[B]:TYR:CD1	3:L:3193[B]:HIS:CE1	2.79	0.70
3:R:2930[A]:LEU:HD22	3:R:2930[A]:LEU:N	2.02	0.70
3:R:2961[A]:HIS:HD2	3:R:2988[A]:TRP:CZ3	2.08	0.70
3:U:3066[A]:TYR:CD1	3:U:3193[A]:HIS:CE1	2.79	0.70
3:U:3089[A]:HIS:NE2	9:U:3401[A]:CUO:CU1	1.54	0.70
3:U:3149[B]:ASN:O	3:d:3154[B]:PRO:C	2.33	0.70
3:U:3153[B]:LYS:HG3	3:d:2979[B]:GLN:HE21	1.54	0.70
3:U:3194[B]:GLY:C	3:U:3195[B]:MET:HG2	2.16	0.70
3:U:3226[A]:ALA:HB1	3:U:3288[A]:MET:O	1.91	0.70
1:V:1137:LYS:HG2	1:V:1240:ILE:HG13	1.73	0.70
3:X:2965[B]:LEU:HG	3:X:2974[B]:ALA:CB	2.21	0.70
3:X:2979[A]:GLN:HE21	3:X:3155[A]:MET:HE2	1.54	0.70
3:X:3133[B]:LEU:O	3:X:3134[B]:GLN:C	2.32	0.70
3:X:3179[B]:ASP:OD1	3:X:3181[B]:GLN:HB2	1.91	0.70
3:X:3221[B]:ALA:HB2	3:X:3256[B]:TRP:H	1.56	0.70
3:X:3293[A]:LYS:HD2	3:X:3293[A]:LYS:C	2.15	0.70
3:a:2979[B]:GLN:HE21	3:a:3155[B]:MET:HE2	1.55	0.70
3:a:3194[B]:GLY:C	3:a:3195[B]:MET:HG2	2.16	0.70
3:d:2965[A]:LEU:HG	3:d:2974[A]:ALA:CB	2.21	0.70
1:A:1242:ASN:ND2	1:A:1245:GLU:OE2	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2982[A]:MET:HE1	3:C:3254[A]:MET:HE2	1.73	0.70
3:C:3066[B]:TYR:CD1	3:C:3193[B]:HIS:CE1	2.79	0.70
3:C:3156[B]:MET:CE	3:L:2979[B]:GLN:CB	2.15	0.70
3:C:3287[B]:ILE:O	3:C:3287[B]:ILE:HD13	1.92	0.70
1:D:401:VAL:HG22	1:D:662:SER:HB3	1.73	0.70
3:F:2982[B]:MET:HE1	3:F:3254[B]:MET:HE2	1.72	0.70
3:F:3287[B]:ILE:O	3:F:3287[B]:ILE:HD13	1.91	0.70
2:K:2556:TYR:HD1	2:K:2557:ALA:H	1.39	0.70
3:L:2935[A]:ILE:HD13	3:L:2936[A]:GLU:N	2.05	0.70
3:L:3293[A]:LYS:HD2	3:L:3293[A]:LYS:C	2.15	0.70
3:O:2961[A]:HIS:HD2	3:O:2988[A]:TRP:CZ3	2.08	0.70
3:O:3221[B]:ALA:HB2	3:O:3256[B]:TRP:H	1.56	0.70
3:O:3293[B]:LYS:HD2	3:O:3293[B]:LYS:C	2.15	0.70
2:Q:2598:PRO:HD3	2:Q:2651:GLN:HB2	1.73	0.70
3:R:2933[B]:SER:O	3:R:2936[B]:GLU:N	2.23	0.70
3:U:2952[A]:ALA:H	3:U:2953[A]:GLY:CA	2.04	0.70
3:U:3066[B]:TYR:CD1	3:U:3193[B]:HIS:CE1	2.79	0.70
3:U:3120[B]:HIS:O	3:U:3121[B]:SER:C	2.29	0.70
3:U:3221[B]:ALA:HB2	3:U:3256[B]:TRP:H	1.57	0.70
3:X:3066[A]:TYR:CD1	3:X:3193[A]:HIS:CE1	2.79	0.70
1:Y:1442:MET:HE1	1:Y:1454:PHE:HA	1.74	0.70
3:a:3221[B]:ALA:HB2	3:a:3256[B]:TRP:H	1.56	0.70
3:a:3293[A]:LYS:HB2	3:a:3294[A]:SER:HB2	0.82	0.70
3:d:2969[B]:TYR:HB3	3:d:2971[B]:ASP:OD1	1.82	0.70
3:d:3194[B]:GLY:C	3:d:3195[B]:MET:HG2	2.16	0.70
3:d:3275[A]:LEU:HD12	3:d:3275[A]:LEU:N	2.04	0.70
3:d:3293[A]:LYS:HD2	3:d:3293[A]:LYS:C	2.15	0.70
3:C:2965[A]:LEU:HG	3:C:2974[A]:ALA:CB	2.21	0.70
3:F:2982[A]:MET:HE1	3:F:3254[A]:MET:HE2	1.73	0.70
3:F:3285[B]:VAL:HG22	3:F:3286[B]:THR:N	2.04	0.70
3:I:2948[A]:ASP:CB	3:I:2949[A]:LYS:HA	2.16	0.70
3:I:3153[B]:LYS:HG2	3:R:3155[B]:MET:HB2	1.67	0.70
3:I:3254[B]:MET:CG	3:R:2966[B]:SER:CB	2.55	0.70
3:I:3287[A]:ILE:O	3:I:3287[A]:ILE:HD13	1.92	0.70
1:M:456:GLN:HG2	1:M:551:GLU:HB2	1.72	0.70
3:O:2952[A]:ALA:H	3:O:2953[A]:GLY:CA	2.04	0.70
3:O:2982[A]:MET:HE1	3:O:3254[A]:MET:HE2	1.73	0.70
3:O:3194[B]:GLY:C	3:O:3195[B]:MET:HG2	2.16	0.70
2:Q:2890:VAL:N	2:Q:2891:LEU:HA	2.07	0.70
3:R:2930[B]:LEU:HD22	3:R:2930[B]:LEU:N	2.02	0.70
3:R:2965[B]:LEU:HG	3:R:2974[B]:ALA:CB	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3221[A]:ALA:HB2	3:R:3256[A]:TRP:H	1.57	0.70
3:U:2965[B]:LEU:HD11	3:d:3221[B]:ALA:H	0.62	0.70
3:U:2982[A]:MET:HE1	3:U:3254[A]:MET:HE2	1.72	0.70
3:U:3179[A]:ASP:OD1	3:U:3181[A]:GLN:HB2	1.91	0.70
3:X:2935[A]:ILE:HD13	3:X:2936[A]:GLU:N	2.05	0.70
3:X:3025[A]:VAL:HG22	3:X:3047[A]:ARG:NH1	2.01	0.70
3:X:3283[A]:ILE:HD13	3:X:3283[A]:ILE:C	2.15	0.70
3:a:2935[B]:ILE:HD13	3:a:2936[B]:GLU:N	2.05	0.70
3:a:3221[A]:ALA:HB2	3:a:3256[A]:TRP:H	1.56	0.70
3:a:3228[B]:VAL:HG22	3:a:3245[B]:PHE:O	1.90	0.70
3:d:2982[A]:MET:HE1	3:d:3254[A]:MET:HE2	1.73	0.70
3:C:2948[A]:ASP:CB	3:C:2949[A]:LYS:HA	2.15	0.70
3:C:3154[B]:PRO:CD	3:L:3173[B]:THR:C	2.63	0.70
3:F:2959[B]:SER:CB	3:a:3255[B]:PRO:CB	2.66	0.70
3:F:2969[B]:TYR:O	3:F:2972[B]:GLY:N	2.21	0.70
3:F:2970[B]:PRO:CG	3:a:2989[B]:HIS:CD2	2.74	0.70
3:F:2985[B]:PHE:CZ	3:a:2970[B]:PRO:CA	2.69	0.70
3:I:2937[A]:ASN:CB	3:I:3006[A]:LYS:HE2	2.14	0.70
3:I:2982[B]:MET:HE1	3:I:3254[B]:MET:HE2	1.73	0.70
3:I:3066[B]:TYR:CD1	3:I:3193[B]:HIS:CE1	2.80	0.70
3:L:2965[A]:LEU:HG	3:L:2974[A]:ALA:CB	2.21	0.70
3:L:3306[B]:LEU:HD12	3:L:3306[B]:LEU:C	2.15	0.70
3:O:2965[A]:LEU:HG	3:O:2974[A]:ALA:CB	2.21	0.70
3:O:2969[B]:TYR:HB2	3:X:3158[B]:PHE:CD2	2.26	0.70
3:O:3179[B]:ASP:OD1	3:O:3181[B]:GLN:HB2	1.92	0.70
3:O:3221[A]:ALA:HB2	3:O:3256[A]:TRP:H	1.56	0.70
3:R:3173[B]:THR:CG2	3:R:3174[B]:GLY:N	2.55	0.70
1:S:838:ARG:NH1	1:S:915:ASN:OD1	2.24	0.70
3:U:2933[A]:SER:O	3:U:2936[A]:GLU:N	2.23	0.70
3:U:3086[B]:GLU:CD	3:d:2970[B]:PRO:HG2	2.16	0.70
3:U:3170[B]:ALA:C	3:d:3148[B]:ILE:CG2	2.64	0.70
3:U:3306[B]:LEU:HD12	3:U:3306[B]:LEU:C	2.15	0.70
3:X:2982[B]:MET:HE1	3:X:3254[B]:MET:HE2	1.73	0.70
3:d:2965[B]:LEU:HG	3:d:2974[B]:ALA:CB	2.20	0.70
3:d:3228[A]:VAL:HG22	3:d:3245[A]:PHE:O	1.90	0.70
1:A:898:GLY:N	1:A:899:MET:HA	2.06	0.70
3:C:3179[A]:ASP:OD1	3:C:3181[A]:GLN:HB2	1.92	0.70
3:F:2960[B]:PHE:CA	3:a:3255[B]:PRO:HD2	2.22	0.70
3:F:3066[A]:TYR:CD1	3:F:3193[A]:HIS:CE1	2.79	0.70
3:I:2961[B]:HIS:HD2	3:I:2988[B]:TRP:CZ3	2.08	0.70
3:I:2965[B]:LEU:HG	3:I:2974[B]:ALA:CB	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2969[B]:TYR:HD2	3:I:2971[B]:ASP:N	1.84	0.70
3:I:2971[B]:ASP:O	3:R:3090[B]:ASN:CA	2.38	0.70
3:I:3194[A]:GLY:C	3:I:3195[A]:MET:HG2	2.16	0.70
3:I:3221[B]:ALA:HB1	3:R:2965[B]:LEU:H	0.87	0.70
3:L:3196[B]:THR:H	3:L:3199[B]:GLN:CB	2.02	0.70
1:M:871:GLN:NE2	1:M:964:ILE:O	2.24	0.70
2:N:2130:PRO:HB2	2:N:2142:ALA:HB3	1.72	0.70
3:O:2975[B]:PHE:HD1	3:X:3156[B]:MET:C	1.98	0.70
1:S:515:ASP:O	1:S:518:LYS:NZ	2.19	0.70
1:S:780:GLU:O	1:S:782:THR:N	2.24	0.70
3:U:3226[B]:ALA:HB1	3:U:3288[B]:MET:O	1.90	0.70
3:X:2935[B]:ILE:HD13	3:X:2936[B]:GLU:N	2.05	0.70
3:X:2948[B]:ASP:H	3:X:2949[B]:LYS:CA	1.98	0.70
3:X:3221[A]:ALA:HB2	3:X:3256[A]:TRP:H	1.56	0.70
2:Z:2149:ALA:HA	2:Z:2260:GLU:HG2	1.72	0.70
3:d:3194[A]:GLY:C	3:d:3195[A]:MET:HG2	2.16	0.70
6:r:1:NAG:O3	6:r:2:NAG:C1	2.39	0.70
3:C:2968[A]:GLN:CB	3:C:2972[A]:GLY:HA2	2.19	0.70
3:C:2979[B]:GLN:HE21	3:C:3155[B]:MET:HE2	1.55	0.70
3:C:3156[B]:MET:HB2	3:L:2982[B]:MET:HB3	1.59	0.70
3:C:3279[B]:ASP:OD1	3:C:3279[B]:ASP:N	2.25	0.70
3:F:3066[B]:TYR:CD1	3:F:3193[B]:HIS:CE1	2.79	0.70
3:F:3155[B]:MET:O	3:a:3153[B]:LYS:HE3	1.90	0.70
3:F:3179[B]:ASP:OD1	3:F:3181[B]:GLN:HB2	1.92	0.70
3:F:3228[B]:VAL:HG22	3:F:3245[B]:PHE:O	1.90	0.70
3:F:3256[B]:TRP:NE1	3:a:2965[B]:LEU:HD13	2.07	0.70
3:F:3279[B]:ASP:OD1	3:F:3279[B]:ASP:N	2.25	0.70
1:G:854:LEU:HD23	1:G:941:LEU:HD21	1.72	0.70
1:G:1442:MET:HE1	1:G:1454:PHE:HA	1.72	0.70
3:I:2964[B]:PRO:CA	3:R:3221[B]:ALA:CB	2.69	0.70
3:I:3157[B]:PRO:HD3	3:R:2982[B]:MET:HE1	1.74	0.70
3:I:3173[A]:THR:CG2	3:I:3174[A]:GLY:N	2.55	0.70
3:I:3255[B]:PRO:HG3	3:R:2963[B]:MET:C	2.16	0.70
3:O:3252[B]:TYR:CB	3:X:3156[B]:MET:SD	2.79	0.70
2:Q:2564:PRO:HA	2:Q:2673:GLU:HG3	1.73	0.70
3:R:3194[A]:GLY:C	3:R:3195[A]:MET:HG2	2.16	0.70
3:U:2974[B]:ALA:HB1	3:d:3220[B]:ARG:CD	2.20	0.70
3:U:3152[B]:LYS:HD2	3:d:3173[B]:THR:OG1	1.90	0.70
3:U:3179[B]:ASP:OD1	3:U:3181[B]:GLN:HB2	1.92	0.70
3:U:3194[A]:GLY:C	3:U:3195[A]:MET:HG2	2.16	0.70
1:V:855:ARG:HH21	1:V:941:LEU:HA	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3066[B]:TYR:CD1	3:X:3193[B]:HIS:CE1	2.79	0.70
3:X:3279[B]:ASP:OD1	3:X:3279[B]:ASP:N	2.25	0.70
3:X:3284[A]:LYS:HA	3:X:3284[A]:LYS:CE	2.22	0.70
1:Y:848:VAL:O	1:Y:852:ASN:ND2	2.24	0.70
1:Y:999:LEU:O	1:Y:1063:ARG:NH2	2.24	0.70
2:Z:2225:ARG:HD2	2:Z:2274:LEU:HD22	1.74	0.70
1:b:2:LEU:HD21	1:b:81:VAL:HG21	1.72	0.70
3:d:3066[B]:TYR:CD1	3:d:3193[B]:HIS:CE1	2.79	0.70
3:C:2965[B]:LEU:CD1	3:C:2974[B]:ALA:HA	2.22	0.70
3:C:3169[A]:LYS:C	3:C:3172[A]:SER:HG	1.99	0.70
3:F:2962[B]:GLY:O	3:a:3255[B]:PRO:HD3	1.90	0.70
3:F:2963[B]:MET:HE1	3:a:3223[B]:GLY:HA3	1.73	0.70
1:G:911:LEU:O	1:G:915:ASN:ND2	2.24	0.70
2:H:2605:LEU:O	2:H:2622:ASN:ND2	2.25	0.70
3:I:3226[B]:ALA:HB1	3:I:3288[B]:MET:O	1.91	0.70
1:J:262:LYS:NZ	1:J:795:GLU:OE1	2.25	0.70
1:J:1170:MET:HB3	1:J:1203:MET:HE2	1.74	0.70
3:L:2933[A]:SER:C	3:L:2935[A]:ILE:HD13	2.17	0.70
3:L:3113[A]:ASP:CG	3:L:3114[A]:PRO:CD	2.56	0.70
3:L:3221[A]:ALA:HB2	3:L:3256[A]:TRP:H	1.56	0.70
3:O:3112[B]:TYR:CD2	3:X:2969[B]:TYR:OH	2.45	0.70
3:R:2982[B]:MET:HE1	3:R:3254[B]:MET:HE2	1.73	0.70
3:R:3194[B]:GLY:C	3:R:3195[B]:MET:HG2	2.16	0.70
3:R:3306[B]:LEU:HD12	3:R:3306[B]:LEU:C	2.15	0.70
3:U:2937[A]:ASN:CB	3:U:3006[A]:LYS:HE2	2.14	0.70
3:U:2969[B]:TYR:OH	3:d:3107[B]:LEU:CD1	2.28	0.70
3:U:3173[A]:THR:CG2	3:U:3174[A]:GLY:N	2.55	0.70
1:V:1033:LEU:HA	1:V:1036:SER:HB3	1.74	0.70
3:X:2930[A]:LEU:H	3:X:2930[A]:LEU:CD2	1.98	0.70
3:X:3194[B]:GLY:C	3:X:3195[B]:MET:HG2	2.16	0.70
3:C:2933[A]:SER:C	3:C:2935[A]:ILE:HD13	2.17	0.70
3:C:2952[B]:ALA:CB	3:C:2953[B]:GLY:C	2.48	0.70
3:C:3066[A]:TYR:CD1	3:C:3193[A]:HIS:CE1	2.79	0.70
3:F:2965[A]:LEU:CD1	3:F:2974[A]:ALA:HA	2.22	0.70
3:F:2974[B]:ALA:HB1	3:a:3253[B]:GLU:CD	2.12	0.70
3:F:3259[B]:ASP:HB3	3:a:3162[B]:ASP:HB3	0.78	0.70
3:F:3287[A]:ILE:O	3:F:3287[A]:ILE:HD13	1.92	0.70
1:G:401:VAL:HG22	1:G:662:SER:HB3	1.74	0.70
1:G:619:SER:HB2	1:G:805:VAL:HG11	1.72	0.70
3:I:3255[B]:PRO:CG	3:R:2962[B]:GLY:O	2.38	0.70
1:J:757:VAL:HG21	1:J:781:ILE:HG22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1215:LEU:HD13	1:J:1229:LYS:HE3	1.72	0.70
3:O:2937[A]:ASN:CB	3:O:3006[A]:LYS:HE2	2.14	0.70
3:R:2933[A]:SER:C	3:R:2935[A]:ILE:HD13	2.17	0.70
3:R:3196[A]:THR:H	3:R:3199[A]:GLN:CB	2.02	0.70
3:R:3221[B]:ALA:HB2	3:R:3256[B]:TRP:H	1.56	0.70
3:R:3287[B]:ILE:O	3:R:3287[B]:ILE:HD13	1.92	0.70
1:S:1000:GLU:HG2	1:S:1133:ILE:HG23	1.74	0.70
2:T:2826:GLU:HA	2:T:2876:LYS:HE3	1.73	0.70
3:U:2933[B]:SER:C	3:U:2935[B]:ILE:HD13	2.17	0.70
1:V:609:TRP:HZ3	1:V:761:ALA:HB2	1.56	0.70
1:V:1583:CYS:SG	1:V:1584:GLY:N	2.63	0.70
3:X:2933[A]:SER:C	3:X:2935[A]:ILE:HD13	2.17	0.70
3:X:2961[B]:HIS:HD2	3:X:2988[B]:TRP:CZ3	2.08	0.70
3:a:3226[B]:ALA:HB1	3:a:3288[B]:MET:O	1.91	0.70
2:B:2191:LEU:O	2:B:2225:ARG:NH2	2.25	0.70
3:C:2965[A]:LEU:CD1	3:C:2974[A]:ALA:HA	2.22	0.70
3:F:3090[B]:ASN:CA	3:a:2971[B]:ASP:O	2.39	0.70
3:F:3173[B]:THR:O	3:a:3154[B]:PRO:CD	2.24	0.70
3:I:3221[B]:ALA:HB2	3:I:3256[B]:TRP:H	1.56	0.70
3:L:2930[B]:LEU:H	3:L:2930[B]:LEU:CD2	1.98	0.70
3:L:2952[A]:ALA:H	3:L:2953[A]:GLY:CA	2.04	0.70
3:L:2965[A]:LEU:CD1	3:L:2974[A]:ALA:HA	2.22	0.70
3:L:3025[B]:VAL:HG22	3:L:3047[B]:ARG:NH1	2.01	0.70
3:L:3133[A]:LEU:O	3:L:3134[A]:GLN:C	2.32	0.70
3:O:3066[B]:TYR:CD1	3:O:3193[B]:HIS:CE1	2.79	0.70
3:O:3196[B]:THR:H	3:O:3199[B]:GLN:CB	2.03	0.70
3:O:3226[B]:ALA:HB1	3:O:3288[B]:MET:O	1.91	0.70
2:Q:2090:LYS:NZ	2:Q:2099:GLU:OE2	2.25	0.70
1:S:456:GLN:HG2	1:S:551:GLU:HB3	1.74	0.70
3:U:2933[A]:SER:C	3:U:2935[A]:ILE:HD13	2.17	0.70
3:U:3133[B]:LEU:O	3:U:3134[B]:GLN:C	2.32	0.70
3:U:3169[B]:LYS:CG	3:d:3147[B]:GLU:CB	2.70	0.70
3:U:3293[A]:LYS:HB2	3:U:3294[A]:SER:HB2	0.82	0.70
3:X:2952[A]:ALA:H	3:X:2953[A]:GLY:CA	2.04	0.70
3:X:3179[A]:ASP:OD1	3:X:3181[A]:GLN:HB2	1.92	0.70
3:a:2933[B]:SER:C	3:a:2935[B]:ILE:HD13	2.17	0.70
3:a:2937[A]:ASN:CB	3:a:3006[A]:LYS:HE2	2.14	0.70
3:a:2982[B]:MET:HE1	3:a:3254[B]:MET:HE2	1.73	0.70
3:a:3179[A]:ASP:OD1	3:a:3181[A]:GLN:HB2	1.92	0.70
3:a:3179[B]:ASP:OD1	3:a:3181[B]:GLN:HB2	1.92	0.70
3:a:3226[A]:ALA:HB1	3:a:3288[A]:MET:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3287[B]:ILE:O	3:a:3287[B]:ILE:HD13	1.92	0.70
3:d:2979[B]:GLN:HE21	3:d:3155[B]:MET:HE2	1.55	0.70
3:d:3179[A]:ASP:OD1	3:d:3181[A]:GLN:HB2	1.92	0.70
4:n:1:NAG:O3	4:n:2:NAG:C7	2.40	0.70
3:C:2933[B]:SER:C	3:C:2935[B]:ILE:HD13	2.17	0.70
3:C:2969[B]:TYR:O	3:C:2972[B]:GLY:N	2.20	0.70
3:C:3194[A]:GLY:C	3:C:3195[A]:MET:HG2	2.16	0.70
1:D:724:LYS:HA	1:D:728:ARG:HH11	1.57	0.70
3:F:3160[B]:SER:O	3:a:3150[B]:LYS:CD	2.40	0.70
3:F:3162[B]:ASP:CA	3:a:3147[B]:GLU:OE1	2.36	0.70
3:I:2966[B]:SER:O	3:R:3256[B]:TRP:CG	2.44	0.70
3:I:3173[B]:THR:CG2	3:I:3174[B]:GLY:N	2.55	0.70
3:L:2937[B]:ASN:HB2	3:L:3006[B]:LYS:CE	2.14	0.70
3:L:2961[B]:HIS:HB3	3:L:3111[B]:SER:HG	1.56	0.70
3:L:3173[B]:THR:CG2	3:L:3174[B]:GLY:N	2.55	0.70
3:L:3179[B]:ASP:OD1	3:L:3181[B]:GLN:HB2	1.91	0.70
3:O:3169[B]:LYS:HE3	3:X:3148[B]:ILE:HA	1.69	0.70
3:O:3169[B]:LYS:NZ	3:X:3148[B]:ILE:H	1.90	0.70
3:O:3254[B]:MET:CG	3:X:3159[B]:SER:OG	2.40	0.70
1:P:997:SER:O	1:P:1001:GLN:NE2	2.24	0.70
1:S:1019:HIS:NE2	1:S:1046:HIS:HE1	1.90	0.70
2:T:2806:ALA:HB2	2:T:2856:ILE:HD11	1.74	0.70
3:U:3173[B]:THR:CG2	3:U:3174[B]:GLY:N	2.55	0.70
3:U:3254[B]:MET:HB2	3:d:3254[B]:MET:CB	2.22	0.70
3:U:3284[B]:LYS:HA	3:U:3284[B]:LYS:CE	2.22	0.70
3:U:3287[A]:ILE:O	3:U:3287[A]:ILE:HD13	1.92	0.70
2:W:2166:LEU:HA	2:W:2169:HIS:HB2	1.73	0.70
1:Y:1471:LEU:HD11	1:Y:1540:LEU:HD23	1.73	0.70
3:a:3196[A]:THR:HG21	1:b:416:ASN:CB	2.20	0.70
3:C:3160[B]:SER:HA	3:L:2983[B]:VAL:HB	1.74	0.69
3:F:2964[B]:PRO:HB2	3:a:3255[B]:PRO:HB3	1.74	0.69
3:F:3090[B]:ASN:HB3	3:a:2971[B]:ASP:O	1.92	0.69
3:F:3160[B]:SER:CA	3:a:2983[B]:VAL:H	2.05	0.69
3:F:3196[A]:THR:H	3:F:3199[A]:GLN:CB	2.02	0.69
3:I:2965[B]:LEU:CD1	3:I:2974[B]:ALA:HA	2.22	0.69
3:L:2961[A]:HIS:HD2	3:L:2988[A]:TRP:CZ3	2.08	0.69
3:L:3287[B]:ILE:O	3:L:3287[B]:ILE:HD13	1.92	0.69
3:O:2965[B]:LEU:HG	3:O:2974[B]:ALA:CB	2.21	0.69
3:O:2982[B]:MET:HE1	3:O:3254[B]:MET:HE2	1.72	0.69
3:O:3109[B]:TYR:CE2	3:X:2969[B]:TYR:O	2.44	0.69
3:O:3120[A]:HIS:O	3:O:3121[A]:SER:C	2.29	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1582:ASN:HB3	1:S:1583:CYS:CB	2.22	0.69
3:U:2980[B]:HIS:CB	3:d:2969[B]:TYR:OH	2.39	0.69
3:U:2982[B]:MET:HE1	3:U:3254[B]:MET:HE2	1.72	0.69
1:V:1390:ASP:HB3	1:Y:1372:ILE:HD11	1.74	0.69
3:X:2965[B]:LEU:CD1	3:X:2974[B]:ALA:HA	2.22	0.69
3:X:3173[A]:THR:CG2	3:X:3174[A]:GLY:N	2.55	0.69
1:Y:1576:THR:CG2	3:d:3196[B]:THR:HG21	2.22	0.69
3:a:3066[A]:TYR:CD1	3:a:3193[A]:HIS:CE1	2.79	0.69
3:d:2933[A]:SER:C	3:d:2935[A]:ILE:HD13	2.17	0.69
2:B:2711:HIS:HA	2:B:2714:VAL:HG22	1.74	0.69
3:C:3173[B]:THR:CG2	3:C:3174[B]:GLY:N	2.55	0.69
3:C:3194[B]:GLY:C	3:C:3195[B]:MET:HG2	2.16	0.69
3:I:3150[B]:LYS:HZ3	3:R:3160[B]:SER:CB	2.04	0.69
3:I:3176[B]:LYS:HZ2	3:I:3176[B]:LYS:HB3	1.56	0.69
3:L:3179[A]:ASP:OD1	3:L:3181[A]:GLN:HB2	1.92	0.69
3:O:2965[B]:LEU:CD1	3:O:2974[B]:ALA:HA	2.22	0.69
3:O:2965[B]:LEU:HD11	3:X:2979[B]:GLN:CD	2.12	0.69
3:O:3066[A]:TYR:CD1	3:O:3193[A]:HIS:CE1	2.79	0.69
2:Q:2180:TRP:HB2	2:Q:2243:LEU:HD13	1.72	0.69
3:R:3173[A]:THR:CG2	3:R:3174[A]:GLY:N	2.55	0.69
3:R:3230[A]:PHE:CB	3:R:3243[A]:GLY:N	2.56	0.69
3:U:3153[B]:LYS:CG	3:d:3153[B]:LYS:HD2	2.22	0.69
1:V:337:ASP:OD1	1:V:337:ASP:N	2.24	0.69
2:W:2890:VAL:N	2:W:2891:LEU:HA	2.06	0.69
3:X:3279[A]:ASP:OD1	3:X:3279[A]:ASP:N	2.25	0.69
3:a:3176[B]:LYS:HZ2	3:a:3176[B]:LYS:HB3	1.58	0.69
3:a:3287[A]:ILE:O	3:a:3287[A]:ILE:HD13	1.92	0.69
3:C:3147[B]:GLU:CG	3:L:3160[B]:SER:C	2.55	0.69
3:C:3169[B]:LYS:O	3:L:3152[B]:LYS:HE3	1.91	0.69
3:F:3162[B]:ASP:CG	3:a:3259[B]:ASP:H	1.99	0.69
3:F:3174[B]:GLY:N	3:a:3154[B]:PRO:HD3	2.01	0.69
3:F:3194[A]:GLY:C	3:F:3195[A]:MET:HG2	2.16	0.69
3:F:3194[B]:GLY:C	3:F:3195[B]:MET:HG2	2.16	0.69
3:F:3226[A]:ALA:HB1	3:F:3288[A]:MET:O	1.91	0.69
3:F:3284[A]:LYS:HA	3:F:3284[A]:LYS:CE	2.22	0.69
1:G:1470:GLU:HG2	1:G:1537:ILE:HD12	1.73	0.69
3:I:3194[B]:GLY:C	3:I:3195[B]:MET:HG2	2.16	0.69
3:I:3255[B]:PRO:CB	3:R:2964[B]:PRO:HD2	2.22	0.69
1:M:984:ASP:OD1	1:M:985:PHE:N	2.25	0.69
3:O:3173[A]:THR:CG2	3:O:3174[A]:GLY:N	2.55	0.69
3:O:3220[A]:ARG:HG3	3:O:3220[A]:ARG:NH1	1.98	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3287[A]:ILE:O	3:O:3287[A]:ILE:HD13	1.92	0.69
1:P:21:SER:HB2	1:P:83:HIS:O	1.92	0.69
3:R:2933[B]:SER:C	3:R:2935[B]:ILE:HD13	2.17	0.69
3:U:2980[B]:HIS:O	3:d:2969[B]:TYR:CD1	2.26	0.69
3:U:3153[B]:LYS:CB	3:d:3154[B]:PRO:O	2.30	0.69
3:X:2933[B]:SER:C	3:X:2935[B]:ILE:HD13	2.17	0.69
3:X:3287[B]:ILE:O	3:X:3287[B]:ILE:HD13	1.92	0.69
3:a:2933[A]:SER:C	3:a:2935[A]:ILE:HD13	2.17	0.69
3:a:2965[A]:LEU:CD1	3:a:2974[A]:ALA:HA	2.22	0.69
3:a:2965[B]:LEU:CD1	3:a:2974[B]:ALA:HA	2.22	0.69
1:A:678:ASN:O	1:A:684:ARG:NH2	2.23	0.69
3:C:2930[B]:LEU:H	3:C:2930[B]:LEU:CD2	1.98	0.69
3:C:3284[B]:LYS:HA	3:C:3284[B]:LYS:CE	2.22	0.69
3:F:2933[A]:SER:C	3:F:2935[A]:ILE:HD13	2.17	0.69
3:F:2948[B]:ASP:H	3:F:2949[B]:LYS:CA	1.98	0.69
3:F:2962[B]:GLY:O	3:a:3255[B]:PRO:CG	2.40	0.69
3:F:2966[B]:SER:N	3:a:3255[B]:PRO:HA	2.07	0.69
3:F:3255[B]:PRO:HG3	3:a:2962[B]:GLY:O	1.91	0.69
3:F:3307[A]:PHE:CE1	3:F:3309[A]:PRO:HG3	2.16	0.69
3:I:3133[A]:LEU:O	3:I:3134[A]:GLN:C	2.32	0.69
3:I:3230[B]:PHE:CB	3:I:3243[B]:GLY:N	2.56	0.69
3:I:3287[B]:ILE:O	3:I:3287[B]:ILE:HD13	1.92	0.69
3:L:3066[A]:TYR:CD1	3:L:3193[A]:HIS:CE1	2.80	0.69
3:L:3077[B]:ASP:HB2	3:L:3080[B]:ASP:OD2	1.93	0.69
3:L:3287[A]:ILE:O	3:L:3287[A]:ILE:HD13	1.92	0.69
1:M:1358:LEU:HD23	1:M:1456:LEU:HD21	1.74	0.69
3:O:2930[A]:LEU:H	3:O:2930[A]:LEU:CD2	1.98	0.69
3:O:2961[B]:HIS:CE1	3:O:2980[B]:HIS:NE2	2.57	0.69
3:O:2965[A]:LEU:CD1	3:O:2974[A]:ALA:HA	2.22	0.69
3:O:3154[B]:PRO:CD	3:X:3176[B]:LYS:HE3	2.22	0.69
3:O:3284[B]:LYS:HA	3:O:3284[B]:LYS:CE	2.22	0.69
3:R:3077[B]:ASP:HB2	3:R:3080[B]:ASP:OD2	1.93	0.69
3:R:3230[B]:PHE:CB	3:R:3243[B]:GLY:N	2.56	0.69
3:R:3284[B]:LYS:HA	3:R:3284[B]:LYS:CE	2.22	0.69
1:S:723:ALA:O	1:S:728:ARG:NH1	2.25	0.69
1:V:588:GLU:OE2	1:V:728:ARG:NH1	2.25	0.69
3:X:2930[B]:LEU:H	3:X:2930[B]:LEU:CD2	1.98	0.69
3:X:3230[A]:PHE:CB	3:X:3243[A]:GLY:N	2.56	0.69
3:X:3230[B]:PHE:CB	3:X:3243[B]:GLY:N	2.56	0.69
3:a:2965[B]:LEU:HG	3:a:2974[B]:ALA:CB	2.21	0.69
1:b:588:GLU:OE2	1:b:728:ARG:NH1	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2933[B]:SER:C	3:d:2935[B]:ILE:HD13	2.17	0.69
3:d:3066[A]:TYR:CD1	3:d:3193[A]:HIS:CE1	2.79	0.69
3:d:3077[B]:ASP:HB2	3:d:3080[B]:ASP:OD2	1.93	0.69
3:d:3169[B]:LYS:C	3:d:3172[B]:SER:HG	1.98	0.69
1:A:416:ASN:OD1	3:F:3196[A]:THR:HG21	1.92	0.69
1:A:567:LEU:HB3	1:A:571:PRO:HG2	1.72	0.69
3:C:2930[B]:LEU:HD22	3:C:2930[B]:LEU:N	2.02	0.69
3:C:3179[B]:ASP:OD1	3:C:3181[B]:GLN:HB2	1.91	0.69
3:F:2933[B]:SER:C	3:F:2935[B]:ILE:HD13	2.17	0.69
3:F:2966[B]:SER:HB2	3:F:2977[B]:CYS:CB	2.21	0.69
3:F:2979[A]:GLN:HE21	3:F:3155[A]:MET:HE2	1.55	0.69
3:F:3077[B]:ASP:HB2	3:F:3080[B]:ASP:OD2	1.93	0.69
3:F:3159[B]:SER:HB3	3:a:2984[B]:THR:CB	2.19	0.69
3:I:2937[A]:ASN:CB	3:I:3006[A]:LYS:HD3	2.23	0.69
3:I:3161[B]:GLU:HG2	3:R:3079[B]:CYS:CA	2.20	0.69
3:I:3179[B]:ASP:OD1	3:I:3181[B]:GLN:HB2	1.92	0.69
3:L:3284[A]:LYS:HA	3:L:3284[A]:LYS:CE	2.21	0.69
1:M:1239:GLY:O	1:M:1242:ASN:ND2	2.25	0.69
3:O:2933[A]:SER:C	3:O:2935[A]:ILE:HD13	2.17	0.69
3:O:2937[B]:ASN:HB2	3:O:3006[B]:LYS:CE	2.14	0.69
3:O:3109[B]:TYR:CG	3:X:2970[B]:PRO:N	1.97	0.69
3:O:3230[B]:PHE:CB	3:O:3243[B]:GLY:N	2.56	0.69
2:Q:2166:LEU:HA	2:Q:2169:HIS:HB2	1.73	0.69
3:R:2935[B]:ILE:HD13	3:R:2936[B]:GLU:N	2.05	0.69
3:R:3179[A]:ASP:OD1	3:R:3181[A]:GLN:HB2	1.92	0.69
3:U:2948[B]:ASP:H	3:U:2949[B]:LYS:CA	1.98	0.69
3:U:2952[A]:ALA:CB	3:U:2953[A]:GLY:C	2.48	0.69
3:U:2979[B]:GLN:HE21	3:U:3155[B]:MET:HE2	1.54	0.69
3:U:3086[B]:GLU:CD	3:d:2970[B]:PRO:HG3	2.12	0.69
3:U:3153[B]:LYS:HG3	3:d:3155[B]:MET:HE3	1.75	0.69
1:V:355:ALA:HA	1:V:734:LEU:HD12	1.74	0.69
3:X:3285[A]:VAL:HG22	3:X:3286[A]:THR:N	2.04	0.69
3:X:3287[A]:ILE:O	3:X:3287[A]:ILE:HD13	1.92	0.69
3:a:3077[B]:ASP:HB2	3:a:3080[B]:ASP:OD2	1.93	0.69
3:d:2965[B]:LEU:CD1	3:d:2974[B]:ALA:HA	2.22	0.69
3:d:3077[A]:ASP:HB2	3:d:3080[A]:ASP:OD2	1.93	0.69
3:d:3173[B]:THR:CG2	3:d:3174[B]:GLY:N	2.55	0.69
3:d:3179[B]:ASP:OD1	3:d:3181[B]:GLN:HB2	1.92	0.69
3:C:3173[A]:THR:CG2	3:C:3174[A]:GLY:N	2.55	0.69
3:C:3287[A]:ILE:O	3:C:3287[A]:ILE:HD13	1.92	0.69
1:D:534:ASP:HB2	1:D:541:LYS:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2942[A]:LEU:HD13	3:F:3033[A]:PHE:CE1	2.28	0.69
3:F:2965[B]:LEU:CD1	3:F:2974[B]:ALA:HA	2.22	0.69
3:F:2970[B]:PRO:CB	3:a:2989[B]:HIS:HD2	2.04	0.69
3:F:3024[B]:LEU:CD1	3:F:3025[B]:VAL:H	1.84	0.69
3:F:3169[B]:LYS:HZ3	3:a:3149[B]:ASN:ND2	1.87	0.69
3:I:2937[B]:ASN:CB	3:I:3006[B]:LYS:HD3	2.23	0.69
3:I:2973[B]:THR:HG23	3:R:3248[B]:LEU:CD1	2.20	0.69
3:I:3160[B]:SER:CB	3:R:2982[B]:MET:HB3	2.20	0.69
3:L:2933[B]:SER:C	3:L:2935[B]:ILE:HD13	2.17	0.69
3:L:2937[A]:ASN:CB	3:L:3006[A]:LYS:HD3	2.23	0.69
3:L:2965[B]:LEU:CD1	3:L:2974[B]:ALA:HA	2.22	0.69
3:L:3230[B]:PHE:CB	3:L:3243[B]:GLY:N	2.56	0.69
3:O:3040[B]:VAL:HG21	3:X:2969[B]:TYR:CE1	2.11	0.69
3:O:3077[B]:ASP:HB2	3:O:3080[B]:ASP:OD2	1.93	0.69
3:O:3179[A]:ASP:OD1	3:O:3181[A]:GLN:HB2	1.92	0.69
3:O:3230[A]:PHE:CB	3:O:3243[A]:GLY:N	2.56	0.69
1:P:484:MET:HE2	1:P:663:GLU:HG3	1.73	0.69
2:Q:2797:LYS:HA	2:Q:2800:LYS:HD3	1.75	0.69
3:R:2937[B]:ASN:CB	3:R:3006[B]:LYS:HD3	2.23	0.69
3:R:3077[A]:ASP:HB2	3:R:3080[A]:ASP:OD2	1.93	0.69
3:U:3077[A]:ASP:HB2	3:U:3080[A]:ASP:OD2	1.93	0.69
2:W:2851:ASN:OD1	2:W:2851:ASN:N	2.24	0.69
3:X:2942[A]:LEU:HD13	3:X:3033[A]:PHE:CE1	2.28	0.69
3:X:2942[B]:LEU:HD13	3:X:3033[B]:PHE:CE1	2.28	0.69
3:X:3077[B]:ASP:HB2	3:X:3080[B]:ASP:OD2	1.93	0.69
3:a:2937[B]:ASN:CB	3:a:3006[B]:LYS:HD3	2.23	0.69
3:a:2937[B]:ASN:CB	3:a:3006[B]:LYS:HE2	2.14	0.69
3:a:3173[A]:THR:CG2	3:a:3174[A]:GLY:N	2.55	0.69
1:b:1063:ARG:HB3	1:b:1065:LYS:HD2	1.73	0.69
3:d:2937[B]:ASN:CB	3:d:3006[B]:LYS:HD3	2.23	0.69
3:d:3226[A]:ALA:HB1	3:d:3288[A]:MET:O	1.90	0.69
3:F:3077[A]:ASP:HB2	3:F:3080[A]:ASP:OD2	1.93	0.69
3:F:3156[B]:MET:CB	3:a:2982[B]:MET:SD	2.81	0.69
3:F:3173[A]:THR:CG2	3:F:3174[A]:GLY:N	2.55	0.69
1:G:1046:HIS:HA	1:G:1049:VAL:HB	1.75	0.69
3:I:3077[B]:ASP:HB2	3:I:3080[B]:ASP:OD2	1.93	0.69
3:I:3110[A]:THR:O	3:I:3112[A]:TYR:N	2.26	0.69
3:I:3153[B]:LYS:HD2	3:R:3155[B]:MET:HB3	1.72	0.69
3:O:2937[A]:ASN:CB	3:O:3006[A]:LYS:HD3	2.23	0.69
3:O:2966[B]:SER:HB2	3:O:2977[B]:CYS:HB2	1.39	0.69
3:O:3077[A]:ASP:HB2	3:O:3080[A]:ASP:OD2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3255[B]:PRO:CD	3:X:3163[B]:ASN:HD22	2.06	0.69
2:Q:2546:LEU:H	2:Q:2557:ALA:HA	1.58	0.69
3:R:2942[A]:LEU:HD13	3:R:3033[A]:PHE:CE1	2.28	0.69
3:R:2965[B]:LEU:CD1	3:R:2974[B]:ALA:HA	2.22	0.69
3:R:3066[A]:TYR:CD1	3:R:3193[A]:HIS:CE1	2.79	0.69
3:R:3179[B]:ASP:OD1	3:R:3181[B]:GLN:HB2	1.91	0.69
3:R:3212[A]:ARG:HG3	3:R:3212[A]:ARG:NH1	2.00	0.69
3:U:2937[A]:ASN:CB	3:U:3006[A]:LYS:HD3	2.23	0.69
3:U:3024[B]:LEU:CD1	3:U:3025[B]:VAL:H	1.84	0.69
1:Y:527:LEU:O	1:Y:561:ARG:NH1	2.26	0.69
2:Z:2823:ILE:HD11	2:Z:2856:ILE:HD12	1.74	0.69
3:d:3221[A]:ALA:HB2	3:d:3256[A]:TRP:H	1.56	0.69
3:d:3287[B]:ILE:O	3:d:3287[B]:ILE:HD13	1.92	0.69
1:A:557:VAL:HG23	1:A:558:HIS:HA	1.74	0.69
2:B:2240:GLN:HE21	2:B:2241:THR:H	1.41	0.69
2:B:2550:THR:O	2:B:2553:ALA:N	2.22	0.69
3:C:2942[B]:LEU:HD13	3:C:3033[B]:PHE:CE1	2.28	0.69
3:C:2966[B]:SER:HB2	3:C:2977[B]:CYS:CB	2.21	0.69
3:C:2975[B]:PHE:CE2	3:L:2979[B]:GLN:N	2.57	0.69
3:C:2975[B]:PHE:O	3:L:3256[B]:TRP:CD1	2.46	0.69
3:C:3110[A]:THR:O	3:C:3112[A]:TYR:N	2.26	0.69
3:C:3217[A]:PHE:HE1	3:C:3230[A]:PHE:HZ	0.80	0.69
3:C:3220[A]:ARG:HG3	3:C:3220[A]:ARG:NH1	1.98	0.69
3:F:2942[B]:LEU:HD13	3:F:3033[B]:PHE:CE1	2.28	0.69
3:F:2968[B]:GLN:CG	3:a:2981[B]:GLY:N	2.54	0.69
3:F:2970[B]:PRO:HB3	3:a:2989[B]:HIS:CD2	2.28	0.69
3:F:3110[A]:THR:O	3:F:3112[A]:TYR:N	2.26	0.69
3:F:3169[B]:LYS:HE3	3:a:3150[B]:LYS:HB2	1.74	0.69
3:F:3179[A]:ASP:OD1	3:F:3181[A]:GLN:HB2	1.92	0.69
3:F:3221[B]:ALA:HB2	3:F:3256[B]:TRP:H	1.56	0.69
3:I:2933[A]:SER:C	3:I:2935[A]:ILE:HD13	2.17	0.69
3:I:2933[B]:SER:C	3:I:2935[B]:ILE:HD13	2.17	0.69
3:I:2966[B]:SER:O	3:R:2981[B]:GLY:HA3	1.93	0.69
3:I:3155[B]:MET:CB	3:R:3153[B]:LYS:CG	2.66	0.69
3:I:3158[B]:PHE:H	3:R:3153[B]:LYS:NZ	1.89	0.69
3:L:2942[A]:LEU:HD13	3:L:3033[A]:PHE:CE1	2.28	0.69
3:L:2966[B]:SER:HB2	3:L:2977[B]:CYS:CB	2.21	0.69
3:L:2979[A]:GLN:HE21	3:L:3155[A]:MET:HE2	1.54	0.69
3:L:3110[B]:THR:O	3:L:3112[B]:TYR:N	2.26	0.69
2:N:2225:ARG:HD2	2:N:2274:LEU:HD22	1.74	0.69
3:O:2942[B]:LEU:HD13	3:O:3033[B]:PHE:CE1	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2952[B]:ALA:H	3:O:2953[B]:GLY:CA	2.04	0.69
3:O:2970[B]:PRO:HD2	3:X:2991[B]:LEU:CD2	2.22	0.69
3:O:2970[B]:PRO:CA	3:X:2991[B]:LEU:N	2.56	0.69
3:O:3156[B]:MET:CE	3:X:3173[B]:THR:CG2	2.70	0.69
3:R:3025[B]:VAL:HG22	3:R:3047[B]:ARG:NH1	2.01	0.69
3:R:3089[B]:HIS:ND1	3:R:3119[B]:HIS:CE1	2.61	0.69
3:R:3287[A]:ILE:O	3:R:3287[A]:ILE:HD13	1.92	0.69
3:U:2942[A]:LEU:HD13	3:U:3033[A]:PHE:CE1	2.28	0.69
3:U:2969[B]:TYR:HD2	3:U:2971[B]:ASP:N	1.85	0.69
3:U:2969[B]:TYR:CE2	3:d:2980[B]:HIS:CD2	2.81	0.69
3:U:3307[B]:PHE:CE1	3:U:3309[B]:PRO:HG3	2.16	0.69
1:V:622:HIS:CE1	1:V:767:LYS:H	2.10	0.69
1:V:944:GLU:O	1:V:957:ASN:ND2	2.25	0.69
2:W:2868:GLU:OE1	3:X:2932[A]:PRO:C	2.34	0.69
3:X:3077[A]:ASP:HB2	3:X:3080[A]:ASP:OD2	1.93	0.69
3:X:3110[B]:THR:O	3:X:3112[B]:TYR:N	2.26	0.69
3:X:3176[A]:LYS:HB3	3:X:3176[A]:LYS:NZ	2.08	0.69
1:Y:1656:ASP:N	3:d:3006[B]:LYS:HB2	2.06	0.69
2:Z:2267:HIS:HD2	2:Z:2297:HIS:HE1	1.40	0.69
3:a:2960[A]:PHE:HD1	3:a:2960[A]:PHE:H	1.41	0.69
3:a:2982[A]:MET:HE1	3:a:3254[A]:MET:HE2	1.73	0.69
1:b:946:GLU:HG2	1:b:955:LYS:HD2	1.75	0.69
2:c:2191:LEU:O	2:c:2225:ARG:NH2	2.25	0.69
3:d:2960[B]:PHE:H	3:d:2960[B]:PHE:HD1	1.41	0.69
3:d:3176[B]:LYS:NZ	3:d:3176[B]:LYS:HB3	2.08	0.69
3:d:3284[A]:LYS:HA	3:d:3284[A]:LYS:CE	2.22	0.69
3:C:2948[B]:ASP:H	3:C:2949[B]:LYS:CA	1.98	0.69
3:C:3150[B]:LYS:O	3:L:3172[B]:SER:HB2	1.92	0.69
1:D:329:ARG:HB2	1:G:1583:CYS:H	1.57	0.69
3:F:3110[B]:THR:O	3:F:3112[B]:TYR:N	2.26	0.69
3:I:3284[A]:LYS:HA	3:I:3284[A]:LYS:CE	2.22	0.69
3:O:2937[B]:ASN:CB	3:O:3006[B]:LYS:HD3	2.23	0.69
3:O:3031[A]:ASN:OD1	3:O:3033[A]:PHE:N	2.26	0.69
3:R:3089[A]:HIS:ND1	3:R:3119[A]:HIS:CE1	2.61	0.69
3:R:3110[B]:THR:O	3:R:3112[B]:TYR:N	2.26	0.69
1:S:460:GLU:HB3	1:S:465:PRO:HG2	1.74	0.69
3:U:2961[A]:HIS:HB3	3:U:3111[A]:SER:HG	1.56	0.69
3:U:3176[B]:LYS:NZ	3:U:3176[B]:LYS:HB3	2.08	0.69
3:U:3258[B]:PHE:C	3:d:2968[B]:GLN:HE21	2.00	0.69
3:U:3287[B]:ILE:O	3:U:3287[B]:ILE:HD13	1.92	0.69
3:X:2965[A]:LEU:CD1	3:X:2974[A]:ALA:HA	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3230[A]:PHE:CB	3:a:3243[A]:GLY:N	2.56	0.69
2:c:2648:ALA:HA	2:c:2654:SER:HB2	1.75	0.69
3:d:3220[A]:ARG:HG2	3:d:3221[A]:ALA:N	2.08	0.69
3:C:2979[A]:GLN:HE21	3:C:3155[A]:MET:HE2	1.55	0.69
3:C:3154[B]:PRO:HB3	3:L:3151[B]:LEU:C	2.17	0.69
3:C:3230[A]:PHE:CB	3:C:3243[A]:GLY:N	2.56	0.69
3:F:3031[A]:ASN:OD1	3:F:3033[A]:PHE:N	2.26	0.69
3:F:3217[A]:PHE:HE1	3:F:3230[A]:PHE:HZ	0.80	0.69
3:F:3256[B]:TRP:CZ2	3:a:2965[B]:LEU:HB3	2.25	0.69
3:F:3279[A]:ASP:OD1	3:F:3279[A]:ASP:N	2.25	0.69
1:G:1650:ILE:HB	2:K:2326:ILE:HG22	1.74	0.69
3:I:2966[B]:SER:HB2	3:I:2977[B]:CYS:CB	2.21	0.69
3:I:2983[B]:VAL:HG22	3:R:3162[B]:ASP:OD1	1.92	0.69
3:I:3176[A]:LYS:HB3	3:I:3176[A]:LYS:NZ	2.08	0.69
1:J:1148:LEU:HB2	1:J:1188:PHE:HD2	1.57	0.69
3:O:2968[B]:GLN:HB2	3:X:2988[B]:TRP:N	2.08	0.69
3:O:3176[B]:LYS:HB3	3:O:3176[B]:LYS:NZ	2.08	0.69
3:O:3255[B]:PRO:HB3	3:X:3161[B]:GLU:C	2.18	0.69
3:O:3287[B]:ILE:O	3:O:3287[B]:ILE:HD13	1.92	0.69
1:P:744:VAL:HG22	1:P:760:ILE:HG12	1.73	0.69
3:R:2942[B]:LEU:HD13	3:R:3033[B]:PHE:CE1	2.28	0.69
3:R:3293[B]:LYS:HB2	3:R:3294[B]:SER:HB2	0.82	0.69
3:U:2937[B]:ASN:CB	3:U:3006[B]:LYS:HD3	2.23	0.69
3:U:3077[B]:ASP:HB2	3:U:3080[B]:ASP:OD2	1.93	0.69
3:U:3110[B]:THR:O	3:U:3112[B]:TYR:N	2.26	0.69
3:X:3089[B]:HIS:ND1	3:X:3119[B]:HIS:CE1	2.61	0.69
3:d:2966[A]:SER:HB2	3:d:2977[A]:CYS:CB	2.21	0.69
3:d:3279[B]:ASP:OD1	3:d:3279[B]:ASP:N	2.25	0.69
3:C:2942[A]:LEU:HD13	3:C:3033[A]:PHE:CE1	2.28	0.68
3:C:3077[A]:ASP:HB2	3:C:3080[A]:ASP:OD2	1.93	0.68
3:C:3160[B]:SER:HB2	3:L:3150[B]:LYS:HZ3	0.55	0.68
3:F:3031[B]:ASN:OD1	3:F:3033[B]:PHE:N	2.27	0.68
1:G:210:HIS:HA	1:G:213:VAL:HG22	1.74	0.68
3:I:2942[A]:LEU:HD13	3:I:3033[A]:PHE:CE1	2.28	0.68
3:I:2942[B]:LEU:HD13	3:I:3033[B]:PHE:CE1	2.28	0.68
3:I:3108[B]:HIS:HE1	3:R:3251[B]:ASP:CG	2.00	0.68
3:L:3176[A]:LYS:NZ	3:L:3176[A]:LYS:HB3	2.08	0.68
1:M:550:ILE:N	1:M:557:VAL:O	2.26	0.68
1:P:105:VAL:HG12	1:P:123:PHE:HB3	1.73	0.68
1:P:152:LYS:HE3	1:P:153:ASN:H	1.58	0.68
3:R:2965[A]:LEU:CD1	3:R:2974[A]:ALA:HA	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2937[B]:ASN:CB	3:X:3006[B]:LYS:HD3	2.23	0.68
1:Y:958:PRO:HA	1:Y:959:PHE:HB2	1.74	0.68
3:a:3230[B]:PHE:CB	3:a:3243[B]:GLY:N	2.56	0.68
3:d:2942[A]:LEU:HD13	3:d:3033[A]:PHE:CE1	2.28	0.68
3:d:2952[A]:ALA:H	3:d:2953[A]:GLY:CA	2.04	0.68
3:d:3173[A]:THR:CG2	3:d:3174[A]:GLY:N	2.55	0.68
4:m:1:NAG:O3	4:m:2:NAG:N2	2.21	0.68
3:C:2964[B]:PRO:N	3:L:3255[B]:PRO:HB3	2.08	0.68
3:F:3221[A]:ALA:HB2	3:F:3256[A]:TRP:H	1.56	0.68
3:I:2965[A]:LEU:CD1	3:I:2974[A]:ALA:HA	2.22	0.68
3:I:3217[B]:PHE:HE1	3:I:3230[B]:PHE:HZ	0.80	0.68
3:I:3230[A]:PHE:CB	3:I:3243[A]:GLY:N	2.56	0.68
3:L:3031[A]:ASN:OD1	3:L:3033[A]:PHE:N	2.27	0.68
3:O:2942[A]:LEU:HD13	3:O:3033[A]:PHE:CE1	2.28	0.68
3:O:3106[B]:THR:HG21	3:X:2970[B]:PRO:C	2.18	0.68
3:O:3173[B]:THR:CG2	3:O:3174[B]:GLY:N	2.55	0.68
1:P:105:VAL:HB	1:P:137:ARG:HH22	1.58	0.68
1:P:1000:GLU:HG2	1:P:1133:ILE:HG23	1.75	0.68
2:T:2872:GLU:O	1:V:1078:ARG:NH1	2.26	0.68
3:U:2952[B]:ALA:H	3:U:2953[B]:GLY:CA	2.04	0.68
3:U:2969[B]:TYR:OH	3:d:2961[B]:HIS:CE1	2.46	0.68
3:U:3220[B]:ARG:HG2	3:d:2974[B]:ALA:H	1.58	0.68
3:U:3221[A]:ALA:HB2	3:U:3256[A]:TRP:H	1.57	0.68
1:V:439:LEU:HD23	1:V:509:ILE:HD12	1.72	0.68
2:W:2180:TRP:HB2	2:W:2243:LEU:HD13	1.75	0.68
3:a:3110[A]:THR:O	3:a:3112[A]:TYR:N	2.26	0.68
3:a:3176[A]:LYS:NZ	3:a:3176[A]:LYS:HB3	2.08	0.68
3:a:3279[A]:ASP:OD1	3:a:3279[A]:ASP:N	2.25	0.68
3:d:3287[A]:ILE:O	3:d:3287[A]:ILE:HD13	1.92	0.68
1:A:1304:ASP:OD1	1:A:1305:GLY:N	2.26	0.68
3:C:2979[A]:GLN:NE2	3:C:3155[A]:MET:HE2	2.09	0.68
3:C:3153[B]:LYS:HD3	3:L:2988[B]:TRP:HD1	1.56	0.68
3:C:3221[A]:ALA:HB2	3:C:3256[A]:TRP:H	1.56	0.68
3:F:2966[A]:SER:HB2	3:F:2977[A]:CYS:CB	2.21	0.68
3:F:2973[B]:THR:HG23	3:a:3248[B]:LEU:HD11	1.75	0.68
3:F:3230[A]:PHE:CB	3:F:3243[A]:GLY:N	2.56	0.68
1:G:355:ALA:HA	1:G:734:LEU:HD12	1.74	0.68
1:G:1296:VAL:HB	1:G:1446:ASP:HB3	1.75	0.68
2:H:2806:ALA:HB2	2:H:2856:ILE:HD11	1.75	0.68
3:I:3089[A]:HIS:ND1	3:I:3119[A]:HIS:CE1	2.61	0.68
3:I:3162[B]:ASP:C	3:R:3150[B]:LYS:HZ1	2.00	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2794:LEU:HD12	2:K:2797:LYS:HD2	1.75	0.68
3:L:3089[A]:HIS:ND1	3:L:3119[A]:HIS:CE1	2.61	0.68
3:L:3176[B]:LYS:NZ	3:L:3176[B]:LYS:HB3	2.08	0.68
3:L:3194[A]:GLY:C	3:L:3195[A]:MET:HG2	2.16	0.68
3:O:2933[B]:SER:C	3:O:2935[B]:ILE:HD13	2.17	0.68
3:O:3110[B]:THR:O	3:O:3112[B]:TYR:N	2.26	0.68
1:S:164:GLU:OE1	1:S:296:ARG:NH1	2.22	0.68
1:S:871:GLN:NE2	1:S:964:ILE:O	2.26	0.68
1:S:1030:MET:HA	1:S:1036:SER:HA	1.75	0.68
3:U:2965[A]:LEU:CD1	3:U:2974[A]:ALA:HA	2.22	0.68
3:U:3153[B]:LYS:HG3	3:d:2979[B]:GLN:NE2	2.08	0.68
3:X:3194[A]:GLY:C	3:X:3195[A]:MET:HG2	2.16	0.68
1:Y:194:MET:HA	1:Y:200:THR:HA	1.75	0.68
3:a:3176[B]:LYS:HB3	3:a:3176[B]:LYS:NZ	2.08	0.68
3:a:3284[A]:LYS:HA	3:a:3284[A]:LYS:CE	2.22	0.68
3:d:2942[B]:LEU:HD13	3:d:3033[B]:PHE:CE1	2.28	0.68
3:d:3284[B]:LYS:HA	3:d:3284[B]:LYS:CE	2.22	0.68
1:A:912:ASN:HD21	1:A:1091:ASN:HD21	1.41	0.68
3:C:3089[B]:HIS:ND1	3:C:3119[B]:HIS:CE1	2.61	0.68
3:C:3253[B]:GLU:HB2	3:L:2975[B]:PHE:CA	2.23	0.68
3:F:2966[B]:SER:CB	3:a:3254[B]:MET:CB	2.71	0.68
2:H:2695:MET:HE1	2:H:2707:PHE:HB2	1.74	0.68
3:I:2961[B]:HIS:CE1	3:I:2980[B]:HIS:NE2	2.57	0.68
3:I:3077[A]:ASP:HB2	3:I:3080[A]:ASP:OD2	1.93	0.68
3:I:3110[B]:THR:HG21	3:R:2971[B]:ASP:OD2	1.93	0.68
3:L:2966[A]:SER:HB2	3:L:2977[A]:CYS:CB	2.21	0.68
3:L:2969[A]:TYR:HD2	3:L:2971[A]:ASP:N	1.84	0.68
3:L:3173[A]:THR:CG2	3:L:3174[A]:GLY:N	2.55	0.68
3:O:3194[A]:GLY:C	3:O:3195[A]:MET:HG2	2.16	0.68
1:P:46:ASP:OD2	1:P:249:ARG:NH2	2.26	0.68
3:R:2979[B]:GLN:HE21	3:R:3155[B]:MET:HE2	1.54	0.68
3:R:3176[A]:LYS:NZ	3:R:3176[A]:LYS:HB3	2.08	0.68
3:U:2960[A]:PHE:HD1	3:U:2960[A]:PHE:H	1.41	0.68
3:U:3089[A]:HIS:ND1	3:U:3119[A]:HIS:CE1	2.61	0.68
3:U:3230[A]:PHE:CB	3:U:3243[A]:GLY:N	2.56	0.68
3:X:3173[B]:THR:CG2	3:X:3174[B]:GLY:N	2.55	0.68
3:a:3089[A]:HIS:ND1	3:a:3119[A]:HIS:CE1	2.61	0.68
3:a:3089[B]:HIS:ND1	3:a:3119[B]:HIS:CE1	2.61	0.68
3:d:2979[B]:GLN:NE2	3:d:3155[B]:MET:HE2	2.09	0.68
3:d:3110[A]:THR:O	3:d:3112[A]:TYR:N	2.26	0.68
1:A:460:GLU:HB3	1:A:465:PRO:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:ASN:HB3	1:A:832:LYS:N	2.09	0.68
2:B:2573:TYR:HE2	2:B:2707:PHE:HE2	1.42	0.68
3:C:3150[B]:LYS:NZ	3:L:3160[B]:SER:CA	2.51	0.68
3:F:2937[B]:ASN:CB	3:F:3006[B]:LYS:HD3	2.23	0.68
2:H:2191:LEU:O	2:H:2225:ARG:NH2	2.25	0.68
3:I:2930[A]:LEU:HD22	3:I:2930[A]:LEU:N	2.02	0.68
3:I:2975[B]:PHE:CZ	3:R:2961[B]:HIS:ND1	2.62	0.68
2:K:2648:ALA:HA	2:K:2654:SER:HB2	1.75	0.68
3:L:2930[A]:LEU:H	3:L:2930[A]:LEU:CD2	1.98	0.68
3:L:3194[B]:GLY:C	3:L:3195[B]:MET:HG2	2.16	0.68
2:N:2344:LEU:HB3	2:Q:2515:ARG:HB3	1.74	0.68
3:O:2930[B]:LEU:HD22	3:O:2930[B]:LEU:N	2.02	0.68
3:O:3110[A]:THR:O	3:O:3112[A]:TYR:N	2.26	0.68
3:O:3169[A]:LYS:C	3:O:3172[A]:SER:HG	1.98	0.68
1:P:1414:THR:HG23	1:P:1477:LEU:HD13	1.76	0.68
3:R:3077[A]:ASP:CB	3:R:3080[A]:ASP:OD2	2.42	0.68
2:T:2890:VAL:N	2:T:2891:LEU:HA	2.08	0.68
3:U:2960[B]:PHE:H	3:U:2960[B]:PHE:HD1	1.41	0.68
3:X:2937[A]:ASN:CB	3:X:3006[A]:LYS:HD3	2.23	0.68
3:X:3110[A]:THR:O	3:X:3112[A]:TYR:N	2.26	0.68
3:a:2942[A]:LEU:HD13	3:a:3033[A]:PHE:CE1	2.28	0.68
3:a:2942[B]:LEU:HD13	3:a:3033[B]:PHE:CE1	2.28	0.68
3:a:3194[A]:GLY:C	3:a:3195[A]:MET:HG2	2.17	0.68
1:b:28:ASP:OD2	1:b:83:HIS:NE2	2.22	0.68
1:b:964:ILE:HG12	1:b:971:THR:HG22	1.76	0.68
2:c:2711:HIS:HA	2:c:2714:VAL:HG22	1.76	0.68
3:d:2961[B]:HIS:CE1	3:d:2980[B]:HIS:NE2	2.57	0.68
3:C:2972[B]:GLY:HA2	3:L:3086[B]:GLU:CG	2.24	0.68
3:C:3077[A]:ASP:CB	3:C:3080[A]:ASP:OD2	2.42	0.68
3:C:3230[B]:PHE:CB	3:C:3243[B]:GLY:N	2.56	0.68
3:F:3161[B]:GLU:HG2	3:a:3079[B]:CYS:CB	2.22	0.68
3:I:3089[B]:HIS:CD2	3:R:2971[B]:ASP:C	2.70	0.68
3:I:3150[B]:LYS:HZ1	3:R:3162[B]:ASP:C	2.01	0.68
3:I:3221[A]:ALA:HB2	3:I:3256[A]:TRP:H	1.57	0.68
3:L:3077[A]:ASP:HB2	3:L:3080[A]:ASP:OD2	1.93	0.68
3:L:3176[A]:LYS:C	3:L:3177[A]:SER:HG	1.98	0.68
1:M:622:HIS:CE1	1:M:767:LYS:H	2.12	0.68
2:N:2900:SER:HA	1:P:1075:GLU:HG2	1.74	0.68
3:O:2937[A]:ASN:HB2	3:O:3006[A]:LYS:CE	2.14	0.68
3:O:3108[B]:HIS:HB2	3:X:2970[B]:PRO:HA	1.75	0.68
3:O:3220[B]:ARG:HG2	3:O:3221[B]:ALA:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2966[B]:SER:HB2	3:R:2977[B]:CYS:CB	2.21	0.68
2:W:2267:HIS:HD2	2:W:2297:HIS:HE1	1.42	0.68
3:X:3031[B]:ASN:OD1	3:X:3033[B]:PHE:N	2.27	0.68
3:X:3284[B]:LYS:HA	3:X:3284[B]:LYS:CE	2.22	0.68
1:Y:1414:THR:HG23	1:Y:1477:LEU:HD13	1.74	0.68
3:a:2930[B]:LEU:H	3:a:2930[B]:LEU:CD2	1.98	0.68
3:a:2952[B]:ALA:H	3:a:2953[B]:GLY:CA	2.04	0.68
3:d:3077[B]:ASP:CB	3:d:3080[B]:ASP:OD2	2.42	0.68
3:d:3110[B]:THR:O	3:d:3112[B]:TYR:N	2.26	0.68
3:d:3176[A]:LYS:HB3	3:d:3176[A]:LYS:HZ2	1.59	0.68
3:d:3279[A]:ASP:OD1	3:d:3279[A]:ASP:N	2.25	0.68
3:C:2937[B]:ASN:CB	3:C:3006[B]:LYS:HD3	2.23	0.68
3:C:3031[B]:ASN:OD1	3:C:3033[B]:PHE:N	2.26	0.68
3:C:3150[B]:LYS:C	3:L:3159[B]:SER:OG	2.37	0.68
3:C:3220[B]:ARG:HG2	3:C:3221[B]:ALA:N	2.09	0.68
3:L:2937[B]:ASN:CB	3:L:3006[B]:LYS:HD3	2.23	0.68
3:L:2948[B]:ASP:CB	3:L:2949[B]:LYS:HA	2.16	0.68
3:L:3089[B]:HIS:ND1	3:L:3119[B]:HIS:CE1	2.61	0.68
3:L:3230[A]:PHE:CB	3:L:3243[A]:GLY:N	2.56	0.68
3:O:2960[B]:PHE:HD1	3:O:2960[B]:PHE:H	1.41	0.68
3:O:2968[B]:GLN:HG2	3:X:2984[B]:THR:HB	1.75	0.68
3:O:2970[B]:PRO:CG	3:X:2991[B]:LEU:HA	1.99	0.68
3:O:3163[B]:ASN:HB3	3:X:3149[B]:ASN:CA	1.99	0.68
3:O:3220[B]:ARG:HG3	3:O:3220[B]:ARG:NH1	1.98	0.68
3:U:3176[B]:LYS:HD3	3:d:3152[B]:LYS:HD2	1.74	0.68
3:U:3230[B]:PHE:CB	3:U:3243[B]:GLY:N	2.56	0.68
3:U:3284[A]:LYS:HA	3:U:3284[A]:LYS:CE	2.22	0.68
3:U:3307[A]:PHE:CE1	3:U:3309[A]:PRO:HG3	2.16	0.68
1:V:1304:ASP:N	1:V:1305:GLY:HA2	2.08	0.68
3:X:2960[B]:PHE:H	3:X:2960[B]:PHE:HD1	1.41	0.68
3:X:3031[A]:ASN:OD1	3:X:3033[A]:PHE:N	2.26	0.68
3:X:3176[B]:LYS:NZ	3:X:3176[B]:LYS:HB3	2.08	0.68
2:Z:2722:GLN:NE2	2:Z:2769:PHE:O	2.24	0.68
3:a:3110[B]:THR:O	3:a:3112[B]:TYR:N	2.26	0.68
3:d:2937[A]:ASN:CB	3:d:3006[A]:LYS:HD3	2.23	0.68
3:d:3089[A]:HIS:ND1	3:d:3119[A]:HIS:CE1	2.61	0.68
3:C:2971[B]:ASP:CG	3:C:2973[B]:THR:OG1	2.37	0.68
3:C:3077[B]:ASP:HB2	3:C:3080[B]:ASP:OD2	1.93	0.68
3:F:2937[A]:ASN:CB	3:F:3006[A]:LYS:HD3	2.23	0.68
3:F:2979[B]:GLN:NE2	3:F:3155[B]:MET:HE2	2.09	0.68
3:F:3089[B]:HIS:ND1	3:F:3119[B]:HIS:CE1	2.61	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3160[B]:SER:O	3:a:3150[B]:LYS:HD2	1.71	0.68
3:F:3173[B]:THR:CG2	3:a:3173[B]:THR:OG1	2.42	0.68
3:I:2983[B]:VAL:CB	3:R:3160[B]:SER:CA	2.70	0.68
3:I:3077[A]:ASP:CB	3:I:3080[A]:ASP:OD2	2.42	0.68
3:I:3107[B]:LEU:CG	3:R:2975[B]:PHE:HD1	2.06	0.68
3:I:3133[B]:LEU:O	3:I:3134[B]:GLN:C	2.32	0.68
2:K:2824:CYS:HA	2:K:2829:CYS:HA	1.75	0.68
3:L:2960[A]:PHE:H	3:L:2960[A]:PHE:HD1	1.41	0.68
3:L:2960[B]:PHE:HD1	3:L:2960[B]:PHE:H	1.41	0.68
3:L:3110[A]:THR:O	3:L:3112[A]:TYR:N	2.26	0.68
2:N:2149:ALA:HA	2:N:2260:GLU:HG2	1.75	0.68
3:O:2968[B]:GLN:HA	3:X:2988[B]:TRP:HD1	1.58	0.68
3:O:2971[A]:ASP:CG	3:O:2973[A]:THR:OG1	2.37	0.68
3:O:3024[A]:LEU:CD1	3:O:3025[A]:VAL:H	1.83	0.68
3:O:3077[B]:ASP:CB	3:O:3080[B]:ASP:OD2	2.42	0.68
3:O:3089[B]:HIS:ND1	3:O:3119[B]:HIS:CE1	2.61	0.68
2:Q:2172:ILE:HG13	2:Q:2173:VAL:HG13	1.74	0.68
2:Q:2903:TYR:OH	3:R:2932[A]:PRO:HD2	1.94	0.68
3:R:2937[A]:ASN:CB	3:R:3006[A]:LYS:HD3	2.23	0.68
3:R:2952[B]:ALA:H	3:R:2953[B]:GLY:CA	2.04	0.68
3:R:3077[B]:ASP:CB	3:R:3080[B]:ASP:OD2	2.42	0.68
3:U:3110[A]:THR:O	3:U:3112[A]:TYR:N	2.26	0.68
3:U:3220[A]:ARG:HG2	3:U:3221[A]:ALA:N	2.09	0.68
2:W:2235:PRO:HG3	2:W:2240:GLN:HE22	1.58	0.68
3:X:3089[A]:HIS:ND1	3:X:3119[A]:HIS:CE1	2.61	0.68
3:X:3298[A]:ASN:HA	3:X:3299[A]:LEU:HB2	1.76	0.68
1:Y:1656:ASP:C	3:d:3006[B]:LYS:HD2	2.19	0.68
3:a:3077[A]:ASP:HB2	3:a:3080[A]:ASP:OD2	1.93	0.68
3:a:3220[A]:ARG:HG2	3:a:3221[A]:ALA:N	2.09	0.68
3:d:3031[A]:ASN:OD1	3:d:3033[A]:PHE:N	2.26	0.68
3:d:3298[A]:ASN:HA	3:d:3299[A]:LEU:HB2	1.76	0.68
1:A:1140:ASN:ND2	1:A:1236:TYR:OH	2.27	0.68
2:B:2226:GLU:OE2	2:B:2277:LYS:N	2.27	0.68
3:C:3110[B]:THR:O	3:C:3112[B]:TYR:N	2.26	0.68
3:C:3153[B]:LYS:O	3:L:3155[B]:MET:N	2.27	0.68
3:C:3298[B]:ASN:HA	3:C:3299[B]:LEU:HB2	1.76	0.68
3:F:2979[A]:GLN:NE2	3:F:3155[A]:MET:HE2	2.09	0.68
3:F:3077[A]:ASP:CB	3:F:3080[A]:ASP:OD2	2.42	0.68
3:F:3153[B]:LYS:HD3	3:a:2988[B]:TRP:HD1	1.58	0.68
3:F:3253[B]:GLU:CA	3:a:3252[B]:TYR:O	2.42	0.68
3:F:3298[B]:ASN:HA	3:F:3299[B]:LEU:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:474:LEU:H	1:G:474:LEU:HD13	1.59	0.68
3:I:3110[B]:THR:O	3:I:3112[B]:TYR:N	2.26	0.68
3:I:3221[B]:ALA:CB	3:R:2965[B]:LEU:H	1.77	0.68
3:I:3288[A]:MET:HA	3:I:3295[A]:LEU:HG	1.76	0.68
1:M:1078:ARG:NH2	2:Q:2875:SER:O	2.26	0.68
1:M:1357:ARG:HH11	1:M:1357:ARG:HB3	1.59	0.68
2:N:2476:LEU:HG	2:N:2480:LEU:HG	1.76	0.68
3:O:3025[B]:VAL:HG22	3:O:3047[B]:ARG:NH1	2.01	0.68
3:O:3185[B]:TYR:C	3:O:3186[B]:GLU:OE2	2.37	0.68
3:O:3298[B]:ASN:HA	3:O:3299[B]:LEU:HB2	1.76	0.68
2:Q:2680:HIS:HD1	2:Q:2714:VAL:HG11	1.57	0.68
1:S:1617:LYS:HE2	3:X:3135[B]:LYS:HZ3	1.59	0.68
3:U:2965[B]:LEU:CG	3:d:3220[B]:ARG:HH11	2.04	0.68
3:U:3031[A]:ASN:OD1	3:U:3033[A]:PHE:N	2.26	0.68
3:U:3077[B]:ASP:CB	3:U:3080[B]:ASP:OD2	2.42	0.68
3:U:3256[B]:TRP:HB3	3:d:2969[B]:TYR:HB2	1.62	0.68
3:X:3133[A]:LEU:O	3:X:3134[A]:GLN:C	2.32	0.68
1:Y:1620:LEU:HD12	3:d:3189[B]:ASN:CB	2.21	0.68
3:a:3077[B]:ASP:CB	3:a:3080[B]:ASP:OD2	2.42	0.68
3:a:3284[B]:LYS:HA	3:a:3284[B]:LYS:CE	2.21	0.68
1:b:11:THR:HG22	1:b:13:ASP:H	1.58	0.68
3:d:2986[A]:PRO:HB2	3:d:3127[A]:TRP:CZ3	2.29	0.68
3:d:3230[B]:PHE:CB	3:d:3243[B]:GLY:N	2.56	0.68
3:C:2937[A]:ASN:CB	3:C:3006[A]:LYS:HD3	2.23	0.68
3:C:3288[A]:MET:HA	3:C:3295[A]:LEU:HG	1.76	0.68
3:F:2965[B]:LEU:CB	3:a:3256[B]:TRP:HE1	2.05	0.68
3:F:3173[B]:THR:CG2	3:F:3174[B]:GLY:N	2.55	0.68
3:F:3249[B]:GLY:N	3:a:2974[B]:ALA:H	1.92	0.68
3:F:3288[A]:MET:HA	3:F:3295[A]:LEU:HG	1.76	0.68
3:L:2942[B]:LEU:HD13	3:L:3033[B]:PHE:CE1	2.28	0.68
3:L:3031[B]:ASN:OD1	3:L:3033[B]:PHE:N	2.26	0.68
2:N:2597:MET:HE2	2:N:2598:PRO:HD2	1.74	0.68
3:O:3288[A]:MET:HA	3:O:3295[A]:LEU:HG	1.76	0.68
1:P:883:CYS:N	1:P:894:CYS:SG	2.67	0.68
3:R:2960[B]:PHE:H	3:R:2960[B]:PHE:HD1	1.41	0.68
3:R:3031[B]:ASN:OD1	3:R:3033[B]:PHE:N	2.26	0.68
3:U:2966[A]:SER:HB2	3:U:2977[A]:CYS:CB	2.21	0.68
3:U:2973[B]:THR:CG2	3:d:3222[B]:ILE:CG2	2.65	0.68
3:U:2986[B]:PRO:HB2	3:U:3127[B]:TRP:CZ3	2.29	0.68
3:X:2986[B]:PRO:HB2	3:X:3127[B]:TRP:CZ3	2.29	0.68
3:X:3220[B]:ARG:HG2	3:X:3221[B]:ALA:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3298[B]:ASN:HA	3:X:3299[B]:LEU:HB2	1.76	0.68
1:Y:418:ASP:OD1	1:Y:418:ASP:N	2.26	0.68
2:Z:2236:ALA:HB3	2:Z:2239:LYS:HB2	1.76	0.68
3:a:2930[A]:LEU:HD22	3:a:2930[A]:LEU:N	2.02	0.68
3:d:3230[A]:PHE:CB	3:d:3243[A]:GLY:N	2.56	0.68
3:d:3288[A]:MET:HA	3:d:3295[A]:LEU:HG	1.76	0.68
1:A:449:ASP:OD2	1:A:1280:GLN:NE2	2.28	0.67
1:A:1189:ASP:HA	2:E:2809:LEU:HD12	1.76	0.67
3:C:2979[B]:GLN:NE2	3:C:3155[B]:MET:HE2	2.09	0.67
3:C:2986[A]:PRO:HB2	3:C:3127[A]:TRP:CZ3	2.30	0.67
3:C:3176[B]:LYS:HB3	3:C:3176[B]:LYS:NZ	2.08	0.67
3:C:3288[B]:MET:HA	3:C:3295[B]:LEU:HG	1.76	0.67
3:F:2961[B]:HIS:CG	3:a:2975[B]:PHE:HZ	2.10	0.67
3:F:3154[B]:PRO:HB3	3:a:3174[B]:GLY:H	1.52	0.67
3:F:3156[B]:MET:SD	3:a:2982[B]:MET:HG3	2.34	0.67
3:F:3176[B]:LYS:NZ	3:F:3176[B]:LYS:HB3	2.08	0.67
3:F:3298[A]:ASN:HA	3:F:3299[A]:LEU:HB2	1.76	0.67
3:I:2971[B]:ASP:CG	3:I:2973[B]:THR:OG1	2.37	0.67
3:I:3152[B]:LYS:CB	3:R:3171[B]:HIS:N	2.53	0.67
3:O:2965[B]:LEU:CG	3:X:2979[B]:GLN:OE1	2.43	0.67
3:O:2986[A]:PRO:HB2	3:O:3127[A]:TRP:CZ3	2.30	0.67
3:O:3176[A]:LYS:HZ2	3:O:3176[A]:LYS:HB3	1.56	0.67
3:O:3298[B]:ASN:HB2	3:O:3299[B]:LEU:C	2.20	0.67
1:P:556:GLY:H	1:P:558:HIS:CE1	2.12	0.67
2:Q:2870:LEU:HA	2:Q:2877:ILE:HD11	1.76	0.67
3:U:2942[B]:LEU:HD13	3:U:3033[B]:PHE:CE1	2.28	0.67
3:U:3185[A]:TYR:C	3:U:3186[A]:GLU:OE2	2.37	0.67
1:V:804:ASP:OD1	1:V:805:VAL:N	2.27	0.67
2:W:2650:GLY:N	2:W:2651:GLN:HA	2.09	0.67
2:Z:2890:VAL:N	2:Z:2891:LEU:HA	2.08	0.67
3:a:3031[A]:ASN:OD1	3:a:3033[A]:PHE:N	2.27	0.67
2:c:2889:ALA:N	2:c:2890:VAL:HA	2.08	0.67
3:d:3176[A]:LYS:HB3	3:d:3176[A]:LYS:NZ	2.08	0.67
3:d:3298[B]:ASN:HA	3:d:3299[B]:LEU:HB2	1.76	0.67
1:A:566:ARG:HH12	1:A:743:ASN:HB3	1.58	0.67
3:C:3025[A]:VAL:HG22	3:C:3047[A]:ARG:NH1	2.02	0.67
3:C:3147[B]:GLU:HB2	3:C:3149[B]:ASN:ND2	2.09	0.67
3:C:3153[B]:LYS:HE2	3:L:3158[B]:PHE:CG	2.25	0.67
3:C:3253[B]:GLU:CA	3:L:3253[B]:GLU:HA	2.24	0.67
1:D:238:ASN:OD1	1:D:238:ASN:N	2.20	0.67
1:D:566:ARG:NH1	1:D:759:SER:OG	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2124:SER:HB2	2:E:2129:PRO:HG2	1.75	0.67
3:F:2971[A]:ASP:CG	3:F:2973[A]:THR:OG1	2.37	0.67
3:F:3149[B]:ASN:CG	3:a:3163[B]:ASN:HD22	1.98	0.67
3:F:3255[B]:PRO:C	3:a:2966[B]:SER:CA	2.67	0.67
3:I:2977[B]:CYS:HB3	3:R:2982[B]:MET:HE3	1.75	0.67
3:L:2986[B]:PRO:HB2	3:L:3127[B]:TRP:CZ3	2.29	0.67
3:O:2971[B]:ASP:CG	3:O:2973[B]:THR:OG1	2.37	0.67
3:O:2986[B]:PRO:HB2	3:O:3127[B]:TRP:CZ3	2.29	0.67
3:O:3256[B]:TRP:NE1	3:X:3161[B]:GLU:CD	2.52	0.67
3:R:3110[A]:THR:O	3:R:3112[A]:TYR:N	2.26	0.67
3:U:2970[B]:PRO:N	3:d:3086[B]:GLU:OE1	2.27	0.67
3:U:2974[B]:ALA:CB	3:d:3220[B]:ARG:HG2	2.22	0.67
3:U:2979[B]:GLN:NE2	3:U:3155[B]:MET:HE2	2.09	0.67
3:U:3298[A]:ASN:HB2	3:U:3299[A]:LEU:C	2.19	0.67
3:X:3011[A]:TYR:HB3	3:X:3121[A]:SER:HB2	1.77	0.67
3:X:3288[B]:MET:HA	3:X:3295[B]:LEU:HG	1.77	0.67
2:Z:2687:ILE:HD11	2:Z:2695:MET:HG2	1.75	0.67
3:a:2937[A]:ASN:CB	3:a:3006[A]:LYS:HD3	2.23	0.67
3:a:3288[B]:MET:HA	3:a:3295[B]:LEU:HG	1.76	0.67
3:d:2965[A]:LEU:CD1	3:d:2974[A]:ALA:HA	2.22	0.67
3:d:2971[A]:ASP:CG	3:d:2973[A]:THR:OG1	2.37	0.67
3:C:2971[A]:ASP:CG	3:C:2973[A]:THR:OG1	2.37	0.67
3:C:3031[A]:ASN:OD1	3:C:3033[A]:PHE:N	2.26	0.67
3:C:3077[B]:ASP:CB	3:C:3080[B]:ASP:OD2	2.42	0.67
3:C:3176[A]:LYS:HZ2	3:C:3176[A]:LYS:HB3	1.59	0.67
3:C:3185[B]:TYR:C	3:C:3186[B]:GLU:OE2	2.37	0.67
3:C:3254[B]:MET:O	3:L:2977[B]:CYS:N	2.03	0.67
3:F:2986[A]:PRO:HB2	3:F:3127[A]:TRP:CZ3	2.30	0.67
1:G:492:ARG:HD2	1:G:692:VAL:HG13	1.76	0.67
1:G:1140:ASN:ND2	1:G:1236:TYR:OH	2.28	0.67
2:H:2542:TYR:HA	2:H:2547:MET:HE1	1.75	0.67
3:I:3077[B]:ASP:CB	3:I:3080[B]:ASP:OD2	2.42	0.67
3:I:3150[B]:LYS:CB	3:R:3169[B]:LYS:HG3	2.22	0.67
3:I:3150[B]:LYS:CG	3:R:3158[B]:PHE:CA	2.40	0.67
3:I:3220[B]:ARG:HG2	3:I:3221[B]:ALA:N	2.08	0.67
3:I:3255[B]:PRO:HG2	3:R:2964[B]:PRO:HD2	1.74	0.67
3:L:2971[A]:ASP:CG	3:L:2973[A]:THR:OG1	2.37	0.67
3:O:2961[A]:HIS:CE1	3:O:2980[A]:HIS:NE2	2.57	0.67
3:O:3254[B]:MET:CB	3:X:3159[B]:SER:OG	2.40	0.67
3:R:2971[A]:ASP:CG	3:R:2973[A]:THR:OG1	2.37	0.67
3:R:2971[B]:ASP:CG	3:R:2973[B]:THR:OG1	2.37	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2979[A]:GLN:NE2	3:R:3155[A]:MET:HE2	2.09	0.67
3:R:3176[B]:LYS:NZ	3:R:3176[B]:LYS:HB3	2.08	0.67
3:R:3298[B]:ASN:HB2	3:R:3299[B]:LEU:C	2.20	0.67
3:U:2969[A]:TYR:HD2	3:U:2971[A]:ASP:N	1.85	0.67
3:U:3197[B]:ILE:HD12	1:V:1617:LYS:O	1.94	0.67
3:U:3255[B]:PRO:HB2	3:d:2975[B]:PHE:CA	2.21	0.67
3:U:3279[B]:ASP:OD1	3:U:3279[B]:ASP:N	2.25	0.67
3:X:2971[A]:ASP:CG	3:X:2973[A]:THR:OG1	2.37	0.67
2:Z:2457:LYS:O	2:Z:2460:SER:OG	2.12	0.67
3:a:3298[A]:ASN:HB2	3:a:3299[A]:LEU:C	2.19	0.67
3:d:2986[B]:PRO:HB2	3:d:3127[B]:TRP:CZ3	2.30	0.67
3:d:3023[B]:ILE:HA	3:d:3026[B]:THR:OG1	1.95	0.67
2:B:2554:PRO:HB3	2:B:2556:TYR:HB2	1.75	0.67
3:C:2982[B]:MET:HB2	3:L:3156[B]:MET:CG	2.23	0.67
3:C:3160[B]:SER:CA	3:L:2983[B]:VAL:HG21	2.13	0.67
3:F:2986[B]:PRO:HB2	3:F:3127[B]:TRP:CZ3	2.30	0.67
3:F:3089[A]:HIS:ND1	3:F:3119[A]:HIS:CE1	2.61	0.67
3:F:3220[A]:ARG:HG2	3:F:3221[A]:ALA:N	2.09	0.67
3:F:3255[B]:PRO:HA	3:a:2965[B]:LEU:CA	2.18	0.67
3:F:3298[B]:ASN:HB2	3:F:3299[B]:LEU:C	2.20	0.67
3:I:3185[A]:TYR:C	3:I:3186[A]:GLU:OE2	2.37	0.67
3:I:3255[B]:PRO:HB3	3:R:2964[B]:PRO:CA	2.20	0.67
3:I:3288[B]:MET:HA	3:I:3295[B]:LEU:HG	1.77	0.67
2:K:2690:HIS:ND1	2:K:2886:VAL:O	2.23	0.67
3:L:2961[A]:HIS:HB3	3:L:3111[A]:SER:HG	1.58	0.67
3:L:2979[A]:GLN:NE2	3:L:3155[A]:MET:HE2	2.09	0.67
3:L:3011[B]:TYR:HB3	3:L:3121[B]:SER:HB2	1.77	0.67
3:L:3137[B]:ARG:CB	3:L:3139[B]:LEU:HD23	2.25	0.67
3:O:2971[B]:ASP:OD1	3:X:3158[B]:PHE:HZ	1.78	0.67
3:O:3176[A]:LYS:HB3	3:O:3176[A]:LYS:NZ	2.08	0.67
1:P:567:LEU:H	1:P:571:PRO:HB3	1.59	0.67
1:P:588:GLU:HG3	1:P:724:LYS:HD2	1.76	0.67
3:R:3011[A]:TYR:HB3	3:R:3121[A]:SER:HB2	1.76	0.67
3:R:3288[B]:MET:HA	3:R:3295[B]:LEU:HG	1.76	0.67
3:U:2979[A]:GLN:NE2	3:U:3155[A]:MET:HE2	2.09	0.67
3:U:3169[B]:LYS:HE3	3:d:3147[B]:GLU:CA	2.21	0.67
3:U:3170[B]:ALA:C	3:d:3148[B]:ILE:HG22	2.18	0.67
3:a:2979[B]:GLN:NE2	3:a:3155[B]:MET:HE2	2.09	0.67
1:b:804:ASP:OD1	1:b:805:VAL:N	2.28	0.67
1:b:871:GLN:NE2	1:b:964:ILE:O	2.28	0.67
1:b:883:CYS:N	1:b:894:CYS:SG	2.66	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3031[B]:ASN:OD1	3:d:3033[B]:PHE:N	2.27	0.67
2:B:2252:GLU:HG2	2:B:2385:ILE:HG23	1.75	0.67
3:C:2961[B]:HIS:HB2	3:C:2992[B]:TYR:CE2	2.30	0.67
3:C:3023[B]:ILE:HA	3:C:3026[B]:THR:OG1	1.95	0.67
2:E:2340:ALA:HB1	2:E:2341:PRO:HD2	1.77	0.67
3:F:2962[B]:GLY:O	3:a:3255[B]:PRO:HG3	1.94	0.67
3:F:2982[B]:MET:HE1	3:a:2977[B]:CYS:HB2	1.75	0.67
3:F:3252[B]:TYR:HA	3:a:3108[B]:HIS:CD2	2.29	0.67
1:G:534:ASP:HB2	1:G:541:LYS:HE2	1.76	0.67
1:G:930:ASP:OD1	1:G:1051:ARG:NH2	2.27	0.67
3:I:3023[B]:ILE:HA	3:I:3026[B]:THR:OG1	1.95	0.67
3:I:3176[B]:LYS:HB3	3:I:3176[B]:LYS:NZ	2.08	0.67
3:I:3298[B]:ASN:HA	3:I:3299[B]:LEU:HB2	1.76	0.67
3:L:3011[A]:TYR:HB3	3:L:3121[A]:SER:HB2	1.76	0.67
3:L:3023[B]:ILE:HA	3:L:3026[B]:THR:OG1	1.95	0.67
3:L:3185[B]:TYR:C	3:L:3186[B]:GLU:OE2	2.37	0.67
1:M:864:ASP:HB3	1:M:869:GLY:HA3	1.76	0.67
2:N:2370:MET:HE1	2:Q:2094:ARG:HD3	1.77	0.67
3:O:2969[B]:TYR:HD2	3:X:2988[B]:TRP:O	1.78	0.67
3:O:3293[B]:LYS:HB2	3:O:3294[B]:SER:HB2	0.82	0.67
1:S:533:VAL:HG12	1:S:540:THR:HG22	1.76	0.67
3:U:2961[B]:HIS:CE1	3:U:2980[B]:HIS:NE2	2.57	0.67
3:U:3089[B]:HIS:ND1	3:U:3119[B]:HIS:CE1	2.61	0.67
3:X:2971[B]:ASP:CG	3:X:2973[B]:THR:OG1	2.37	0.67
3:a:2986[A]:PRO:HB2	3:a:3127[A]:TRP:CZ3	2.30	0.67
3:a:3077[A]:ASP:CB	3:a:3080[A]:ASP:OD2	2.42	0.67
3:d:2960[A]:PHE:HD1	3:d:2960[A]:PHE:H	1.41	0.67
3:d:3137[B]:ARG:CB	3:d:3139[B]:LEU:HD23	2.25	0.67
3:C:2986[B]:PRO:HB2	3:C:3127[B]:TRP:CZ3	2.30	0.67
3:C:3089[A]:HIS:ND1	3:C:3119[A]:HIS:CE1	2.61	0.67
3:C:3153[B]:LYS:C	3:L:3173[B]:THR:CA	2.65	0.67
3:C:3176[A]:LYS:HB3	3:C:3176[A]:LYS:NZ	2.08	0.67
3:C:3220[A]:ARG:HG2	3:C:3221[A]:ALA:N	2.09	0.67
3:C:3252[B]:TYR:CZ	3:L:3223[B]:GLY:C	2.72	0.67
2:E:2303:ARG:NH2	2:E:2372:GLU:O	2.27	0.67
3:F:2980[B]:HIS:CB	3:a:2968[B]:GLN:HG2	2.22	0.67
3:F:3108[B]:HIS:CD2	3:a:3252[B]:TYR:H	2.08	0.67
3:F:3137[B]:ARG:CB	3:F:3139[B]:LEU:HD23	2.25	0.67
3:F:3230[B]:PHE:CB	3:F:3243[B]:GLY:N	2.56	0.67
3:I:2986[A]:PRO:HB2	3:I:3127[A]:TRP:CZ3	2.29	0.67
3:I:3031[B]:ASN:OD1	3:I:3033[B]:PHE:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3256[B]:TRP:CG	3:R:2966[B]:SER:C	2.60	0.67
1:J:479:CYS:HB3	1:J:670:PRO:HG3	1.76	0.67
2:K:2107:LEU:HD23	2:K:2208:PRO:HB2	1.76	0.67
2:K:2235:PRO:HG3	2:K:2240:GLN:HE22	1.58	0.67
3:L:2961[A]:HIS:HB2	3:L:2992[A]:TYR:CE2	2.30	0.67
3:L:3147[A]:GLU:HB2	3:L:3149[A]:ASN:ND2	2.09	0.67
1:M:46:ASP:OD2	1:M:249:ARG:NH2	2.28	0.67
2:N:2806:ALA:HB2	2:N:2856:ILE:HD11	1.77	0.67
3:O:2970[B]:PRO:C	3:X:2991[B]:LEU:N	2.52	0.67
3:O:2979[A]:GLN:NE2	3:O:3155[A]:MET:HE2	2.09	0.67
3:O:3031[B]:ASN:OD1	3:O:3033[B]:PHE:N	2.26	0.67
3:R:2961[A]:HIS:HB2	3:R:2992[A]:TYR:CE2	2.30	0.67
3:R:2984[B]:THR:HG22	3:R:3151[B]:LEU:HD23	1.77	0.67
3:R:2986[B]:PRO:HB2	3:R:3127[B]:TRP:CZ3	2.30	0.67
3:R:3220[B]:ARG:HG2	3:R:3221[B]:ALA:N	2.08	0.67
3:R:3279[B]:ASP:OD1	3:R:3279[B]:ASP:N	2.25	0.67
3:U:3023[A]:ILE:HA	3:U:3026[A]:THR:OG1	1.95	0.67
3:U:3077[A]:ASP:CB	3:U:3080[A]:ASP:OD2	2.42	0.67
3:X:2984[A]:THR:HG22	3:X:3151[A]:LEU:HD23	1.77	0.67
3:X:3077[A]:ASP:CB	3:X:3080[A]:ASP:OD2	2.42	0.67
3:X:3298[A]:ASN:HB2	3:X:3299[A]:LEU:C	2.20	0.67
3:a:2986[B]:PRO:HB2	3:a:3127[B]:TRP:CZ3	2.30	0.67
3:a:3147[A]:GLU:HB2	3:a:3149[A]:ASN:ND2	2.09	0.67
2:c:2107:LEU:HD23	2:c:2208:PRO:HB2	1.77	0.67
2:B:2877:ILE:H	1:D:1078:ARG:NH1	1.92	0.67
3:C:2960[A]:PHE:H	3:C:2960[A]:PHE:HD1	1.41	0.67
3:C:3011[B]:TYR:HB3	3:C:3121[B]:SER:HB2	1.77	0.67
3:C:3156[B]:MET:CG	3:L:2982[B]:MET:CG	2.73	0.67
3:C:3298[B]:ASN:HB2	3:C:3299[B]:LEU:C	2.20	0.67
1:D:1498:ASN:ND2	1:D:1500:THR:O	2.27	0.67
3:F:3011[B]:TYR:HB3	3:F:3121[B]:SER:HB2	1.77	0.67
3:F:3023[A]:ILE:HA	3:F:3026[A]:THR:OG1	1.95	0.67
3:F:3077[B]:ASP:CB	3:F:3080[B]:ASP:OD2	2.42	0.67
3:F:3137[A]:ARG:CB	3:F:3139[A]:LEU:HD23	2.25	0.67
3:I:2966[B]:SER:C	3:R:3256[B]:TRP:HB3	2.20	0.67
3:I:3176[A]:LYS:HB3	3:I:3176[A]:LYS:HZ2	1.59	0.67
1:J:245:GLU:OE2	1:J:249:ARG:NH1	2.27	0.67
3:L:2930[B]:LEU:HD22	3:L:2930[B]:LEU:N	2.02	0.67
3:L:2984[B]:THR:HG22	3:L:3151[B]:LEU:HD23	1.77	0.67
3:L:3023[A]:ILE:HA	3:L:3026[A]:THR:OG1	1.95	0.67
3:O:3077[A]:ASP:CB	3:O:3080[A]:ASP:OD2	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3137[B]:ARG:CB	3:O:3139[B]:LEU:HD23	2.25	0.67
3:O:3255[B]:PRO:HA	3:X:3161[B]:GLU:N	2.09	0.67
1:P:1304:ASP:N	1:P:1305:GLY:HA2	2.10	0.67
3:R:3023[A]:ILE:HA	3:R:3026[A]:THR:OG1	1.95	0.67
1:S:11:THR:HG22	1:S:13:ASP:H	1.58	0.67
3:U:3279[A]:ASP:OD1	3:U:3279[A]:ASP:N	2.25	0.67
3:X:3220[A]:ARG:HG2	3:X:3221[A]:ALA:N	2.08	0.67
1:Y:829:ALA:HA	1:Y:830:ASN:C	2.19	0.67
1:Y:1401:ARG:HD2	3:d:3182[B]:GLN:OE1	1.92	0.67
3:a:3211[B]:ASP:OD1	3:a:3211[B]:ASP:N	2.27	0.67
1:b:1033:LEU:HD21	1:b:1183:GLU:HB3	1.76	0.67
1:b:1301:PRO:HB3	1:b:1308:VAL:HG22	1.77	0.67
3:F:3147[A]:GLU:HB2	3:F:3149[A]:ASN:ND2	2.10	0.67
3:F:3169[B]:LYS:C	3:a:3152[B]:LYS:HG3	2.19	0.67
3:I:2960[A]:PHE:HD1	3:I:2960[A]:PHE:H	1.41	0.67
3:I:2988[A]:TRP:CE3	3:I:2989[A]:HIS:CE1	2.83	0.67
3:I:3149[B]:ASN:HD22	3:R:3163[B]:ASN:C	2.02	0.67
3:I:3255[B]:PRO:HB3	3:R:2964[B]:PRO:CD	2.24	0.67
3:I:3298[A]:ASN:HD21	3:I:3301[A]:PRO:HA	1.60	0.67
3:L:3169[A]:LYS:C	3:L:3172[A]:SER:HG	1.98	0.67
3:L:3220[A]:ARG:HG2	3:L:3221[A]:ALA:N	2.08	0.67
3:O:3147[B]:GLU:HB2	3:O:3149[B]:ASN:ND2	2.09	0.67
3:O:3169[B]:LYS:HZ1	3:X:3148[B]:ILE:HB	1.60	0.67
3:R:2960[A]:PHE:H	3:R:2960[A]:PHE:HD1	1.41	0.67
3:R:3147[B]:GLU:HB2	3:R:3149[B]:ASN:ND2	2.09	0.67
1:S:401:VAL:HG22	1:S:662:SER:HB3	1.76	0.67
3:U:3031[B]:ASN:OD1	3:U:3033[B]:PHE:N	2.26	0.67
3:U:3185[B]:TYR:C	3:U:3186[B]:GLU:OE2	2.37	0.67
3:U:3254[B]:MET:HE3	3:d:3254[B]:MET:CE	1.90	0.67
1:V:325:THR:OG1	1:V:329:ARG:O	2.07	0.67
3:X:2965[A]:LEU:CD1	3:X:2975[A]:PHE:H	2.08	0.67
3:X:2986[A]:PRO:HB2	3:X:3127[A]:TRP:CZ3	2.30	0.67
3:X:3298[B]:ASN:HB2	3:X:3299[B]:LEU:C	2.20	0.67
1:Y:863:ALA:O	1:Y:865:LYS:NZ	2.27	0.67
3:a:2956[B]:LYS:C	3:a:2960[B]:PHE:CE1	2.47	0.67
3:a:2969[A]:TYR:HD2	3:a:2971[A]:ASP:N	1.85	0.67
3:a:2971[A]:ASP:CG	3:a:2973[A]:THR:OG1	2.37	0.67
3:a:2971[B]:ASP:CG	3:a:2973[B]:THR:OG1	2.37	0.67
3:a:2988[B]:TRP:CE3	3:a:2989[B]:HIS:CE1	2.83	0.67
3:a:3137[B]:ARG:CB	3:a:3139[B]:LEU:HD23	2.25	0.67
3:d:3011[A]:TYR:HB3	3:d:3121[A]:SER:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3077[A]:ASP:CB	3:d:3080[A]:ASP:OD2	2.42	0.67
3:d:3220[B]:ARG:HG2	3:d:3221[B]:ALA:N	2.09	0.67
3:C:2930[A]:LEU:HD22	3:C:2930[A]:LEU:N	2.02	0.67
3:C:2966[A]:SER:HB2	3:C:2977[A]:CYS:CB	2.21	0.67
1:D:1520:GLN:HE21	1:D:1526:LYS:HG3	1.60	0.67
2:E:2525:LYS:HE2	2:E:2620:ILE:HG21	1.76	0.67
3:F:2969[A]:TYR:HD2	3:F:2971[A]:ASP:N	1.84	0.67
3:F:2969[B]:TYR:CE1	3:a:2961[B]:HIS:CG	2.80	0.67
3:F:2984[A]:THR:HG22	3:F:3151[A]:LEU:HD23	1.77	0.67
3:F:2988[B]:TRP:CH2	3:a:2975[B]:PHE:HE2	2.13	0.67
1:G:164:GLU:OE1	1:G:296:ARG:NH1	2.27	0.67
3:I:2979[B]:GLN:NE2	3:I:3155[B]:MET:HE2	2.09	0.67
3:I:3220[A]:ARG:HG2	3:I:3221[A]:ALA:N	2.09	0.67
3:I:3221[B]:ALA:HB2	3:R:2965[B]:LEU:N	2.05	0.67
3:L:2988[A]:TRP:CE3	3:L:2989[A]:HIS:CE1	2.83	0.67
3:L:3077[B]:ASP:CB	3:L:3080[B]:ASP:OD2	2.42	0.67
3:L:3284[B]:LYS:HA	3:L:3284[B]:LYS:CE	2.22	0.67
3:O:2930[A]:LEU:HD22	3:O:2930[A]:LEU:N	2.02	0.67
3:O:2988[B]:TRP:CE3	3:O:2989[B]:HIS:CE1	2.83	0.67
3:O:3137[A]:ARG:CB	3:O:3139[A]:LEU:HD23	2.25	0.67
3:O:3284[A]:LYS:HA	3:O:3284[A]:LYS:CE	2.22	0.67
3:R:2957[B]:ILE:CA	3:R:2960[B]:PHE:CE1	2.78	0.67
3:U:2975[B]:PHE:HE1	3:d:3253[B]:GLU:CD	2.02	0.67
3:U:2975[B]:PHE:HE1	3:d:3253[B]:GLU:CG	2.08	0.67
3:U:3011[A]:TYR:HB3	3:U:3121[A]:SER:HB2	1.77	0.67
3:U:3137[A]:ARG:CB	3:U:3139[A]:LEU:HD23	2.25	0.67
2:W:2569:TRP:CD1	2:W:2746:MET:HG2	2.29	0.67
2:W:2800:LYS:HB3	3:X:3023[A]:ILE:HD13	1.77	0.67
3:X:2960[A]:PHE:H	3:X:2960[A]:PHE:HD1	1.41	0.67
3:X:3011[B]:TYR:HB3	3:X:3121[B]:SER:HB2	1.77	0.67
3:X:3077[B]:ASP:CB	3:X:3080[B]:ASP:OD2	2.42	0.67
1:Y:1616:LYS:HZ2	3:d:3188[B]:ASP:HA	1.58	0.67
3:a:2960[B]:PHE:H	3:a:2960[B]:PHE:HD1	1.41	0.67
3:a:2984[A]:THR:HG22	3:a:3151[A]:LEU:HD23	1.77	0.67
3:d:2930[B]:LEU:HD22	3:d:2930[B]:LEU:N	2.02	0.67
3:d:3023[A]:ILE:HA	3:d:3026[A]:THR:OG1	1.95	0.67
3:d:3147[A]:GLU:HB2	3:d:3149[A]:ASN:ND2	2.09	0.67
2:B:2226:GLU:N	2:B:2226:GLU:OE1	2.28	0.67
3:C:2961[A]:HIS:HB2	3:C:2992[A]:TYR:CE2	2.30	0.67
3:F:2983[B]:VAL:H	3:a:3160[B]:SER:CB	2.07	0.67
3:F:3023[B]:ILE:HA	3:F:3026[B]:THR:OG1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3298[A]:ASN:HB2	3:F:3299[A]:LEU:C	2.19	0.67
1:G:240:PHE:HA	1:G:263:ALA:HB3	1.76	0.67
3:I:2961[A]:HIS:HB2	3:I:2992[A]:TYR:CE2	2.30	0.67
3:I:3011[B]:TYR:HB3	3:I:3121[B]:SER:HB2	1.77	0.67
3:I:3089[B]:HIS:ND1	3:I:3119[B]:HIS:CE1	2.61	0.67
3:I:3090[B]:ASN:CB	3:R:2972[B]:GLY:HA3	2.20	0.67
3:I:3147[A]:GLU:HB2	3:I:3149[A]:ASN:ND2	2.09	0.67
1:M:92:TRP:O	1:M:212:ASN:ND2	2.27	0.67
1:M:944:GLU:O	1:M:957:ASN:ND2	2.28	0.67
2:N:2565:THR:HA	2:N:2568:HIS:HD2	1.59	0.67
3:O:2961[B]:HIS:HB2	3:O:2992[B]:TYR:CE2	2.30	0.67
3:O:2963[B]:MET:CE	3:X:2975[B]:PHE:CE1	2.78	0.67
3:O:3011[B]:TYR:HB3	3:O:3121[B]:SER:HB2	1.77	0.67
3:O:3220[A]:ARG:HG2	3:O:3221[A]:ALA:N	2.09	0.67
3:O:3254[B]:MET:HG2	3:X:3159[B]:SER:OG	1.95	0.67
3:O:3298[A]:ASN:HA	3:O:3299[A]:LEU:HB2	1.76	0.67
3:R:2988[A]:TRP:CE3	3:R:2989[A]:HIS:CE1	2.83	0.67
3:R:2988[B]:TRP:CE3	3:R:2989[B]:HIS:CE1	2.83	0.67
2:T:2107:LEU:HA	2:T:2110:MET:HG2	1.77	0.67
3:U:2961[A]:HIS:HB2	3:U:2992[A]:TYR:CE2	2.30	0.67
3:U:2961[B]:HIS:HB2	3:U:2992[B]:TYR:CE2	2.30	0.67
3:U:2971[B]:ASP:O	3:d:3247[B]:VAL:C	2.38	0.67
3:U:2986[A]:PRO:HB2	3:U:3127[A]:TRP:CZ3	2.29	0.67
3:U:3025[B]:VAL:HG22	3:U:3047[B]:ARG:NH1	2.01	0.67
3:X:2984[B]:THR:HG22	3:X:3151[B]:LEU:HD23	1.77	0.67
3:X:3185[A]:TYR:C	3:X:3186[A]:GLU:OE2	2.37	0.67
3:a:3023[B]:ILE:HA	3:a:3026[B]:THR:OG1	1.95	0.67
3:a:3185[A]:TYR:C	3:a:3186[A]:GLU:OE2	2.38	0.67
3:a:3298[B]:ASN:CB	3:a:3300[B]:LEU:CD2	2.61	0.67
3:a:3298[B]:ASN:HB2	3:a:3299[B]:LEU:C	2.20	0.67
2:c:2800:LYS:HB3	3:d:3023[A]:ILE:HD13	1.77	0.67
3:d:3185[A]:TYR:C	3:d:3186[A]:GLU:OE2	2.37	0.67
3:d:3217[A]:PHE:HE1	3:d:3230[A]:PHE:HZ	0.80	0.67
6:r:1:NAG:H4	6:r:2:NAG:O7	1.94	0.67
1:D:1019:HIS:NE2	1:D:1046:HIS:CE1	2.63	0.66
2:E:2570:HIS:CD2	2:E:2711:HIS:HE1	2.13	0.66
2:E:2711:HIS:HA	2:E:2714:VAL:HG22	1.77	0.66
3:F:2961[B]:HIS:HB2	3:F:2992[B]:TYR:CE2	2.30	0.66
3:F:2988[B]:TRP:CE3	3:F:2989[B]:HIS:CE1	2.83	0.66
3:I:2960[B]:PHE:H	3:I:2960[B]:PHE:HD1	1.41	0.66
3:I:2970[B]:PRO:HA	3:R:2985[B]:PHE:HZ	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2984[A]:THR:HG22	3:I:3151[A]:LEU:HD23	1.77	0.66
3:I:3137[B]:ARG:CB	3:I:3139[B]:LEU:HD23	2.25	0.66
3:L:3288[B]:MET:HA	3:L:3295[B]:LEU:HG	1.76	0.66
1:M:327:ASP:OD1	1:M:328:LYS:N	2.27	0.66
3:O:3023[B]:ILE:HA	3:O:3026[B]:THR:OG1	1.95	0.66
3:O:3149[B]:ASN:OD1	3:O:3150[B]:LYS:HB2	1.96	0.66
3:O:3196[B]:THR:OG1	3:O:3199[B]:GLN:CG	2.44	0.66
3:O:3211[A]:ASP:OD1	3:O:3211[A]:ASP:N	2.27	0.66
2:Q:2217:ILE:HG22	2:Q:2218:SER:H	1.60	0.66
3:R:2961[B]:HIS:HB2	3:R:2992[B]:TYR:CE2	2.30	0.66
3:R:3176[A]:LYS:HB3	3:R:3176[A]:LYS:HZ2	1.60	0.66
3:R:3220[A]:ARG:HG2	3:R:3221[A]:ALA:N	2.09	0.66
2:T:2107:LEU:HD23	2:T:2208:PRO:HB2	1.76	0.66
3:U:2971[A]:ASP:CG	3:U:2973[A]:THR:OG1	2.37	0.66
3:U:2979[A]:GLN:HE21	3:U:3155[A]:MET:HE2	1.55	0.66
3:U:3176[A]:LYS:HB3	3:U:3176[A]:LYS:NZ	2.09	0.66
3:U:3255[B]:PRO:CB	3:d:2975[B]:PHE:HA	2.20	0.66
1:V:492:ARG:NH1	1:V:701:TYR:OH	2.27	0.66
3:X:2961[A]:HIS:HB2	3:X:2992[A]:TYR:CE2	2.30	0.66
3:X:2988[A]:TRP:CE3	3:X:2989[A]:HIS:CE1	2.83	0.66
3:X:3036[B]:GLY:O	3:X:3044[B]:LYS:HA	1.96	0.66
3:a:2979[A]:GLN:NE2	3:a:3155[A]:MET:HE2	2.09	0.66
3:a:3023[A]:ILE:HA	3:a:3026[A]:THR:OG1	1.95	0.66
3:a:3185[B]:TYR:C	3:a:3186[B]:GLU:OE2	2.37	0.66
3:d:3011[B]:TYR:HB3	3:d:3121[B]:SER:HB2	1.77	0.66
3:d:3259[B]:ASP:OD1	3:d:3260[B]:ARG:HD2	1.95	0.66
1:A:562:GLN:HG3	1:A:563:ILE:HG13	1.77	0.66
3:C:2956[A]:LYS:C	3:C:2960[A]:PHE:CE1	2.47	0.66
3:F:2961[A]:HIS:HB2	3:F:2992[A]:TYR:CE2	2.30	0.66
3:F:3036[B]:GLY:O	3:F:3044[B]:LYS:HA	1.96	0.66
3:F:3155[B]:MET:CG	3:a:3153[B]:LYS:C	2.68	0.66
3:F:3185[B]:TYR:C	3:F:3186[B]:GLU:OE2	2.37	0.66
2:H:2643:GLU:HA	2:H:2646:ALA:HB3	1.75	0.66
3:I:2961[B]:HIS:HB2	3:I:2992[B]:TYR:CE2	2.30	0.66
3:I:2966[A]:SER:HB2	3:I:2977[A]:CYS:CB	2.21	0.66
3:I:2967[B]:CYS:SG	3:R:2982[B]:MET:HG3	2.34	0.66
3:I:2969[B]:TYR:CD1	3:R:2961[B]:HIS:ND1	2.44	0.66
3:I:2971[A]:ASP:CG	3:I:2973[A]:THR:OG1	2.37	0.66
3:I:3093[B]:HIS:CD2	3:R:2973[B]:THR:OG1	2.44	0.66
3:L:3077[A]:ASP:CB	3:L:3080[A]:ASP:OD2	2.42	0.66
3:L:3298[B]:ASN:HA	3:L:3299[B]:LEU:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:2252:GLU:CD	2:N:2393:ARG:HH12	2.03	0.66
3:O:2975[B]:PHE:CE2	3:X:3172[B]:SER:HB2	2.30	0.66
3:O:2994[B]:LYS:O	3:O:2995[B]:GLN:C	2.38	0.66
3:O:3023[A]:ILE:HA	3:O:3026[A]:THR:OG1	1.95	0.66
1:P:965:ASP:N	1:P:965:ASP:OD1	2.26	0.66
3:R:3011[B]:TYR:HB3	3:R:3121[B]:SER:HB2	1.77	0.66
3:U:3147[B]:GLU:HB2	3:U:3149[B]:ASN:ND2	2.09	0.66
3:U:3259[A]:ASP:OD1	3:U:3260[A]:ARG:HD2	1.96	0.66
3:U:3298[B]:ASN:HB2	3:U:3299[B]:LEU:C	2.20	0.66
2:W:2823:ILE:HG22	2:W:2879:LEU:HG	1.75	0.66
3:X:2961[B]:HIS:HB2	3:X:2992[B]:TYR:CE2	2.30	0.66
3:X:3147[A]:GLU:HB2	3:X:3149[A]:ASN:ND2	2.10	0.66
3:X:3298[B]:ASN:HD21	3:X:3301[B]:PRO:HA	1.60	0.66
3:a:2952[A]:ALA:H	3:a:2953[A]:GLY:CA	2.04	0.66
3:a:2961[A]:HIS:HB2	3:a:2992[A]:TYR:CE2	2.30	0.66
3:a:3024[B]:LEU:CD1	3:a:3025[B]:VAL:H	1.83	0.66
3:a:3031[B]:ASN:OD1	3:a:3033[B]:PHE:N	2.27	0.66
3:a:3036[A]:GLY:O	3:a:3044[A]:LYS:HA	1.95	0.66
3:a:3217[A]:PHE:HE1	3:a:3230[A]:PHE:HZ	0.80	0.66
3:d:2979[A]:GLN:HE21	3:d:3155[A]:MET:HE2	1.55	0.66
3:d:2984[A]:THR:HG22	3:d:3151[A]:LEU:HD23	1.77	0.66
3:C:2984[B]:THR:HG22	3:C:3151[B]:LEU:HD23	1.77	0.66
3:C:3023[A]:ILE:HA	3:C:3026[A]:THR:OG1	1.95	0.66
3:C:3036[B]:GLY:O	3:C:3044[B]:LYS:HA	1.96	0.66
3:C:3137[A]:ARG:CB	3:C:3139[A]:LEU:HD23	2.25	0.66
3:C:3154[B]:PRO:O	3:L:3155[B]:MET:CG	2.43	0.66
3:C:3155[B]:MET:HE2	3:L:3153[B]:LYS:HD3	1.77	0.66
3:F:3107[B]:LEU:CD1	3:a:2975[B]:PHE:CD1	2.52	0.66
3:F:3251[B]:ASP:CG	3:a:3251[B]:ASP:CB	2.67	0.66
3:F:3259[A]:ASP:OD1	3:F:3260[A]:ARG:HD2	1.96	0.66
1:G:1166:THR:N	1:G:1167:ASP:HA	2.08	0.66
3:I:3196[B]:THR:OG1	3:I:3199[B]:GLN:CG	2.44	0.66
1:J:881:GLN:NE2	1:J:888:ALA:O	2.28	0.66
3:L:2961[B]:HIS:HB2	3:L:2992[B]:TYR:CE2	2.30	0.66
3:L:3036[B]:GLY:O	3:L:3044[B]:LYS:HA	1.95	0.66
3:L:3137[A]:ARG:CB	3:L:3139[A]:LEU:HD23	2.25	0.66
3:L:3185[A]:TYR:C	3:L:3186[A]:GLU:OE2	2.37	0.66
3:L:3298[A]:ASN:HA	3:L:3299[A]:LEU:HB2	1.76	0.66
3:O:2967[B]:CYS:N	3:X:2979[B]:GLN:NE2	2.42	0.66
3:O:2971[B]:ASP:H	3:X:2992[B]:TYR:H	1.44	0.66
3:O:3185[A]:TYR:C	3:O:3186[A]:GLU:OE2	2.37	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:2500:ILE:HG12	2:Q:2501:PRO:HD2	1.76	0.66
3:U:3149[A]:ASN:OD1	3:U:3150[A]:LYS:HB2	1.96	0.66
3:U:3170[B]:ALA:O	3:d:3152[B]:LYS:CE	2.44	0.66
3:U:3259[B]:ASP:OD1	3:U:3260[B]:ARG:HD2	1.96	0.66
2:W:2142:ALA:HB2	2:W:2433:THR:HG23	1.77	0.66
3:X:3137[B]:ARG:CB	3:X:3139[B]:LEU:HD23	2.25	0.66
3:a:3149[A]:ASN:OD1	3:a:3150[A]:LYS:HB2	1.96	0.66
1:b:949:ASP:HB2	1:b:953:GLU:HB2	1.76	0.66
2:c:2090:LYS:NZ	2:c:2099:GLU:OE2	2.28	0.66
3:d:2933[B]:SER:O	3:d:2936[B]:GLU:HB3	1.96	0.66
3:d:2961[A]:HIS:HB3	3:d:3111[A]:SER:HG	1.59	0.66
3:d:2988[B]:TRP:CE3	3:d:2989[B]:HIS:CE1	2.83	0.66
3:d:3036[A]:GLY:O	3:d:3044[A]:LYS:HA	1.95	0.66
3:d:3137[A]:ARG:CB	3:d:3139[A]:LEU:HD23	2.25	0.66
3:C:3036[A]:GLY:O	3:C:3044[A]:LYS:HA	1.95	0.66
3:F:2960[A]:PHE:HD1	3:F:2960[A]:PHE:H	1.41	0.66
3:F:2960[B]:PHE:H	3:F:2960[B]:PHE:HD1	1.41	0.66
3:F:2981[B]:GLY:N	3:a:2968[B]:GLN:CG	2.47	0.66
3:F:2988[A]:TRP:CE3	3:F:2989[A]:HIS:CE1	2.83	0.66
3:F:3284[B]:LYS:HA	3:F:3284[B]:LYS:CE	2.22	0.66
1:G:1263:LEU:HD11	1:G:1358:LEU:HD22	1.76	0.66
3:I:2966[B]:SER:HB3	3:I:2977[B]:CYS:HB2	1.78	0.66
3:I:2979[B]:GLN:OE1	3:R:2977[B]:CYS:SG	2.53	0.66
3:I:2994[A]:LYS:O	3:I:2995[A]:GLN:C	2.38	0.66
3:I:3132[A]:ALA:HB1	3:I:3197[A]:ILE:CD1	2.26	0.66
3:I:3185[B]:TYR:C	3:I:3186[B]:GLU:OE2	2.37	0.66
3:I:3252[B]:TYR:CG	3:R:3108[B]:HIS:CE1	2.84	0.66
1:J:949:ASP:HB2	1:J:953:GLU:HB2	1.76	0.66
3:L:2957[A]:ILE:CA	3:L:2960[A]:PHE:CE1	2.78	0.66
3:L:2984[A]:THR:HG22	3:L:3151[A]:LEU:HD23	1.77	0.66
3:L:3036[A]:GLY:O	3:L:3044[A]:LYS:HA	1.96	0.66
3:L:3149[B]:ASN:OD1	3:L:3150[B]:LYS:HB2	1.96	0.66
3:L:3288[A]:MET:HA	3:L:3295[A]:LEU:HG	1.76	0.66
3:O:2975[B]:PHE:HE2	3:X:3172[B]:SER:HB3	1.49	0.66
3:O:3036[A]:GLY:O	3:O:3044[A]:LYS:HA	1.96	0.66
3:O:3180[B]:TYR:CA	3:O:3183[B]:LEU:HD22	2.26	0.66
3:O:3298[A]:ASN:HB2	3:O:3299[A]:LEU:C	2.20	0.66
3:R:2965[A]:LEU:CD1	3:R:2975[A]:PHE:H	2.08	0.66
3:R:3298[B]:ASN:HA	3:R:3299[B]:LEU:HB2	1.76	0.66
1:S:1442:MET:HE1	1:S:1454:PHE:HA	1.76	0.66
3:U:2967[B]:CYS:O	3:d:3256[B]:TRP:CD2	2.47	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2970[B]:PRO:CB	3:d:2985[B]:PHE:CE2	2.75	0.66
3:U:3150[B]:LYS:CG	3:d:3156[B]:MET:HG2	2.24	0.66
3:U:3150[B]:LYS:HA	3:d:3154[B]:PRO:O	1.94	0.66
3:U:3196[B]:THR:OG1	3:U:3199[B]:GLN:CG	2.44	0.66
3:U:3298[B]:ASN:HA	3:U:3299[B]:LEU:HB2	1.76	0.66
1:V:240:PHE:HA	1:V:263:ALA:HB3	1.77	0.66
1:V:450:LYS:HB3	1:V:454:GLY:HA3	1.75	0.66
3:X:3023[A]:ILE:HA	3:X:3026[A]:THR:OG1	1.95	0.66
3:X:3137[A]:ARG:CB	3:X:3139[A]:LEU:HD23	2.25	0.66
1:Y:1612:THR:C	3:d:3186[B]:GLU:CB	2.60	0.66
3:a:3036[B]:GLY:O	3:a:3044[B]:LYS:HA	1.95	0.66
3:a:3149[B]:ASN:OD1	3:a:3150[B]:LYS:HB2	1.96	0.66
3:a:3173[B]:THR:CG2	3:a:3174[B]:GLY:N	2.55	0.66
3:d:3036[B]:GLY:O	3:d:3044[B]:LYS:HA	1.96	0.66
3:d:3180[B]:TYR:CA	3:d:3183[B]:LEU:HD22	2.26	0.66
3:d:3196[B]:THR:OG1	3:d:3199[B]:GLN:CG	2.44	0.66
1:A:516:TRP:HB2	1:A:579:LEU:HD13	1.77	0.66
3:C:2975[B]:PHE:CD2	3:L:2979[B]:GLN:N	2.37	0.66
3:C:3153[B]:LYS:CE	3:L:3158[B]:PHE:CE2	2.71	0.66
3:C:3185[A]:TYR:C	3:C:3186[A]:GLU:OE2	2.37	0.66
3:F:3036[A]:GLY:O	3:F:3044[A]:LYS:HA	1.95	0.66
3:F:3157[B]:PRO:HB3	3:a:2982[B]:MET:SD	2.34	0.66
3:F:3196[B]:THR:OG1	3:F:3199[B]:GLN:CG	2.44	0.66
2:H:2251:LEU:O	2:H:2315:ARG:NH2	2.27	0.66
3:I:2961[B]:HIS:HB3	3:I:3111[B]:SER:HG	1.59	0.66
3:I:2970[B]:PRO:CA	3:R:2989[B]:HIS:CD2	2.79	0.66
3:I:2979[A]:GLN:NE2	3:I:3155[A]:MET:HE2	2.09	0.66
3:I:3152[B]:LYS:HB3	3:R:3171[B]:HIS:CA	2.25	0.66
1:J:875:ALA:O	1:J:878:GLY:N	2.20	0.66
1:J:1258:ARG:NH2	1:J:1332:ASP:OD1	2.29	0.66
3:L:2986[A]:PRO:HB2	3:L:3127[A]:TRP:CZ3	2.29	0.66
3:L:3147[B]:GLU:HB2	3:L:3149[B]:ASN:ND2	2.09	0.66
3:L:3180[A]:TYR:CA	3:L:3183[A]:LEU:HD22	2.26	0.66
3:O:2933[B]:SER:O	3:O:2936[B]:GLU:HB3	1.96	0.66
3:O:2961[A]:HIS:HB2	3:O:2992[A]:TYR:CE2	2.30	0.66
3:O:3011[A]:TYR:HB3	3:O:3121[A]:SER:HB2	1.77	0.66
3:O:3036[B]:GLY:O	3:O:3044[B]:LYS:HA	1.95	0.66
3:O:3253[B]:GLU:HG2	3:X:3160[B]:SER:OG	1.96	0.66
2:Q:2824:CYS:HB2	2:Q:2878:ARG:HD2	1.77	0.66
3:R:3298[A]:ASN:HB2	3:R:3299[A]:LEU:C	2.20	0.66
3:U:2966[B]:SER:HB2	3:U:2977[B]:CYS:CB	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2984[A]:THR:HG22	3:U:3151[A]:LEU:HD23	1.77	0.66
3:U:2984[B]:THR:HG22	3:U:3151[B]:LEU:HD23	1.77	0.66
3:U:2994[A]:LYS:O	3:U:2995[A]:GLN:C	2.38	0.66
3:U:3147[A]:GLU:HB2	3:U:3149[A]:ASN:ND2	2.09	0.66
3:U:3155[B]:MET:N	3:d:3150[B]:LYS:CB	2.58	0.66
3:X:2933[A]:SER:O	3:X:2936[A]:GLU:HB3	1.96	0.66
3:X:2988[B]:TRP:CE3	3:X:2989[B]:HIS:CE1	2.83	0.66
3:X:3132[A]:ALA:HB1	3:X:3197[A]:ILE:CD1	2.26	0.66
3:X:3259[B]:ASP:OD1	3:X:3260[B]:ARG:HD2	1.95	0.66
1:Y:1550:ARG:NE	3:d:3008[B]:GLY:O	2.29	0.66
3:a:2961[B]:HIS:HB2	3:a:2992[B]:TYR:CE2	2.30	0.66
3:a:3132[A]:ALA:HB1	3:a:3197[A]:ILE:CD1	2.26	0.66
1:b:1172:ALA:HB1	1:b:1196:ILE:HG13	1.78	0.66
3:d:2957[B]:ILE:CA	3:d:2960[B]:PHE:CE1	2.78	0.66
3:d:2965[B]:LEU:CD1	3:d:2975[B]:PHE:H	2.08	0.66
3:C:2988[B]:TRP:CE3	3:C:2989[B]:HIS:CE1	2.83	0.66
3:C:3132[A]:ALA:HB1	3:C:3197[A]:ILE:CD1	2.26	0.66
3:C:3132[B]:ALA:HB1	3:C:3197[B]:ILE:CD1	2.26	0.66
3:C:3298[A]:ASN:HB2	3:C:3299[A]:LEU:C	2.20	0.66
1:D:930:ASP:OD1	1:D:1051:ARG:NH2	2.29	0.66
2:E:2252:GLU:HG2	2:E:2385:ILE:HG23	1.77	0.66
3:F:2971[B]:ASP:CG	3:F:2973[B]:THR:OG1	2.37	0.66
3:F:3132[B]:ALA:HB1	3:F:3197[B]:ILE:CD1	2.26	0.66
3:F:3169[A]:LYS:C	3:F:3172[A]:SER:HG	2.00	0.66
3:F:3196[A]:THR:OG1	3:F:3199[A]:GLN:CG	2.44	0.66
3:F:3248[B]:LEU:C	3:a:2974[B]:ALA:N	2.53	0.66
3:F:3259[B]:ASP:OD1	3:F:3260[B]:ARG:HD2	1.96	0.66
2:H:2415:PRO:HD3	2:H:2454:MET:HE1	1.77	0.66
2:H:2903:TYR:OH	3:I:2932[A]:PRO:HD2	1.96	0.66
3:I:2964[B]:PRO:CB	3:R:3221[B]:ALA:CB	2.70	0.66
3:I:2986[B]:PRO:HB2	3:I:3127[B]:TRP:CZ3	2.30	0.66
3:I:2988[B]:TRP:CE3	3:I:2989[B]:HIS:CE1	2.83	0.66
3:I:3137[A]:ARG:CB	3:I:3139[A]:LEU:HD23	2.25	0.66
3:I:3150[B]:LYS:HD2	3:R:3160[B]:SER:O	1.96	0.66
3:I:3163[B]:ASN:CB	3:R:3150[B]:LYS:NZ	2.58	0.66
3:I:3259[B]:ASP:OD1	3:I:3260[B]:ARG:HD2	1.96	0.66
3:I:3298[B]:ASN:HB2	3:I:3299[B]:LEU:C	2.19	0.66
1:J:1427:HIS:CE1	1:J:1458:HIS:HE2	2.13	0.66
3:L:3132[A]:ALA:HB1	3:L:3197[A]:ILE:CD1	2.26	0.66
3:L:3196[A]:THR:OG1	3:L:3199[A]:GLN:CG	2.43	0.66
2:N:2472:ASN:ND2	4:2:1:NAG:O7	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2988[A]:TRP:CE3	3:O:2989[A]:HIS:CE1	2.83	0.66
3:O:3038[B]:ILE:HG23	3:X:2969[B]:TYR:CZ	2.26	0.66
3:O:3196[A]:THR:OG1	3:O:3199[A]:GLN:CG	2.44	0.66
3:O:3259[B]:ASP:OD1	3:O:3260[B]:ARG:HD2	1.96	0.66
3:O:3279[A]:ASP:OD1	3:O:3279[A]:ASP:N	2.25	0.66
1:P:673:PHE:HB3	1:P:677:LEU:HB2	1.78	0.66
3:R:2933[A]:SER:O	3:R:2936[A]:GLU:HB3	1.96	0.66
3:R:2979[B]:GLN:NE2	3:R:3155[B]:MET:HE2	2.09	0.66
3:U:2994[B]:LYS:O	3:U:2995[B]:GLN:C	2.38	0.66
3:U:3154[B]:PRO:C	3:d:3150[B]:LYS:CG	2.67	0.66
3:X:3036[A]:GLY:O	3:X:3044[A]:LYS:HA	1.95	0.66
3:a:2957[A]:ILE:CA	3:a:2960[A]:PHE:CE1	2.78	0.66
3:a:2988[A]:TRP:CE3	3:a:2989[A]:HIS:CE1	2.83	0.66
3:a:3011[A]:TYR:HB3	3:a:3121[A]:SER:HB2	1.77	0.66
3:a:3137[A]:ARG:CB	3:a:3139[A]:LEU:HD23	2.25	0.66
3:a:3180[A]:TYR:CA	3:a:3183[A]:LEU:HD22	2.26	0.66
3:a:3180[B]:TYR:CA	3:a:3183[B]:LEU:HD22	2.26	0.66
3:a:3259[A]:ASP:OD1	3:a:3260[A]:ARG:HD2	1.96	0.66
3:d:2961[B]:HIS:HB2	3:d:2992[B]:TYR:CE2	2.30	0.66
3:d:3185[B]:TYR:C	3:d:3186[B]:GLU:OE2	2.37	0.66
3:d:3293[B]:LYS:HB2	3:d:3294[B]:SER:HB2	0.82	0.66
3:d:3298[B]:ASN:HB2	3:d:3299[B]:LEU:C	2.19	0.66
1:A:70:ARG:HA	1:A:214:GLU:OE1	1.95	0.66
3:C:3161[B]:GLU:HA	3:L:3147[B]:GLU:N	2.09	0.66
3:C:3298[A]:ASN:HA	3:C:3299[A]:LEU:HB2	1.76	0.66
3:F:2960[B]:PHE:C	3:a:3255[B]:PRO:HD2	2.20	0.66
3:F:2965[A]:LEU:CD1	3:F:2975[A]:PHE:H	2.08	0.66
3:F:3176[A]:LYS:NZ	3:F:3176[A]:LYS:HB3	2.08	0.66
3:F:3180[A]:TYR:CA	3:F:3183[A]:LEU:HD22	2.26	0.66
3:F:3185[A]:TYR:C	3:F:3186[A]:GLU:OE2	2.37	0.66
3:F:3288[B]:MET:HA	3:F:3295[B]:LEU:HG	1.76	0.66
1:G:305:ASN:HB3	1:G:400:ILE:HG12	1.76	0.66
3:I:3298[A]:ASN:HB2	3:I:3299[A]:LEU:C	2.20	0.66
3:L:2933[B]:SER:O	3:L:2936[B]:GLU:HB3	1.96	0.66
3:L:3279[A]:ASP:N	3:L:3279[A]:ASP:OD1	2.25	0.66
3:L:3298[B]:ASN:HB2	3:L:3299[B]:LEU:C	2.20	0.66
1:M:533:VAL:HG12	1:M:540:THR:HG22	1.77	0.66
3:O:2969[B]:TYR:CB	3:X:3158[B]:PHE:CE2	2.79	0.66
1:P:1315:GLY:HA3	1:P:1601:TRP:HB2	1.78	0.66
3:R:2986[A]:PRO:HB2	3:R:3127[A]:TRP:CZ3	2.30	0.66
3:R:3023[B]:ILE:HA	3:R:3026[B]:THR:OG1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3137[A]:ARG:CB	3:R:3139[A]:LEU:HD23	2.25	0.66
3:R:3137[B]:ARG:CB	3:R:3139[B]:LEU:HD23	2.25	0.66
3:R:3288[A]:MET:HA	3:R:3295[A]:LEU:HG	1.77	0.66
3:U:2979[B]:GLN:HE22	3:d:3153[B]:LYS:HZ1	0.69	0.66
3:U:2988[A]:TRP:CE3	3:U:2989[A]:HIS:CE1	2.83	0.66
3:U:2988[B]:TRP:CE3	3:U:2989[B]:HIS:CE1	2.83	0.66
3:U:3036[B]:GLY:O	3:U:3044[B]:LYS:HA	1.95	0.66
3:U:3132[A]:ALA:HB1	3:U:3197[A]:ILE:CD1	2.26	0.66
3:U:3298[A]:ASN:HA	3:U:3299[A]:LEU:HB2	1.76	0.66
1:V:105:VAL:HG12	1:V:123:PHE:HB3	1.77	0.66
1:V:1023:GLY:HA3	1:V:1031:ALA:HB2	1.77	0.66
3:X:2957[B]:ILE:CA	3:X:2960[B]:PHE:CE1	2.78	0.66
3:a:2957[B]:ILE:CA	3:a:2960[B]:PHE:CE1	2.78	0.66
1:b:324:PRO:HG2	1:b:376:ASN:HD21	1.61	0.66
3:d:3089[B]:HIS:ND1	3:d:3119[B]:HIS:CE1	2.61	0.66
3:d:3180[A]:TYR:CA	3:d:3183[A]:LEU:HD22	2.26	0.66
1:A:221:GLN:NE2	1:A:267:PHE:O	2.27	0.66
3:C:2964[B]:PRO:O	3:L:3255[B]:PRO:C	2.38	0.66
3:C:2966[A]:SER:HB3	3:C:2977[A]:CYS:HB2	1.78	0.66
3:C:3148[B]:ILE:HG22	3:L:3170[B]:ALA:HA	1.77	0.66
3:C:3196[B]:THR:OG1	3:C:3199[B]:GLN:CG	2.44	0.66
2:E:2799:LYS:HA	2:E:2803:ARG:HH12	1.60	0.66
3:F:3147[B]:GLU:HB2	3:F:3149[B]:ASN:ND2	2.09	0.66
3:F:3149[A]:ASN:OD1	3:F:3150[A]:LYS:HB2	1.96	0.66
3:I:3031[A]:ASN:OD1	3:I:3033[A]:PHE:N	2.26	0.66
3:I:3132[B]:ALA:HB1	3:I:3197[B]:ILE:CD1	2.26	0.66
3:I:3162[B]:ASP:C	3:R:3150[B]:LYS:NZ	2.54	0.66
3:O:2957[B]:ILE:CA	3:O:2960[B]:PHE:CE1	2.78	0.66
3:O:2984[B]:THR:HG22	3:O:3151[B]:LEU:HD23	1.77	0.66
3:R:2982[A]:MET:CE	3:R:3254[A]:MET:HE2	2.26	0.66
3:R:3031[A]:ASN:OD1	3:R:3033[A]:PHE:N	2.26	0.66
3:R:3149[A]:ASN:OD1	3:R:3150[A]:LYS:HB2	1.96	0.66
1:S:1567:ASP:OD1	1:S:1591:SER:OG	2.11	0.66
2:T:2090:LYS:NZ	2:T:2099:GLU:OE2	2.28	0.66
3:U:3011[B]:TYR:HB3	3:U:3121[B]:SER:HB2	1.76	0.66
3:U:3023[B]:ILE:HA	3:U:3026[B]:THR:OG1	1.95	0.66
3:X:2957[A]:ILE:CA	3:X:2960[A]:PHE:CE1	2.78	0.66
1:Y:1546:LYS:CB	3:d:3001[B]:LYS:HZ2	2.02	0.66
3:a:2982[B]:MET:CE	3:a:3254[B]:MET:HE2	2.26	0.66
3:a:2984[B]:THR:HG22	3:a:3151[B]:LEU:HD23	1.77	0.66
3:a:3196[A]:THR:OG1	3:a:3199[A]:GLN:CG	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3298[A]:ASN:HA	3:a:3299[A]:LEU:HB2	1.77	0.66
3:a:3298[B]:ASN:HA	3:a:3299[B]:LEU:HB2	1.76	0.66
3:d:2988[A]:TRP:CE3	3:d:2989[A]:HIS:CE1	2.83	0.66
2:B:2472:ASN:HD21	4:i:1:NAG:C7	2.08	0.66
3:C:2982[A]:MET:CE	3:C:3254[A]:MET:HE2	2.26	0.66
3:C:3147[A]:GLU:HB2	3:C:3149[A]:ASN:ND2	2.10	0.66
1:D:110:PHE:N	1:D:119:LYS:O	2.29	0.66
1:D:1329:LEU:HB2	1:D:1507:THR:HG21	1.78	0.66
3:F:2937[B]:ASN:ND2	3:F:3006[B]:LYS:HD3	2.11	0.66
3:F:2965[B]:LEU:O	3:a:3256[B]:TRP:N	2.29	0.66
3:F:2965[B]:LEU:CG	3:a:3256[B]:TRP:HE1	2.09	0.66
3:F:2970[B]:PRO:CA	3:a:2989[B]:HIS:HD2	2.09	0.66
3:F:3155[B]:MET:C	3:a:3153[B]:LYS:CD	2.64	0.66
1:G:606:ILE:O	1:G:610:THR:OG1	2.12	0.66
3:I:2937[B]:ASN:HD22	3:I:3006[B]:LYS:HD3	1.61	0.66
3:I:3116[B]:PHE:CE2	3:R:2969[B]:TYR:CG	2.36	0.66
3:I:3147[B]:GLU:HB2	3:I:3149[B]:ASN:ND2	2.09	0.66
1:J:527:LEU:HD22	1:J:629:MET:HG3	1.77	0.66
2:K:2800:LYS:HB3	3:L:3023[A]:ILE:HD13	1.78	0.66
3:L:2933[A]:SER:O	3:L:2936[A]:GLU:HB3	1.96	0.66
3:L:2937[A]:ASN:HB3	3:L:3006[A]:LYS:HD3	1.78	0.66
3:L:2988[B]:TRP:CE3	3:L:2989[B]:HIS:CE1	2.83	0.66
3:L:3132[B]:ALA:HB1	3:L:3197[B]:ILE:CD1	2.26	0.66
3:L:3180[B]:TYR:CA	3:L:3183[B]:LEU:HD22	2.26	0.66
3:L:3259[B]:ASP:OD1	3:L:3260[B]:ARG:HD2	1.96	0.66
1:M:1617:LYS:O	3:R:3197[B]:ILE:HD12	1.96	0.66
3:O:2960[A]:PHE:H	3:O:2960[A]:PHE:HD1	1.41	0.66
3:O:3112[B]:TYR:CE2	3:X:2969[B]:TYR:OH	2.46	0.66
3:O:3147[A]:GLU:HB2	3:O:3149[A]:ASN:ND2	2.09	0.66
1:P:1639:LYS:HD2	1:S:472:ASP:HB3	1.77	0.66
1:S:1639:LYS:HD2	4:BA:1:NAG:C1	2.26	0.66
3:U:2937[A]:ASN:ND2	3:U:3006[A]:LYS:HD3	2.11	0.66
3:U:3180[B]:TYR:CA	3:U:3183[B]:LEU:HD22	2.26	0.66
3:X:2930[B]:LEU:HD22	3:X:2930[B]:LEU:N	2.02	0.66
3:X:2952[B]:ALA:H	3:X:2953[B]:GLY:CA	2.04	0.66
1:Y:1348:TRP:HD1	1:Y:1403:LEU:HD13	1.61	0.66
3:a:2937[B]:ASN:HD22	3:a:3006[B]:LYS:HD3	1.61	0.66
3:a:3196[B]:THR:OG1	3:a:3199[B]:GLN:CG	2.43	0.66
3:a:3220[B]:ARG:HG2	3:a:3221[B]:ALA:N	2.09	0.66
3:d:2937[A]:ASN:ND2	3:d:3006[A]:LYS:HD3	2.11	0.66
3:d:2937[B]:ASN:ND2	3:d:3006[B]:LYS:HD3	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2952[B]:ALA:H	3:d:2953[B]:GLY:CA	2.04	0.66
3:d:2982[B]:MET:CE	3:d:3254[B]:MET:HE2	2.26	0.66
3:d:3259[A]:ASP:OD1	3:d:3260[A]:ARG:HD2	1.96	0.66
3:C:2937[A]:ASN:HD22	3:C:3006[A]:LYS:HD3	1.61	0.66
3:C:2966[B]:SER:HB3	3:C:2977[B]:CYS:HB2	1.77	0.66
3:C:3152[B]:LYS:HB2	3:L:3173[B]:THR:N	2.11	0.66
3:C:3180[B]:TYR:CA	3:C:3183[B]:LEU:HD22	2.26	0.66
1:D:456:GLN:NE2	1:D:549:PRO:O	2.29	0.66
1:D:518:LYS:NZ	1:D:519:PRO:O	2.29	0.66
2:E:2412:GLN:HG2	2:E:2422:GLU:HA	1.77	0.66
3:F:2970[B]:PRO:HB3	3:a:2989[B]:HIS:HD2	1.58	0.66
3:F:3220[B]:ARG:HG2	3:F:3221[B]:ALA:N	2.09	0.66
1:G:126:GLY:HA3	1:G:127:GLU:HG3	1.77	0.66
3:I:3150[B]:LYS:CE	3:R:3163[B]:ASN:HB3	2.12	0.66
3:L:3220[B]:ARG:HG2	3:L:3221[B]:ALA:N	2.08	0.66
2:N:2830:GLN:OE1	2:N:2863:ARG:NH1	2.27	0.66
3:O:2968[B]:GLN:CA	3:X:2988[B]:TRP:CB	2.67	0.66
3:O:3160[B]:SER:CA	3:X:3151[B]:LEU:CD1	2.59	0.66
1:P:841:LYS:HA	1:P:1117:ASP:HB2	1.78	0.66
3:R:3196[A]:THR:OG1	3:R:3199[A]:GLN:CG	2.44	0.66
3:R:3196[B]:THR:OG1	3:R:3199[B]:GLN:CG	2.44	0.66
1:S:1618:LEU:CD2	3:X:3136[B]:TYR:HE2	2.08	0.66
3:U:2930[B]:LEU:HD22	3:U:2930[B]:LEU:N	2.02	0.66
3:U:2957[B]:ILE:CA	3:U:2960[B]:PHE:CE1	2.78	0.66
3:U:3132[B]:ALA:HB1	3:U:3197[B]:ILE:CD1	2.26	0.66
3:U:3171[B]:HIS:HA	3:d:3152[B]:LYS:HZ3	1.55	0.66
3:U:3217[B]:PHE:HB2	3:U:3219[B]:LEU:HD21	1.78	0.66
3:X:2937[B]:ASN:ND2	3:X:3006[B]:LYS:HD3	2.11	0.66
3:X:3151[A]:LEU:O	3:X:3174[A]:GLY:HA3	1.96	0.66
3:X:3185[B]:TYR:C	3:X:3186[B]:GLU:OE2	2.37	0.66
1:Y:1250:ILE:O	1:Y:1473:ARG:NH2	2.29	0.66
3:a:3132[B]:ALA:HB1	3:a:3197[B]:ILE:CD1	2.26	0.66
3:a:3217[B]:PHE:HB2	3:a:3219[B]:LEU:HD21	1.78	0.66
3:d:2957[A]:ILE:CA	3:d:2960[A]:PHE:CE1	2.78	0.66
3:d:3196[A]:THR:OG1	3:d:3199[A]:GLN:CG	2.44	0.66
3:C:2957[B]:ILE:CA	3:C:2960[B]:PHE:CE1	2.78	0.65
3:C:2968[B]:GLN:HE21	3:L:3086[B]:GLU:CG	2.09	0.65
3:C:2988[A]:TRP:CE3	3:C:2989[A]:HIS:CE1	2.83	0.65
3:C:3217[B]:PHE:HE1	3:C:3230[B]:PHE:HZ	0.80	0.65
3:C:3259[B]:ASP:OD1	3:C:3260[B]:ARG:HD2	1.96	0.65
2:E:2149:ALA:HA	2:E:2260:GLU:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2961[B]:HIS:CD2	3:a:2975[B]:PHE:CZ	2.83	0.65
3:F:3256[B]:TRP:N	3:a:2965[B]:LEU:O	2.17	0.65
3:I:2964[B]:PRO:CA	3:R:3221[B]:ALA:HB1	2.24	0.65
3:I:2984[B]:THR:HG22	3:I:3151[B]:LEU:HD23	1.77	0.65
3:I:3298[A]:ASN:HA	3:I:3299[A]:LEU:HB2	1.76	0.65
3:L:2957[B]:ILE:CA	3:L:2960[B]:PHE:CE1	2.78	0.65
3:L:3259[A]:ASP:OD1	3:L:3260[A]:ARG:HD2	1.96	0.65
3:L:3298[B]:ASN:HD21	3:L:3301[B]:PRO:HA	1.60	0.65
1:M:926:LEU:HD11	1:M:1043:MET:HB3	1.77	0.65
3:O:2937[A]:ASN:ND2	3:O:3006[A]:LYS:HD3	2.11	0.65
3:O:2937[B]:ASN:ND2	3:O:3006[B]:LYS:HD3	2.11	0.65
3:O:2973[B]:THR:C	3:X:2979[B]:GLN:HB2	2.21	0.65
3:O:2982[B]:MET:CE	3:O:3254[B]:MET:HE2	2.26	0.65
3:R:2937[B]:ASN:ND2	3:R:3006[B]:LYS:HD3	2.11	0.65
3:R:3036[A]:GLY:O	3:R:3044[A]:LYS:HA	1.95	0.65
3:R:3180[B]:TYR:CA	3:R:3183[B]:LEU:HD22	2.26	0.65
2:T:2885:SER:HB3	2:T:2890:VAL:HG22	1.77	0.65
3:U:2933[B]:SER:O	3:U:2936[B]:GLU:HB3	1.96	0.65
3:U:3180[A]:TYR:CA	3:U:3183[A]:LEU:HD22	2.26	0.65
3:U:3196[A]:THR:OG1	3:U:3199[A]:GLN:CG	2.44	0.65
1:V:1573:CYS:HB2	1:V:1627:ARG:HG2	1.78	0.65
3:X:2937[A]:ASN:ND2	3:X:3006[A]:LYS:HD3	2.11	0.65
1:Y:958:PRO:HB2	1:Y:960:PHE:N	2.12	0.65
3:a:2933[B]:SER:O	3:a:2936[B]:GLU:HB3	1.96	0.65
3:a:2937[A]:ASN:HB3	3:a:3006[A]:LYS:HD3	1.79	0.65
3:a:3151[B]:LEU:O	3:a:3174[B]:GLY:HA3	1.97	0.65
3:d:3132[B]:ALA:HB1	3:d:3197[B]:ILE:CD1	2.26	0.65
1:A:70:ARG:NH1	1:A:266:LEU:O	2.29	0.65
3:C:2933[B]:SER:O	3:C:2936[B]:GLU:HB3	1.96	0.65
3:C:2937[B]:ASN:HD22	3:C:3006[B]:LYS:HD3	1.61	0.65
3:C:3011[A]:TYR:HB3	3:C:3121[A]:SER:HB2	1.77	0.65
3:C:3151[B]:LEU:O	3:C:3174[B]:GLY:HA3	1.97	0.65
3:F:2957[A]:ILE:CA	3:F:2960[A]:PHE:CE1	2.78	0.65
3:F:2984[B]:THR:HG22	3:F:3151[B]:LEU:HD23	1.77	0.65
3:F:3180[B]:TYR:CA	3:F:3183[B]:LEU:HD22	2.26	0.65
3:F:3298[B]:ASN:HD21	3:F:3301[B]:PRO:HA	1.60	0.65
3:I:2957[A]:ILE:CA	3:I:2960[A]:PHE:CE1	2.78	0.65
3:I:3023[A]:ILE:HA	3:I:3026[A]:THR:OG1	1.95	0.65
3:I:3149[A]:ASN:OD1	3:I:3150[A]:LYS:HB2	1.96	0.65
3:I:3171[B]:HIS:C	3:R:3152[B]:LYS:CB	2.68	0.65
3:I:3248[B]:LEU:C	3:R:2974[B]:ALA:N	2.54	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2937[A]:ASN:ND2	3:L:3006[A]:LYS:HD3	2.11	0.65
3:L:3298[A]:ASN:HB2	3:L:3299[A]:LEU:C	2.20	0.65
3:O:3151[A]:LEU:O	3:O:3174[A]:GLY:HA3	1.96	0.65
3:O:3180[A]:TYR:CA	3:O:3183[A]:LEU:HD22	2.26	0.65
3:O:3288[B]:MET:HA	3:O:3295[B]:LEU:HG	1.76	0.65
1:P:534:ASP:HB2	1:P:541:LYS:HE2	1.79	0.65
3:R:3036[B]:GLY:O	3:R:3044[B]:LYS:HA	1.96	0.65
3:R:3147[A]:GLU:HB2	3:R:3149[A]:ASN:ND2	2.09	0.65
3:U:2937[B]:ASN:ND2	3:U:3006[B]:LYS:HD3	2.11	0.65
3:U:2967[B]:CYS:HB2	3:d:3256[B]:TRP:HA	1.79	0.65
3:U:2975[B]:PHE:HD2	3:d:3255[B]:PRO:O	1.79	0.65
2:W:2687:ILE:HD11	2:W:2695:MET:HG2	1.79	0.65
3:X:2982[B]:MET:CE	3:X:3254[B]:MET:HE2	2.26	0.65
3:X:3196[B]:THR:OG1	3:X:3199[B]:GLN:CG	2.43	0.65
3:d:2951[B]:ASP:O	3:d:2956[B]:LYS:CE	2.45	0.65
3:C:2937[A]:ASN:ND2	3:C:3006[A]:LYS:HD3	2.11	0.65
1:D:1573:CYS:HB2	1:D:1627:ARG:HG2	1.79	0.65
3:F:2933[B]:SER:O	3:F:2936[B]:GLU:HB3	1.96	0.65
3:F:2951[B]:ASP:O	3:F:2956[B]:LYS:CE	2.45	0.65
3:F:2952[A]:ALA:H	3:F:2953[A]:GLY:CA	2.04	0.65
3:F:2965[B]:LEU:CD1	3:F:2975[B]:PHE:H	2.08	0.65
3:F:2982[B]:MET:HE3	3:a:2977[B]:CYS:HB3	1.76	0.65
3:F:3011[A]:TYR:HB3	3:F:3121[A]:SER:HB2	1.77	0.65
3:F:3149[B]:ASN:OD1	3:F:3150[B]:LYS:HB2	1.95	0.65
3:F:3255[B]:PRO:HG2	3:a:2962[B]:GLY:C	2.19	0.65
3:I:2937[A]:ASN:HD22	3:I:3006[A]:LYS:HD3	1.61	0.65
3:I:3151[A]:LEU:O	3:I:3174[A]:GLY:HA3	1.97	0.65
3:I:3171[B]:HIS:CA	3:R:3152[B]:LYS:CB	2.74	0.65
3:I:3180[A]:TYR:CA	3:I:3183[A]:LEU:HD22	2.26	0.65
3:I:3196[A]:THR:OG1	3:I:3199[A]:GLN:CG	2.44	0.65
3:I:3217[A]:PHE:HB2	3:I:3219[A]:LEU:HD21	1.78	0.65
1:J:450:LYS:HB3	1:J:454:GLY:HA3	1.79	0.65
1:J:898:GLY:N	1:J:899:MET:HA	2.10	0.65
3:L:2937[B]:ASN:ND2	3:L:3006[B]:LYS:HD3	2.11	0.65
1:M:1280:GLN:NE2	1:M:1337:ARG:HB3	2.10	0.65
3:O:2963[B]:MET:HG2	3:O:3108[B]:HIS:CG	2.23	0.65
3:R:2933[B]:SER:O	3:R:2936[B]:GLU:HB3	1.96	0.65
3:R:2969[A]:TYR:HD2	3:R:2971[A]:ASP:N	1.84	0.65
3:R:3089[B]:HIS:CE1	3:R:3119[B]:HIS:CE1	2.81	0.65
3:R:3132[B]:ALA:HB1	3:R:3197[B]:ILE:CD1	2.26	0.65
3:R:3259[A]:ASP:OD1	3:R:3260[A]:ARG:HD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3259[B]:ASP:OD1	3:R:3260[B]:ARG:HD2	1.96	0.65
3:U:2951[A]:ASP:O	3:U:2956[A]:LYS:CE	2.45	0.65
3:U:3288[A]:MET:HA	3:U:3295[A]:LEU:HG	1.76	0.65
2:W:2889:ALA:N	2:W:2890:VAL:HA	2.12	0.65
3:X:2966[A]:SER:HB3	3:X:2977[A]:CYS:HB2	1.78	0.65
3:X:3293[B]:LYS:HB2	3:X:3294[B]:SER:HB2	0.82	0.65
1:Y:492:ARG:HD2	1:Y:692:VAL:HG22	1.78	0.65
1:Y:1140:ASN:ND2	1:Y:1236:TYR:OH	2.30	0.65
3:a:3288[A]:MET:HA	3:a:3295[A]:LEU:HG	1.76	0.65
3:d:2961[A]:HIS:HB2	3:d:2992[A]:TYR:CE2	2.30	0.65
3:d:2979[A]:GLN:NE2	3:d:3155[A]:MET:HE2	2.09	0.65
3:d:3132[A]:ALA:HB1	3:d:3197[A]:ILE:CD1	2.26	0.65
3:C:3137[B]:ARG:CB	3:C:3139[B]:LEU:HD23	2.25	0.65
3:C:3180[A]:TYR:CA	3:C:3183[A]:LEU:HD22	2.26	0.65
3:C:3196[A]:THR:OG1	3:C:3199[A]:GLN:CG	2.44	0.65
3:C:3284[A]:LYS:HA	3:C:3284[A]:LYS:CE	2.22	0.65
1:D:1019:HIS:NE2	1:D:1046:HIS:HE1	1.95	0.65
1:D:1153:LYS:HB2	1:D:1155:LEU:HD23	1.78	0.65
3:F:2937[B]:ASN:HB3	3:F:3006[B]:LYS:HD3	1.79	0.65
3:F:2957[B]:ILE:CA	3:F:2960[B]:PHE:CE1	2.78	0.65
3:F:3248[B]:LEU:HD11	3:a:2973[B]:THR:HG23	1.78	0.65
2:H:2889:ALA:N	2:H:2890:VAL:HA	2.11	0.65
3:I:2933[A]:SER:O	3:I:2936[A]:GLU:HB3	1.96	0.65
3:I:2957[B]:ILE:CA	3:I:2960[B]:PHE:CE1	2.78	0.65
3:I:2970[B]:PRO:HA	3:R:2985[B]:PHE:CZ	2.31	0.65
3:I:2982[B]:MET:SD	3:R:3157[B]:PRO:N	2.70	0.65
3:I:3036[B]:GLY:O	3:I:3044[B]:LYS:HA	1.95	0.65
3:I:3150[B]:LYS:NZ	3:R:3162[B]:ASP:C	2.54	0.65
3:I:3217[B]:PHE:HB2	3:I:3219[B]:LEU:HD21	1.78	0.65
3:I:3256[B]:TRP:HE1	3:R:2965[B]:LEU:HB3	1.15	0.65
3:L:3066[B]:TYR:CE1	3:L:3193[B]:HIS:HE1	2.15	0.65
3:L:3149[A]:ASN:OD1	3:L:3150[A]:LYS:HB2	1.96	0.65
3:L:3217[A]:PHE:HB2	3:L:3219[A]:LEU:HD21	1.78	0.65
3:O:2965[B]:LEU:C	3:X:3153[B]:LYS:HZ3	2.05	0.65
3:O:2966[A]:SER:HB3	3:O:2977[A]:CYS:HB2	1.78	0.65
3:O:3132[A]:ALA:HB1	3:O:3197[A]:ILE:CD1	2.26	0.65
3:O:3217[B]:PHE:HB2	3:O:3219[B]:LEU:HD21	1.78	0.65
3:O:3259[A]:ASP:OD1	3:O:3260[A]:ARG:HD2	1.96	0.65
1:P:1195:ASP:OD1	1:P:1196:ILE:N	2.29	0.65
1:P:1280:GLN:HG2	1:P:1337:ARG:HD2	1.77	0.65
3:R:3285[B]:VAL:HG22	3:R:3286[B]:THR:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2933[A]:SER:O	3:U:2936[A]:GLU:HB3	1.96	0.65
3:U:2937[A]:ASN:HD22	3:U:3006[A]:LYS:HD3	1.61	0.65
3:U:2937[B]:ASN:HD22	3:U:3006[B]:LYS:HD3	1.61	0.65
3:U:2973[B]:THR:N	3:d:3247[B]:VAL:HG12	2.09	0.65
3:U:2975[B]:PHE:CE1	3:d:3253[B]:GLU:CG	2.80	0.65
3:U:3151[B]:LEU:O	3:U:3174[B]:GLY:HA3	1.97	0.65
2:W:2317:LEU:HB3	2:W:2318:PRO:HD2	1.79	0.65
3:X:2951[A]:ASP:O	3:X:2956[A]:LYS:CE	2.45	0.65
3:X:2979[A]:GLN:NE2	3:X:3155[A]:MET:HE2	2.09	0.65
3:X:3023[B]:ILE:HA	3:X:3026[B]:THR:OG1	1.95	0.65
2:Z:2509:ILE:HD11	2:Z:2605:LEU:HD23	1.78	0.65
3:a:2966[B]:SER:HB2	3:a:2977[B]:CYS:CB	2.21	0.65
3:a:3011[B]:TYR:HB3	3:a:3121[B]:SER:HB2	1.77	0.65
2:c:2867:PRO:HG2	3:d:2932[A]:PRO:HG2	1.73	0.65
3:d:2933[A]:SER:O	3:d:2936[A]:GLU:HB3	1.96	0.65
3:d:2937[A]:ASN:HD22	3:d:3006[A]:LYS:HD3	1.62	0.65
3:d:2937[B]:ASN:HB3	3:d:3006[B]:LYS:HD3	1.79	0.65
3:d:3151[B]:LEU:O	3:d:3174[B]:GLY:HA3	1.97	0.65
3:C:2937[B]:ASN:ND2	3:C:3006[B]:LYS:HD3	2.11	0.65
3:C:3151[A]:LEU:O	3:C:3174[A]:GLY:HA3	1.97	0.65
3:C:3174[B]:GLY:HA2	3:L:3154[B]:PRO:HG3	1.79	0.65
3:C:3217[B]:PHE:HB2	3:C:3219[B]:LEU:HD21	1.78	0.65
3:F:2937[A]:ASN:ND2	3:F:3006[A]:LYS:HD3	2.11	0.65
3:F:2980[B]:HIS:HB3	3:a:2968[B]:GLN:HG2	1.75	0.65
3:F:3252[B]:TYR:O	3:a:3252[B]:TYR:C	2.40	0.65
3:I:2966[B]:SER:CB	3:R:3254[B]:MET:CG	2.54	0.65
3:I:3011[A]:TYR:HB3	3:I:3121[A]:SER:HB2	1.76	0.65
3:I:3169[A]:LYS:C	3:I:3172[A]:SER:HG	1.98	0.65
1:J:327:ASP:OD1	1:J:328:LYS:N	2.27	0.65
1:J:1286:ARG:NH1	1:J:1333:GLU:OE1	2.30	0.65
2:K:2470:ALA:HB2	2:K:2476:LEU:HD11	1.77	0.65
3:L:3285[B]:VAL:HG22	3:L:3286[B]:THR:H	1.62	0.65
1:M:1421:VAL:HG23	1:M:1422:HIS:HD1	1.61	0.65
2:N:2687:ILE:HD11	2:N:2695:MET:HG2	1.79	0.65
3:O:3089[A]:HIS:ND1	3:O:3119[A]:HIS:CE1	2.61	0.65
3:O:3156[B]:MET:HG2	3:X:3173[B]:THR:HG23	1.61	0.65
3:O:3169[B]:LYS:HZ1	3:X:3148[B]:ILE:CB	2.05	0.65
1:P:891:LYS:HB3	1:P:892:TYR:CD2	2.31	0.65
1:P:1143:ALA:HA	1:P:1195:ASP:HA	1.77	0.65
2:Q:2394:VAL:H	2:Q:2448:THR:HG22	1.60	0.65
3:R:2937[A]:ASN:HD22	3:R:3006[A]:LYS:HD3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2982[B]:MET:CE	3:R:3254[B]:MET:HE2	2.26	0.65
3:R:3228[B]:VAL:HG21	3:R:3245[B]:PHE:CE1	2.32	0.65
3:R:3298[A]:ASN:HD21	3:R:3301[A]:PRO:HA	1.60	0.65
1:S:1414:THR:HG23	1:S:1477:LEU:HD13	1.78	0.65
2:T:2252:GLU:O	2:T:2389:ARG:NH2	2.28	0.65
3:U:2957[A]:ILE:CA	3:U:2960[A]:PHE:CE1	2.78	0.65
3:U:3137[B]:ARG:CB	3:U:3139[B]:LEU:HD23	2.25	0.65
3:U:3284[A]:LYS:CD	3:U:3285[A]:VAL:H	2.10	0.65
3:U:3288[B]:MET:HA	3:U:3295[B]:LEU:HG	1.76	0.65
3:X:3066[A]:TYR:CE1	3:X:3193[A]:HIS:HE1	2.15	0.65
3:X:3217[B]:PHE:HB2	3:X:3219[B]:LEU:HD21	1.78	0.65
3:X:3228[B]:VAL:HG21	3:X:3245[B]:PHE:CE1	2.32	0.65
1:Y:1621:ASN:N	3:d:3189[B]:ASN:HD22	1.93	0.65
3:a:2982[A]:MET:CE	3:a:3254[A]:MET:HE2	2.26	0.65
3:a:3259[B]:ASP:OD1	3:a:3260[B]:ARG:HD2	1.96	0.65
1:b:23:ARG:HD3	1:b:120:LYS:HG2	1.79	0.65
1:b:1086:LEU:HB3	1:b:1090:ILE:HD11	1.78	0.65
3:d:2984[B]:THR:HG22	3:d:3151[B]:LEU:HD23	1.77	0.65
3:d:3217[A]:PHE:HB2	3:d:3219[A]:LEU:HD21	1.79	0.65
1:A:1492:PRO:HB2	1:A:1497:SER:HB2	1.78	0.65
3:C:2988[B]:TRP:CD1	3:L:3153[B]:LYS:CE	2.79	0.65
3:C:3149[B]:ASN:CB	3:L:3158[B]:PHE:O	2.45	0.65
3:C:3149[B]:ASN:OD1	3:C:3150[B]:LYS:HB2	1.96	0.65
3:C:3228[A]:VAL:HG21	3:C:3245[A]:PHE:CE1	2.32	0.65
3:F:2966[B]:SER:CB	3:a:3254[B]:MET:HB2	2.26	0.65
3:F:2985[B]:PHE:CE2	3:a:2969[B]:TYR:C	2.74	0.65
3:F:3155[B]:MET:N	3:a:3153[B]:LYS:C	2.47	0.65
3:F:3173[B]:THR:HG23	3:a:3173[B]:THR:OG1	1.95	0.65
3:F:3228[A]:VAL:HG21	3:F:3245[A]:PHE:CE1	2.32	0.65
3:I:2937[B]:ASN:ND2	3:I:3006[B]:LYS:HD3	2.11	0.65
3:I:3180[B]:TYR:CA	3:I:3183[B]:LEU:HD22	2.26	0.65
1:J:1219:ASP:OD1	1:J:1223:ALA:N	2.30	0.65
3:L:3200[A]:LEU:HD22	3:L:3204[A]:LEU:CD1	2.27	0.65
1:M:1060:GLN:OE1	1:M:1063:ARG:NH1	2.30	0.65
3:O:2933[A]:SER:O	3:O:2936[A]:GLU:HB3	1.96	0.65
3:O:2937[A]:ASN:HB3	3:O:3006[A]:LYS:HD3	1.79	0.65
3:O:2957[A]:ILE:CA	3:O:2960[A]:PHE:CE1	2.78	0.65
3:O:2984[A]:THR:HG22	3:O:3151[A]:LEU:HD23	1.77	0.65
3:O:3149[A]:ASN:OD1	3:O:3150[A]:LYS:HB2	1.96	0.65
3:O:3158[B]:PHE:O	3:X:3148[B]:ILE:O	2.13	0.65
3:O:3217[A]:PHE:HB2	3:O:3219[A]:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:2545:SER:HA	2:Q:2546:LEU:HB3	1.78	0.65
3:R:2984[A]:THR:HG22	3:R:3151[A]:LEU:HD23	1.77	0.65
3:R:3132[A]:ALA:HB1	3:R:3197[A]:ILE:CD1	2.26	0.65
3:R:3185[A]:TYR:C	3:R:3186[A]:GLU:OE2	2.37	0.65
3:R:3217[B]:PHE:HB2	3:R:3219[B]:LEU:HD21	1.78	0.65
2:T:2403:PHE:HD1	2:T:2405:SER:H	1.45	0.65
3:U:2982[A]:MET:CE	3:U:3254[A]:MET:HE2	2.26	0.65
3:X:2937[B]:ASN:HD22	3:X:3006[B]:LYS:HD3	1.61	0.65
3:X:3288[A]:MET:HA	3:X:3295[A]:LEU:HG	1.76	0.65
3:a:2994[A]:LYS:O	3:a:2995[A]:GLN:C	2.38	0.65
3:a:3176[A]:LYS:HB3	3:a:3176[A]:LYS:HZ2	1.62	0.65
3:a:3228[A]:VAL:HG21	3:a:3245[A]:PHE:CE1	2.32	0.65
3:a:3298[A]:ASN:ND2	3:a:3301[A]:PRO:O	2.30	0.65
3:d:2982[A]:MET:CE	3:d:3254[A]:MET:HE2	2.26	0.65
3:d:3288[B]:MET:HA	3:d:3295[B]:LEU:HG	1.76	0.65
1:A:133:LYS:HG3	1:A:134:VAL:HG22	1.78	0.65
1:A:327:ASP:OD1	1:A:328:LYS:N	2.29	0.65
2:B:2283:ASN:O	2:B:2406:SER:OG	2.07	0.65
3:C:3120[A]:HIS:HA	3:C:3123[A]:THR:HG1	1.61	0.65
3:C:3154[B]:PRO:HD2	3:L:3155[B]:MET:SD	2.37	0.65
3:C:3217[A]:PHE:HB2	3:C:3219[A]:LEU:HD21	1.79	0.65
3:C:3255[B]:PRO:HG2	3:L:2959[B]:SER:O	1.96	0.65
3:F:2937[A]:ASN:HD22	3:F:3006[A]:LYS:HD3	1.62	0.65
3:F:2966[B]:SER:HB2	3:a:3254[B]:MET:CB	2.26	0.65
3:F:3176[A]:LYS:HB3	3:F:3176[A]:LYS:HZ2	1.60	0.65
3:F:3298[B]:ASN:ND2	3:F:3301[B]:PRO:O	2.30	0.65
3:I:2951[A]:ASP:O	3:I:2956[A]:LYS:CE	2.45	0.65
3:I:2965[B]:LEU:CD1	3:I:2975[B]:PHE:H	2.08	0.65
3:I:2982[A]:MET:CE	3:I:3254[A]:MET:HE2	2.26	0.65
3:I:3036[A]:GLY:O	3:I:3044[A]:LYS:HA	1.96	0.65
3:I:3171[B]:HIS:N	3:R:3152[B]:LYS:CB	2.45	0.65
3:I:3248[B]:LEU:HB2	3:R:2972[B]:GLY:C	2.19	0.65
3:I:3256[B]:TRP:CB	3:R:2966[B]:SER:O	2.45	0.65
3:I:3259[A]:ASP:OD1	3:I:3260[A]:ARG:HD2	1.96	0.65
3:L:2979[B]:GLN:NE2	3:L:3155[B]:MET:HE2	2.09	0.65
3:L:3089[B]:HIS:CE1	3:L:3119[B]:HIS:CE1	2.81	0.65
3:L:3151[A]:LEU:O	3:L:3174[A]:GLY:HA3	1.97	0.65
3:L:3196[B]:THR:OG1	3:L:3199[B]:GLN:CG	2.44	0.65
3:L:3217[B]:PHE:HB2	3:L:3219[B]:LEU:HD21	1.78	0.65
1:M:664:VAL:HG12	1:M:690:THR:HG22	1.79	0.65
3:O:2965[B]:LEU:HD12	3:X:2979[B]:GLN:NE2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2979[B]:GLN:NE2	3:O:3155[B]:MET:HE2	2.09	0.65
3:O:2994[A]:LYS:O	3:O:2995[A]:GLN:C	2.38	0.65
1:P:450:LYS:NZ	1:P:1273:SER:OG	2.26	0.65
1:P:1304:ASP:N	1:P:1304:ASP:OD1	2.23	0.65
3:R:2957[A]:ILE:CA	3:R:2960[A]:PHE:CE1	2.78	0.65
3:R:3180[A]:TYR:CA	3:R:3183[A]:LEU:HD22	2.26	0.65
3:R:3217[A]:PHE:HB2	3:R:3219[A]:LEU:HD21	1.79	0.65
3:R:3298[A]:ASN:HA	3:R:3299[A]:LEU:HB2	1.76	0.65
3:U:2965[B]:LEU:CD1	3:U:2975[B]:PHE:H	2.08	0.65
3:U:3036[A]:GLY:O	3:U:3044[A]:LYS:HA	1.95	0.65
1:V:1631:GLU:OE1	1:Y:328:LYS:NZ	2.29	0.65
3:X:3180[B]:TYR:CA	3:X:3183[B]:LEU:HD22	2.26	0.65
1:b:1140:ASN:ND2	1:b:1236:TYR:OH	2.30	0.65
3:d:3284[A]:LYS:CD	3:d:3285[A]:VAL:H	2.10	0.65
6:GA:1:NAG:O3	6:GA:2:NAG:N2	2.30	0.65
1:A:931:TRP:CG	1:A:1018:ILE:HD11	2.32	0.65
3:C:3160[B]:SER:CB	3:L:2983[B]:VAL:CG2	2.55	0.65
3:C:3169[B]:LYS:C	3:C:3172[B]:SER:HG	1.98	0.65
3:C:3298[A]:ASN:ND2	3:C:3301[A]:PRO:O	2.30	0.65
3:C:3298[B]:ASN:ND2	3:C:3301[B]:PRO:O	2.30	0.65
3:F:2982[A]:MET:CE	3:F:3254[A]:MET:HE2	2.26	0.65
3:F:3066[B]:TYR:CE1	3:F:3193[B]:HIS:HE1	2.15	0.65
3:F:3217[B]:PHE:HE1	3:F:3230[B]:PHE:HZ	0.80	0.65
1:G:580:TYR:O	1:G:584:SER:OG	2.14	0.65
3:I:2982[B]:MET:CE	3:I:3254[B]:MET:HE2	2.26	0.65
3:I:3014[A]:TRP:CG	3:I:3092[A]:ILE:HD11	2.32	0.65
3:I:3014[B]:TRP:CG	3:I:3092[B]:ILE:HD11	2.32	0.65
3:I:3228[A]:VAL:HG21	3:I:3245[A]:PHE:CE1	2.32	0.65
3:I:3298[B]:ASN:ND2	3:I:3301[B]:PRO:O	2.30	0.65
3:L:3176[B]:LYS:HB3	3:L:3176[B]:LYS:HZ2	1.60	0.65
3:L:3228[B]:VAL:HG21	3:L:3245[B]:PHE:CE1	2.32	0.65
3:L:3298[A]:ASN:HD21	3:L:3301[A]:PRO:HA	1.60	0.65
3:O:3217[A]:PHE:HE1	3:O:3230[A]:PHE:HZ	0.81	0.65
2:Q:2648:ALA:HA	2:Q:2654:SER:HB2	1.78	0.65
3:R:2966[A]:SER:HB3	3:R:2977[A]:CYS:HB2	1.78	0.65
3:R:3014[B]:TRP:CG	3:R:3092[B]:ILE:HD11	2.32	0.65
3:R:3149[B]:ASN:OD1	3:R:3150[B]:LYS:HB2	1.96	0.65
3:R:3284[A]:LYS:HA	3:R:3284[A]:LYS:CE	2.22	0.65
3:R:3285[A]:VAL:HG22	3:R:3286[A]:THR:H	1.61	0.65
2:T:2638:ARG:NH2	2:T:2704:ASP:OD1	2.30	0.65
3:U:3066[B]:TYR:CE1	3:U:3193[B]:HIS:HE1	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:2867:PRO:HB2	3:X:2932[A]:PRO:HG2	1.79	0.65
3:X:3180[A]:TYR:CB	3:X:3183[A]:LEU:HD22	2.27	0.65
3:X:3259[A]:ASP:OD1	3:X:3260[A]:ARG:HD2	1.96	0.65
3:d:3285[B]:VAL:HG22	3:d:3286[B]:THR:H	1.62	0.65
3:d:3298[A]:ASN:ND2	3:d:3301[A]:PRO:O	2.30	0.65
1:A:930:ASP:OD1	1:A:1051:ARG:NH2	2.29	0.65
3:C:2957[A]:ILE:CA	3:C:2960[A]:PHE:CE1	2.78	0.65
3:C:3149[A]:ASN:OD1	3:C:3150[A]:LYS:HB2	1.96	0.65
3:C:3248[B]:LEU:HD21	3:L:2971[B]:ASP:OD2	1.97	0.65
3:C:3285[A]:VAL:HG22	3:C:3286[A]:THR:H	1.61	0.65
3:F:2961[B]:HIS:CA	3:a:2975[B]:PHE:CZ	2.69	0.65
3:F:3117[B]:TYR:O	3:F:3120[B]:HIS:HB2	1.97	0.65
3:F:3200[B]:LEU:HD22	3:F:3204[B]:LEU:CD1	2.27	0.65
3:F:3217[B]:PHE:HB2	3:F:3219[B]:LEU:HD21	1.79	0.65
2:H:2509:ILE:HD11	2:H:2605:LEU:HD23	1.78	0.65
3:I:2965[B]:LEU:HB3	3:R:3256[B]:TRP:CZ2	2.31	0.65
3:I:3025[B]:VAL:HG22	3:I:3047[B]:ARG:NH1	2.02	0.65
1:J:1576:THR:H	1:J:1581:GLU:HB3	1.60	0.65
3:L:2961[B]:HIS:CE1	3:L:2980[B]:HIS:NE2	2.57	0.65
3:L:2982[A]:MET:CE	3:L:3254[A]:MET:HE2	2.26	0.65
3:L:3014[A]:TRP:CG	3:L:3092[A]:ILE:HD11	2.32	0.65
1:M:460:GLU:HB3	1:M:465:PRO:HG2	1.79	0.65
3:O:2937[A]:ASN:HD22	3:O:3006[A]:LYS:HD3	1.61	0.65
3:O:2967[B]:CYS:C	3:X:2979[B]:GLN:CG	2.61	0.65
1:P:329:ARG:O	1:S:1583:CYS:N	2.29	0.65
1:P:883:CYS:O	1:P:885:SER:OG	2.14	0.65
2:Q:2109:ARG:NH1	2:Q:2169:HIS:O	2.30	0.65
3:R:2937[B]:ASN:HD22	3:R:3006[B]:LYS:HD3	1.62	0.65
3:R:3180[A]:TYR:CB	3:R:3183[A]:LEU:HD22	2.27	0.65
3:R:3185[B]:TYR:C	3:R:3186[B]:GLU:OE2	2.37	0.65
1:S:545:PHE:O	1:S:561:ARG:NH2	2.28	0.65
3:U:3228[B]:VAL:HG21	3:U:3245[B]:PHE:CE1	2.32	0.65
1:V:136:ALA:O	1:V:193:SER:OG	2.14	0.65
1:V:452:ILE:HD12	1:V:1367:SER:HB2	1.79	0.65
3:X:2982[A]:MET:CE	3:X:3254[A]:MET:HE2	2.26	0.65
3:a:2966[B]:SER:HB3	3:a:2977[B]:CYS:HB2	1.78	0.65
3:a:2994[B]:LYS:O	3:a:2995[B]:GLN:C	2.38	0.65
3:a:3151[A]:LEU:O	3:a:3174[A]:GLY:HA3	1.97	0.65
3:a:3228[B]:VAL:HG21	3:a:3245[B]:PHE:CE1	2.32	0.65
3:d:3298[A]:ASN:HB2	3:d:3299[A]:LEU:C	2.20	0.65
8:0:1:NAG:C6	8:0:2:NAG:N2	2.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3153[B]:LYS:NZ	3:L:2988[B]:TRP:HE1	1.93	0.65
3:C:3154[B]:PRO:CG	3:L:3174[B]:GLY:HA3	2.09	0.65
3:C:3176[B]:LYS:HB3	3:C:3176[B]:LYS:HZ2	1.62	0.65
3:C:3232[A]:VAL:CG2	3:C:3273[A]:LEU:HD11	2.27	0.65
3:C:3251[B]:ASP:O	3:L:3253[B]:GLU:N	2.22	0.65
1:D:855:ARG:NH2	1:D:941:LEU:O	2.30	0.65
2:E:2858:ASP:OD2	2:E:2862:LYS:NZ	2.30	0.65
3:F:3170[B]:ALA:C	3:a:3152[B]:LYS:CG	2.70	0.65
3:F:3172[B]:SER:CB	3:a:3150[B]:LYS:C	2.70	0.65
3:F:3200[A]:LEU:HD22	3:F:3204[A]:LEU:CD1	2.27	0.65
2:H:2185:THR:HG23	2:H:2186:GLU:HG3	1.79	0.65
3:I:2937[B]:ASN:HB3	3:I:3006[B]:LYS:HD3	1.79	0.65
3:I:2955[B]:GLN:OE1	3:I:3037[B]:TYR:CE1	2.50	0.65
3:I:2965[B]:LEU:CA	3:R:3221[B]:ALA:HB1	2.18	0.65
3:I:2966[B]:SER:C	3:R:3256[B]:TRP:CB	2.70	0.65
3:I:2975[B]:PHE:CZ	3:R:2961[B]:HIS:O	2.50	0.65
3:I:3146[B]:CYS:O	3:R:3161[B]:GLU:HG3	1.97	0.65
3:I:3153[B]:LYS:HB3	3:R:3155[B]:MET:CB	2.26	0.65
1:J:1182:ASN:HD22	1:J:1182:ASN:H	1.44	0.65
3:L:2937[A]:ASN:HD22	3:L:3006[A]:LYS:HD3	1.62	0.65
1:M:450:LYS:NZ	1:M:1273:SER:OG	2.30	0.65
3:O:3066[B]:TYR:CE1	3:O:3193[B]:HIS:HE1	2.15	0.65
3:O:3089[B]:HIS:CE1	3:O:3119[B]:HIS:CE1	2.81	0.65
3:O:3124[A]:ASP:OD2	3:O:3187[A]:TYR:OH	2.15	0.65
1:P:61:GLY:HA3	1:P:352:TRP:HB2	1.78	0.65
3:R:2951[B]:ASP:O	3:R:2956[B]:LYS:CE	2.45	0.65
3:R:3066[A]:TYR:CE1	3:R:3193[A]:HIS:HE1	2.15	0.65
3:R:3298[B]:ASN:HD21	3:R:3301[B]:PRO:HA	1.60	0.65
3:U:3232[B]:VAL:CG2	3:U:3273[B]:LEU:HD11	2.27	0.65
3:U:3254[B]:MET:HB3	3:d:3254[B]:MET:C	2.20	0.65
3:U:3298[B]:ASN:ND2	3:U:3301[B]:PRO:O	2.30	0.65
3:X:3014[A]:TRP:CG	3:X:3092[A]:ILE:HD11	2.32	0.65
3:X:3014[B]:TRP:CG	3:X:3092[B]:ILE:HD11	2.32	0.65
3:X:3298[B]:ASN:ND2	3:X:3301[B]:PRO:O	2.30	0.65
3:a:2937[A]:ASN:ND2	3:a:3006[A]:LYS:HD3	2.11	0.65
3:a:3025[B]:VAL:HG22	3:a:3047[B]:ARG:NH1	2.02	0.65
3:a:3066[B]:TYR:CE1	3:a:3193[B]:HIS:HE1	2.15	0.65
3:a:3117[B]:TYR:O	3:a:3120[B]:HIS:HB2	1.97	0.65
3:a:3124[B]:ASP:OD2	3:a:3187[B]:TYR:OH	2.15	0.65
3:a:3200[A]:LEU:HD22	3:a:3204[A]:LEU:CD1	2.27	0.65
3:a:3232[A]:VAL:CG2	3:a:3273[A]:LEU:HD11	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3232[B]:VAL:CG2	3:a:3273[B]:LEU:HD11	2.27	0.65
3:a:3284[A]:LYS:CD	3:a:3285[A]:VAL:H	2.09	0.65
3:a:3298[A]:ASN:CB	3:a:3300[A]:LEU:CD2	2.61	0.65
3:d:2937[B]:ASN:HD22	3:d:3006[B]:LYS:HD3	1.62	0.65
3:d:3124[B]:ASP:OD2	3:d:3187[B]:TYR:OH	2.15	0.65
4:m:1:NAG:H4	4:m:2:NAG:N2	2.11	0.65
1:A:1013:ILE:HD11	1:A:1175:PHE:CD2	2.31	0.64
1:A:1604:ASP:OD1	1:A:1605:ARG:NH1	2.30	0.64
3:C:3014[B]:TRP:CG	3:C:3092[B]:ILE:HD11	2.32	0.64
1:D:984:ASP:N	1:D:984:ASP:OD1	2.30	0.64
3:F:2933[A]:SER:O	3:F:2936[A]:GLU:HB3	1.96	0.64
3:F:3124[B]:ASP:OD2	3:F:3187[B]:TYR:OH	2.15	0.64
3:F:3151[B]:LEU:O	3:F:3174[B]:GLY:HA3	1.97	0.64
3:F:3174[B]:GLY:H	3:a:3154[B]:PRO:CB	1.82	0.64
3:I:2960[B]:PHE:CA	3:R:3255[B]:PRO:HD2	2.18	0.64
3:I:2969[A]:TYR:HD2	3:I:2971[A]:ASP:N	1.84	0.64
3:I:3259[B]:ASP:N	3:R:3162[B]:ASP:HB3	2.11	0.64
1:J:534:ASP:HB2	1:J:541:LYS:HE2	1.77	0.64
3:L:2994[A]:LYS:O	3:L:2995[A]:GLN:C	2.38	0.64
3:L:3151[B]:LEU:O	3:L:3174[B]:GLY:HA3	1.97	0.64
3:L:3298[A]:ASN:ND2	3:L:3301[A]:PRO:O	2.30	0.64
3:O:2951[A]:ASP:O	3:O:2956[A]:LYS:CE	2.45	0.64
3:O:3117[B]:TYR:O	3:O:3120[B]:HIS:HB2	1.98	0.64
3:R:3298[B]:ASN:ND2	3:R:3301[B]:PRO:O	2.30	0.64
3:U:3124[B]:ASP:OD2	3:U:3187[B]:TYR:OH	2.15	0.64
3:U:3217[A]:PHE:HB2	3:U:3219[A]:LEU:HD21	1.79	0.64
3:U:3285[A]:VAL:HG22	3:U:3286[A]:THR:H	1.62	0.64
3:X:2955[A]:GLN:OE1	3:X:3037[A]:TYR:CE1	2.51	0.64
3:X:3132[B]:ALA:HB1	3:X:3197[B]:ILE:CD1	2.26	0.64
3:X:3180[A]:TYR:CA	3:X:3183[A]:LEU:HD22	2.26	0.64
3:X:3180[B]:TYR:CB	3:X:3183[B]:LEU:HD22	2.27	0.64
3:X:3232[B]:VAL:CG2	3:X:3273[B]:LEU:HD11	2.27	0.64
1:Y:1613:ASP:OD1	3:d:3185[B]:TYR:C	2.40	0.64
2:Z:2833:GLY:HA3	2:Z:2854:MET:HE1	1.79	0.64
3:a:2933[A]:SER:O	3:a:2936[A]:GLU:HB3	1.96	0.64
3:a:2966[A]:SER:HB3	3:a:2977[A]:CYS:HB2	1.77	0.64
1:b:105:VAL:HB	1:b:137:ARG:NH2	2.12	0.64
1:b:589:GLN:HG2	1:b:594:ASP:HB3	1.78	0.64
1:b:898:GLY:N	1:b:899:MET:SD	2.64	0.64
1:b:1296:VAL:HB	1:b:1446:ASP:HB3	1.78	0.64
3:d:3120[A]:HIS:NE2	9:d:3401[A]:CUO:O1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3149[A]:ASN:OD1	3:d:3150[A]:LYS:HB2	1.96	0.64
3:d:3232[A]:VAL:CG2	3:d:3273[A]:LEU:HD11	2.27	0.64
3:d:3232[B]:VAL:CG2	3:d:3273[B]:LEU:HD11	2.27	0.64
1:A:1618:LEU:O	3:F:3198[B]:PRO:HD3	1.98	0.64
3:C:2952[A]:ALA:H	3:C:2953[A]:GLY:CA	2.04	0.64
3:C:3066[A]:TYR:CE1	3:C:3193[A]:HIS:HE1	2.15	0.64
3:C:3149[B]:ASN:ND2	3:L:3163[B]:ASN:CB	2.60	0.64
1:D:1013:ILE:HD11	1:D:1175:PHE:CD2	2.32	0.64
3:F:3217[A]:PHE:HB2	3:F:3219[A]:LEU:HD21	1.78	0.64
3:I:2930[B]:LEU:HD22	3:I:2930[B]:LEU:N	2.02	0.64
3:I:3120[A]:HIS:NE2	9:R:3401[A]:CUO:O1	2.30	0.64
3:I:3251[B]:ASP:CB	3:R:3251[B]:ASP:CG	2.70	0.64
3:I:3298[A]:ASN:ND2	3:I:3301[A]:PRO:O	2.30	0.64
3:L:2966[B]:SER:HB3	3:L:2977[B]:CYS:HB2	1.78	0.64
3:L:3200[B]:LEU:HD22	3:L:3204[B]:LEU:CD1	2.27	0.64
3:O:2951[B]:ASP:O	3:O:2956[B]:LYS:CE	2.45	0.64
3:O:2982[A]:MET:CE	3:O:3254[A]:MET:HE2	2.26	0.64
3:O:3132[B]:ALA:HB1	3:O:3197[B]:ILE:CD1	2.26	0.64
3:O:3157[B]:PRO:HD3	3:X:3153[B]:LYS:HA	1.80	0.64
3:O:3298[A]:ASN:ND2	3:O:3301[A]:PRO:O	2.30	0.64
3:O:3298[B]:ASN:ND2	3:O:3301[B]:PRO:O	2.30	0.64
3:R:3151[B]:LEU:O	3:R:3174[B]:GLY:HA3	1.97	0.64
3:R:3232[B]:VAL:CG2	3:R:3273[B]:LEU:HD11	2.27	0.64
3:R:3298[A]:ASN:ND2	3:R:3301[A]:PRO:O	2.30	0.64
1:S:573:LYS:HD2	1:S:574:GLY:HA2	1.77	0.64
3:U:2937[A]:ASN:HB3	3:U:3006[A]:LYS:HD3	1.78	0.64
3:U:3117[A]:TYR:O	3:U:3120[A]:HIS:HB2	1.97	0.64
3:U:3228[A]:VAL:HG21	3:U:3245[A]:PHE:CE1	2.32	0.64
1:V:912:ASN:ND2	1:V:1093:ASP:OD2	2.30	0.64
1:V:1029:SER:OG	1:V:1030:MET:N	2.30	0.64
3:X:2961[A]:HIS:CE1	3:X:2980[A]:HIS:NE2	2.57	0.64
3:X:3149[A]:ASN:OD1	3:X:3150[A]:LYS:HB2	1.96	0.64
3:X:3232[A]:VAL:CG2	3:X:3273[A]:LEU:HD11	2.27	0.64
3:a:2951[A]:ASP:O	3:a:2956[A]:LYS:CE	2.45	0.64
3:d:2994[A]:LYS:O	3:d:2995[A]:GLN:C	2.38	0.64
3:d:3066[B]:TYR:HD1	3:d:3193[B]:HIS:CE1	2.16	0.64
3:d:3149[B]:ASN:OD1	3:d:3150[B]:LYS:HB2	1.96	0.64
3:d:3157[B]:PRO:O	3:d:3160[B]:SER:N	2.30	0.64
3:d:3217[B]:PHE:HB2	3:d:3219[B]:LEU:HD21	1.78	0.64
3:C:2971[B]:ASP:CB	3:L:3089[B]:HIS:CE1	2.59	0.64
3:C:3180[A]:TYR:CB	3:C:3183[A]:LEU:HD22	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3259[A]:ASP:OD1	3:C:3260[A]:ARG:HD2	1.96	0.64
2:E:2142:ALA:HB1	2:E:2143:CYS:HB2	1.77	0.64
3:F:2937[B]:ASN:HD22	3:F:3006[B]:LYS:HD3	1.61	0.64
3:F:2975[B]:PHE:CE1	3:a:3107[B]:LEU:HG	2.32	0.64
3:F:3014[A]:TRP:CG	3:F:3092[A]:ILE:HD11	2.32	0.64
3:F:3014[B]:TRP:CG	3:F:3092[B]:ILE:HD11	2.32	0.64
3:F:3180[A]:TYR:CB	3:F:3183[A]:LEU:HD22	2.27	0.64
3:F:3255[B]:PRO:HB2	3:a:2959[B]:SER:CA	2.28	0.64
3:I:2965[A]:LEU:CD1	3:I:2975[A]:PHE:H	2.08	0.64
3:I:3180[A]:TYR:CB	3:I:3183[A]:LEU:HD22	2.27	0.64
3:I:3259[B]:ASP:CA	3:R:3162[B]:ASP:HB3	2.26	0.64
1:J:105:VAL:HG12	1:J:123:PHE:HB3	1.80	0.64
3:L:2951[A]:ASP:O	3:L:2956[A]:LYS:CE	2.45	0.64
3:L:2961[A]:HIS:CE1	3:L:2980[A]:HIS:NE2	2.57	0.64
3:L:3180[B]:TYR:CB	3:L:3183[B]:LEU:HD22	2.27	0.64
3:L:3232[B]:VAL:CG2	3:L:3273[B]:LEU:HD11	2.27	0.64
3:O:2969[B]:TYR:CG	3:X:3158[B]:PHE:HE1	2.12	0.64
3:O:3120[B]:HIS:NE2	9:O:3401[B]:CUO:O1	2.30	0.64
3:O:3180[A]:TYR:CB	3:O:3183[A]:LEU:HD22	2.27	0.64
3:O:3253[B]:GLU:OE2	3:X:3161[B]:GLU:CD	2.40	0.64
1:P:450:LYS:HB3	1:P:454:GLY:HA3	1.79	0.64
3:R:2955[B]:GLN:OE1	3:R:3037[B]:TYR:CE1	2.51	0.64
3:R:2966[A]:SER:HB2	3:R:2977[A]:CYS:CB	2.21	0.64
1:S:1284:GLU:OE1	1:S:1337:ARG:NH1	2.30	0.64
3:U:2955[B]:GLN:OE1	3:U:3037[B]:TYR:CE1	2.51	0.64
3:U:3014[A]:TRP:CG	3:U:3092[A]:ILE:HD11	2.32	0.64
3:U:3151[A]:LEU:O	3:U:3174[A]:GLY:HA3	1.97	0.64
1:V:804:ASP:OD2	6:EA:1:NAG:O6	2.14	0.64
3:X:3298[A]:ASN:ND2	3:X:3301[A]:PRO:O	2.30	0.64
3:a:2937[A]:ASN:HD22	3:a:3006[A]:LYS:HD3	1.61	0.64
3:a:2965[A]:LEU:CD1	3:a:2975[A]:PHE:H	2.08	0.64
3:a:3200[B]:LEU:HD22	3:a:3204[B]:LEU:CD1	2.27	0.64
3:a:3279[B]:ASP:OD1	3:a:3279[B]:ASP:N	2.25	0.64
3:d:2955[A]:GLN:OE1	3:d:3037[A]:TYR:CE1	2.51	0.64
3:d:3066[B]:TYR:CE1	3:d:3193[B]:HIS:HE1	2.15	0.64
1:A:533:VAL:HG12	1:A:540:THR:HG22	1.80	0.64
3:C:2937[B]:ASN:HB3	3:C:3006[B]:LYS:HD3	1.79	0.64
3:C:2955[A]:GLN:OE1	3:C:3037[A]:TYR:CE1	2.51	0.64
3:C:2975[B]:PHE:HD1	3:L:3107[B]:LEU:HD13	1.54	0.64
3:C:3066[B]:TYR:CE1	3:C:3193[B]:HIS:HE1	2.15	0.64
3:F:2954[A]:TYR:HA	3:F:2957[A]:ILE:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3117[A]:TYR:O	3:F:3120[A]:HIS:HB2	1.98	0.64
3:F:3151[A]:LEU:O	3:F:3174[A]:GLY:HA3	1.97	0.64
3:F:3232[A]:VAL:CG2	3:F:3273[A]:LEU:HD11	2.27	0.64
3:F:3255[B]:PRO:CG	3:a:2964[B]:PRO:HD2	2.27	0.64
3:F:3285[A]:VAL:HG22	3:F:3286[A]:THR:H	1.62	0.64
1:G:164:GLU:HG3	1:G:297:ARG:HE	1.63	0.64
3:I:2961[A]:HIS:CE1	3:I:2980[A]:HIS:NE2	2.57	0.64
3:I:3025[A]:VAL:HG22	3:I:3047[A]:ARG:NH1	2.01	0.64
3:I:3151[B]:LEU:O	3:I:3174[B]:GLY:HA3	1.96	0.64
3:I:3153[B]:LYS:CB	3:R:3155[B]:MET:CB	2.71	0.64
3:L:3240[A]:THR:HG22	3:L:3241[A]:PHE:N	2.13	0.64
3:L:3279[B]:ASP:OD1	3:L:3279[B]:ASP:N	2.25	0.64
3:L:3285[A]:VAL:HG22	3:L:3286[A]:THR:H	1.62	0.64
1:M:439:LEU:HD23	1:M:509:ILE:HD12	1.80	0.64
1:M:873:VAL:HA	1:M:876:PHE:CE1	2.32	0.64
3:O:2937[B]:ASN:HB3	3:O:3006[B]:LYS:HD3	1.79	0.64
3:O:2969[B]:TYR:CD2	3:X:2988[B]:TRP:O	2.50	0.64
3:O:3285[B]:VAL:HG22	3:O:3286[B]:THR:H	1.62	0.64
1:P:325:THR:HB	1:P:332:ASP:H	1.62	0.64
2:Q:2687:ILE:HD11	2:Q:2695:MET:HG2	1.77	0.64
3:R:2961[B]:HIS:CE1	3:R:2980[B]:HIS:NE2	2.57	0.64
3:U:2937[B]:ASN:HB3	3:U:3006[B]:LYS:HD3	1.79	0.64
3:U:2969[B]:TYR:OH	3:d:2980[B]:HIS:NE2	2.30	0.64
3:U:3149[B]:ASN:OD1	3:U:3150[B]:LYS:HB2	1.96	0.64
3:U:3157[B]:PRO:O	3:U:3160[B]:SER:N	2.30	0.64
3:U:3298[A]:ASN:ND2	3:U:3301[A]:PRO:O	2.30	0.64
1:Y:1505:ARG:HG3	1:Y:1508:PHE:HB3	1.79	0.64
3:d:2930[A]:LEU:H	3:d:2930[A]:LEU:CD2	1.98	0.64
3:d:3120[B]:HIS:NE2	9:d:3401[B]:CUO:O1	2.30	0.64
3:d:3200[A]:LEU:HD22	3:d:3204[A]:LEU:CD1	2.27	0.64
3:d:3228[B]:VAL:HG21	3:d:3245[B]:PHE:CE1	2.32	0.64
3:d:3298[B]:ASN:ND2	3:d:3301[B]:PRO:O	2.30	0.64
6:LA:2:NAG:H62	6:LA:3:BMA:H2	1.80	0.64
3:C:2933[A]:SER:O	3:C:2936[A]:GLU:HB3	1.96	0.64
3:C:2951[A]:ASP:O	3:C:2956[A]:LYS:CE	2.45	0.64
3:C:2984[A]:THR:HG22	3:C:3151[A]:LEU:HD23	1.77	0.64
3:C:3147[B]:GLU:CD	3:L:3160[B]:SER:O	2.40	0.64
3:C:3211[B]:ASP:OD1	3:C:3211[B]:ASP:N	2.27	0.64
3:C:3252[B]:TYR:HB3	3:L:3253[B]:GLU:CB	2.27	0.64
3:F:2955[B]:GLN:OE1	3:F:3037[B]:TYR:CE1	2.51	0.64
3:F:2982[B]:MET:CE	3:F:3254[B]:MET:HE2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2983[B]:VAL:HB	3:a:3160[B]:SER:HA	1.79	0.64
3:F:3252[B]:TYR:HE1	3:a:3251[B]:ASP:CG	2.04	0.64
3:F:3298[A]:ASN:ND2	3:F:3301[A]:PRO:O	2.30	0.64
1:G:834:ASP:OD1	1:G:834:ASP:N	2.20	0.64
3:I:2969[B]:TYR:CA	3:R:2989[B]:HIS:NE2	2.61	0.64
3:I:3066[B]:TYR:CE1	3:I:3193[B]:HIS:HE1	2.15	0.64
3:I:3149[B]:ASN:OD1	3:I:3150[B]:LYS:HB2	1.96	0.64
3:I:3200[A]:LEU:HD22	3:I:3204[A]:LEU:CD1	2.27	0.64
3:I:3200[B]:LEU:HD22	3:I:3204[B]:LEU:CD1	2.27	0.64
3:I:3228[B]:VAL:HG21	3:I:3245[B]:PHE:CE1	2.32	0.64
2:K:2549:PRO:HG2	2:K:2747:LYS:HD2	1.78	0.64
3:L:2937[B]:ASN:HD22	3:L:3006[B]:LYS:HD3	1.61	0.64
3:L:2965[A]:LEU:CD1	3:L:2975[A]:PHE:H	2.08	0.64
3:L:3066[A]:TYR:CE1	3:L:3193[A]:HIS:HE1	2.15	0.64
3:L:3066[B]:TYR:HD1	3:L:3193[B]:HIS:CE1	2.16	0.64
1:M:260:ASN:OD1	1:M:271:HIS:NE2	2.30	0.64
2:N:2133:PRO:HD3	2:N:2142:ALA:HB2	1.78	0.64
2:N:2390:GLN:NE2	2:N:2494:GLN:O	2.29	0.64
3:O:2937[B]:ASN:HD22	3:O:3006[B]:LYS:HD3	1.61	0.64
3:O:2957[B]:ILE:CA	3:O:2960[B]:PHE:HE1	2.11	0.64
3:O:2965[A]:LEU:CD1	3:O:2975[A]:PHE:H	2.08	0.64
3:O:3014[A]:TRP:CG	3:O:3092[A]:ILE:HD11	2.32	0.64
1:P:588:GLU:OE2	1:P:728:ARG:NH2	2.30	0.64
3:R:2955[A]:GLN:OE1	3:R:3037[A]:TYR:CE1	2.51	0.64
3:R:2969[B]:TYR:HD2	3:R:2971[B]:ASP:N	1.84	0.64
3:R:3066[B]:TYR:CE1	3:R:3193[B]:HIS:HE1	2.15	0.64
3:R:3200[A]:LEU:HD22	3:R:3204[A]:LEU:CD1	2.27	0.64
1:S:37:ILE:HD13	1:S:75:GLN:HG3	1.80	0.64
1:S:909:ILE:HG12	1:S:1084:PHE:HZ	1.62	0.64
3:U:2982[B]:MET:CE	3:U:3254[B]:MET:HE2	2.26	0.64
3:U:3180[A]:TYR:CB	3:U:3183[A]:LEU:HD22	2.27	0.64
2:W:2548:CYS:O	2:W:2554:PRO:HB3	1.97	0.64
3:X:2937[B]:ASN:HB3	3:X:3006[B]:LYS:HD3	1.79	0.64
3:X:3149[B]:ASN:OD1	3:X:3150[B]:LYS:HB2	1.96	0.64
3:X:3196[A]:THR:OG1	3:X:3199[A]:GLN:CG	2.44	0.64
3:X:3200[B]:LEU:HD22	3:X:3204[B]:LEU:CD1	2.27	0.64
3:a:3217[B]:PHE:HE1	3:a:3230[B]:PHE:HZ	0.81	0.64
3:d:2937[A]:ASN:HB3	3:d:3006[A]:LYS:HD3	1.78	0.64
3:d:3066[A]:TYR:HD1	3:d:3193[A]:HIS:CE1	2.16	0.64
1:A:157:GLU:OE2	1:A:296:ARG:NH2	2.31	0.64
3:C:3066[A]:TYR:HD1	3:C:3193[A]:HIS:CE1	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3285[B]:VAL:HG22	3:C:3286[B]:THR:H	1.62	0.64
3:F:2951[A]:ASP:O	3:F:2956[A]:LYS:CE	2.45	0.64
3:F:2955[A]:GLN:OE1	3:F:3037[A]:TYR:CE1	2.51	0.64
3:F:2975[B]:PHE:HA	3:a:3107[B]:LEU:HD21	1.79	0.64
3:F:3066[A]:TYR:HD1	3:F:3193[A]:HIS:CE1	2.16	0.64
3:F:3120[A]:HIS:NE2	9:a:3401[A]:CUO:O1	2.30	0.64
3:F:3132[A]:ALA:HB1	3:F:3197[A]:ILE:CD1	2.26	0.64
1:G:104:LEU:O	1:G:121:ASN:ND2	2.30	0.64
1:G:127:GLU:HG2	1:G:135:THR:H	1.61	0.64
3:I:2937[A]:ASN:ND2	3:I:3006[A]:LYS:HD3	2.11	0.64
3:I:2951[B]:ASP:O	3:I:2956[B]:LYS:CE	2.45	0.64
3:I:2954[A]:TYR:HA	3:I:2957[A]:ILE:HG22	1.80	0.64
3:I:2975[B]:PHE:HA	3:R:3107[B]:LEU:HD22	1.80	0.64
3:I:3066[A]:TYR:CE1	3:I:3193[A]:HIS:HE1	2.15	0.64
3:I:3089[B]:HIS:CE1	3:I:3119[B]:HIS:CE1	2.81	0.64
3:I:3163[B]:ASN:CB	3:R:3149[B]:ASN:ND2	2.61	0.64
3:I:3256[B]:TRP:CB	3:R:2966[B]:SER:C	2.70	0.64
9:I:3401[A]:CUO:O1	3:R:3120[A]:HIS:NE2	2.30	0.64
1:J:118:ALA:HB1	1:J:119:LYS:HA	1.79	0.64
3:L:2965[B]:LEU:CD1	3:L:2975[B]:PHE:H	2.08	0.64
1:M:1164:ASP:CG	1:M:1212:HIS:HE2	2.06	0.64
3:O:2955[A]:GLN:OE1	3:O:3037[A]:TYR:CE1	2.51	0.64
3:O:2965[B]:LEU:CD1	3:O:2975[B]:PHE:H	2.08	0.64
3:O:2971[B]:ASP:N	3:X:2992[B]:TYR:H	1.96	0.64
3:O:3200[A]:LEU:HD22	3:O:3204[A]:LEU:CD1	2.27	0.64
3:O:3200[B]:LEU:HD22	3:O:3204[B]:LEU:CD1	2.27	0.64
3:O:3284[A]:LYS:CD	3:O:3285[A]:VAL:H	2.10	0.64
1:P:1355:LEU:HD11	1:P:1393:THR:HG21	1.77	0.64
3:R:3151[A]:LEU:O	3:R:3174[A]:GLY:HA3	1.96	0.64
3:R:3180[B]:TYR:CB	3:R:3183[B]:LEU:HD22	2.27	0.64
3:R:3228[A]:VAL:HG21	3:R:3245[A]:PHE:CE1	2.32	0.64
1:S:896:HIS:HB2	1:S:905:TRP:CG	2.32	0.64
3:U:2961[A]:HIS:CE1	3:U:2980[A]:HIS:NE2	2.57	0.64
3:U:2969[B]:TYR:CZ	3:d:2980[B]:HIS:CD2	2.86	0.64
3:U:3154[B]:PRO:CA	3:d:3153[B]:LYS:H	2.11	0.64
3:U:3240[B]:THR:HG22	3:U:3241[B]:PHE:N	2.13	0.64
3:U:3254[B]:MET:HE1	3:d:3254[B]:MET:HE3	0.65	0.64
3:U:3258[B]:PHE:HA	3:d:2969[B]:TYR:O	1.98	0.64
1:V:450:LYS:HE3	1:V:505:ARG:HH21	1.61	0.64
2:W:2572:VAL:HG22	2:W:2768:LEU:HD22	1.80	0.64
3:X:2933[B]:SER:O	3:X:2936[B]:GLU:HB3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2951[B]:ASP:O	3:X:2956[B]:LYS:CE	2.45	0.64
3:X:2954[A]:TYR:HA	3:X:2957[A]:ILE:HG22	1.80	0.64
3:X:2955[B]:GLN:OE1	3:X:3037[B]:TYR:CE1	2.50	0.64
3:X:2966[B]:SER:HB2	3:X:2977[B]:CYS:CB	2.21	0.64
3:X:3200[A]:LEU:HD22	3:X:3204[A]:LEU:CD1	2.27	0.64
3:X:3217[B]:PHE:HE1	3:X:3230[B]:PHE:HZ	0.80	0.64
3:X:3298[A]:ASN:HD21	3:X:3301[A]:PRO:HA	1.60	0.64
1:Y:830:ASN:HA	1:Y:831:VAL:C	2.22	0.64
2:Z:2711:HIS:HA	2:Z:2714:VAL:HG22	1.79	0.64
3:a:2948[A]:ASP:HB3	3:a:2953[A]:GLY:CA	2.24	0.64
3:a:3014[A]:TRP:CG	3:a:3092[A]:ILE:HD11	2.32	0.64
3:a:3217[A]:PHE:HB2	3:a:3219[A]:LEU:HD21	1.79	0.64
3:a:3298[B]:ASN:ND2	3:a:3301[B]:PRO:O	2.30	0.64
3:d:3014[A]:TRP:CG	3:d:3092[A]:ILE:HD11	2.32	0.64
3:d:3117[B]:TYR:O	3:d:3120[B]:HIS:HB2	1.97	0.64
3:d:3228[A]:VAL:HG21	3:d:3245[A]:PHE:CE1	2.32	0.64
1:A:630:PHE:O	1:A:633:HIS:HB3	1.98	0.64
2:B:2149:ALA:HA	2:B:2260:GLU:HG2	1.77	0.64
3:C:2982[B]:MET:H	3:L:2967[B]:CYS:HB3	1.62	0.64
3:C:3066[B]:TYR:HD1	3:C:3193[B]:HIS:CE1	2.16	0.64
3:C:3224[B]:GLN:HA	3:L:3252[B]:TYR:OH	1.97	0.64
1:D:1301:PRO:HB3	1:D:1308:VAL:HG12	1.79	0.64
3:F:3092[A]:ILE:HG23	3:F:3096[A]:VAL:CG2	2.28	0.64
3:F:3159[B]:SER:CB	3:a:3150[B]:LYS:O	2.45	0.64
3:F:3232[B]:VAL:CG2	3:F:3273[B]:LEU:HD11	2.27	0.64
1:G:166:GLU:OE2	1:G:297:ARG:NH1	2.31	0.64
3:I:2933[B]:SER:O	3:I:2936[B]:GLU:HB3	1.96	0.64
3:I:2937[A]:ASN:HB3	3:I:3006[A]:LYS:HD3	1.79	0.64
3:I:2952[A]:ALA:H	3:I:2953[A]:GLY:CA	2.04	0.64
3:I:3156[B]:MET:HB3	3:R:2982[B]:MET:HB2	1.80	0.64
3:I:3159[B]:SER:N	3:R:3150[B]:LYS:O	2.31	0.64
3:L:2994[B]:LYS:O	3:L:2995[B]:GLN:C	2.38	0.64
1:M:1018:ILE:HA	1:M:1021:LEU:HB2	1.78	0.64
2:N:2889:ALA:N	2:N:2890:VAL:HA	2.12	0.64
3:R:2937[A]:ASN:HB3	3:R:3006[A]:LYS:HD3	1.79	0.64
3:R:3279[A]:ASP:OD1	3:R:3279[A]:ASP:N	2.25	0.64
3:U:2971[B]:ASP:OD1	3:U:2973[B]:THR:OG1	2.04	0.64
3:U:3117[B]:TYR:O	3:U:3120[B]:HIS:HB2	1.98	0.64
3:U:3162[B]:ASP:CG	3:d:3260[B]:ARG:NH1	2.54	0.64
3:X:3066[A]:TYR:HD1	3:X:3193[A]:HIS:CE1	2.16	0.64
3:a:2937[B]:ASN:ND2	3:a:3006[B]:LYS:HD3	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:2954[A]:TYR:HA	3:a:2957[A]:ILE:HG22	1.80	0.64
3:a:2966[A]:SER:HB2	3:a:2977[A]:CYS:CB	2.21	0.64
3:a:3117[A]:TYR:O	3:a:3120[A]:HIS:HB2	1.97	0.64
3:d:2951[A]:ASP:O	3:d:2956[A]:LYS:CE	2.45	0.64
3:d:3117[A]:TYR:O	3:d:3120[A]:HIS:HB2	1.98	0.64
3:d:3273[A]:LEU:CB	3:d:3275[A]:LEU:HD13	2.28	0.64
3:d:3298[B]:ASN:HD21	3:d:3301[B]:PRO:HA	1.60	0.64
3:C:2937[A]:ASN:HB3	3:C:3006[A]:LYS:HD3	1.79	0.64
3:C:3200[A]:LEU:HD22	3:C:3204[A]:LEU:CD1	2.27	0.64
3:C:3200[B]:LEU:HD22	3:C:3204[B]:LEU:CD1	2.27	0.64
3:F:2965[B]:LEU:C	3:a:3221[B]:ALA:CB	2.71	0.64
3:F:2979[B]:GLN:C	3:a:2967[B]:CYS:HB2	2.23	0.64
3:F:3152[B]:LYS:HD3	3:a:3170[B]:ALA:O	1.89	0.64
3:F:3180[B]:TYR:CB	3:F:3183[B]:LEU:HD22	2.27	0.64
3:F:3259[B]:ASP:CA	3:a:3162[B]:ASP:HB3	2.26	0.64
1:G:729:VAL:HG11	1:G:785:LEU:HD12	1.80	0.64
3:I:2954[B]:TYR:HA	3:I:2957[B]:ILE:HG22	1.80	0.64
3:I:2988[B]:TRP:NE1	3:I:3158[B]:PHE:HE2	1.96	0.64
3:I:2990[A]:ARG:CZ	3:I:3180[A]:TYR:HB3	2.28	0.64
3:I:3116[B]:PHE:HE2	3:R:2969[B]:TYR:CG	1.98	0.64
3:I:3254[B]:MET:O	3:R:2966[B]:SER:OG	2.15	0.64
3:I:3259[B]:ASP:HB3	3:R:3162[B]:ASP:CA	2.27	0.64
3:L:2952[B]:ALA:H	3:L:2953[B]:GLY:CA	2.04	0.64
3:L:2966[A]:SER:HB3	3:L:2977[A]:CYS:HB2	1.78	0.64
3:L:3232[A]:VAL:CG2	3:L:3273[A]:LEU:HD11	2.27	0.64
1:M:567:LEU:HB3	1:M:570:GLN:O	1.97	0.64
3:O:3066[A]:TYR:CE1	3:O:3193[A]:HIS:HE1	2.15	0.64
3:O:3066[B]:TYR:HD1	3:O:3193[B]:HIS:CE1	2.16	0.64
1:P:1348:TRP:HH2	1:P:1461:VAL:HG23	1.63	0.64
1:P:1492:PRO:HB2	1:P:1497:SER:HB3	1.78	0.64
3:R:3014[A]:TRP:CG	3:R:3092[A]:ILE:HD11	2.32	0.64
2:T:2180:TRP:HB2	2:T:2243:LEU:HD22	1.79	0.64
2:T:2240:GLN:HE21	2:T:2241:THR:HG22	1.61	0.64
3:U:2966[B]:SER:HB3	3:U:2977[B]:CYS:HB2	1.78	0.64
3:U:2988[A]:TRP:NE1	3:U:3158[A]:PHE:HE2	1.96	0.64
3:U:3014[B]:TRP:CG	3:U:3092[B]:ILE:HD11	2.32	0.64
3:U:3255[B]:PRO:CD	3:d:3252[B]:TYR:O	2.45	0.64
3:U:3285[B]:VAL:HG22	3:U:3286[B]:THR:H	1.62	0.64
3:X:2948[A]:ASP:HB3	3:X:2953[A]:GLY:CA	2.24	0.64
3:X:2954[B]:TYR:HA	3:X:2957[B]:ILE:HG22	1.80	0.64
3:X:2969[A]:TYR:HD2	3:X:2971[A]:ASP:N	1.84	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3228[A]:VAL:HG21	3:X:3245[A]:PHE:CE1	2.32	0.64
3:X:3284[B]:LYS:CD	3:X:3285[B]:VAL:H	2.10	0.64
1:Y:1620:LEU:C	3:d:3189[B]:ASN:ND2	2.55	0.64
3:a:2990[B]:ARG:CZ	3:a:3180[B]:TYR:HB3	2.28	0.64
3:d:3014[B]:TRP:CG	3:d:3092[B]:ILE:HD11	2.32	0.64
3:C:2928[A]:ASN:OD1	3:C:2929[A]:SER:N	2.31	0.64
3:C:2928[B]:ASN:OD1	3:C:2929[B]:SER:N	2.31	0.64
3:C:2955[B]:GLN:OE1	3:C:3037[B]:TYR:CE1	2.51	0.64
3:C:3157[B]:PRO:N	3:L:2982[B]:MET:SD	2.71	0.64
3:F:3066[A]:TYR:CE1	3:F:3193[A]:HIS:HE1	2.15	0.64
1:G:567:LEU:HB3	1:G:570:GLN:O	1.97	0.64
1:G:1031:ALA:O	1:G:1154:SER:OG	2.10	0.64
3:I:2981[B]:GLY:CA	3:R:2968[B]:GLN:OE1	2.46	0.64
3:I:3090[B]:ASN:HB3	3:R:2972[B]:GLY:C	2.23	0.64
3:I:3153[B]:LYS:C	3:R:3155[B]:MET:N	2.53	0.64
1:J:1358:LEU:HD23	1:J:1456:LEU:HD21	1.79	0.64
1:J:1565:SER:HB3	1:J:1594:GLY:H	1.63	0.64
3:L:3014[B]:TRP:CG	3:L:3092[B]:ILE:HD11	2.32	0.64
3:L:3298[B]:ASN:ND2	3:L:3301[B]:PRO:O	2.30	0.64
2:N:2833:GLY:HA3	2:N:2854:MET:HE1	1.80	0.64
3:O:3120[A]:HIS:NE2	9:O:3401[A]:CUO:O1	2.30	0.64
3:O:3151[B]:LEU:O	3:O:3174[B]:GLY:HA3	1.97	0.64
3:O:3240[B]:THR:HG22	3:O:3241[B]:PHE:N	2.13	0.64
3:R:2951[A]:ASP:O	3:R:2956[A]:LYS:CE	2.45	0.64
3:R:3092[A]:ILE:HG23	3:R:3096[A]:VAL:CG2	2.28	0.64
3:R:3200[B]:LEU:HD22	3:R:3204[B]:LEU:CD1	2.27	0.64
3:R:3273[A]:LEU:CB	3:R:3275[A]:LEU:HD13	2.28	0.64
1:S:749:VAL:HB	1:S:754:GLU:HB3	1.80	0.64
3:U:2948[A]:ASP:CB	3:U:2949[A]:LYS:HA	2.15	0.64
3:U:3212[A]:ARG:HH11	3:U:3212[A]:ARG:CG	2.11	0.64
3:U:3217[A]:PHE:CE2	3:U:3303[A]:PRO:HG3	2.33	0.64
3:U:3298[B]:ASN:HD21	3:U:3301[B]:PRO:HA	1.60	0.64
2:W:2800:LYS:O	3:X:3023[A]:ILE:HD11	1.97	0.64
3:X:2928[B]:ASN:OD1	3:X:2929[B]:SER:N	2.31	0.64
3:X:2988[A]:TRP:NE1	3:X:3158[A]:PHE:HE2	1.96	0.64
3:X:2988[B]:TRP:NE1	3:X:3158[B]:PHE:HE2	1.96	0.64
3:X:3120[A]:HIS:NE2	9:X:3401[A]:CUO:O1	2.30	0.64
3:X:3217[B]:PHE:CE2	3:X:3303[B]:PRO:HG3	2.33	0.64
3:a:2965[B]:LEU:CD1	3:a:2975[B]:PHE:H	2.08	0.64
3:a:2988[A]:TRP:NE1	3:a:3158[A]:PHE:HE2	1.96	0.64
3:a:3092[B]:ILE:HG23	3:a:3096[B]:VAL:CG2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3157[A]:PRO:O	3:a:3160[A]:SER:N	2.30	0.64
1:b:450:LYS:HE3	1:b:451:SER:H	1.61	0.64
3:d:3066[A]:TYR:CE1	3:d:3193[A]:HIS:HE1	2.15	0.64
3:d:3092[B]:ILE:HG23	3:d:3096[B]:VAL:CG2	2.28	0.64
3:d:3200[B]:LEU:HD22	3:d:3204[B]:LEU:CD1	2.27	0.64
1:A:928:TYR:HB3	1:A:1047:SER:HB3	1.80	0.64
3:C:2982[B]:MET:SD	3:L:3156[B]:MET:CA	2.85	0.64
3:C:2990[A]:ARG:CZ	3:C:3180[A]:TYR:HB3	2.28	0.64
3:C:3092[B]:ILE:HG23	3:C:3096[B]:VAL:CG2	2.28	0.64
3:C:3117[A]:TYR:O	3:C:3120[A]:HIS:HB2	1.97	0.64
3:C:3223[B]:GLY:H	3:L:2963[B]:MET:CE	2.07	0.64
3:C:3228[B]:VAL:HG21	3:C:3245[B]:PHE:CE1	2.32	0.64
1:D:1585:ASN:OD1	1:G:329:ARG:NH2	2.32	0.64
3:F:2961[B]:HIS:HB3	3:F:3111[B]:SER:CB	2.28	0.64
3:F:2966[B]:SER:CA	3:a:3255[B]:PRO:O	2.45	0.64
3:F:2982[B]:MET:SD	3:a:3156[B]:MET:HB2	2.37	0.64
3:F:3155[B]:MET:CA	3:a:3153[B]:LYS:HB3	2.28	0.64
3:F:3217[B]:PHE:CE2	3:F:3303[B]:PRO:HG3	2.33	0.64
3:F:3240[A]:THR:HG22	3:F:3241[A]:PHE:N	2.13	0.64
3:F:3255[B]:PRO:O	3:a:2966[B]:SER:CB	2.46	0.64
1:G:911:LEU:HG	1:G:915:ASN:HD21	1.63	0.64
1:G:1471:LEU:HD12	1:G:1537:ILE:HG23	1.79	0.64
3:I:3117[A]:TYR:O	3:I:3120[A]:HIS:HB2	1.98	0.64
3:I:3255[B]:PRO:CD	3:R:2962[B]:GLY:C	2.64	0.64
2:K:2451:LEU:HD22	2:K:2456:LEU:HD11	1.78	0.64
3:O:2955[B]:GLN:OE1	3:O:3037[B]:TYR:CE1	2.51	0.64
3:O:2971[B]:ASP:O	3:X:2988[B]:TRP:CE3	2.50	0.64
3:O:3014[B]:TRP:CG	3:O:3092[B]:ILE:HD11	2.32	0.64
3:O:3089[A]:HIS:CE1	3:O:3119[A]:HIS:CE1	2.81	0.64
3:O:3254[B]:MET:SD	3:X:3154[B]:PRO:HB2	2.37	0.64
1:P:1130:SER:O	1:P:1134:ASN:ND2	2.31	0.64
1:P:1301:PRO:O	1:P:1494:ARG:NH2	2.29	0.64
3:R:2937[B]:ASN:HB3	3:R:3006[B]:LYS:HD3	1.79	0.64
3:R:3066[A]:TYR:HD1	3:R:3193[A]:HIS:CE1	2.16	0.64
1:S:678:ASN:O	1:S:684:ARG:NH1	2.31	0.64
3:U:2928[B]:ASN:OD1	3:U:2929[B]:SER:N	2.31	0.64
3:U:2957[B]:ILE:CA	3:U:2960[B]:PHE:HE1	2.11	0.64
3:U:3066[A]:TYR:CE1	3:U:3193[A]:HIS:HE1	2.15	0.64
3:U:3169[B]:LYS:HD3	3:d:3147[B]:GLU:HA	1.77	0.64
3:U:3298[A]:ASN:HD21	3:U:3301[A]:PRO:HA	1.60	0.64
3:X:2990[B]:ARG:CZ	3:X:3180[B]:TYR:HB3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3117[B]:TYR:O	3:X:3120[B]:HIS:HB2	1.98	0.64
3:X:3217[A]:PHE:HB2	3:X:3219[A]:LEU:HD21	1.78	0.64
3:a:3066[B]:TYR:HD1	3:a:3193[B]:HIS:CE1	2.16	0.64
3:d:2948[B]:ASP:HB3	3:d:2953[B]:GLY:CA	2.24	0.64
3:d:2987[A]:HIS:NE2	3:d:3178[A]:PHE:HE1	1.95	0.64
3:C:2951[B]:ASP:O	3:C:2956[B]:LYS:CE	2.45	0.63
3:C:2965[B]:LEU:HD22	3:L:3253[B]:GLU:CD	2.11	0.63
3:C:2985[B]:PHE:HE2	3:L:2970[B]:PRO:N	1.81	0.63
3:C:3014[A]:TRP:CG	3:C:3092[A]:ILE:HD11	2.32	0.63
3:C:3120[B]:HIS:NE2	3:L:2969[B]:TYR:OH	2.26	0.63
3:C:3124[A]:ASP:OD2	3:C:3187[A]:TYR:OH	2.15	0.63
3:C:3149[B]:ASN:C	3:L:3172[B]:SER:HG	2.05	0.63
3:C:3153[B]:LYS:HZ3	3:L:2988[B]:TRP:HE1	1.44	0.63
3:C:3162[B]:ASP:OD1	3:C:3162[B]:ASP:N	2.31	0.63
3:C:3217[B]:PHE:CE2	3:C:3303[B]:PRO:HG3	2.33	0.63
3:C:3284[B]:LYS:CD	3:C:3285[B]:VAL:H	2.10	0.63
3:F:3176[B]:LYS:HB3	3:F:3176[B]:LYS:HZ2	1.60	0.63
3:F:3217[A]:PHE:CE2	3:F:3303[A]:PRO:HG3	2.33	0.63
1:G:468:CYS:SG	1:G:669:LYS:HB3	2.39	0.63
2:H:2252:GLU:O	2:H:2389:ARG:NH2	2.31	0.63
3:I:2962[B]:GLY:O	3:R:3255[B]:PRO:HG3	1.98	0.63
3:I:2977[B]:CYS:HB2	3:R:2982[B]:MET:CE	2.28	0.63
3:I:3173[B]:THR:C	3:R:3154[B]:PRO:CB	2.68	0.63
3:I:3211[A]:ASP:OD1	3:I:3211[A]:ASP:N	2.27	0.63
3:I:3255[B]:PRO:CB	3:R:2959[B]:SER:HB2	2.15	0.63
1:J:883:CYS:N	1:J:894:CYS:SG	2.70	0.63
1:J:1506:LEU:O	1:J:1510:ASN:ND2	2.28	0.63
3:L:3162[A]:ASP:N	3:L:3162[A]:ASP:OD1	2.31	0.63
3:L:3217[B]:PHE:CE2	3:L:3303[B]:PRO:HG3	2.33	0.63
3:O:2966[A]:SER:HB2	3:O:2977[A]:CYS:CB	2.21	0.63
3:O:2970[B]:PRO:HD2	3:X:2991[B]:LEU:HD13	1.35	0.63
3:O:3092[A]:ILE:HG23	3:O:3096[A]:VAL:CG2	2.28	0.63
3:O:3157[A]:PRO:O	3:O:3160[A]:SER:N	2.30	0.63
3:O:3157[B]:PRO:O	3:O:3160[B]:SER:N	2.30	0.63
3:O:3180[B]:TYR:CB	3:O:3183[B]:LEU:HD22	2.27	0.63
3:R:2937[A]:ASN:ND2	3:R:3006[A]:LYS:HD3	2.11	0.63
3:R:2954[A]:TYR:HA	3:R:2957[A]:ILE:HG22	1.80	0.63
3:R:2965[B]:LEU:CD1	3:R:2975[B]:PHE:H	2.08	0.63
3:R:2987[B]:HIS:NE2	3:R:3178[B]:PHE:HE1	1.96	0.63
3:R:3232[A]:VAL:CG2	3:R:3273[A]:LEU:HD11	2.27	0.63
1:S:806:ASN:OD1	4:9:1:NAG:N2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2969[B]:TYR:CZ	3:d:2980[B]:HIS:NE2	2.66	0.63
3:U:3066[A]:TYR:HD1	3:U:3193[A]:HIS:CE1	2.16	0.63
1:V:327:ASP:OD1	1:V:328:LYS:N	2.31	0.63
3:X:2928[A]:ASN:OD1	3:X:2929[A]:SER:N	2.31	0.63
3:X:2949[A]:LYS:HD3	3:X:2949[A]:LYS:C	2.24	0.63
1:Y:534:ASP:HB2	1:Y:541:LYS:HE2	1.80	0.63
3:a:2930[A]:LEU:H	3:a:2930[A]:LEU:CD2	1.97	0.63
3:a:2990[A]:ARG:CZ	3:a:3180[A]:TYR:HB3	2.28	0.63
3:a:3240[A]:THR:HG22	3:a:3241[A]:PHE:N	2.13	0.63
1:b:1536:SER:N	1:b:1539:GLN:OE1	2.30	0.63
3:d:2949[A]:LYS:HD3	3:d:2949[A]:LYS:C	2.24	0.63
8:0:1:NAG:H61	8:0:2:NAG:N2	2.11	0.63
6:GA:1:NAG:C4	6:GA:2:NAG:C7	2.75	0.63
3:C:2952[B]:ALA:H	3:C:2953[B]:GLY:CA	2.04	0.63
3:C:2954[B]:TYR:HA	3:C:2957[B]:ILE:HG22	1.80	0.63
3:C:2957[A]:ILE:CA	3:C:2960[A]:PHE:HE1	2.11	0.63
3:C:3090[B]:ASN:CB	3:L:2972[B]:GLY:HA3	2.25	0.63
3:C:3217[A]:PHE:CE2	3:C:3303[A]:PRO:HG3	2.33	0.63
3:F:2928[B]:ASN:OD1	3:F:2929[B]:SER:N	2.31	0.63
3:F:2965[B]:LEU:HA	3:a:3253[B]:GLU:HG3	1.78	0.63
3:F:3273[B]:LEU:CB	3:F:3275[B]:LEU:HD13	2.28	0.63
1:G:983:PRO:HG3	1:G:989:THR:HB	1.81	0.63
3:I:2955[A]:GLN:OE1	3:I:3037[A]:TYR:CE1	2.51	0.63
3:I:3066[B]:TYR:HD1	3:I:3193[B]:HIS:CE1	2.16	0.63
3:I:3124[A]:ASP:OD2	3:I:3187[A]:TYR:OH	2.15	0.63
3:L:2937[B]:ASN:HB3	3:L:3006[B]:LYS:HD3	1.79	0.63
3:L:2957[B]:ILE:CA	3:L:2960[B]:PHE:HE1	2.11	0.63
3:L:3066[A]:TYR:HD1	3:L:3193[A]:HIS:CE1	2.16	0.63
3:L:3092[B]:ILE:HG23	3:L:3096[B]:VAL:CG2	2.28	0.63
3:L:3117[A]:TYR:O	3:L:3120[A]:HIS:HB2	1.98	0.63
3:L:3117[B]:TYR:O	3:L:3120[B]:HIS:HB2	1.97	0.63
3:L:3180[A]:TYR:CB	3:L:3183[A]:LEU:HD22	2.27	0.63
3:L:3240[B]:THR:HG22	3:L:3241[B]:PHE:N	2.13	0.63
2:N:2107:LEU:HD23	2:N:2208:PRO:HB2	1.80	0.63
3:O:2928[A]:ASN:OD1	3:O:2929[A]:SER:N	2.31	0.63
3:O:2975[B]:PHE:CD1	3:X:3156[B]:MET:C	2.77	0.63
3:O:2988[A]:TRP:NE1	3:O:3158[A]:PHE:HE2	1.96	0.63
3:O:2990[B]:ARG:CZ	3:O:3180[B]:TYR:HB3	2.28	0.63
3:O:3228[A]:VAL:HG21	3:O:3245[A]:PHE:CE1	2.32	0.63
3:R:3092[B]:ILE:HG23	3:R:3096[B]:VAL:CG2	2.28	0.63
3:R:3117[B]:TYR:O	3:R:3120[B]:HIS:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3240[B]:THR:HG22	3:R:3241[B]:PHE:N	2.13	0.63
2:T:2117:ASP:OD2	2:T:2168:ARG:NH2	2.30	0.63
3:U:2951[B]:ASP:O	3:U:2956[B]:LYS:CE	2.45	0.63
3:U:3066[B]:TYR:HD1	3:U:3193[B]:HIS:CE1	2.16	0.63
3:U:3173[A]:THR:CG2	3:U:3174[A]:GLY:H	2.12	0.63
3:U:3232[A]:VAL:CG2	3:U:3273[A]:LEU:HD11	2.27	0.63
3:U:3256[B]:TRP:CB	3:d:2969[B]:TYR:CA	2.52	0.63
1:V:1627:ARG:NH2	1:V:1629:GLU:OE1	2.30	0.63
3:X:3092[A]:ILE:HG23	3:X:3096[A]:VAL:CG2	2.28	0.63
3:X:3157[B]:PRO:O	3:X:3160[B]:SER:N	2.30	0.63
1:Y:465:PRO:HG2	1:Y:467:LYS:HG2	1.79	0.63
1:Y:563:ILE:HG23	1:Y:565:GLU:HB2	1.80	0.63
1:Y:622:HIS:HE1	1:Y:767:LYS:H	1.46	0.63
3:a:2928[B]:ASN:OD1	3:a:2929[B]:SER:N	2.31	0.63
3:a:3162[B]:ASP:N	3:a:3162[B]:ASP:OD1	2.31	0.63
3:a:3173[B]:THR:CG2	3:a:3174[B]:GLY:H	2.12	0.63
3:a:3285[B]:VAL:HG22	3:a:3286[B]:THR:H	1.61	0.63
3:d:2954[B]:TYR:HA	3:d:2957[B]:ILE:HG22	1.80	0.63
1:A:907:ARG:NH2	1:A:1057:GLN:OE1	2.31	0.63
1:A:1286:ARG:NH2	1:A:1333:GLU:OE2	2.30	0.63
3:C:3120[A]:HIS:NE2	9:L:3401[A]:CUO:O1	2.30	0.63
3:C:3149[B]:ASN:C	3:L:3172[B]:SER:OG	2.40	0.63
3:C:3157[A]:PRO:O	3:C:3160[A]:SER:N	2.30	0.63
3:C:3180[B]:TYR:CB	3:C:3183[B]:LEU:HD22	2.27	0.63
3:C:3232[B]:VAL:CG2	3:C:3273[B]:LEU:HD11	2.27	0.63
3:F:3173[B]:THR:HB	3:F:3176[B]:LYS:HG2	1.81	0.63
3:F:3211[A]:ASP:OD1	3:F:3211[A]:ASP:N	2.28	0.63
9:F:3401[A]:CUO:O1	3:a:3120[A]:HIS:NE2	2.30	0.63
1:G:460:GLU:HB3	1:G:465:PRO:HG2	1.81	0.63
1:G:757:VAL:HG21	1:G:781:ILE:HG22	1.79	0.63
3:I:3180[B]:TYR:CB	3:I:3183[B]:LEU:HD22	2.27	0.63
3:I:3232[B]:VAL:CG2	3:I:3273[B]:LEU:HD11	2.27	0.63
3:L:2949[A]:LYS:HD3	3:L:2949[A]:LYS:C	2.24	0.63
3:L:2951[B]:ASP:O	3:L:2956[B]:LYS:CE	2.45	0.63
3:L:2954[A]:TYR:HA	3:L:2957[A]:ILE:HG22	1.80	0.63
3:L:2955[B]:GLN:OE1	3:L:3037[B]:TYR:CE1	2.51	0.63
3:L:2987[A]:HIS:NE2	3:L:3178[A]:PHE:HE1	1.96	0.63
3:L:2988[A]:TRP:NE1	3:L:3158[A]:PHE:HE2	1.96	0.63
3:O:2954[A]:TYR:HA	3:O:2957[A]:ILE:HG22	1.80	0.63
3:O:2961[B]:HIS:HB3	3:O:3111[B]:SER:CB	2.28	0.63
3:O:3298[A]:ASN:HD21	3:O:3301[A]:PRO:HA	1.60	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:843:VAL:HG13	1:P:927:PRO:HB2	1.81	0.63
3:R:3066[B]:TYR:HD1	3:R:3193[B]:HIS:CE1	2.16	0.63
3:R:3117[A]:TYR:O	3:R:3120[A]:HIS:HB2	1.98	0.63
3:U:2955[A]:GLN:OE1	3:U:3037[A]:TYR:CE1	2.51	0.63
3:U:2961[B]:HIS:HB3	3:U:3111[B]:SER:CB	2.28	0.63
3:U:3200[B]:LEU:HD22	3:U:3204[B]:LEU:CD1	2.27	0.63
3:U:3252[B]:TYR:CE2	3:d:3222[B]:ILE:HD12	2.22	0.63
1:V:972:SER:HA	1:V:1028:VAL:HG22	1.80	0.63
3:X:2949[B]:LYS:HD3	3:X:2949[B]:LYS:C	2.23	0.63
3:X:2961[B]:HIS:CE1	3:X:2980[B]:HIS:NE2	2.57	0.63
3:X:2961[B]:HIS:HB3	3:X:3111[B]:SER:CB	2.29	0.63
3:X:2994[A]:LYS:O	3:X:2995[A]:GLN:C	2.38	0.63
3:X:3066[B]:TYR:CE1	3:X:3193[B]:HIS:HE1	2.15	0.63
3:X:3089[A]:HIS:CE1	3:X:3119[A]:HIS:CE1	2.81	0.63
1:Y:675:SER:O	1:Y:679:ASN:ND2	2.31	0.63
3:a:3014[B]:TRP:CG	3:a:3092[B]:ILE:HD11	2.32	0.63
3:a:3096[A]:VAL:HG11	3:a:3115[A]:LEU:HD13	1.81	0.63
3:a:3180[A]:TYR:CB	3:a:3183[A]:LEU:HD22	2.27	0.63
1:b:43:GLU:HG3	1:b:44:PRO:HA	1.81	0.63
3:d:2961[B]:HIS:HB3	3:d:3111[B]:SER:CB	2.28	0.63
3:d:2988[A]:TRP:NE1	3:d:3158[A]:PHE:HE2	1.96	0.63
3:d:3173[B]:THR:HB	3:d:3176[B]:LYS:HG2	1.81	0.63
3:d:3217[A]:PHE:CE2	3:d:3303[A]:PRO:HG3	2.33	0.63
3:d:3217[B]:PHE:HE1	3:d:3230[B]:PHE:HZ	0.80	0.63
1:A:1210:LYS:HA	1:A:1211:TYR:CD2	2.34	0.63
3:C:3096[B]:VAL:HG11	3:C:3115[B]:LEU:HD13	1.81	0.63
3:C:3298[B]:ASN:CB	3:C:3300[B]:LEU:N	2.60	0.63
3:F:3228[B]:VAL:HG21	3:F:3245[B]:PHE:CE1	2.32	0.63
1:G:1321:HIS:HD2	1:G:1465:TRP:CH2	2.17	0.63
3:I:3092[B]:ILE:HG23	3:I:3096[B]:VAL:CG2	2.28	0.63
3:I:3173[A]:THR:CG2	3:I:3174[A]:GLY:H	2.12	0.63
3:I:3232[A]:VAL:CG2	3:I:3273[A]:LEU:HD11	2.27	0.63
3:L:2954[B]:TYR:HA	3:L:2957[B]:ILE:HG22	1.80	0.63
1:M:167:ASP:OD1	1:M:167:ASP:N	2.31	0.63
2:N:2166:LEU:HA	2:N:2169:HIS:HB2	1.80	0.63
3:O:2949[A]:LYS:C	3:O:2949[A]:LYS:HD3	2.24	0.63
3:O:2990[A]:ARG:CZ	3:O:3180[A]:TYR:HB3	2.28	0.63
3:O:3155[B]:MET:HG3	3:O:3172[B]:SER:O	1.99	0.63
1:P:757:VAL:HG21	1:P:781:ILE:HG23	1.80	0.63
3:R:2928[B]:ASN:OD1	3:R:2929[B]:SER:N	2.31	0.63
3:R:2988[B]:TRP:NE1	3:R:3158[B]:PHE:HE2	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:566:ARG:HG3	1:S:567:LEU:HB2	1.79	0.63
3:U:2971[B]:ASP:C	3:d:3090[B]:ASN:ND2	2.57	0.63
3:U:2988[B]:TRP:NE1	3:U:3158[B]:PHE:HE2	1.96	0.63
3:U:3092[A]:ILE:HG23	3:U:3096[A]:VAL:CG2	2.28	0.63
3:U:3155[B]:MET:HG3	3:U:3172[B]:SER:O	1.99	0.63
2:W:2472:ASN:HD21	4:HA:1:NAG:C6	2.06	0.63
3:X:2957[A]:ILE:CA	3:X:2960[A]:PHE:HE1	2.11	0.63
3:X:2966[A]:SER:HB2	3:X:2977[A]:CYS:CB	2.21	0.63
3:X:3120[B]:HIS:NE2	9:X:3401[B]:CUO:O1	2.30	0.63
3:X:3124[B]:ASP:OD2	3:X:3187[B]:TYR:OH	2.15	0.63
3:X:3169[B]:LYS:C	3:X:3172[B]:SER:HG	2.00	0.63
3:X:3217[A]:PHE:CE2	3:X:3303[A]:PRO:HG3	2.33	0.63
3:X:3285[B]:VAL:HG22	3:X:3286[B]:THR:H	1.62	0.63
1:Y:1301:PRO:HB3	1:Y:1308:VAL:HG12	1.81	0.63
2:Z:2166:LEU:HA	2:Z:2169:HIS:HB2	1.80	0.63
3:a:2928[A]:ASN:OD1	3:a:2929[A]:SER:N	2.31	0.63
3:a:2957[B]:ILE:CA	3:a:2960[B]:PHE:HE1	2.11	0.63
3:a:3066[A]:TYR:HD1	3:a:3193[A]:HIS:CE1	2.16	0.63
3:a:3066[A]:TYR:CE1	3:a:3193[A]:HIS:HE1	2.15	0.63
3:a:3217[B]:PHE:CE2	3:a:3303[B]:PRO:HG3	2.33	0.63
1:b:1046:HIS:HA	1:b:1049:VAL:HB	1.79	0.63
3:d:2966[B]:SER:HB2	3:d:2977[B]:CYS:CB	2.21	0.63
3:C:2994[B]:LYS:O	3:C:2995[B]:GLN:C	2.38	0.63
3:C:3154[B]:PRO:HB2	3:L:3151[B]:LEU:C	2.22	0.63
3:C:3162[A]:ASP:OD1	3:C:3162[A]:ASP:N	2.31	0.63
1:D:1067:TYR:H	1:D:1067:TYR:HD1	1.45	0.63
3:F:2928[A]:ASN:OD1	3:F:2929[A]:SER:N	2.31	0.63
3:F:2961[A]:HIS:HB3	3:F:3111[A]:SER:CB	2.29	0.63
3:F:2988[B]:TRP:NE1	3:F:3158[B]:PHE:HE2	1.96	0.63
3:F:3096[B]:VAL:HG11	3:F:3115[B]:LEU:HD13	1.81	0.63
3:F:3153[B]:LYS:C	3:a:3155[B]:MET:CB	2.69	0.63
1:G:437:TYR:HB3	1:G:985:PHE:HZ	1.64	0.63
3:I:2961[A]:HIS:HB3	3:I:3111[A]:SER:CB	2.29	0.63
3:I:2961[B]:HIS:HB3	3:I:3111[B]:SER:CB	2.29	0.63
3:I:2969[B]:TYR:HD2	3:R:3093[B]:HIS:NE2	1.95	0.63
3:I:2994[B]:LYS:O	3:I:2995[B]:GLN:C	2.38	0.63
3:I:3066[A]:TYR:HD1	3:I:3193[A]:HIS:CE1	2.16	0.63
3:I:3252[B]:TYR:O	3:R:2976[B]:ALA:CB	2.47	0.63
3:I:3273[B]:LEU:CB	3:I:3275[B]:LEU:HD13	2.28	0.63
3:I:3285[B]:VAL:HG22	3:I:3286[B]:THR:H	1.61	0.63
1:J:1427:HIS:HE1	1:J:1458:HIS:NE2	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2955[A]:GLN:OE1	3:L:3037[A]:TYR:CE1	2.51	0.63
3:L:3212[B]:ARG:HH11	3:L:3212[B]:ARG:CG	2.12	0.63
3:L:3217[A]:PHE:HE1	3:L:3230[A]:PHE:HZ	0.81	0.63
3:L:3284[A]:LYS:CD	3:L:3285[A]:VAL:H	2.10	0.63
1:M:961:SER:OG	1:M:974:ALA:N	2.31	0.63
3:O:2954[B]:TYR:HA	3:O:2957[B]:ILE:HG22	1.80	0.63
3:O:2957[A]:ILE:CA	3:O:2960[A]:PHE:HE1	2.11	0.63
3:O:3117[A]:TYR:O	3:O:3120[A]:HIS:HB2	1.97	0.63
3:O:3155[A]:MET:HG3	3:O:3172[A]:SER:O	1.99	0.63
3:O:3198[B]:PRO:HD3	1:P:1618:LEU:O	1.97	0.63
3:O:3228[A]:VAL:HG12	3:O:3287[A]:ILE:CG1	2.29	0.63
3:O:3232[B]:VAL:CG2	3:O:3273[B]:LEU:HD11	2.27	0.63
3:O:3255[B]:PRO:HG2	3:X:3163[B]:ASN:CG	2.24	0.63
3:O:3256[B]:TRP:HE1	3:X:3161[B]:GLU:CD	2.07	0.63
3:O:3285[A]:VAL:HG22	3:O:3286[A]:THR:H	1.62	0.63
3:R:3066[B]:TYR:CD1	3:R:3193[B]:HIS:HE1	2.17	0.63
2:T:2630:LYS:O	2:T:2632:GLU:N	2.30	0.63
3:U:2928[A]:ASN:OD1	3:U:2929[A]:SER:N	2.31	0.63
3:U:3155[A]:MET:HG3	3:U:3172[A]:SER:O	1.99	0.63
3:U:3162[B]:ASP:N	3:U:3162[B]:ASP:OD1	2.31	0.63
3:U:3217[B]:PHE:CE2	3:U:3303[B]:PRO:HG3	2.33	0.63
3:U:3228[A]:VAL:HG12	3:U:3287[A]:ILE:CG1	2.29	0.63
3:U:3284[B]:LYS:CD	3:U:3285[B]:VAL:H	2.09	0.63
2:W:2684:HIS:NE2	2:W:2711:HIS:CE1	2.66	0.63
3:X:2965[B]:LEU:CD1	3:X:2975[B]:PHE:H	2.08	0.63
3:X:3120[B]:HIS:C	3:X:3122[B]:ASN:N	2.55	0.63
3:X:3173[B]:THR:HB	3:X:3176[B]:LYS:HG2	1.81	0.63
3:X:3285[A]:VAL:HG22	3:X:3286[A]:THR:H	1.62	0.63
1:Y:932:THR:HG22	1:Y:995:ILE:HD12	1.80	0.63
3:a:2951[B]:ASP:O	3:a:2956[B]:LYS:CE	2.45	0.63
3:a:2988[B]:TRP:NE1	3:a:3158[B]:PHE:HE2	1.96	0.63
3:a:3092[A]:ILE:HG23	3:a:3096[A]:VAL:CG2	2.28	0.63
3:a:3173[B]:THR:HB	3:a:3176[B]:LYS:HG2	1.81	0.63
3:a:3212[A]:ARG:HH11	3:a:3212[A]:ARG:CG	2.12	0.63
1:b:533:VAL:HG12	1:b:540:THR:HG22	1.81	0.63
2:c:2800:LYS:HB3	3:d:3023[A]:ILE:CD1	2.29	0.63
3:d:3155[A]:MET:HG3	3:d:3172[A]:SER:O	1.99	0.63
1:A:804:ASP:OD2	4:f:1:NAG:O6	2.16	0.63
2:B:2799:LYS:HB3	2:B:2907:LYS:HD3	1.79	0.63
3:C:2965[B]:LEU:CD1	3:C:2975[B]:PHE:H	2.08	0.63
3:C:2971[B]:ASP:CG	3:L:3248[B]:LEU:CD2	2.71	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2972[B]:GLY:C	3:L:3090[B]:ASN:HB3	2.23	0.63
3:C:3149[B]:ASN:CB	3:L:3169[B]:LYS:N	2.34	0.63
3:C:3211[A]:ASP:OD1	3:C:3211[A]:ASP:N	2.28	0.63
1:D:898:GLY:HA2	1:D:1186:TRP:HB2	1.80	0.63
1:D:1244:GLY:HA2	1:D:1476:LYS:HD3	1.79	0.63
3:F:3135[B]:LYS:HG3	3:F:3141[B]:TYR:CD1	2.33	0.63
1:G:931:TRP:CG	1:G:1018:ILE:HD11	2.34	0.63
1:G:1396:GLU:OE2	1:G:1569:ARG:NH2	2.32	0.63
3:I:2988[A]:TRP:NE1	3:I:3158[A]:PHE:HE2	1.96	0.63
3:I:3092[A]:ILE:HG23	3:I:3096[A]:VAL:CG2	2.28	0.63
3:I:3161[B]:GLU:HG2	3:R:3079[B]:CYS:CB	2.29	0.63
3:I:3217[B]:PHE:CE2	3:I:3303[B]:PRO:HG3	2.33	0.63
3:I:3240[A]:THR:HG22	3:I:3241[A]:PHE:N	2.13	0.63
3:I:3284[B]:LYS:HA	3:I:3284[B]:LYS:CE	2.22	0.63
3:I:3285[A]:VAL:HG22	3:I:3286[A]:THR:H	1.62	0.63
1:J:119:LYS:HB2	1:J:120:LYS:C	2.24	0.63
1:J:838:ARG:NH2	1:J:915:ASN:OD1	2.31	0.63
3:L:2988[B]:TRP:NE1	3:L:3158[B]:PHE:HE2	1.96	0.63
3:L:3092[A]:ILE:HG23	3:L:3096[A]:VAL:CG2	2.28	0.63
3:L:3124[B]:ASP:OD2	3:L:3187[B]:TYR:OH	2.15	0.63
3:L:3228[A]:VAL:HG21	3:L:3245[A]:PHE:CE1	2.32	0.63
3:L:3228[A]:VAL:HG12	3:L:3287[A]:ILE:CG1	2.29	0.63
3:O:2961[A]:HIS:HB3	3:O:3111[A]:SER:CB	2.29	0.63
3:O:2988[B]:TRP:NE1	3:O:3158[B]:PHE:HE2	1.96	0.63
3:O:3066[A]:TYR:CD1	3:O:3193[A]:HIS:HE1	2.17	0.63
3:O:3109[B]:TYR:CZ	3:X:2969[B]:TYR:O	2.52	0.63
3:O:3284[B]:LYS:CD	3:O:3285[B]:VAL:H	2.10	0.63
1:P:401:VAL:HG22	1:P:662:SER:HB3	1.80	0.63
1:P:1170:MET:HB3	1:P:1203:MET:HE2	1.81	0.63
1:P:1470:GLU:HG3	1:P:1530:LEU:HD12	1.80	0.63
3:R:2949[B]:LYS:HD3	3:R:2949[B]:LYS:C	2.24	0.63
3:R:2957[B]:ILE:CA	3:R:2960[B]:PHE:HE1	2.11	0.63
3:R:3240[A]:THR:HG22	3:R:3241[A]:PHE:N	2.13	0.63
3:U:2969[B]:TYR:N	3:d:3256[B]:TRP:CD1	2.66	0.63
3:U:3200[A]:LEU:HD22	3:U:3204[A]:LEU:CD1	2.27	0.63
3:X:2937[A]:ASN:HD22	3:X:3006[A]:LYS:HD3	1.61	0.63
3:X:2961[A]:HIS:HB3	3:X:3111[A]:SER:CB	2.29	0.63
1:Y:327:ASP:OD1	1:Y:328:LYS:N	2.30	0.63
1:Y:622:HIS:CE1	1:Y:767:LYS:H	2.16	0.63
3:a:2949[B]:LYS:C	3:a:2949[B]:LYS:HD3	2.24	0.63
3:a:3180[B]:TYR:CB	3:a:3183[B]:LEU:HD22	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:1462:ASP:OD2	1:b:1525:TYR:OH	2.15	0.63
3:d:2955[B]:GLN:OE1	3:d:3037[B]:TYR:CE1	2.51	0.63
3:d:2988[B]:TRP:NE1	3:d:3158[B]:PHE:HE2	1.96	0.63
3:d:3228[A]:VAL:HG12	3:d:3287[A]:ILE:CG1	2.29	0.63
3:d:3285[A]:VAL:HG22	3:d:3286[A]:THR:H	1.62	0.63
2:B:2851:ASN:HD21	1:D:1189:ASP:HB2	1.62	0.63
3:C:3086[B]:GLU:CG	3:L:2968[B]:GLN:HE21	2.12	0.63
3:C:3153[B]:LYS:C	3:L:3155[B]:MET:HG2	2.22	0.63
3:C:3228[B]:VAL:HG12	3:C:3287[B]:ILE:CG1	2.29	0.63
1:D:1290:ILE:HD13	1:D:1329:LEU:HG	1.79	0.63
2:E:2868:GLU:CD	2:E:2868:GLU:H	2.07	0.63
3:F:2949[A]:LYS:HD3	3:F:2949[A]:LYS:C	2.24	0.63
3:F:2954[B]:TYR:HA	3:F:2957[B]:ILE:HG22	1.80	0.63
3:F:3092[B]:ILE:HG23	3:F:3096[B]:VAL:CG2	2.28	0.63
3:F:3163[B]:ASN:HB2	3:a:3150[B]:LYS:CE	2.26	0.63
3:F:3252[B]:TYR:HA	3:a:3108[B]:HIS:NE2	2.12	0.63
3:F:3255[B]:PRO:C	3:a:2966[B]:SER:HA	2.24	0.63
3:F:3273[A]:LEU:CB	3:F:3275[A]:LEU:HD13	2.28	0.63
3:I:2990[B]:ARG:CZ	3:I:3180[B]:TYR:HB3	2.28	0.63
3:I:3228[A]:VAL:HG12	3:I:3287[A]:ILE:CG1	2.29	0.63
1:J:590:ASP:O	1:J:648:GLN:NE2	2.32	0.63
3:L:2961[B]:HIS:HB3	3:L:3111[B]:SER:CB	2.28	0.63
1:M:965:ASP:OD2	1:M:969:ALA:N	2.31	0.63
1:M:1212:HIS:H	1:M:1212:HIS:CD2	2.15	0.63
1:M:1427:HIS:CE1	1:M:1458:HIS:NE2	2.66	0.63
3:O:3124[B]:ASP:OD2	3:O:3187[B]:TYR:OH	2.15	0.63
3:O:3232[A]:VAL:CG2	3:O:3273[A]:LEU:HD11	2.27	0.63
3:R:2957[A]:ILE:HA	3:R:2960[A]:PHE:HE1	1.64	0.63
2:T:2746:MET:HE3	2:T:2765:PRO:HG3	1.80	0.63
3:U:2975[B]:PHE:CE2	3:d:3254[B]:MET:CB	2.79	0.63
3:U:2980[B]:HIS:CB	3:d:2969[B]:TYR:CE1	2.69	0.63
3:U:3169[B]:LYS:CD	3:d:3148[B]:ILE:H	2.08	0.63
3:U:3173[A]:THR:HB	3:U:3176[A]:LYS:HG2	1.81	0.63
3:U:3173[B]:THR:HB	3:U:3176[B]:LYS:HG2	1.81	0.63
3:U:3240[A]:THR:HG22	3:U:3241[A]:PHE:N	2.13	0.63
3:X:2990[A]:ARG:CZ	3:X:3180[A]:TYR:HB3	2.28	0.63
3:X:3155[B]:MET:HG3	3:X:3172[B]:SER:O	1.99	0.63
1:Y:1335:LEU:HD23	1:Y:1339:SER:HB3	1.80	0.63
3:a:2937[B]:ASN:HB3	3:a:3006[B]:LYS:HD3	1.79	0.63
3:a:3228[B]:VAL:HG12	3:a:3287[B]:ILE:CG1	2.29	0.63
1:b:898:GLY:N	1:b:899:MET:HA	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:1438:ASP:OD1	1:b:1439:VAL:N	2.32	0.63
3:d:2961[A]:HIS:HB3	3:d:3111[A]:SER:CB	2.29	0.63
3:d:2966[A]:SER:HB3	3:d:2977[A]:CYS:HB2	1.78	0.63
3:d:3151[A]:LEU:O	3:d:3174[A]:GLY:HA3	1.97	0.63
3:d:3180[A]:TYR:CB	3:d:3183[A]:LEU:HD22	2.27	0.63
3:d:3217[B]:PHE:CE2	3:d:3303[B]:PRO:HG3	2.34	0.63
1:A:460:GLU:OE2	1:A:1368:ARG:NH2	2.30	0.63
3:C:3092[A]:ILE:HG23	3:C:3096[A]:VAL:CG2	2.28	0.63
3:C:3146[B]:CYS:SG	3:L:3161[B]:GLU:HG3	2.34	0.63
3:C:3159[B]:SER:CB	3:L:3150[B]:LYS:O	2.46	0.63
3:C:3173[A]:THR:CG2	3:C:3174[A]:GLY:H	2.12	0.63
3:C:3240[B]:THR:HG22	3:C:3241[B]:PHE:N	2.13	0.63
1:D:949:ASP:OD1	1:D:950:ALA:N	2.26	0.63
3:F:2930[A]:LEU:HD22	3:F:2930[A]:LEU:N	2.02	0.63
3:F:2988[B]:TRP:CH2	3:a:2975[B]:PHE:CE2	2.86	0.63
3:F:3066[B]:TYR:HD1	3:F:3193[B]:HIS:CE1	2.16	0.63
3:F:3160[B]:SER:CA	3:a:3150[B]:LYS:HZ2	2.12	0.63
3:F:3169[B]:LYS:CD	3:a:3148[B]:ILE:C	2.30	0.63
3:F:3284[B]:LYS:CD	3:F:3285[B]:VAL:H	2.10	0.63
1:G:1576:THR:HG23	1:G:1581:GLU:HG2	1.80	0.63
3:I:2957[A]:ILE:CA	3:I:2960[A]:PHE:HE1	2.11	0.63
3:I:3147[B]:GLU:HG3	3:R:3160[B]:SER:O	1.97	0.63
1:J:730:PHE:HA	1:J:780:GLU:HA	1.79	0.63
1:J:804:ASP:OD1	1:J:805:VAL:N	2.32	0.63
1:J:1472:GLN:OE1	1:J:1475:ARG:NH1	2.32	0.63
3:L:3124[A]:ASP:OD2	3:L:3187[A]:TYR:OH	2.15	0.63
3:L:3217[A]:PHE:CE2	3:L:3303[A]:PRO:HG3	2.33	0.63
3:O:3240[A]:THR:HG22	3:O:3241[A]:PHE:N	2.13	0.63
3:R:2957[A]:ILE:CA	3:R:2960[A]:PHE:HE1	2.11	0.63
3:U:2957[A]:ILE:CA	3:U:2960[A]:PHE:HE1	2.11	0.63
3:U:2965[A]:LEU:CD1	3:U:2975[A]:PHE:H	2.08	0.63
3:U:3089[B]:HIS:CE1	3:U:3119[B]:HIS:CE1	2.81	0.63
3:U:3092[B]:ILE:HG23	3:U:3096[B]:VAL:CG2	2.28	0.63
3:U:3096[B]:VAL:HG11	3:U:3115[B]:LEU:HD13	1.81	0.63
3:U:3120[B]:HIS:NE2	9:U:3401[B]:CUO:O1	2.30	0.63
3:U:3173[B]:THR:CG2	3:U:3174[B]:GLY:H	2.12	0.63
1:V:898:GLY:N	1:V:899:MET:HA	2.14	0.63
3:X:3155[A]:MET:HG3	3:X:3172[A]:SER:O	1.99	0.63
3:X:3173[A]:THR:HB	3:X:3176[A]:LYS:HG2	1.81	0.63
3:X:3173[A]:THR:CG2	3:X:3174[A]:GLY:H	2.12	0.63
3:X:3240[A]:THR:HG22	3:X:3241[A]:PHE:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1655:SER:C	3:d:3006[B]:LYS:HZ3	2.05	0.63
2:Z:2345:ASN:HB3	2:Z:2348:THR:HB	1.81	0.63
3:a:2961[B]:HIS:HB3	3:a:3111[B]:SER:CB	2.29	0.63
3:a:3162[A]:ASP:OD1	3:a:3162[A]:ASP:N	2.31	0.63
3:a:3173[A]:THR:CG2	3:a:3174[A]:GLY:H	2.12	0.63
2:c:2133:PRO:HG2	2:c:2140:ARG:HA	1.81	0.63
3:d:2957[A]:ILE:CA	3:d:2960[A]:PHE:HE1	2.11	0.63
3:d:2957[B]:ILE:CA	3:d:2960[B]:PHE:HE1	2.11	0.63
3:d:2990[A]:ARG:CZ	3:d:3180[A]:TYR:HB3	2.28	0.63
3:d:3240[A]:THR:HG22	3:d:3241[A]:PHE:N	2.13	0.63
1:A:639:ARG:NH2	1:A:707:PHE:O	2.31	0.63
3:C:2965[A]:LEU:CD1	3:C:2975[A]:PHE:H	2.08	0.63
3:C:3156[B]:MET:CG	3:L:2982[B]:MET:CB	2.77	0.63
3:C:3253[B]:GLU:HG3	3:L:2976[B]:ALA:HB2	1.79	0.63
1:D:1494:ARG:HG3	1:D:1494:ARG:NH1	2.05	0.63
3:F:2971[B]:ASP:C	3:a:3093[B]:HIS:CD2	2.48	0.63
3:F:3212[A]:ARG:HH11	3:F:3212[A]:ARG:CG	2.11	0.63
1:G:804:ASP:OD2	1:G:806:ASN:ND2	2.32	0.63
3:I:2982[B]:MET:HG3	3:R:3156[B]:MET:CB	2.21	0.63
3:I:3117[B]:TYR:O	3:I:3120[B]:HIS:HB2	1.98	0.63
3:I:3279[B]:ASP:OD1	3:I:3279[B]:ASP:N	2.25	0.63
2:K:2128:LEU:HD23	2:K:2216:PHE:HZ	1.62	0.63
3:L:2928[A]:ASN:OD1	3:L:2929[A]:SER:N	2.31	0.63
3:L:2949[B]:LYS:HD3	3:L:2949[B]:LYS:C	2.23	0.63
3:L:2961[A]:HIS:HB3	3:L:3111[A]:SER:CB	2.29	0.63
2:N:2446:GLU:HG2	2:N:2448:THR:HG22	1.81	0.63
3:O:3066[B]:TYR:CD1	3:O:3193[B]:HIS:HE1	2.17	0.63
3:O:3135[B]:LYS:CB	3:O:3141[B]:TYR:HD1	2.12	0.63
3:O:3162[A]:ASP:N	3:O:3162[A]:ASP:OD1	2.31	0.63
3:O:3211[B]:ASP:OD1	3:O:3211[B]:ASP:N	2.28	0.63
3:O:3212[B]:ARG:HH11	3:O:3212[B]:ARG:CG	2.12	0.63
3:R:2988[A]:TRP:NE1	3:R:3158[A]:PHE:HE2	1.96	0.63
3:R:3114[A]:PRO:CD	3:R:3115[A]:LEU:H	2.12	0.63
3:R:3217[A]:PHE:CE2	3:R:3303[A]:PRO:HG3	2.33	0.63
3:R:3273[B]:LEU:CB	3:R:3275[B]:LEU:HD13	2.28	0.63
3:U:2990[B]:ARG:CZ	3:U:3180[B]:TYR:HB3	2.28	0.63
3:U:3066[A]:TYR:CD1	3:U:3193[A]:HIS:HE1	2.17	0.63
3:U:3066[B]:TYR:CD1	3:U:3193[B]:HIS:HE1	2.17	0.63
3:U:3120[A]:HIS:NE2	9:U:3401[A]:CUO:O1	2.30	0.63
3:U:3157[A]:PRO:O	3:U:3160[A]:SER:N	2.30	0.63
3:U:3307[B]:PHE:HE1	3:U:3309[B]:PRO:CG	2.08	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:965:ASP:OD1	1:V:965:ASP:N	2.28	0.63
1:Y:930:ASP:OD1	1:Y:1051:ARG:NH2	2.32	0.63
2:Z:2107:LEU:HD23	2:Z:2208:PRO:HB2	1.80	0.63
2:Z:2866:PRO:HG3	3:a:2933[A]:SER:OG	1.99	0.63
3:a:2957[A]:ILE:CA	3:a:2960[A]:PHE:HE1	2.11	0.63
3:a:3155[A]:MET:HG3	3:a:3172[A]:SER:O	1.99	0.63
2:c:2235:PRO:HG3	2:c:2240:GLN:HE22	1.64	0.63
3:d:3066[A]:TYR:CD1	3:d:3193[A]:HIS:HE1	2.17	0.63
3:d:3114[B]:PRO:CD	3:d:3115[B]:LEU:H	2.12	0.63
3:d:3157[A]:PRO:O	3:d:3160[A]:SER:N	2.30	0.63
3:d:3173[A]:THR:CG2	3:d:3174[A]:GLY:H	2.12	0.63
3:d:3212[A]:ARG:HH11	3:d:3212[A]:ARG:CG	2.12	0.63
3:d:3240[B]:THR:HG22	3:d:3241[B]:PHE:N	2.13	0.63
3:C:2960[B]:PHE:H	3:C:2960[B]:PHE:HD1	1.41	0.62
3:C:2988[B]:TRP:NE1	3:C:3158[B]:PHE:HE2	1.96	0.62
3:C:2990[B]:ARG:CZ	3:C:3180[B]:TYR:HB3	2.28	0.62
3:C:3066[B]:TYR:CD1	3:C:3193[B]:HIS:HE1	2.17	0.62
3:C:3173[B]:THR:CG2	3:C:3174[B]:GLY:H	2.12	0.62
1:D:1636:ASN:OD1	1:D:1636:ASN:N	2.29	0.62
3:F:2937[A]:ASN:HB3	3:F:3006[A]:LYS:HD3	1.78	0.62
3:F:2957[A]:ILE:N	3:F:2960[A]:PHE:HE1	1.97	0.62
3:F:2990[A]:ARG:CZ	3:F:3180[A]:TYR:HB3	2.28	0.62
1:G:104:LEU:HB3	1:G:123:PHE:HD2	1.64	0.62
1:G:1240:ILE:HG13	1:G:1247:ARG:HG3	1.80	0.62
1:G:1329:LEU:HB2	1:G:1507:THR:HG21	1.80	0.62
3:I:2928[A]:ASN:OD1	3:I:2929[A]:SER:N	2.31	0.62
3:I:2957[B]:ILE:CA	3:I:2960[B]:PHE:HE1	2.11	0.62
3:I:2965[B]:LEU:CB	3:R:3253[B]:GLU:OE2	2.40	0.62
3:I:2987[A]:HIS:NE2	3:I:3178[A]:PHE:HE1	1.96	0.62
3:I:3066[B]:TYR:CD1	3:I:3193[B]:HIS:HE1	2.17	0.62
3:I:3162[B]:ASP:H	3:R:2983[B]:VAL:CG2	2.12	0.62
3:I:3212[B]:ARG:HH11	3:I:3212[B]:ARG:CG	2.12	0.62
3:I:3217[A]:PHE:CE2	3:I:3303[A]:PRO:HG3	2.33	0.62
1:J:392:PRO:HB2	1:J:394:GLN:HG2	1.79	0.62
1:J:1013:ILE:HD11	1:J:1175:PHE:CD2	2.33	0.62
1:M:1441:SER:OG	1:M:1442:MET:N	2.31	0.62
2:N:2728:ARG:NH1	2:N:2792:GLU:OE1	2.28	0.62
2:N:2825:ILE:HB	2:N:2865:ILE:HD11	1.80	0.62
2:N:2890:VAL:N	2:N:2891:LEU:HA	2.12	0.62
3:O:2957[A]:ILE:HA	3:O:2960[A]:PHE:HE1	1.64	0.62
3:O:2957[B]:ILE:HA	3:O:2960[B]:PHE:HE1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3169[B]:LYS:CG	3:X:3148[B]:ILE:HG23	1.85	0.62
3:R:2966[B]:SER:HB3	3:R:2977[B]:CYS:HB2	1.78	0.62
3:R:2990[B]:ARG:CZ	3:R:3180[B]:TYR:HB3	2.28	0.62
3:R:3066[A]:TYR:CD1	3:R:3193[A]:HIS:HE1	2.17	0.62
3:R:3135[B]:LYS:HG3	3:R:3141[B]:TYR:CD1	2.33	0.62
1:S:416:ASN:CG	3:X:3196[A]:THR:CG2	2.32	0.62
3:U:2954[A]:TYR:HA	3:U:2957[A]:ILE:HG22	1.80	0.62
3:X:3092[B]:ILE:HG23	3:X:3096[B]:VAL:CG2	2.28	0.62
3:X:3117[A]:TYR:O	3:X:3120[A]:HIS:HB2	1.98	0.62
3:a:2949[A]:LYS:HD3	3:a:2949[A]:LYS:C	2.24	0.62
3:a:2961[A]:HIS:HB3	3:a:3111[A]:SER:CB	2.28	0.62
3:a:3027[A]:GLU:CD	3:a:3028[A]:PRO:HD2	2.24	0.62
3:a:3228[A]:VAL:HG12	3:a:3287[A]:ILE:CG1	2.29	0.62
3:d:2928[B]:ASN:OD1	3:d:2929[B]:SER:N	2.31	0.62
3:d:2949[B]:LYS:HD3	3:d:2949[B]:LYS:C	2.24	0.62
3:d:3169[A]:LYS:C	3:d:3172[A]:SER:HG	2.00	0.62
3:d:3180[B]:TYR:CB	3:d:3183[B]:LEU:HD22	2.27	0.62
3:C:2954[A]:TYR:HA	3:C:2957[A]:ILE:HG22	1.80	0.62
3:C:3027[B]:GLU:CD	3:C:3028[B]:PRO:HD2	2.25	0.62
3:C:3148[B]:ILE:O	3:L:3170[B]:ALA:N	2.30	0.62
3:C:3153[B]:LYS:NZ	3:L:3156[B]:MET:O	2.27	0.62
3:C:3155[B]:MET:SD	3:L:3154[B]:PRO:O	2.57	0.62
1:D:898:GLY:N	1:D:899:MET:HA	2.12	0.62
2:E:2507:ARG:HA	2:E:2779:ASP:HB2	1.81	0.62
3:F:2988[A]:TRP:NE1	3:F:3158[A]:PHE:HE2	1.96	0.62
3:F:3027[B]:GLU:CD	3:F:3028[B]:PRO:HD2	2.24	0.62
3:F:3093[B]:HIS:HD2	3:a:2973[B]:THR:OG1	1.83	0.62
3:F:3173[B]:THR:CG2	3:F:3174[B]:GLY:H	2.12	0.62
3:F:3285[B]:VAL:HG22	3:F:3286[B]:THR:H	1.62	0.62
1:G:1358:LEU:HD23	1:G:1456:LEU:HD21	1.80	0.62
3:I:3259[B]:ASP:H	3:R:3162[B]:ASP:HB3	1.65	0.62
1:J:195:SER:HB2	1:J:386:ILE:HD11	1.81	0.62
3:L:2957[A]:ILE:CA	3:L:2960[A]:PHE:HE1	2.11	0.62
3:L:3066[B]:TYR:CD1	3:L:3193[B]:HIS:HE1	2.17	0.62
3:L:3162[B]:ASP:OD1	3:L:3162[B]:ASP:N	2.31	0.62
3:O:3027[A]:GLU:CD	3:O:3028[A]:PRO:HD2	2.24	0.62
3:O:3092[B]:ILE:HG23	3:O:3096[B]:VAL:CG2	2.28	0.62
3:O:3217[B]:PHE:CE2	3:O:3303[B]:PRO:HG3	2.33	0.62
3:O:3228[B]:VAL:HG21	3:O:3245[B]:PHE:CE1	2.32	0.62
3:R:2928[A]:ASN:OD1	3:R:2929[A]:SER:N	2.31	0.62
3:R:3217[A]:PHE:HE1	3:R:3230[A]:PHE:HZ	0.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3228[A]:VAL:HG12	3:R:3287[A]:ILE:CG1	2.29	0.62
3:U:3135[A]:LYS:CB	3:U:3141[A]:TYR:HD1	2.13	0.62
3:U:3154[B]:PRO:C	3:d:3150[B]:LYS:CB	2.61	0.62
3:U:3162[A]:ASP:OD1	3:U:3162[A]:ASP:N	2.31	0.62
3:X:2957[B]:ILE:CA	3:X:2960[B]:PHE:HE1	2.11	0.62
2:Z:2524:LEU:HA	2:Z:2581:MET:HE1	1.81	0.62
3:a:2954[B]:TYR:HA	3:a:2957[B]:ILE:HG22	1.80	0.62
3:a:3124[A]:ASP:OD2	3:a:3187[A]:TYR:OH	2.16	0.62
3:a:3217[A]:PHE:CE2	3:a:3303[A]:PRO:HG3	2.33	0.62
1:b:277:ASP:OD1	1:b:278:ASP:N	2.31	0.62
3:d:2990[B]:ARG:CZ	3:d:3180[B]:TYR:HB3	2.28	0.62
3:d:2994[B]:LYS:O	3:d:2995[B]:GLN:C	2.38	0.62
3:d:3092[A]:ILE:HG23	3:d:3096[A]:VAL:CG2	2.28	0.62
1:A:804:ASP:OD1	1:A:805:VAL:N	2.32	0.62
3:C:2957[B]:ILE:CA	3:C:2960[B]:PHE:HE1	2.11	0.62
3:C:2961[A]:HIS:HB3	3:C:3111[A]:SER:CB	2.29	0.62
3:C:3155[A]:MET:HG3	3:C:3172[A]:SER:O	1.99	0.62
3:C:3160[B]:SER:O	3:L:3149[B]:ASN:ND2	2.30	0.62
9:C:3401[A]:CUO:O1	3:L:3120[A]:HIS:NE2	2.30	0.62
1:D:1140:ASN:OD1	1:D:1239:GLY:N	2.25	0.62
1:D:1639:LYS:HG3	4:m:1:NAG:O5	1.98	0.62
3:F:2957[B]:ILE:CA	3:F:2960[B]:PHE:HE1	2.11	0.62
3:F:2990[B]:ARG:CZ	3:F:3180[B]:TYR:HB3	2.28	0.62
3:F:3173[A]:THR:CG2	3:F:3174[A]:GLY:H	2.12	0.62
1:G:104:LEU:HD23	1:G:123:PHE:HE2	1.64	0.62
2:H:2887:ASP:OD1	2:H:2887:ASP:N	2.32	0.62
3:I:2957[B]:ILE:HA	3:I:2960[B]:PHE:HE1	1.64	0.62
3:I:2962[B]:GLY:O	3:R:3255[B]:PRO:CG	2.47	0.62
3:I:3038[A]:ILE:HG22	3:I:3041[A]:ALA:H	1.65	0.62
3:I:3124[B]:ASP:OD2	3:I:3187[B]:TYR:OH	2.15	0.62
3:I:3155[B]:MET:HB2	3:R:3153[B]:LYS:HB3	1.80	0.62
3:I:3173[B]:THR:CG2	3:I:3174[B]:GLY:H	2.12	0.62
3:I:3174[B]:GLY:CA	3:R:3154[B]:PRO:CG	2.47	0.62
1:J:240:PHE:HA	1:J:263:ALA:HB3	1.81	0.62
1:J:806:ASN:OD1	4:u:1:NAG:H82	1.99	0.62
3:L:2957[A]:ILE:N	3:L:2960[A]:PHE:HE1	1.97	0.62
3:L:2990[A]:ARG:CZ	3:L:3180[A]:TYR:HB3	2.28	0.62
3:L:2990[B]:ARG:CZ	3:L:3180[B]:TYR:HB3	2.28	0.62
3:L:3135[B]:LYS:HG3	3:L:3141[B]:TYR:CD1	2.33	0.62
3:L:3228[B]:VAL:HG12	3:L:3287[B]:ILE:CG1	2.29	0.62
1:M:450:LYS:HB3	1:M:454:GLY:HA3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:2625:LEU:O	2:N:2638:ARG:NH1	2.32	0.62
2:N:2643:GLU:O	2:N:2647:LEU:N	2.32	0.62
3:O:2949[B]:LYS:HD3	3:O:2949[B]:LYS:C	2.24	0.62
3:O:3120[A]:HIS:C	3:O:3122[A]:ASN:N	2.55	0.62
3:O:3153[B]:LYS:HG3	3:X:3176[B]:LYS:NZ	2.12	0.62
3:O:3228[B]:VAL:HG12	3:O:3287[B]:ILE:CG1	2.29	0.62
1:P:1582:ASN:HB3	1:P:1583:CYS:CB	2.27	0.62
3:R:2949[A]:LYS:HD3	3:R:2949[A]:LYS:C	2.24	0.62
3:R:2957[B]:ILE:N	3:R:2960[B]:PHE:HE1	1.97	0.62
3:R:3162[B]:ASP:OD1	3:R:3162[B]:ASP:N	2.31	0.62
3:R:3211[A]:ASP:OD1	3:R:3211[A]:ASP:N	2.28	0.62
1:S:2:LEU:HD21	1:S:81:VAL:HG21	1.81	0.62
2:T:2191:LEU:O	2:T:2225:ARG:NH2	2.31	0.62
3:U:2974[B]:ALA:CB	3:d:3220[B]:ARG:CD	2.77	0.62
3:U:3135[B]:LYS:CB	3:U:3141[B]:TYR:HD1	2.12	0.62
3:U:3180[B]:TYR:CB	3:U:3183[B]:LEU:HD22	2.27	0.62
1:V:127:GLU:HG3	1:V:133:LYS:HB3	1.80	0.62
3:X:3038[B]:ILE:HG22	3:X:3041[B]:ALA:H	1.65	0.62
1:Y:932:THR:O	1:Y:989:THR:OG1	2.17	0.62
2:Z:2142:ALA:HB2	2:Z:2433:THR:HG23	1.82	0.62
3:a:2955[B]:GLN:OE1	3:a:3037[B]:TYR:CE1	2.51	0.62
3:a:3038[B]:ILE:HG22	3:a:3041[B]:ALA:H	1.65	0.62
3:a:3273[B]:LEU:CB	3:a:3275[B]:LEU:HD13	2.29	0.62
1:b:979:LEU:HB2	1:b:980:TYR:CB	2.29	0.62
3:d:2966[B]:SER:HB3	3:d:2977[B]:CYS:HB2	1.78	0.62
3:d:2969[A]:TYR:HD2	3:d:2971[A]:ASP:N	1.84	0.62
3:d:3124[A]:ASP:OD2	3:d:3187[A]:TYR:OH	2.15	0.62
3:d:3135[B]:LYS:HG3	3:d:3141[B]:TYR:CD1	2.33	0.62
3:d:3162[B]:ASP:OD1	3:d:3162[B]:ASP:N	2.31	0.62
3:d:3300[A]:LEU:HD23	3:d:3300[A]:LEU:N	2.14	0.62
6:5:1:NAG:O4	6:5:2:NAG:O7	2.16	0.62
2:B:2667:GLU:HB3	2:B:2730:LEU:HD22	1.81	0.62
3:C:2989[B]:HIS:NE2	3:L:2969[B]:TYR:HA	2.15	0.62
3:C:3096[A]:VAL:HG11	3:C:3115[A]:LEU:HD13	1.81	0.62
3:C:3114[A]:PRO:CD	3:C:3115[A]:LEU:H	2.12	0.62
3:C:3151[B]:LEU:HA	3:L:3154[B]:PRO:CB	2.30	0.62
3:C:3252[B]:TYR:CD2	3:L:3223[B]:GLY:O	2.53	0.62
2:E:2665:GLU:OE1	2:E:2798:GLN:NE2	2.31	0.62
3:F:2983[B]:VAL:HB	3:a:3161[B]:GLU:N	2.14	0.62
3:F:3153[B]:LYS:HG2	3:a:3155[B]:MET:SD	2.38	0.62
1:G:11:THR:HG22	1:G:13:ASP:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:THR:HG21	1:G:239:LEU:HB2	1.81	0.62
1:G:157:GLU:OE2	1:G:296:ARG:NH2	2.32	0.62
2:H:2426:PHE:HB3	2:H:2445:MET:HE1	1.80	0.62
3:I:2930[A]:LEU:H	3:I:2930[A]:LEU:CD2	1.98	0.62
3:I:3066[A]:TYR:CD1	3:I:3193[A]:HIS:HE1	2.17	0.62
3:I:3096[A]:VAL:HG11	3:I:3115[A]:LEU:HD13	1.81	0.62
3:I:3107[B]:LEU:HD11	3:R:2975[B]:PHE:CG	2.30	0.62
3:I:3155[B]:MET:O	3:R:3153[B]:LYS:HB3	2.00	0.62
3:L:2928[B]:ASN:OD1	3:L:2929[B]:SER:N	2.31	0.62
3:L:3027[A]:GLU:CD	3:L:3028[A]:PRO:HD2	2.24	0.62
3:L:3135[B]:LYS:CB	3:L:3141[B]:TYR:HD1	2.13	0.62
3:L:3155[A]:MET:HG3	3:L:3172[A]:SER:O	1.99	0.62
2:N:2650:GLY:HA3	2:N:2653:GLU:H	1.63	0.62
3:O:2928[B]:ASN:OD1	3:O:2929[B]:SER:N	2.31	0.62
3:O:3066[A]:TYR:HD1	3:O:3193[A]:HIS:CE1	2.16	0.62
3:O:3273[A]:LEU:CB	3:O:3275[A]:LEU:HD13	2.28	0.62
3:R:2961[A]:HIS:CE1	3:R:2980[A]:HIS:NE2	2.57	0.62
3:R:2961[B]:HIS:HB3	3:R:3111[B]:SER:HG	1.63	0.62
3:R:2994[A]:LYS:O	3:R:2995[A]:GLN:C	2.38	0.62
3:R:3212[B]:ARG:HH11	3:R:3212[B]:ARG:CG	2.11	0.62
3:U:3038[B]:ILE:HG22	3:U:3041[B]:ALA:H	1.65	0.62
3:U:3162[B]:ASP:HB3	3:d:3260[B]:ARG:NH2	2.14	0.62
1:V:926:LEU:HD12	1:V:927:PRO:HD2	1.80	0.62
2:W:2090:LYS:NZ	2:W:2099:GLU:OE2	2.32	0.62
3:X:2987[B]:HIS:NE2	3:X:3178[B]:PHE:HE1	1.95	0.62
3:X:3135[B]:LYS:CB	3:X:3141[B]:TYR:HD1	2.13	0.62
3:X:3240[B]:THR:HG22	3:X:3241[B]:PHE:N	2.13	0.62
1:Y:757:VAL:HG21	1:Y:781:ILE:HG22	1.81	0.62
3:a:3300[B]:LEU:HD23	3:a:3300[B]:LEU:N	2.14	0.62
3:d:2952[B]:ALA:N	3:d:2953[B]:GLY:HA2	2.06	0.62
3:d:3228[B]:VAL:HG12	3:d:3287[B]:ILE:CG1	2.29	0.62
1:A:883:CYS:HB2	1:A:891:LYS:HD3	1.81	0.62
2:B:2877:ILE:O	1:D:1078:ARG:NH1	2.32	0.62
3:C:2949[A]:LYS:HD3	3:C:2949[A]:LYS:C	2.23	0.62
3:F:3155[A]:MET:HG3	3:F:3172[A]:SER:O	1.99	0.62
3:F:3169[B]:LYS:C	3:a:3148[B]:ILE:O	2.43	0.62
3:F:3228[B]:VAL:HG12	3:F:3287[B]:ILE:CG1	2.29	0.62
1:G:161:ASN:ND2	1:G:174:GLN:OE1	2.32	0.62
1:G:164:GLU:OE2	1:G:301:ARG:NH2	2.33	0.62
1:G:304:ALA:HB1	1:G:306:PHE:HE1	1.65	0.62
3:I:2928[B]:ASN:OD1	3:I:2929[B]:SER:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3162[A]:ASP:OD1	3:I:3162[A]:ASP:N	2.31	0.62
3:I:3298[B]:ASN:CB	3:I:3300[B]:LEU:N	2.60	0.62
3:L:3114[B]:PRO:CD	3:L:3115[B]:LEU:H	2.12	0.62
3:L:3173[B]:THR:CG2	3:L:3174[B]:GLY:H	2.12	0.62
1:M:527:LEU:HD13	1:M:629:MET:HG3	1.82	0.62
3:O:2957[A]:ILE:N	3:O:2960[A]:PHE:HE1	1.97	0.62
3:O:3041[B]:ALA:CB	3:X:2971[B]:ASP:OD2	2.48	0.62
1:P:500:ASN:O	1:P:504:THR:OG1	2.18	0.62
1:P:1372:ILE:HD12	1:S:1438:ASP:HB2	1.80	0.62
3:R:3135[B]:LYS:CB	3:R:3141[B]:TYR:HD1	2.12	0.62
3:U:2954[B]:TYR:HA	3:U:2957[B]:ILE:HG22	1.80	0.62
3:U:2994[A]:LYS:HD2	3:U:2998[A]:ASP:OD2	2.00	0.62
3:U:3228[B]:VAL:HG12	3:U:3287[B]:ILE:CG1	2.29	0.62
3:U:3273[A]:LEU:CB	3:U:3275[A]:LEU:HD13	2.28	0.62
3:U:3273[B]:LEU:CB	3:U:3275[B]:LEU:HD13	2.28	0.62
3:X:3027[A]:GLU:CD	3:X:3028[A]:PRO:HD2	2.24	0.62
3:X:3300[A]:LEU:HD23	3:X:3300[A]:LEU:N	2.15	0.62
1:Y:157:GLU:OE2	1:Y:296:ARG:NH2	2.33	0.62
3:a:2955[A]:GLN:OE1	3:a:3037[A]:TYR:CE1	2.50	0.62
3:d:2928[A]:ASN:OD1	3:d:2929[A]:SER:N	2.31	0.62
3:C:2959[B]:SER:O	3:L:3255[B]:PRO:CG	2.47	0.62
3:C:3117[B]:TYR:O	3:C:3120[B]:HIS:HB2	1.98	0.62
3:C:3149[B]:ASN:HB2	3:L:3158[B]:PHE:O	1.99	0.62
3:C:3156[B]:MET:CG	3:L:2979[B]:GLN:HG3	2.30	0.62
3:C:3156[B]:MET:CG	3:L:2982[B]:MET:HB2	2.30	0.62
3:C:3220[B]:ARG:HH11	3:C:3220[B]:ARG:CG	2.12	0.62
3:C:3240[A]:THR:HG22	3:C:3241[A]:PHE:N	2.13	0.62
3:C:3298[B]:ASN:HD21	3:C:3301[B]:PRO:HA	1.60	0.62
3:F:2957[B]:ILE:N	3:F:2960[B]:PHE:HE1	1.98	0.62
3:F:3114[A]:PRO:CD	3:F:3115[A]:LEU:H	2.12	0.62
3:F:3156[B]:MET:HB3	3:a:2982[B]:MET:CB	2.29	0.62
3:F:3259[B]:ASP:HB3	3:a:3162[B]:ASP:CA	2.30	0.62
3:F:3270[A]:LEU:O	3:F:3274[A]:ARG:N	2.33	0.62
3:I:2994[B]:LYS:HD2	3:I:2998[B]:ASP:OD2	2.00	0.62
3:I:3027[A]:GLU:CD	3:I:3028[A]:PRO:HD2	2.24	0.62
3:I:3152[B]:LYS:HB2	3:R:3171[B]:HIS:N	2.10	0.62
3:I:3240[B]:THR:HG22	3:I:3241[B]:PHE:N	2.13	0.62
3:L:2948[A]:ASP:HB3	3:L:2953[A]:GLY:CA	2.24	0.62
3:L:3173[B]:THR:HB	3:L:3176[B]:LYS:HG2	1.81	0.62
1:M:1219:ASP:OD1	1:M:1223:ALA:N	2.33	0.62
1:P:447:MET:HA	1:P:455:TYR:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3027[A]:GLU:CD	3:R:3028[A]:PRO:HD2	2.24	0.62
3:U:2957[A]:ILE:N	3:U:2960[A]:PHE:HE1	1.97	0.62
3:U:3222[A]:ILE:HD11	3:U:3224[A]:GLN:OE1	2.00	0.62
1:V:484:MET:HE2	1:V:663:GLU:HG3	1.80	0.62
3:X:2994[A]:LYS:HD2	3:X:2998[A]:ASP:OD2	2.00	0.62
3:X:3162[A]:ASP:OD1	3:X:3162[A]:ASP:N	2.32	0.62
3:X:3220[A]:ARG:HH11	3:X:3220[A]:ARG:CG	2.12	0.62
3:a:2957[B]:ILE:HA	3:a:2960[B]:PHE:HE1	1.64	0.62
3:a:3220[B]:ARG:HH11	3:a:3220[B]:ARG:CG	2.12	0.62
3:a:3240[B]:THR:HG22	3:a:3241[B]:PHE:N	2.13	0.62
3:a:3298[B]:ASN:HD21	3:a:3301[B]:PRO:HA	1.60	0.62
3:a:3300[A]:LEU:HD23	3:a:3300[A]:LEU:N	2.15	0.62
3:d:3038[A]:ILE:HG22	3:d:3041[A]:ALA:H	1.65	0.62
3:d:3222[A]:ILE:HD11	3:d:3224[A]:GLN:OE1	2.00	0.62
3:d:3298[A]:ASN:CB	3:d:3300[A]:LEU:N	2.60	0.62
3:C:2961[B]:HIS:HB3	3:C:3111[B]:SER:CB	2.28	0.62
3:C:2994[A]:LYS:O	3:C:2995[A]:GLN:C	2.38	0.62
3:C:2994[B]:LYS:HD2	3:C:2998[B]:ASP:OD2	2.00	0.62
3:C:3038[B]:ILE:HG12	3:C:3112[B]:TYR:CE2	2.35	0.62
3:C:3155[B]:MET:CG	3:L:3154[B]:PRO:O	2.47	0.62
3:C:3252[B]:TYR:CB	3:L:3253[B]:GLU:CG	2.77	0.62
3:C:3279[A]:ASP:OD1	3:C:3279[A]:ASP:N	2.25	0.62
1:D:1499:SER:HA	1:D:1508:PHE:HE2	1.65	0.62
3:F:2957[A]:ILE:CA	3:F:2960[A]:PHE:HE1	2.11	0.62
3:F:3038[B]:ILE:HG22	3:F:3041[B]:ALA:H	1.65	0.62
3:F:3090[B]:ASN:CB	3:a:2971[B]:ASP:O	2.48	0.62
3:F:3124[A]:ASP:OD2	3:F:3187[A]:TYR:OH	2.15	0.62
3:F:3135[A]:LYS:CB	3:F:3141[A]:TYR:HD1	2.12	0.62
3:F:3222[A]:ILE:HD11	3:F:3224[A]:GLN:OE1	2.00	0.62
3:F:3240[B]:THR:HG22	3:F:3241[B]:PHE:N	2.13	0.62
3:F:3251[B]:ASP:HB2	3:a:3251[B]:ASP:CG	2.24	0.62
3:F:3256[B]:TRP:CD1	3:a:2967[B]:CYS:N	2.67	0.62
1:G:1286:ARG:NH2	1:G:1333:GLU:OE2	2.33	0.62
3:I:2949[A]:LYS:HD3	3:I:2949[A]:LYS:C	2.23	0.62
3:I:3135[A]:LYS:CB	3:I:3141[A]:TYR:HD1	2.13	0.62
3:I:3135[B]:LYS:CB	3:I:3141[B]:TYR:HD1	2.12	0.62
3:I:3157[A]:PRO:O	3:I:3160[A]:SER:N	2.30	0.62
3:I:3222[A]:ILE:HD11	3:I:3224[A]:GLN:OE1	2.00	0.62
3:I:3270[A]:LEU:O	3:I:3274[A]:ARG:N	2.33	0.62
3:I:3298[B]:ASN:HD21	3:I:3301[B]:PRO:HA	1.60	0.62
3:L:3066[A]:TYR:CD1	3:L:3193[A]:HIS:HE1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3114[A]:PRO:CD	3:L:3115[A]:LEU:H	2.12	0.62
3:L:3120[B]:HIS:C	3:L:3122[B]:ASN:N	2.55	0.62
3:L:3270[A]:LEU:O	3:L:3274[A]:ARG:N	2.33	0.62
3:L:3270[B]:LEU:O	3:L:3274[B]:ARG:N	2.33	0.62
3:O:2968[B]:GLN:CB	3:O:2972[B]:GLY:HA2	2.19	0.62
3:O:2994[B]:LYS:HD2	3:O:2998[B]:ASP:OD2	2.00	0.62
3:O:3038[B]:ILE:HG12	3:O:3112[B]:TYR:CE2	2.35	0.62
3:O:3217[A]:PHE:CE2	3:O:3303[A]:PRO:HG3	2.33	0.62
1:P:452:ILE:HD11	1:P:676:PRO:O	2.00	0.62
1:P:909:ILE:HG12	1:P:1084:PHE:HZ	1.64	0.62
3:R:2990[A]:ARG:CZ	3:R:3180[A]:TYR:HB3	2.28	0.62
3:R:2994[A]:LYS:HD2	3:R:2998[A]:ASP:OD2	2.00	0.62
3:R:3155[A]:MET:HG3	3:R:3172[A]:SER:O	1.99	0.62
3:R:3173[B]:THR:CG2	3:R:3174[B]:GLY:H	2.12	0.62
3:R:3212[A]:ARG:HH11	3:R:3212[A]:ARG:CG	2.12	0.62
3:R:3270[A]:LEU:O	3:R:3274[A]:ARG:N	2.33	0.62
3:R:3284[A]:LYS:CD	3:R:3285[A]:VAL:H	2.10	0.62
1:S:1140:ASN:OD1	1:S:1239:GLY:N	2.22	0.62
2:T:2345:ASN:O	2:T:2349:THR:OG1	2.16	0.62
2:T:2756:ASN:HD21	2:T:2759:THR:HG23	1.65	0.62
3:U:2949[A]:LYS:HD3	3:U:2949[A]:LYS:C	2.24	0.62
3:U:3027[B]:GLU:CD	3:U:3028[B]:PRO:HD2	2.25	0.62
3:U:3038[A]:ILE:HG22	3:U:3041[A]:ALA:H	1.65	0.62
3:U:3038[B]:ILE:HG12	3:U:3112[B]:TYR:CE2	2.35	0.62
3:U:3270[A]:LEU:O	3:U:3274[A]:ARG:N	2.33	0.62
1:V:1195:ASP:O	1:V:1196:ILE:HG12	1.99	0.62
1:V:1286:ARG:NH2	1:V:1333:GLU:OE2	2.33	0.62
2:W:2345:ASN:O	2:W:2349:THR:OG1	2.18	0.62
3:X:2937[A]:ASN:HB3	3:X:3006[A]:LYS:HD3	1.79	0.62
3:X:3222[A]:ILE:HD11	3:X:3224[A]:GLN:OE1	2.00	0.62
3:X:3228[B]:VAL:HG12	3:X:3287[B]:ILE:CG1	2.29	0.62
1:Y:589:GLN:HG2	1:Y:594:ASP:HB3	1.82	0.62
1:Y:1317:PRO:HD2	1:Y:1488:LEU:HD12	1.82	0.62
1:Y:1613:ASP:OD2	3:d:3184[B]:ASN:OD1	2.16	0.62
3:a:2961[A]:HIS:CE1	3:a:2980[A]:HIS:NE2	2.57	0.62
3:a:3066[A]:TYR:CD1	3:a:3193[A]:HIS:HE1	2.17	0.62
3:a:3147[B]:GLU:HG3	3:a:3149[B]:ASN:HD21	1.65	0.62
1:b:1470:GLU:OE2	1:b:1473:ARG:NH1	2.33	0.62
3:d:2987[B]:HIS:NE2	3:d:3178[B]:PHE:HE1	1.95	0.62
3:d:3024[A]:LEU:CD1	3:d:3025[A]:VAL:H	1.83	0.62
3:C:2948[B]:ASP:HB3	3:C:2953[B]:GLY:CA	2.24	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3086[B]:GLU:HB3	3:L:2968[B]:GLN:HE21	1.63	0.62
3:C:3114[B]:PRO:CD	3:C:3115[B]:LEU:H	2.12	0.62
3:C:3135[B]:LYS:CB	3:C:3141[B]:TYR:HD1	2.13	0.62
3:C:3173[B]:THR:HB	3:C:3176[B]:LYS:HG2	1.81	0.62
3:F:2949[B]:LYS:C	3:F:2949[B]:LYS:HD3	2.24	0.62
3:F:3066[B]:TYR:CD1	3:F:3193[B]:HIS:HE1	2.17	0.62
3:F:3162[A]:ASP:OD1	3:F:3162[A]:ASP:N	2.31	0.62
3:F:3222[B]:ILE:HD11	3:F:3224[B]:GLN:OE1	2.00	0.62
1:G:1441:SER:OG	1:G:1442:MET:N	2.31	0.62
3:I:2957[A]:ILE:N	3:I:2960[A]:PHE:HE1	1.97	0.62
3:I:3114[A]:PRO:CD	3:I:3115[A]:LEU:H	2.12	0.62
3:I:3155[B]:MET:SD	3:R:3154[B]:PRO:CD	2.88	0.62
3:I:3249[B]:GLY:N	3:R:2974[B]:ALA:H	1.96	0.62
3:L:3038[A]:ILE:HG12	3:L:3112[A]:TYR:CE2	2.35	0.62
3:L:3038[B]:ILE:HG22	3:L:3041[B]:ALA:H	1.65	0.62
2:N:2882:GLU:OE1	2:N:2884:LYS:NZ	2.32	0.62
3:O:2974[B]:ALA:HB2	3:X:2978[B]:CYS:N	2.15	0.62
3:O:3135[A]:LYS:CB	3:O:3141[A]:TYR:HD1	2.13	0.62
3:O:3270[B]:LEU:O	3:O:3274[B]:ARG:N	2.33	0.62
3:R:2954[B]:TYR:HA	3:R:2957[B]:ILE:HG22	1.80	0.62
3:R:2961[B]:HIS:HB3	3:R:3111[B]:SER:CB	2.29	0.62
3:U:3027[A]:GLU:CD	3:U:3028[A]:PRO:HD2	2.24	0.62
3:U:3114[B]:PRO:CD	3:U:3115[B]:LEU:H	2.12	0.62
2:W:2500:ILE:HG12	2:W:2501:PRO:HD2	1.81	0.62
3:X:2957[A]:ILE:N	3:X:2960[A]:PHE:HE1	1.98	0.62
3:X:2994[B]:LYS:O	3:X:2995[B]:GLN:C	2.38	0.62
3:X:3038[A]:ILE:HG22	3:X:3041[A]:ALA:H	1.65	0.62
3:X:3066[B]:TYR:HD1	3:X:3193[B]:HIS:CE1	2.16	0.62
2:Z:2564:PRO:HA	2:Z:2673:GLU:HG3	1.82	0.62
3:a:2948[B]:ASP:CB	3:a:2949[B]:LYS:HA	2.16	0.62
3:a:2949[A]:LYS:HZ2	3:a:2950[A]:THR:HA	1.65	0.62
3:a:3270[B]:LEU:O	3:a:3274[B]:ARG:N	2.33	0.62
1:b:105:VAL:HG12	1:b:123:PHE:HB3	1.82	0.62
3:d:3038[B]:ILE:HG12	3:d:3112[B]:TYR:CE2	2.35	0.62
3:d:3114[A]:PRO:CD	3:d:3115[A]:LEU:H	2.12	0.62
1:A:492:ARG:HD2	1:A:692:VAL:HG22	1.82	0.62
3:C:3152[B]:LYS:HG3	3:L:3172[B]:SER:OG	1.99	0.62
3:C:3154[B]:PRO:HB3	3:L:3174[B]:GLY:N	2.14	0.62
3:C:3155[B]:MET:N	3:L:3153[B]:LYS:C	2.57	0.62
3:C:3212[B]:ARG:HH11	3:C:3212[B]:ARG:CG	2.12	0.62
1:D:43:GLU:HG3	1:D:44:PRO:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2966[B]:SER:HB3	3:F:2977[B]:CYS:HB2	1.78	0.62
3:F:2967[B]:CYS:SG	3:a:2982[B]:MET:HG3	2.38	0.62
3:I:2965[B]:LEU:HB2	3:R:3253[B]:GLU:OE2	1.99	0.62
3:I:2975[B]:PHE:CE1	3:R:2961[B]:HIS:CE1	2.87	0.62
3:I:3155[A]:MET:HG3	3:I:3172[A]:SER:O	1.99	0.62
3:I:3162[B]:ASP:OD1	3:I:3162[B]:ASP:N	2.31	0.62
3:I:3228[B]:VAL:HG12	3:I:3287[B]:ILE:CG1	2.29	0.62
1:J:238:ASN:OD1	1:J:238:ASN:N	2.33	0.62
1:J:325:THR:HG22	1:J:327:ASP:H	1.62	0.62
3:L:3027[B]:GLU:CD	3:L:3028[B]:PRO:HD2	2.24	0.62
3:L:3038[A]:ILE:HG22	3:L:3041[A]:ALA:H	1.65	0.62
3:L:3273[A]:LEU:CB	3:L:3275[A]:LEU:HD13	2.28	0.62
3:O:3027[B]:GLU:CD	3:O:3028[B]:PRO:HD2	2.25	0.62
3:R:2994[B]:LYS:HD2	3:R:2998[B]:ASP:OD2	2.00	0.62
1:S:164:GLU:O	1:S:297:ARG:NH2	2.32	0.62
3:U:3169[A]:LYS:C	3:U:3172[A]:SER:HG	1.99	0.62
1:V:329:ARG:HH22	1:Y:1574:VAL:H	1.46	0.62
2:W:2128:LEU:HB2	2:W:2286:HIS:HB3	1.82	0.62
3:X:3066[A]:TYR:CD1	3:X:3193[A]:HIS:HE1	2.17	0.62
3:X:3066[B]:TYR:CD1	3:X:3193[B]:HIS:HE1	2.17	0.62
3:X:3270[B]:LEU:O	3:X:3274[B]:ARG:N	2.33	0.62
2:Z:2497:GLU:HB2	2:Z:2498:VAL:HA	1.82	0.62
3:a:2994[B]:LYS:HD2	3:a:2998[B]:ASP:OD2	2.00	0.62
3:a:3027[B]:GLU:CD	3:a:3028[B]:PRO:HD2	2.24	0.62
3:d:2954[A]:TYR:HA	3:d:2957[A]:ILE:HG22	1.80	0.62
3:d:3135[A]:LYS:CB	3:d:3141[A]:TYR:HD1	2.12	0.62
3:d:3220[B]:ARG:HH11	3:d:3220[B]:ARG:CG	2.12	0.62
2:B:2109:ARG:NH1	2:B:2169:HIS:O	2.33	0.62
3:C:2949[B]:LYS:HD3	3:C:2949[B]:LYS:C	2.24	0.62
3:C:2957[B]:ILE:N	3:C:2960[B]:PHE:HE1	1.97	0.62
3:C:3147[A]:GLU:HG3	3:C:3149[A]:ASN:HD21	1.65	0.62
3:C:3212[A]:ARG:HH11	3:C:3212[A]:ARG:CG	2.12	0.62
3:C:3256[B]:TRP:HZ2	3:L:2965[B]:LEU:CG	2.10	0.62
3:F:2979[B]:GLN:HA	3:a:2977[B]:CYS:SG	2.38	0.62
3:F:3228[A]:VAL:HG12	3:F:3287[A]:ILE:CG1	2.29	0.62
1:G:402:THR:HG23	1:G:659:CYS:HA	1.81	0.62
3:I:2948[B]:ASP:HB3	3:I:2953[B]:GLY:CA	2.24	0.62
3:I:3270[B]:LEU:O	3:I:3274[B]:ARG:N	2.33	0.62
3:L:3147[A]:GLU:HG3	3:L:3149[A]:ASN:HD21	1.65	0.62
3:L:3173[A]:THR:CG2	3:L:3174[A]:GLY:H	2.12	0.62
3:L:3222[B]:ILE:HD11	3:L:3224[B]:GLN:OE1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3300[B]:LEU:HD23	3:L:3300[B]:LEU:N	2.15	0.62
3:O:2964[A]:PRO:HG3	3:O:3040[A]:VAL:HG11	1.82	0.62
3:O:3173[A]:THR:CG2	3:O:3174[A]:GLY:H	2.12	0.62
3:O:3298[A]:ASN:CB	3:O:3300[A]:LEU:CD2	2.61	0.62
1:P:474:LEU:HD23	1:P:475:ASN:H	1.65	0.62
2:Q:2889:ALA:N	2:Q:2890:VAL:HA	2.14	0.62
3:R:2961[A]:HIS:HB3	3:R:3111[A]:SER:CB	2.29	0.62
3:R:3024[B]:LEU:CD1	3:R:3025[B]:VAL:H	1.84	0.62
3:R:3147[A]:GLU:HG3	3:R:3149[A]:ASN:HD21	1.65	0.62
3:R:3173[A]:THR:HB	3:R:3176[A]:LYS:HG2	1.81	0.62
3:R:3222[B]:ILE:HD11	3:R:3224[B]:GLN:OE1	2.00	0.62
3:R:3298[A]:ASN:CB	3:R:3300[A]:LEU:N	2.60	0.62
1:S:757:VAL:HG21	1:S:781:ILE:HG13	1.80	0.62
2:T:2800:LYS:HB3	3:U:3023[A]:ILE:HD13	1.76	0.62
3:U:2975[B]:PHE:CB	3:d:3256[B]:TRP:CD1	2.81	0.62
3:U:2990[A]:ARG:CZ	3:U:3180[A]:TYR:HB3	2.28	0.62
3:U:3170[B]:ALA:C	3:d:3152[B]:LYS:NZ	2.55	0.62
3:U:3259[B]:ASP:N	3:d:2968[B]:GLN:HG3	2.14	0.62
2:W:2884:LYS:HG3	2:W:2889:ALA:O	2.00	0.62
3:X:2957[A]:ILE:HA	3:X:2960[A]:PHE:HE1	1.64	0.62
3:X:3228[A]:VAL:HG12	3:X:3287[A]:ILE:CG1	2.29	0.62
3:X:3270[A]:LEU:O	3:X:3274[A]:ARG:N	2.33	0.62
1:Y:673:PHE:HB3	1:Y:677:LEU:HB2	1.82	0.62
3:a:2964[B]:PRO:HG3	3:a:3040[B]:VAL:HG11	1.82	0.62
3:a:3120[A]:HIS:C	3:a:3122[A]:ASN:N	2.55	0.62
3:a:3285[A]:VAL:HG22	3:a:3286[A]:THR:H	1.61	0.62
1:b:46:ASP:OD2	1:b:249:ARG:NH2	2.33	0.62
3:d:2994[A]:LYS:HD2	3:d:2998[A]:ASP:OD2	2.00	0.62
3:d:3270[A]:LEU:O	3:d:3274[A]:ARG:N	2.33	0.62
4:i:1:NAG:O3	4:i:2:NAG:N2	2.33	0.62
6:DA:1:NAG:H61	6:DA:2:NAG:C7	2.30	0.62
3:C:2976[B]:ALA:N	3:L:3253[B]:GLU:CA	2.61	0.61
3:C:3025[A]:VAL:HG22	3:C:3025[A]:VAL:O	2.00	0.61
3:C:3273[A]:LEU:CB	3:C:3275[A]:LEU:HD13	2.28	0.61
1:D:1317:PRO:HA	1:D:1420:GLU:HG3	1.82	0.61
3:F:2962[B]:GLY:O	3:a:3255[B]:PRO:CD	2.48	0.61
3:F:2965[B]:LEU:C	3:a:3256[B]:TRP:N	2.58	0.61
3:F:3114[B]:PRO:CD	3:F:3115[B]:LEU:H	2.12	0.61
3:F:3150[B]:LYS:HG3	3:a:3163[B]:ASN:ND2	2.10	0.61
3:F:3155[B]:MET:HG3	3:F:3172[B]:SER:O	1.99	0.61
3:F:3162[B]:ASP:CB	3:a:3259[B]:ASP:N	2.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1082:SER:O	1:G:1086:LEU:HG	2.00	0.61
1:G:1163:ALA:O	1:G:1167:ASP:HB2	2.00	0.61
2:H:2226:GLU:HG2	2:H:2276:GLY:HA3	1.81	0.61
2:H:2725:GLN:OE1	2:H:2728:ARG:NH2	2.31	0.61
3:I:2964[B]:PRO:CB	3:R:3255[B]:PRO:HB3	2.30	0.61
3:I:2966[A]:SER:HB3	3:I:2977[A]:CYS:HB2	1.78	0.61
3:I:3025[B]:VAL:HG22	3:I:3025[B]:VAL:O	2.00	0.61
3:I:3171[B]:HIS:CA	3:R:3152[B]:LYS:HB3	2.30	0.61
1:M:931:TRP:CG	1:M:1018:ILE:HD11	2.34	0.61
3:O:2977[B]:CYS:N	3:X:3153[B]:LYS:HG2	2.15	0.61
3:O:3173[B]:THR:CG2	3:O:3174[B]:GLY:H	2.12	0.61
3:R:2994[B]:LYS:O	3:R:2995[B]:GLN:C	2.38	0.61
1:S:492:ARG:NH1	1:S:701:TYR:OH	2.32	0.61
1:S:946:GLU:HG2	1:S:955:LYS:HD2	1.81	0.61
3:U:2961[A]:HIS:HB3	3:U:3111[A]:SER:CB	2.29	0.61
3:U:3114[A]:PRO:CD	3:U:3115[A]:LEU:H	2.12	0.61
2:W:2625:LEU:HG	2:W:2626:ARG:HG2	1.81	0.61
3:X:2987[A]:HIS:NE2	3:X:3178[A]:PHE:HE1	1.95	0.61
1:Y:946:GLU:HA	1:Y:956:PRO:HB3	1.82	0.61
2:Z:2545:SER:CA	2:Z:2546:LEU:HB2	2.30	0.61
3:a:3038[A]:ILE:HG12	3:a:3112[A]:TYR:CE2	2.35	0.61
3:a:3096[B]:VAL:HG11	3:a:3115[B]:LEU:HD13	1.81	0.61
3:d:3066[B]:TYR:CD1	3:d:3193[B]:HIS:HE1	2.17	0.61
3:d:3155[B]:MET:HG3	3:d:3172[B]:SER:O	1.99	0.61
3:d:3173[B]:THR:CG2	3:d:3174[B]:GLY:H	2.12	0.61
3:C:2957[A]:ILE:N	3:C:2960[A]:PHE:HE1	1.97	0.61
3:C:2975[B]:PHE:HE1	3:L:3107[B]:LEU:CD1	2.03	0.61
3:C:3027[A]:GLU:CD	3:C:3028[A]:PRO:HD2	2.24	0.61
3:C:3155[B]:MET:HG2	3:L:3154[B]:PRO:N	2.07	0.61
3:C:3158[B]:PHE:HE2	3:L:3153[B]:LYS:NZ	1.93	0.61
3:C:3300[A]:LEU:HD23	3:C:3300[A]:LEU:N	2.15	0.61
2:E:2394:VAL:HG11	2:E:2451:LEU:HD12	1.82	0.61
3:F:2964[A]:PRO:HG3	3:F:3040[A]:VAL:HG11	1.82	0.61
3:F:2994[B]:LYS:HD2	3:F:2998[B]:ASP:OD2	2.00	0.61
3:F:3066[A]:TYR:CD1	3:F:3193[A]:HIS:HE1	2.17	0.61
3:F:3253[B]:GLU:CD	3:a:2974[B]:ALA:HB1	2.21	0.61
3:I:2949[B]:LYS:HD3	3:I:2949[B]:LYS:C	2.24	0.61
3:I:2964[B]:PRO:HD2	3:R:3255[B]:PRO:CG	2.30	0.61
3:I:2994[A]:LYS:HD2	3:I:2998[A]:ASP:OD2	2.00	0.61
3:I:3169[B]:LYS:O	3:R:3152[B]:LYS:N	2.30	0.61
3:L:2994[A]:LYS:HD2	3:L:2998[A]:ASP:OD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3135[A]:LYS:CB	3:L:3141[A]:TYR:HD1	2.13	0.61
1:M:293:LEU:HB3	1:M:297:ARG:HH21	1.65	0.61
3:O:3025[A]:VAL:HG22	3:O:3025[A]:VAL:O	2.00	0.61
3:O:3038[A]:ILE:HG12	3:O:3112[A]:TYR:CE2	2.35	0.61
3:O:3038[A]:ILE:HG22	3:O:3041[A]:ALA:H	1.65	0.61
3:O:3038[B]:ILE:HG22	3:O:3041[B]:ALA:H	1.65	0.61
1:P:780:GLU:O	1:P:782:THR:N	2.33	0.61
3:R:3038[A]:ILE:HG12	3:R:3112[A]:TYR:CE2	2.35	0.61
3:R:3200[A]:LEU:HD22	3:R:3204[A]:LEU:HD13	1.82	0.61
3:R:3228[B]:VAL:HG12	3:R:3287[B]:ILE:CG1	2.29	0.61
1:V:957:ASN:HD22	1:V:960:PHE:HB2	1.64	0.61
3:X:3027[B]:GLU:CD	3:X:3028[B]:PRO:HD2	2.24	0.61
3:X:3038[B]:ILE:HG12	3:X:3112[B]:TYR:CE2	2.35	0.61
3:a:3114[B]:PRO:CD	3:a:3115[B]:LEU:H	2.12	0.61
1:b:115:GLY:HA2	1:b:116:LYS:HB2	1.82	0.61
3:d:3300[B]:LEU:HD23	3:d:3300[B]:LEU:N	2.15	0.61
3:C:3038[B]:ILE:HG22	3:C:3041[B]:ALA:H	1.65	0.61
1:D:1304:ASP:N	1:D:1305:GLY:HA2	2.15	0.61
2:E:2107:LEU:HD23	2:E:2208:PRO:HB2	1.80	0.61
3:F:2994[A]:LYS:O	3:F:2995[A]:GLN:C	2.38	0.61
3:F:3270[B]:LEU:O	3:F:3274[B]:ARG:N	2.33	0.61
3:I:2969[B]:TYR:O	3:R:2980[B]:HIS:HD2	1.84	0.61
1:J:573:LYS:HB3	1:J:574:GLY:HA2	1.83	0.61
1:J:930:ASP:OD1	1:J:1051:ARG:NH2	2.34	0.61
1:J:1144:VAL:HG23	1:J:1234:VAL:HG22	1.82	0.61
3:L:3200[B]:LEU:HD22	3:L:3204[B]:LEU:HD13	1.83	0.61
1:M:1414:THR:HG23	1:M:1477:LEU:HD13	1.82	0.61
3:O:3256[B]:TRP:CE2	3:X:3161[B]:GLU:HG3	2.35	0.61
3:O:3276[B]:ASP:HB3	3:O:3278[B]:HIS:HB2	1.83	0.61
3:O:3298[B]:ASN:CB	3:O:3300[B]:LEU:N	2.60	0.61
1:P:1641:THR:HG21	1:P:1644:ILE:HD11	1.83	0.61
3:R:3124[B]:ASP:OD2	3:R:3187[B]:TYR:OH	2.15	0.61
3:R:3217[B]:PHE:CE2	3:R:3303[B]:PRO:HG3	2.33	0.61
3:R:3300[B]:LEU:HD23	3:R:3300[B]:LEU:N	2.15	0.61
1:S:221:GLN:NE2	1:S:267:PHE:O	2.30	0.61
1:S:865:LYS:HE2	1:S:964:ILE:HD11	1.81	0.61
3:U:2930[A]:LEU:HD22	3:U:2930[A]:LEU:N	2.02	0.61
3:U:2957[B]:ILE:N	3:U:2960[B]:PHE:HE1	1.98	0.61
3:U:3025[A]:VAL:HG22	3:U:3025[A]:VAL:O	2.00	0.61
3:U:3155[B]:MET:O	3:d:3149[B]:ASN:CB	2.48	0.61
3:U:3220[B]:ARG:HB2	3:d:2973[B]:THR:HA	1.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:11:THR:HG22	1:V:13:ASP:H	1.65	0.61
3:X:3024[A]:LEU:CD1	3:X:3025[A]:VAL:H	1.83	0.61
3:X:3025[A]:VAL:HG22	3:X:3025[A]:VAL:O	2.00	0.61
1:Y:1358:LEU:HD23	1:Y:1456:LEU:HD21	1.80	0.61
3:a:2957[A]:ILE:N	3:a:2960[A]:PHE:HE1	1.97	0.61
3:a:2987[A]:HIS:NE2	3:a:3178[A]:PHE:HE1	1.95	0.61
3:a:3276[B]:ASP:HB3	3:a:3278[B]:HIS:HB2	1.83	0.61
3:d:3027[B]:GLU:CD	3:d:3028[B]:PRO:HD2	2.24	0.61
3:d:3135[B]:LYS:CB	3:d:3141[B]:TYR:HD1	2.13	0.61
3:d:3270[B]:LEU:O	3:d:3274[B]:ARG:N	2.33	0.61
3:d:3273[B]:LEU:CB	3:d:3275[B]:LEU:HD13	2.28	0.61
3:d:3284[B]:LYS:CD	3:d:3285[B]:VAL:H	2.09	0.61
1:A:304:ALA:HB1	1:A:306:PHE:HE1	1.64	0.61
3:C:2961[A]:HIS:CE1	3:C:2980[A]:HIS:NE2	2.57	0.61
3:C:2988[A]:TRP:NE1	3:C:3158[A]:PHE:HE2	1.96	0.61
3:C:3154[B]:PRO:O	3:L:3155[B]:MET:HE3	1.99	0.61
3:C:3270[A]:LEU:O	3:C:3274[A]:ARG:N	2.33	0.61
1:D:1462:ASP:OD2	1:D:1525:TYR:OH	2.14	0.61
2:E:2344:LEU:HD23	2:E:2346:PRO:HA	1.82	0.61
3:F:3027[A]:GLU:CD	3:F:3028[A]:PRO:HD2	2.25	0.61
3:F:3160[B]:SER:CA	3:a:3150[B]:LYS:NZ	2.63	0.61
3:F:3276[A]:ASP:HB3	3:F:3278[A]:HIS:HB2	1.83	0.61
3:F:3276[B]:ASP:HB3	3:F:3278[B]:HIS:HB2	1.83	0.61
3:F:3300[A]:LEU:HD23	3:F:3300[A]:LEU:N	2.14	0.61
1:G:456:GLN:HG2	1:G:551:GLU:HB2	1.81	0.61
1:G:1026:GLU:OE1	1:G:1029:SER:N	2.32	0.61
3:I:2964[B]:PRO:C	3:R:3221[B]:ALA:HB3	2.16	0.61
3:I:3027[B]:GLU:CD	3:I:3028[B]:PRO:HD2	2.24	0.61
3:I:3038[B]:ILE:HG12	3:I:3112[B]:TYR:CE2	2.35	0.61
3:I:3150[B]:LYS:NZ	3:R:3160[B]:SER:CB	2.55	0.61
3:I:3152[B]:LYS:HB3	3:R:3172[B]:SER:N	2.04	0.61
3:I:3155[B]:MET:HB3	3:R:3153[B]:LYS:HD2	1.74	0.61
3:I:3222[B]:ILE:HD11	3:I:3224[B]:GLN:OE1	2.00	0.61
3:I:3300[B]:LEU:HD23	3:I:3300[B]:LEU:N	2.15	0.61
2:K:2122:ILE:O	2:K:2125:PHE:HB2	1.99	0.61
2:K:2344:LEU:HA	2:K:2345:ASN:C	2.25	0.61
2:K:2472:ASN:N	2:K:2473:GLY:HA2	2.16	0.61
3:O:2987[A]:HIS:NE2	3:O:3178[A]:PHE:HE1	1.95	0.61
3:O:2994[A]:LYS:HD2	3:O:2998[A]:ASP:OD2	2.00	0.61
3:O:3101[B]:PRO:CB	3:X:2971[B]:ASP:C	2.53	0.61
3:O:3114[B]:PRO:CD	3:O:3115[B]:LEU:H	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3147[A]:GLU:HG3	3:O:3149[A]:ASN:HD21	1.65	0.61
3:O:3273[B]:LEU:CB	3:O:3275[B]:LEU:HD13	2.28	0.61
2:Q:2419:ASP:OD1	2:Q:2419:ASP:N	2.33	0.61
3:R:3027[B]:GLU:CD	3:R:3028[B]:PRO:HD2	2.24	0.61
3:R:3038[A]:ILE:HG22	3:R:3041[A]:ALA:H	1.65	0.61
3:R:3120[B]:HIS:C	3:R:3122[B]:ASN:N	2.55	0.61
3:U:2970[B]:PRO:HB3	3:d:2980[B]:HIS:HB3	1.72	0.61
3:U:3300[A]:LEU:HD23	3:U:3300[A]:LEU:N	2.15	0.61
3:X:3096[A]:VAL:HG11	3:X:3115[A]:LEU:HD13	1.81	0.61
3:X:3169[A]:LYS:C	3:X:3172[A]:SER:HG	2.00	0.61
3:X:3300[B]:LEU:HD23	3:X:3300[B]:LEU:N	2.15	0.61
1:Y:1627:ARG:NH2	1:Y:1629:GLU:OE1	2.31	0.61
1:Y:1655:SER:C	3:d:3006[B]:LYS:HD2	2.26	0.61
3:a:3135[B]:LYS:CB	3:a:3141[B]:TYR:HD1	2.12	0.61
3:a:3222[A]:ILE:HD11	3:a:3224[A]:GLN:OE1	2.00	0.61
3:a:3270[A]:LEU:O	3:a:3274[A]:ARG:N	2.33	0.61
3:d:3162[A]:ASP:OD1	3:d:3162[A]:ASP:N	2.31	0.61
3:d:3173[A]:THR:HB	3:d:3176[A]:LYS:HG2	1.81	0.61
3:C:2974[B]:ALA:C	3:L:3249[B]:GLY:HA2	2.25	0.61
3:C:2984[B]:THR:HB	3:L:3154[B]:PRO:CG	2.30	0.61
3:C:2994[A]:LYS:HD2	3:C:2998[A]:ASP:OD2	2.00	0.61
3:C:3200[B]:LEU:HD22	3:C:3204[B]:LEU:HD13	1.83	0.61
2:E:2567:MET:HE3	2:E:2718:TRP:HB2	1.82	0.61
3:F:2984[B]:THR:CG2	3:a:3159[B]:SER:OG	2.15	0.61
3:F:3157[A]:PRO:O	3:F:3160[A]:SER:N	2.30	0.61
2:H:2820:HIS:HB3	2:H:2822:LYS:HE2	1.83	0.61
3:I:2957[B]:ILE:N	3:I:2960[B]:PHE:HE1	1.98	0.61
3:I:2964[A]:PRO:HG3	3:I:3040[A]:VAL:HG11	1.82	0.61
3:I:2987[B]:HIS:NE2	3:I:3178[B]:PHE:HE1	1.96	0.61
3:I:3120[B]:HIS:C	3:I:3122[B]:ASN:N	2.55	0.61
3:I:3147[B]:GLU:HG3	3:I:3149[B]:ASN:HD21	1.65	0.61
3:I:3150[B]:LYS:CA	3:R:3159[B]:SER:HA	2.18	0.61
3:I:3194[A]:GLY:O	3:I:3195[A]:MET:HG2	2.01	0.61
1:J:332:ASP:OD2	1:J:378:TYR:OH	2.16	0.61
3:L:3194[B]:GLY:O	3:L:3195[B]:MET:HG2	2.01	0.61
1:M:1140:ASN:ND2	1:M:1236:TYR:OH	2.34	0.61
1:M:1210:LYS:HA	1:M:1211:TYR:HB2	1.82	0.61
3:O:3173[A]:THR:HB	3:O:3176[A]:LYS:HG2	1.81	0.61
3:O:3270[A]:LEU:O	3:O:3274[A]:ARG:N	2.33	0.61
3:O:3300[B]:LEU:HD23	3:O:3300[B]:LEU:N	2.15	0.61
1:P:1639:LYS:HE3	1:S:473:ALA:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3124[A]:ASP:OD2	3:R:3187[A]:TYR:OH	2.16	0.61
3:R:3135[A]:LYS:CB	3:R:3141[A]:TYR:HD1	2.13	0.61
3:R:3173[A]:THR:CG2	3:R:3174[A]:GLY:H	2.12	0.61
3:R:3293[B]:LYS:CB	3:R:3294[B]:SER:CB	2.54	0.61
3:U:3252[B]:TYR:O	3:d:3255[B]:PRO:HG3	2.00	0.61
3:U:3257[B]:ALA:CB	3:d:2973[B]:THR:C	2.52	0.61
3:U:3300[B]:LEU:HD23	3:U:3300[B]:LEU:N	2.15	0.61
2:W:2263:PHE:HE1	2:W:2304:LEU:HB3	1.65	0.61
3:X:2994[B]:LYS:HD2	3:X:2998[B]:ASP:OD2	2.00	0.61
3:X:3124[A]:ASP:OD2	3:X:3187[A]:TYR:OH	2.15	0.61
3:X:3139[A]:LEU:N	3:X:3139[A]:LEU:HD22	2.16	0.61
2:Z:2876:LYS:HA	1:b:1078:ARG:HH22	1.65	0.61
2:Z:2878:ARG:NH1	2:Z:2880:GLU:OE2	2.34	0.61
3:a:3066[B]:TYR:CD1	3:a:3193[B]:HIS:HE1	2.17	0.61
3:a:3173[A]:THR:HB	3:a:3176[A]:LYS:HG2	1.81	0.61
2:c:2476:LEU:HB3	2:c:2480:LEU:HD21	1.81	0.61
3:d:3027[A]:GLU:CD	3:d:3028[A]:PRO:HD2	2.24	0.61
3:d:3222[B]:ILE:HD11	3:d:3224[B]:GLN:OE1	2.00	0.61
3:d:3276[A]:ASP:HB3	3:d:3278[A]:HIS:HB2	1.83	0.61
1:A:126:GLY:HA3	1:A:202:TYR:O	2.00	0.61
1:A:1486:LEU:HB2	2:E:2486:ILE:HB	1.81	0.61
3:C:3147[B]:GLU:HG3	3:C:3149[B]:ASN:HD21	1.65	0.61
3:C:3200[A]:LEU:HD22	3:C:3204[A]:LEU:HD13	1.83	0.61
3:C:3228[A]:VAL:HG12	3:C:3287[A]:ILE:CG1	2.29	0.61
1:G:1492:PRO:HB2	1:G:1497:SER:HB3	1.82	0.61
3:I:3173[B]:THR:HB	3:I:3176[B]:LYS:HG2	1.81	0.61
3:I:3200[B]:LEU:HD22	3:I:3204[B]:LEU:HD13	1.83	0.61
3:I:3254[B]:MET:CA	3:R:2966[B]:SER:OG	2.48	0.61
3:I:3273[A]:LEU:CB	3:I:3275[A]:LEU:HD13	2.28	0.61
3:L:2957[B]:ILE:N	3:L:2960[B]:PHE:HE1	1.97	0.61
3:L:2994[B]:LYS:HD2	3:L:2998[B]:ASP:OD2	2.00	0.61
3:L:3120[A]:HIS:C	3:L:3122[A]:ASN:N	2.55	0.61
3:O:2968[B]:GLN:HB2	3:X:2988[B]:TRP:CA	2.29	0.61
1:P:1321:HIS:HD2	1:P:1465:TRP:CH2	2.18	0.61
1:P:1562:ILE:HD13	1:P:1644:ILE:HD12	1.81	0.61
2:Q:2181:THR:HB	2:Q:2374:ASN:H	1.66	0.61
3:R:3147[B]:GLU:HG3	3:R:3149[B]:ASN:HD21	1.65	0.61
3:R:3194[A]:GLY:O	3:R:3195[A]:MET:HG2	2.01	0.61
3:R:3200[B]:LEU:HD22	3:R:3204[B]:LEU:HD13	1.83	0.61
3:R:3300[A]:LEU:HD23	3:R:3300[A]:LEU:N	2.15	0.61
1:S:505:ARG:NE	1:S:1339:SER:OG	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:2128:LEU:HD23	2:T:2216:PHE:HZ	1.65	0.61
3:U:2949[B]:LYS:HD3	3:U:2949[B]:LYS:C	2.24	0.61
3:U:2973[B]:THR:OG1	3:d:3248[B]:LEU:C	2.43	0.61
3:U:3270[B]:LEU:O	3:U:3274[B]:ARG:N	2.33	0.61
1:V:1018:ILE:HA	1:V:1021:LEU:HB2	1.81	0.61
1:V:1143:ALA:HB3	1:V:1235:ILE:HG13	1.83	0.61
2:W:2849:ASP:OD2	2:W:2850:ARG:NH2	2.33	0.61
3:X:3096[B]:VAL:HG11	3:X:3115[B]:LEU:HD13	1.81	0.61
3:X:3114[B]:PRO:CD	3:X:3115[B]:LEU:H	2.12	0.61
3:X:3135[A]:LYS:CB	3:X:3141[A]:TYR:HD1	2.13	0.61
2:Z:2394:VAL:HG11	2:Z:2451:LEU:HD12	1.82	0.61
3:a:2930[B]:LEU:HD22	3:a:2930[B]:LEU:N	2.02	0.61
3:a:2994[A]:LYS:HD2	3:a:2998[A]:ASP:OD2	2.00	0.61
3:a:3222[B]:ILE:HD11	3:a:3224[B]:GLN:OE1	2.00	0.61
3:a:3307[A]:PHE:HE1	3:a:3309[A]:PRO:CG	2.08	0.61
1:b:22:LEU:HD12	1:b:25:MET:HG2	1.83	0.61
2:c:2567:MET:HE3	2:c:2718:TRP:HB2	1.83	0.61
3:d:3038[B]:ILE:HG22	3:d:3041[B]:ALA:H	1.65	0.61
3:C:3152[B]:LYS:N	3:L:3172[B]:SER:CB	2.62	0.61
3:C:3173[A]:THR:HB	3:C:3176[A]:LYS:HG2	1.81	0.61
3:C:3300[B]:LEU:HD23	3:C:3300[B]:LEU:N	2.15	0.61
3:F:2948[A]:ASP:HB3	3:F:2953[A]:GLY:CA	2.24	0.61
3:F:3025[A]:VAL:HG22	3:F:3025[A]:VAL:O	2.00	0.61
3:F:3194[A]:GLY:O	3:F:3195[A]:MET:HG2	2.01	0.61
2:K:2819:VAL:HB	2:K:2835:ILE:HG23	1.82	0.61
3:L:3025[A]:VAL:HG22	3:L:3025[A]:VAL:O	2.00	0.61
3:L:3194[A]:GLY:O	3:L:3195[A]:MET:HG2	2.01	0.61
3:O:3120[B]:HIS:C	3:O:3122[B]:ASN:N	2.55	0.61
1:P:439:LEU:HD23	1:P:509:ILE:HD12	1.82	0.61
1:P:488:PRO:HB2	1:P:641:TRP:CE3	2.36	0.61
1:P:935:ILE:HD11	1:P:980:TYR:HE2	1.65	0.61
3:R:3038[B]:ILE:HG12	3:R:3112[B]:TYR:CE2	2.35	0.61
3:R:3114[B]:PRO:CD	3:R:3115[B]:LEU:H	2.13	0.61
1:S:1429:THR:HG23	1:S:1433:TRP:CZ2	2.36	0.61
3:U:3254[B]:MET:HA	3:d:3253[B]:GLU:O	2.00	0.61
3:U:3274[A]:ARG:NE	3:U:3274[A]:ARG:HA	2.16	0.61
1:V:906:HIS:CD2	9:V:5003:CUO:O1	2.53	0.61
1:V:1441:SER:OG	1:V:1442:MET:N	2.30	0.61
1:Y:1656:ASP:N	3:d:3006[B]:LYS:CB	2.63	0.61
3:a:3135[A]:LYS:CB	3:a:3141[A]:TYR:HD1	2.13	0.61
1:b:622:HIS:CE1	1:b:767:LYS:H	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2957[B]:ILE:N	3:d:2960[B]:PHE:HE1	1.97	0.61
3:d:2994[B]:LYS:HD2	3:d:2998[B]:ASP:OD2	2.00	0.61
3:d:3096[B]:VAL:HG11	3:d:3115[B]:LEU:HD13	1.81	0.61
3:d:3307[A]:PHE:HE1	3:d:3309[A]:PRO:CG	2.08	0.61
3:C:3276[B]:ASP:HB3	3:C:3278[B]:HIS:HB2	1.83	0.61
1:D:909:ILE:HG12	1:D:1084:PHE:HZ	1.64	0.61
2:E:2356:ASP:O	2:E:2363:ASN:ND2	2.33	0.61
3:F:2964[B]:PRO:CB	3:a:3221[B]:ALA:HB3	2.31	0.61
3:F:3038[A]:ILE:HG12	3:F:3112[A]:TYR:CE2	2.35	0.61
3:F:3162[B]:ASP:N	3:F:3162[B]:ASP:OD1	2.31	0.61
1:G:684:ARG:O	1:G:687:SER:OG	2.18	0.61
3:I:2949[B]:LYS:HZ2	3:I:2950[B]:THR:HA	1.66	0.61
3:I:2967[B]:CYS:SG	3:R:2982[B]:MET:HE3	2.40	0.61
3:I:3120[A]:HIS:C	3:I:3122[A]:ASN:N	2.55	0.61
3:I:3156[B]:MET:HB3	3:R:2982[B]:MET:CB	2.31	0.61
3:I:3220[B]:ARG:HH11	3:I:3220[B]:ARG:CG	2.12	0.61
2:K:2109:ARG:NH1	2:K:2169:HIS:O	2.34	0.61
3:L:3222[A]:ILE:HD11	3:L:3224[A]:GLN:OE1	2.00	0.61
1:M:946:GLU:HA	1:M:955:LYS:HB3	1.82	0.61
3:O:3194[B]:GLY:O	3:O:3195[B]:MET:HG2	2.01	0.61
3:O:3254[B]:MET:HB3	3:X:3159[B]:SER:OG	2.00	0.61
1:P:1498:ASN:ND2	1:P:1500:THR:O	2.33	0.61
3:R:3270[B]:LEU:O	3:R:3274[B]:ARG:N	2.33	0.61
3:R:3276[B]:ASP:HB3	3:R:3278[B]:HIS:HB2	1.83	0.61
1:S:1162:ALA:HB2	1:S:1169:LYS:HG2	1.83	0.61
1:S:1394:GLN:HB2	1:S:1433:TRP:HB2	1.83	0.61
3:U:3200[A]:LEU:HD22	3:U:3204[A]:LEU:HD13	1.83	0.61
1:V:133:LYS:HB2	1:V:134:VAL:HG22	1.82	0.61
3:X:2957[B]:ILE:HA	3:X:2960[B]:PHE:HE1	1.64	0.61
1:Y:594:ASP:OD1	1:Y:775:ARG:NH1	2.34	0.61
1:Y:639:ARG:NH2	1:Y:707:PHE:O	2.33	0.61
2:Z:2243:LEU:HD11	2:Z:2273:TRP:HZ3	1.64	0.61
3:a:3194[A]:GLY:O	3:a:3195[A]:MET:HG2	2.01	0.61
3:a:3200[B]:LEU:HD22	3:a:3204[B]:LEU:HD13	1.83	0.61
2:c:2885:SER:HB3	2:c:2890:VAL:HG22	1.83	0.61
3:d:2930[A]:LEU:HD22	3:d:2930[A]:LEU:N	2.02	0.61
3:d:3298[A]:ASN:HD21	3:d:3301[A]:PRO:HA	1.60	0.61
3:d:3307[B]:PHE:HE1	3:d:3309[B]:PRO:CG	2.08	0.61
2:B:2619:VAL:HG23	1:b:190:PHE:HD2	1.66	0.61
3:C:2985[B]:PHE:HE2	3:L:2969[B]:TYR:CA	2.12	0.61
3:C:3222[B]:ILE:HD11	3:C:3224[B]:GLN:OE1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3270[B]:LEU:O	3:C:3274[B]:ARG:N	2.33	0.61
3:C:3272[A]:HIS:CD2	1:D:1543:ILE:HD11	2.36	0.61
3:C:3281[A]:PHE:CE1	3:C:3305[A]:ILE:HG21	2.36	0.61
9:C:3401[B]:CUO:O1	3:L:3120[B]:HIS:NE2	2.30	0.61
1:D:465:PRO:HD2	1:D:467:LYS:NZ	2.16	0.61
1:D:619:SER:HB2	1:D:805:VAL:HG11	1.81	0.61
1:D:804:ASP:OD1	1:D:805:VAL:N	2.33	0.61
3:F:3038[B]:ILE:HG12	3:F:3112[B]:TYR:CE2	2.35	0.61
3:F:3173[A]:THR:HB	3:F:3176[A]:LYS:HG2	1.81	0.61
2:H:2472:ASN:N	2:H:2473:GLY:HA2	2.16	0.61
3:I:2964[B]:PRO:HG3	3:I:3040[B]:VAL:HG11	1.82	0.61
3:I:2969[B]:TYR:CD2	3:R:3093[B]:HIS:NE2	2.68	0.61
3:I:3114[B]:PRO:CD	3:I:3115[B]:LEU:H	2.12	0.61
3:I:3139[A]:LEU:N	3:I:3139[A]:LEU:HD22	2.16	0.61
3:I:3147[A]:GLU:HG3	3:I:3149[A]:ASN:HD21	1.65	0.61
3:I:3163[B]:ASN:HB3	3:R:3150[B]:LYS:NZ	2.16	0.61
1:J:517:THR:HG21	1:J:708:PHE:HE1	1.65	0.61
1:J:926:LEU:HD11	1:J:1043:MET:HB3	1.83	0.61
3:O:2967[B]:CYS:H	3:X:2979[B]:GLN:NE2	1.98	0.61
3:O:3038[B]:ILE:CD1	3:X:2969[B]:TYR:HE2	2.05	0.61
3:O:3157[B]:PRO:CA	3:X:3153[B]:LYS:H	2.11	0.61
3:O:3300[A]:LEU:HD23	3:O:3300[A]:LEU:N	2.14	0.61
2:Q:2130:PRO:O	2:Q:2140:ARG:HD2	2.01	0.61
3:R:2948[A]:ASP:CB	3:R:2949[A]:LYS:CA	2.78	0.61
3:R:2987[A]:HIS:NE2	3:R:3178[A]:PHE:HE1	1.96	0.61
3:R:3173[B]:THR:HB	3:R:3176[B]:LYS:HG2	1.81	0.61
3:R:3194[B]:GLY:O	3:R:3195[B]:MET:HG2	2.01	0.61
2:T:2201:THR:O	2:T:2203:ILE:N	2.32	0.61
3:U:2965[B]:LEU:H	3:d:3220[B]:ARG:NH2	1.98	0.61
3:U:2979[B]:GLN:NE2	3:d:3153[B]:LYS:CE	2.64	0.61
3:U:2994[B]:LYS:HD2	3:U:2998[B]:ASP:OD2	2.00	0.61
3:U:3194[B]:GLY:O	3:U:3195[B]:MET:HG2	2.01	0.61
3:U:3252[B]:TYR:C	3:d:3255[B]:PRO:CG	2.73	0.61
3:U:3256[B]:TRP:CG	3:d:2969[B]:TYR:CG	2.86	0.61
3:X:2957[B]:ILE:N	3:X:2960[B]:PHE:HE1	1.98	0.61
3:X:2964[A]:PRO:HG3	3:X:3040[A]:VAL:HG11	1.82	0.61
3:X:3156[B]:MET:HA	3:X:3157[B]:PRO:C	2.26	0.61
3:X:3222[B]:ILE:HD11	3:X:3224[B]:GLN:OE1	2.00	0.61
3:X:3298[B]:ASN:CA	3:X:3300[B]:LEU:HD23	2.31	0.61
1:Y:1551:ASP:OD1	3:d:3007[B]:ILE:CD1	2.49	0.61
3:a:3200[A]:LEU:HD22	3:a:3204[A]:LEU:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:2128:LEU:HD13	2:c:2286:HIS:CG	2.35	0.61
2:c:2800:LYS:O	3:d:3023[A]:ILE:HD11	2.00	0.61
3:d:3025[A]:VAL:HG22	3:d:3025[A]:VAL:O	2.00	0.61
1:A:562:GLN:HG2	1:A:614:GLU:HG3	1.81	0.61
3:C:2963[B]:MET:HE1	3:L:3222[B]:ILE:CD1	2.24	0.61
3:C:2964[A]:PRO:HG3	3:C:3040[A]:VAL:HG11	1.82	0.61
3:C:3038[A]:ILE:HG22	3:C:3041[A]:ALA:H	1.65	0.61
3:F:2977[B]:CYS:HB2	3:a:2982[B]:MET:CE	2.31	0.61
3:F:3135[B]:LYS:CB	3:F:3141[B]:TYR:HD1	2.13	0.61
3:F:3149[B]:ASN:ND2	3:a:3163[B]:ASN:O	2.32	0.61
3:F:3300[B]:LEU:HD23	3:F:3300[B]:LEU:N	2.15	0.61
3:I:2998[B]:ASP:O	3:I:3001[B]:LYS:HB2	2.01	0.61
3:I:3171[B]:HIS:CA	3:R:3152[B]:LYS:HB2	2.30	0.61
2:K:2421:TYR:HB2	2:K:2454:MET:HE3	1.83	0.61
3:L:3157[A]:PRO:O	3:L:3160[A]:SER:N	2.30	0.61
3:L:3200[A]:LEU:HD22	3:L:3204[A]:LEU:HD13	1.83	0.61
2:N:2851:ASN:OD1	2:N:2851:ASN:N	2.34	0.61
3:O:3139[B]:LEU:N	3:O:3139[B]:LEU:HD22	2.16	0.61
2:Q:2795:ILE:O	2:Q:2798:GLN:HG2	2.00	0.61
3:R:2948[A]:ASP:HB3	3:R:2953[A]:GLY:CA	2.24	0.61
1:S:240:PHE:HA	1:S:263:ALA:HB3	1.82	0.61
1:S:1301:PRO:HB3	1:S:1308:VAL:HG12	1.83	0.61
3:U:2939[A]:ARG:HH11	3:U:2939[A]:ARG:HG3	1.66	0.61
3:X:2948[A]:ASP:CB	3:X:2949[A]:LYS:CA	2.78	0.61
3:X:3120[A]:HIS:C	3:X:3122[A]:ASN:N	2.55	0.61
3:X:3194[A]:GLY:O	3:X:3195[A]:MET:HG2	2.01	0.61
3:X:3274[B]:ARG:NE	3:X:3274[B]:ARG:HA	2.16	0.61
3:X:3276[A]:ASP:HB3	3:X:3278[A]:HIS:HB2	1.83	0.61
2:Z:2889:ALA:N	2:Z:2890:VAL:HA	2.15	0.61
3:a:2957[B]:ILE:N	3:a:2960[B]:PHE:HE1	1.97	0.61
3:a:3194[B]:GLY:O	3:a:3195[B]:MET:HG2	2.01	0.61
3:a:3273[A]:LEU:CB	3:a:3275[A]:LEU:HD13	2.28	0.61
3:d:3038[A]:ILE:HG12	3:d:3112[A]:TYR:CE2	2.35	0.61
3:d:3139[A]:LEU:N	3:d:3139[A]:LEU:HD22	2.16	0.61
3:d:3218[B]:LEU:O	3:d:3219[B]:LEU:HD13	2.01	0.61
2:B:2094:ARG:HH21	2:E:2094:ARG:HH21	1.49	0.60
3:C:2985[B]:PHE:CE2	3:L:2968[B]:GLN:O	2.54	0.60
3:C:3066[A]:TYR:CD1	3:C:3193[A]:HIS:HE1	2.17	0.60
3:C:3276[A]:ASP:HB3	3:C:3278[A]:HIS:HB2	1.83	0.60
1:D:135:THR:HG21	1:D:192:HIS:HB3	1.83	0.60
3:F:2964[B]:PRO:HG3	3:F:3040[B]:VAL:HG11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2975[B]:PHE:HD1	3:a:3107[B]:LEU:CD2	2.13	0.60
3:F:3147[A]:GLU:HG3	3:F:3149[A]:ASN:HD21	1.65	0.60
3:F:3170[B]:ALA:O	3:a:3152[B]:LYS:CG	2.48	0.60
1:G:1242:ASN:HB3	1:G:1479:TYR:OH	2.02	0.60
3:I:2965[B]:LEU:HA	3:R:3253[B]:GLU:CG	2.31	0.60
3:I:3191[A]:ASN:ND2	3:I:3191[A]:ASN:H	1.99	0.60
3:I:3281[B]:PHE:CE1	3:I:3305[B]:ILE:HG21	2.36	0.60
3:I:3298[B]:ASN:CA	3:I:3300[B]:LEU:HD23	2.31	0.60
2:K:2166:LEU:HA	2:K:2169:HIS:HB2	1.83	0.60
3:L:2939[A]:ARG:HG3	3:L:2939[A]:ARG:HH11	1.66	0.60
3:L:2945[A]:VAL:HG22	3:L:2945[A]:VAL:O	2.01	0.60
3:L:2964[A]:PRO:HG3	3:L:3040[A]:VAL:HG11	1.82	0.60
3:L:3025[B]:VAL:HG22	3:L:3025[B]:VAL:O	2.00	0.60
3:L:3211[B]:ASP:OD1	3:L:3211[B]:ASP:N	2.28	0.60
3:L:3212[A]:ARG:HH11	3:L:3212[A]:ARG:CG	2.12	0.60
3:O:3025[B]:VAL:HG22	3:O:3025[B]:VAL:O	2.00	0.60
3:O:3114[A]:PRO:CD	3:O:3115[A]:LEU:H	2.12	0.60
3:O:3218[A]:LEU:O	3:O:3219[A]:LEU:HD13	2.01	0.60
3:R:3025[B]:VAL:HG22	3:R:3025[B]:VAL:O	2.00	0.60
3:R:3134[B]:GLN:O	3:R:3135[B]:LYS:C	2.44	0.60
1:S:452:ILE:HD12	1:S:1367:SER:HB2	1.83	0.60
1:S:881:GLN:OE1	1:S:888:ALA:HB3	2.01	0.60
3:U:2949[B]:LYS:HZ2	3:U:2950[B]:THR:HA	1.66	0.60
3:U:2969[B]:TYR:HE2	3:d:3248[B]:LEU:HD23	1.66	0.60
3:U:3169[B]:LYS:CD	3:d:3146[B]:CYS:HA	2.31	0.60
1:V:1019:HIS:HE2	1:V:1046:HIS:CE1	2.19	0.60
1:V:1582:ASN:HB3	1:V:1583:CYS:CB	2.26	0.60
3:X:2964[B]:PRO:HG3	3:X:3040[B]:VAL:HG11	1.82	0.60
3:X:3114[A]:PRO:CD	3:X:3115[A]:LEU:H	2.12	0.60
3:X:3218[A]:LEU:O	3:X:3219[A]:LEU:HD13	2.01	0.60
3:a:3038[B]:ILE:HG12	3:a:3112[B]:TYR:CE2	2.35	0.60
1:b:1067:TYR:H	1:b:1067:TYR:HD1	1.48	0.60
1:b:1595:GLY:O	1:b:1598:GLU:HG2	2.01	0.60
3:d:3274[A]:ARG:NE	3:d:3274[A]:ARG:HA	2.16	0.60
3:d:3281[B]:PHE:CE1	3:d:3305[B]:ILE:HG21	2.36	0.60
3:d:3298[B]:ASN:CB	3:d:3300[B]:LEU:N	2.60	0.60
3:C:2998[B]:ASP:O	3:C:3001[B]:LYS:HB2	2.01	0.60
3:C:3135[A]:LYS:CB	3:C:3141[A]:TYR:HD1	2.12	0.60
3:C:3218[A]:LEU:O	3:C:3219[A]:LEU:HD13	2.01	0.60
3:C:3222[A]:ILE:HD11	3:C:3224[A]:GLN:OE1	2.00	0.60
3:C:3281[B]:PHE:CE1	3:C:3305[B]:ILE:HG21	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3155[B]:MET:HB3	3:a:3153[B]:LYS:HD3	1.71	0.60
3:F:3157[B]:PRO:HD3	3:a:3254[B]:MET:HE2	1.83	0.60
3:F:3212[B]:ARG:HH11	3:F:3212[B]:ARG:CG	2.12	0.60
3:F:3281[A]:PHE:CE1	3:F:3305[A]:ILE:HG21	2.36	0.60
1:G:488:PRO:HB2	1:G:641:TRP:CE3	2.36	0.60
2:H:2670:CYS:N	2:H:2737:CYS:SG	2.74	0.60
3:I:2945[A]:VAL:HG22	3:I:2945[A]:VAL:O	2.02	0.60
3:I:2948[A]:ASP:HB3	3:I:2953[A]:GLY:CA	2.24	0.60
3:I:2948[A]:ASP:CB	3:I:2949[A]:LYS:CA	2.78	0.60
3:I:2975[B]:PHE:CZ	3:R:2961[B]:HIS:C	2.79	0.60
3:I:3156[A]:MET:HA	3:I:3157[A]:PRO:C	2.26	0.60
3:I:3194[B]:GLY:O	3:I:3195[B]:MET:HG2	2.01	0.60
3:I:3300[A]:LEU:HD23	3:I:3300[A]:LEU:N	2.15	0.60
3:L:3298[A]:ASN:CA	3:L:3300[A]:LEU:HD23	2.31	0.60
3:O:3222[A]:ILE:HD11	3:O:3224[A]:GLN:OE1	2.00	0.60
3:O:3222[B]:ILE:HD11	3:O:3224[B]:GLN:OE1	2.00	0.60
3:O:3274[B]:ARG:NE	3:O:3274[B]:ARG:HA	2.16	0.60
3:O:3307[A]:PHE:HE1	3:O:3309[A]:PRO:CG	2.08	0.60
2:Q:2225:ARG:HD2	2:Q:2274:LEU:HD22	1.83	0.60
3:R:2949[A]:LYS:HZ2	3:R:2950[A]:THR:HA	1.65	0.60
3:R:2957[A]:ILE:N	3:R:2960[A]:PHE:HE1	1.97	0.60
3:R:2964[A]:PRO:HG3	3:R:3040[A]:VAL:HG11	1.82	0.60
3:R:3218[A]:LEU:O	3:R:3219[A]:LEU:HD13	2.01	0.60
3:R:3281[B]:PHE:CE1	3:R:3305[B]:ILE:HG21	2.36	0.60
1:S:1195:ASP:HA	1:S:1196:ILE:HB	1.82	0.60
1:S:1304:ASP:N	1:S:1305:GLY:HA2	2.15	0.60
3:U:2949[A]:LYS:HZ2	3:U:2950[A]:THR:HA	1.66	0.60
3:U:3038[A]:ILE:HG12	3:U:3112[A]:TYR:CE2	2.35	0.60
3:U:3139[A]:LEU:N	3:U:3139[A]:LEU:HD22	2.16	0.60
3:U:3176[B]:LYS:HB3	3:U:3176[B]:LYS:HZ2	1.66	0.60
3:U:3194[A]:GLY:O	3:U:3195[A]:MET:HG2	2.01	0.60
3:U:3222[B]:ILE:HD11	3:U:3224[B]:GLN:OE1	2.00	0.60
3:X:2939[B]:ARG:HH11	3:X:2939[B]:ARG:HG3	1.66	0.60
3:X:3200[B]:LEU:HD22	3:X:3204[B]:LEU:HD13	1.83	0.60
2:Z:2849:ASP:OD2	2:Z:2850:ARG:NH2	2.34	0.60
3:a:3114[A]:PRO:CD	3:a:3115[A]:LEU:H	2.12	0.60
3:a:3134[B]:GLN:O	3:a:3135[B]:LYS:C	2.44	0.60
3:a:3218[A]:LEU:O	3:a:3219[A]:LEU:HD13	2.01	0.60
3:a:3281[A]:PHE:CE1	3:a:3305[A]:ILE:HG21	2.36	0.60
2:c:2903:TYR:OH	3:d:2932[A]:PRO:HD2	2.00	0.60
3:d:3298[B]:ASN:CA	3:d:3300[B]:LEU:HD23	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2830:GLN:HB2	2:B:2863:ARG:HH12	1.66	0.60
3:C:2945[B]:VAL:HG22	3:C:2945[B]:VAL:O	2.02	0.60
3:C:3124[B]:ASP:OD2	3:C:3187[B]:TYR:OH	2.15	0.60
3:C:3134[B]:GLN:O	3:C:3135[B]:LYS:C	2.44	0.60
3:C:3154[B]:PRO:CB	3:L:3174[B]:GLY:N	2.65	0.60
3:C:3273[B]:LEU:CB	3:C:3275[B]:LEU:HD13	2.28	0.60
3:C:3284[A]:LYS:CD	3:C:3285[A]:VAL:H	2.09	0.60
1:D:325:THR:HG21	1:D:329:ARG:O	2.00	0.60
2:E:2210:ASN:O	2:E:2225:ARG:NH2	2.34	0.60
3:F:2939[A]:ARG:HH11	3:F:2939[A]:ARG:HG3	1.66	0.60
3:F:2939[B]:ARG:HG3	3:F:2939[B]:ARG:HH11	1.66	0.60
3:F:2994[A]:LYS:HD2	3:F:2998[A]:ASP:OD2	2.00	0.60
3:F:3038[A]:ILE:HG22	3:F:3041[A]:ALA:H	1.65	0.60
3:F:3135[A]:LYS:HG3	3:F:3141[A]:TYR:CD1	2.33	0.60
3:F:3139[B]:LEU:N	3:F:3139[B]:LEU:HD22	2.16	0.60
1:G:71:LEU:HD22	1:G:266:LEU:HD21	1.82	0.60
3:I:2965[B]:LEU:HD21	3:R:3250[B]:GLY:H	1.65	0.60
3:I:3221[B]:ALA:CB	3:R:2964[B]:PRO:CB	2.62	0.60
2:K:2300:ASN:OD1	2:K:2303:ARG:NH1	2.34	0.60
3:L:3038[B]:ILE:HG12	3:L:3112[B]:TYR:CE2	2.35	0.60
1:M:898:GLY:N	1:M:899:MET:HA	2.16	0.60
3:O:2973[B]:THR:CB	3:X:3158[B]:PHE:CZ	2.82	0.60
3:O:2998[B]:ASP:O	3:O:3001[B]:LYS:HB2	2.01	0.60
3:O:3272[A]:HIS:CD2	1:P:1542:ARG:HH22	2.19	0.60
1:P:622:HIS:CE1	1:P:767:LYS:H	2.19	0.60
3:R:3096[B]:VAL:HG11	3:R:3115[B]:LEU:HD13	1.81	0.60
3:R:3120[A]:HIS:C	3:R:3122[A]:ASN:N	2.55	0.60
3:R:3139[B]:LEU:N	3:R:3139[B]:LEU:HD22	2.16	0.60
3:R:3156[B]:MET:HA	3:R:3157[B]:PRO:C	2.26	0.60
3:R:3191[B]:ASN:ND2	3:R:3191[B]:ASN:H	1.99	0.60
3:R:3274[B]:ARG:HA	3:R:3274[B]:ARG:NE	2.16	0.60
3:R:3307[A]:PHE:HE1	3:R:3309[A]:PRO:CG	2.08	0.60
1:S:494:VAL:HG23	1:S:671:PHE:HZ	1.67	0.60
1:S:1639:LYS:HE3	4:BA:2:NAG:H82	1.83	0.60
2:T:2830:GLN:HE22	2:T:2863:ARG:HH11	1.49	0.60
2:T:2879:LEU:HD21	2:T:2901:LEU:HD11	1.83	0.60
3:U:2987[B]:HIS:NE2	3:U:3178[B]:PHE:HE1	1.95	0.60
3:U:3218[B]:LEU:O	3:U:3219[B]:LEU:HD13	2.01	0.60
1:V:555:ALA:HB3	1:V:557:VAL:HG12	1.83	0.60
3:X:3212[B]:ARG:HH11	3:X:3212[B]:ARG:CG	2.12	0.60
3:X:3276[B]:ASP:HB3	3:X:3278[B]:HIS:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:545:PHE:O	1:Y:561:ARG:NH2	2.34	0.60
1:Y:606:ILE:O	1:Y:610:THR:OG1	2.18	0.60
1:Y:729:VAL:HG11	1:Y:785:LEU:HD12	1.84	0.60
2:Z:2745:PRO:HB2	2:Z:2750:ILE:HD11	1.82	0.60
3:a:2998[A]:ASP:O	3:a:3001[A]:LYS:HB2	2.01	0.60
3:a:3139[B]:LEU:N	3:a:3139[B]:LEU:HD22	2.16	0.60
3:a:3156[B]:MET:HA	3:a:3157[B]:PRO:C	2.26	0.60
3:a:3218[B]:LEU:O	3:a:3219[B]:LEU:HD13	2.02	0.60
3:a:3298[A]:ASN:CA	3:a:3300[A]:LEU:HD23	2.31	0.60
3:a:3298[B]:ASN:ND2	3:a:3301[B]:PRO:C	2.60	0.60
3:d:2949[A]:LYS:HZ2	3:d:2950[A]:THR:HA	1.66	0.60
3:d:2957[A]:ILE:N	3:d:2960[A]:PHE:HE1	1.98	0.60
3:d:3139[B]:LEU:HD22	3:d:3139[B]:LEU:N	2.16	0.60
3:d:3218[A]:LEU:O	3:d:3219[A]:LEU:HD13	2.01	0.60
6:LA:1:NAG:O4	6:LA:2:NAG:C7	2.49	0.60
3:C:3139[A]:LEU:HD22	3:C:3139[A]:LEU:N	2.16	0.60
3:C:3154[B]:PRO:N	3:L:3173[B]:THR:C	2.59	0.60
3:C:3194[A]:GLY:O	3:C:3195[A]:MET:HG2	2.01	0.60
1:D:262:LYS:NZ	1:D:795:GLU:OE1	2.35	0.60
1:D:411:ASP:OD1	1:D:658:TYR:OH	2.16	0.60
3:F:2994[B]:LYS:O	3:F:2995[B]:GLN:C	2.38	0.60
3:F:3155[B]:MET:CB	3:a:3153[B]:LYS:CB	2.76	0.60
3:F:3255[B]:PRO:CG	3:a:2964[B]:PRO:CD	2.80	0.60
3:F:3255[B]:PRO:C	3:a:2965[B]:LEU:C	2.67	0.60
1:G:238:ASN:OD1	1:G:238:ASN:N	2.33	0.60
3:I:2964[B]:PRO:CA	3:R:3221[B]:ALA:HB3	2.30	0.60
3:I:2977[B]:CYS:SG	3:R:2982[B]:MET:HE3	2.41	0.60
3:I:3025[A]:VAL:HG22	3:I:3025[A]:VAL:O	2.00	0.60
3:I:3222[A]:ILE:HG13	3:I:3224[A]:GLN:HG2	1.84	0.60
1:J:444:GLU:HG3	1:J:544:PRO:HG3	1.84	0.60
1:J:456:GLN:HG2	1:J:551:GLU:HB2	1.84	0.60
3:L:2998[B]:ASP:O	3:L:3001[B]:LYS:HB2	2.01	0.60
3:L:3134[B]:GLN:O	3:L:3135[B]:LYS:C	2.44	0.60
3:L:3139[A]:LEU:N	3:L:3139[A]:LEU:HD22	2.16	0.60
3:L:3274[A]:ARG:HA	3:L:3274[A]:ARG:NE	2.16	0.60
3:L:3300[A]:LEU:HD23	3:L:3300[A]:LEU:N	2.15	0.60
3:O:3102[B]:TYR:CA	3:X:2971[B]:ASP:CA	2.78	0.60
3:O:3139[A]:LEU:N	3:O:3139[A]:LEU:HD22	2.16	0.60
3:O:3298[B]:ASN:ND2	3:O:3301[B]:PRO:C	2.60	0.60
3:R:2939[A]:ARG:HH11	3:R:2939[A]:ARG:HG3	1.66	0.60
3:R:3038[B]:ILE:HG22	3:R:3041[B]:ALA:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3222[A]:ILE:HD11	3:R:3224[A]:GLN:OE1	2.00	0.60
3:R:3222[B]:ILE:HG13	3:R:3224[B]:GLN:HG2	1.84	0.60
3:R:3298[B]:ASN:CB	3:R:3300[B]:LEU:CD2	2.61	0.60
1:S:575:ASP:N	1:S:576:HIS:HA	2.16	0.60
3:U:3298[A]:ASN:ND2	3:U:3301[A]:PRO:C	2.60	0.60
1:V:533:VAL:HG12	1:V:540:THR:HG22	1.82	0.60
1:V:1143:ALA:HA	1:V:1195:ASP:O	2.01	0.60
3:X:3025[B]:VAL:HG22	3:X:3025[B]:VAL:O	2.00	0.60
1:Y:1296:VAL:HB	1:Y:1446:ASP:HB3	1.82	0.60
3:a:2952[A]:ALA:N	3:a:2953[A]:GLY:HA2	2.06	0.60
3:a:3038[A]:ILE:HG22	3:a:3041[A]:ALA:H	1.65	0.60
3:a:3155[B]:MET:HG3	3:a:3172[B]:SER:O	1.99	0.60
1:b:589:GLN:O	1:b:651:ARG:NH1	2.34	0.60
3:d:3096[A]:VAL:HG11	3:d:3115[A]:LEU:HD13	1.81	0.60
3:d:3200[A]:LEU:HD22	3:d:3204[A]:LEU:HD13	1.83	0.60
1:A:1242:ASN:OD1	1:A:1243:PHE:N	2.35	0.60
2:B:2133:PRO:HG2	2:B:2140:ARG:HA	1.82	0.60
3:C:2978[B]:CYS:H	3:L:3254[B]:MET:CB	1.76	0.60
3:C:3154[B]:PRO:N	3:L:3155[B]:MET:CG	2.64	0.60
3:C:3194[B]:GLY:O	3:C:3195[B]:MET:HG2	2.01	0.60
1:D:979:LEU:HB3	1:D:980:TYR:CD2	2.36	0.60
3:F:2948[B]:ASP:CB	3:F:2949[B]:LYS:CA	2.78	0.60
3:F:3220[A]:ARG:HH11	3:F:3220[A]:ARG:CG	2.12	0.60
3:F:3298[B]:ASN:ND2	3:F:3301[B]:PRO:C	2.60	0.60
1:G:221:GLN:NE2	1:G:267:PHE:O	2.32	0.60
1:G:1427:HIS:HD2	1:G:1457:HIS:HE1	1.49	0.60
3:I:2966[B]:SER:CB	3:R:2982[B]:MET:HE2	2.27	0.60
3:I:3160[B]:SER:CB	3:R:2982[B]:MET:CA	2.79	0.60
3:I:3298[B]:ASN:ND2	3:I:3301[B]:PRO:C	2.60	0.60
3:L:3218[B]:LEU:O	3:L:3219[B]:LEU:HD13	2.01	0.60
3:L:3274[B]:ARG:NE	3:L:3274[B]:ARG:HA	2.16	0.60
3:O:2957[B]:ILE:N	3:O:2960[B]:PHE:HE1	1.97	0.60
3:O:3101[B]:PRO:CG	3:X:2971[B]:ASP:O	2.48	0.60
3:O:3173[B]:THR:HB	3:O:3176[B]:LYS:HG2	1.81	0.60
3:O:3274[A]:ARG:HA	3:O:3274[A]:ARG:NE	2.16	0.60
3:O:3276[A]:ASP:HB3	3:O:3278[A]:HIS:HB2	1.83	0.60
3:O:3281[B]:PHE:CE1	3:O:3305[B]:ILE:HG21	2.36	0.60
1:P:23:ARG:HD3	1:P:120:LYS:HD3	1.83	0.60
1:P:1417:CYS:N	1:P:1484:CYS:SG	2.73	0.60
1:P:1639:LYS:HG2	4:6:1:NAG:HN2	1.66	0.60
2:Q:2684:HIS:HA	2:Q:2695:MET:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2964[B]:PRO:HG3	3:R:3040[B]:VAL:HG11	1.82	0.60
3:R:3025[A]:VAL:HG22	3:R:3025[A]:VAL:O	2.00	0.60
3:R:3134[A]:GLN:O	3:R:3135[A]:LYS:C	2.44	0.60
3:R:3191[A]:ASN:ND2	3:R:3191[A]:ASN:H	2.00	0.60
1:S:975:PRO:HG3	1:S:1026:GLU:HG3	1.83	0.60
1:S:1296:VAL:HB	1:S:1446:ASP:HB3	1.83	0.60
3:U:3025[B]:VAL:HG22	3:U:3025[B]:VAL:O	2.00	0.60
3:U:3154[B]:PRO:CG	3:d:2984[B]:THR:HG23	2.26	0.60
3:U:3220[A]:ARG:HH11	3:U:3220[A]:ARG:CG	2.12	0.60
3:U:3259[B]:ASP:N	3:d:2968[B]:GLN:HE21	1.98	0.60
3:U:3298[A]:ASN:CA	3:U:3300[A]:LEU:HD23	2.31	0.60
3:X:2949[A]:LYS:HZ2	3:X:2950[A]:THR:HA	1.65	0.60
3:X:3273[B]:LEU:CB	3:X:3275[B]:LEU:HD13	2.28	0.60
3:X:3298[B]:ASN:ND2	3:X:3301[B]:PRO:C	2.60	0.60
3:a:3025[B]:VAL:HG22	3:a:3025[B]:VAL:O	2.00	0.60
3:a:3139[A]:LEU:N	3:a:3139[A]:LEU:HD22	2.16	0.60
3:a:3147[A]:GLU:HG3	3:a:3149[A]:ASN:HD21	1.65	0.60
2:c:2406:SER:HB3	2:c:2429:LEU:HA	1.83	0.60
2:c:2509:ILE:HD11	2:c:2605:LEU:HD23	1.83	0.60
1:A:717:GLN:O	1:A:721:GLU:HG2	2.02	0.60
2:B:2863:ARG:HB2	2:B:2865:ILE:HG13	1.83	0.60
3:C:2949[A]:LYS:C	3:C:2949[A]:LYS:HZ3	2.09	0.60
3:C:3134[A]:GLN:O	3:C:3135[A]:LYS:C	2.44	0.60
3:C:3147[B]:GLU:CD	3:L:3163[B]:ASN:N	2.46	0.60
3:C:3222[A]:ILE:HG13	3:C:3224[A]:GLN:HG2	1.84	0.60
3:C:3253[B]:GLU:OE1	3:L:2974[B]:ALA:HB1	2.01	0.60
1:D:177:VAL:HA	1:D:180:ASN:HD22	1.65	0.60
1:D:931:TRP:CG	1:D:1018:ILE:HD11	2.36	0.60
3:F:2961[B]:HIS:HB3	3:F:3111[B]:SER:HG	1.67	0.60
3:F:2966[A]:SER:HB3	3:F:2977[A]:CYS:HB2	1.78	0.60
3:F:2966[B]:SER:HB3	3:a:2982[B]:MET:CE	2.30	0.60
3:F:3025[B]:VAL:HG22	3:F:3025[B]:VAL:O	2.00	0.60
3:F:3281[B]:PHE:CE1	3:F:3305[B]:ILE:HG21	2.36	0.60
3:F:3298[A]:ASN:CB	3:F:3300[A]:LEU:N	2.60	0.60
3:F:3298[A]:ASN:HD21	3:F:3301[A]:PRO:HA	1.60	0.60
1:G:829:ALA:HA	1:G:830:ASN:C	2.27	0.60
3:I:3158[B]:PHE:H	3:R:3153[B]:LYS:CE	2.13	0.60
3:I:3281[A]:PHE:CE1	3:I:3305[A]:ILE:HG21	2.36	0.60
3:I:3284[B]:LYS:CD	3:I:3285[B]:VAL:H	2.10	0.60
3:I:3298[A]:ASN:CB	3:I:3300[A]:LEU:N	2.60	0.60
3:L:3169[B]:LYS:C	3:L:3172[B]:SER:HG	2.03	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:392:PRO:O	1:M:395:THR:OG1	2.18	0.60
1:M:896:HIS:HB2	1:M:905:TRP:CG	2.36	0.60
3:O:2963[B]:MET:CE	3:X:2975[B]:PHE:CB	2.56	0.60
3:O:3156[B]:MET:HA	3:O:3157[B]:PRO:C	2.26	0.60
3:O:3194[A]:GLY:O	3:O:3195[A]:MET:HG2	2.01	0.60
3:O:3298[A]:ASN:ND2	3:O:3301[A]:PRO:C	2.60	0.60
3:O:3298[B]:ASN:HD21	3:O:3301[B]:PRO:HA	1.60	0.60
3:R:2939[B]:ARG:HG3	3:R:2939[B]:ARG:HH11	1.66	0.60
3:R:3139[A]:LEU:HD22	3:R:3139[A]:LEU:N	2.16	0.60
3:U:2964[A]:PRO:HG3	3:U:3040[A]:VAL:HG11	1.83	0.60
3:U:2964[B]:PRO:HG3	3:U:3040[B]:VAL:HG11	1.82	0.60
3:U:3200[B]:LEU:HD22	3:U:3204[B]:LEU:HD13	1.82	0.60
3:U:3276[A]:ASP:HB3	3:U:3278[A]:HIS:HB2	1.83	0.60
3:U:3281[A]:PHE:CE1	3:U:3305[A]:ILE:HG21	2.36	0.60
3:U:3281[B]:PHE:CE1	3:U:3305[B]:ILE:HG21	2.36	0.60
3:X:3281[B]:PHE:CE1	3:X:3305[B]:ILE:HG21	2.36	0.60
1:Y:1411:PHE:O	1:Y:1475:ARG:NH2	2.29	0.60
1:Y:1655:SER:HB3	3:d:3007[B]:ILE:CG2	2.30	0.60
3:a:2998[B]:ASP:O	3:a:3001[B]:LYS:HB2	2.02	0.60
2:c:2891:LEU:H	2:c:2891:LEU:HD12	1.66	0.60
3:d:2948[B]:ASP:CB	3:d:2949[B]:LYS:HA	2.16	0.60
2:B:2166:LEU:HA	2:B:2169:HIS:HB2	1.82	0.60
3:C:2972[B]:GLY:CA	3:L:3090[B]:ASN:HB3	2.31	0.60
3:C:3139[B]:LEU:N	3:C:3139[B]:LEU:HD22	2.16	0.60
3:C:3274[B]:ARG:HA	3:C:3274[B]:ARG:NE	2.16	0.60
3:C:3307[A]:PHE:HE1	3:C:3309[A]:PRO:CG	2.08	0.60
2:E:2141:HIS:ND1	2:E:2141:HIS:O	2.35	0.60
3:F:2979[B]:GLN:OE1	3:a:2977[B]:CYS:SG	2.60	0.60
3:F:3191[A]:ASN:ND2	3:F:3191[A]:ASN:H	1.99	0.60
3:F:3200[B]:LEU:HD22	3:F:3204[B]:LEU:HD13	1.83	0.60
3:F:3218[A]:LEU:O	3:F:3219[A]:LEU:HD13	2.01	0.60
1:G:1138:ALA:HA	1:G:1240:ILE:HG22	1.84	0.60
3:I:3139[B]:LEU:HD22	3:I:3139[B]:LEU:N	2.16	0.60
1:J:133:LYS:HA	1:J:133:LYS:HE3	1.82	0.60
3:L:2964[B]:PRO:HG3	3:L:3040[B]:VAL:HG11	1.82	0.60
3:L:3014[A]:TRP:CE3	3:L:3092[A]:ILE:HD12	2.37	0.60
3:O:2970[B]:PRO:CG	3:X:2991[B]:LEU:CD1	2.80	0.60
3:O:3298[A]:ASN:CA	3:O:3300[A]:LEU:HD23	2.31	0.60
2:Q:2303:ARG:NH2	2:Q:2372:GLU:O	2.34	0.60
2:Q:2830:GLN:HB2	2:Q:2863:ARG:HH12	1.67	0.60
3:R:2998[A]:ASP:O	3:R:3001[A]:LYS:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3182[B]:GLN:O	3:R:3183[B]:LEU:HD12	2.02	0.60
1:S:871:GLN:NE2	1:S:964:ILE:HG13	2.13	0.60
1:S:1157:VAL:HB	1:S:1217:ILE:HD13	1.84	0.60
2:T:2180:TRP:HB3	2:T:2184:MET:HE1	1.84	0.60
2:T:2800:LYS:C	3:U:3023[A]:ILE:CD1	2.75	0.60
3:U:3218[A]:LEU:O	3:U:3219[A]:LEU:HD13	2.01	0.60
3:U:3274[B]:ARG:HA	3:U:3274[B]:ARG:NE	2.16	0.60
3:X:2998[A]:ASP:O	3:X:3001[A]:LYS:HB2	2.01	0.60
3:X:3104[A]:MET:SD	3:X:3110[A]:THR:HG22	2.42	0.60
3:a:3025[A]:VAL:HG22	3:a:3025[A]:VAL:O	2.00	0.60
3:a:3104[B]:MET:SD	3:a:3110[B]:THR:HG22	2.42	0.60
3:a:3281[B]:PHE:CE1	3:a:3305[B]:ILE:HG21	2.36	0.60
3:a:3298[B]:ASN:CA	3:a:3300[B]:LEU:HD23	2.31	0.60
1:b:324:PRO:HG2	1:b:376:ASN:ND2	2.16	0.60
2:c:2644:LEU:HD22	2:c:2687:ILE:HG22	1.84	0.60
2:c:2874:ASP:OD1	2:c:2874:ASP:N	2.18	0.60
3:d:3147[A]:GLU:HG3	3:d:3149[A]:ASN:HD21	1.65	0.60
3:d:3194[A]:GLY:O	3:d:3195[A]:MET:HG2	2.01	0.60
1:A:1156:LEU:HD13	1:A:1176:TYR:CZ	2.36	0.60
3:C:2949[B]:LYS:HZ2	3:C:2950[B]:THR:HA	1.66	0.60
3:C:2952[A]:ALA:N	3:C:2953[A]:GLY:HA2	2.06	0.60
3:C:2998[A]:ASP:O	3:C:3001[A]:LYS:HB2	2.01	0.60
3:C:3224[B]:GLN:HA	3:L:3252[B]:TYR:CZ	2.36	0.60
1:D:1304:ASP:OD2	1:D:1306:THR:OG1	2.20	0.60
2:E:2828:ASP:OD2	2:E:2830:GLN:NE2	2.35	0.60
3:F:2981[B]:GLY:N	3:a:2968[B]:GLN:CD	2.56	0.60
3:F:3182[B]:GLN:O	3:F:3183[B]:LEU:HD12	2.02	0.60
3:F:3218[B]:LEU:O	3:F:3219[B]:LEU:HD13	2.01	0.60
1:G:327:ASP:OD1	1:G:328:LYS:N	2.32	0.60
3:I:2975[B]:PHE:HE2	3:R:2988[B]:TRP:CH2	2.19	0.60
3:I:3158[B]:PHE:H	3:R:3153[B]:LYS:HE3	1.67	0.60
3:I:3200[A]:LEU:HD22	3:I:3204[A]:LEU:HD13	1.83	0.60
1:J:898:GLY:HA2	1:J:1186:TRP:HB2	1.84	0.60
3:L:3096[B]:VAL:HG11	3:L:3115[B]:LEU:HD13	1.81	0.60
3:L:3222[A]:ILE:HG13	3:L:3224[A]:GLN:HG2	1.84	0.60
1:M:126:GLY:CA	1:M:127:GLU:HB3	2.31	0.60
1:M:757:VAL:HG21	1:M:781:ILE:HG22	1.83	0.60
1:M:881:GLN:HE21	1:M:888:ALA:HB3	1.65	0.60
3:O:2939[A]:ARG:HG3	3:O:2939[A]:ARG:HH11	1.67	0.60
3:O:2945[B]:VAL:HG22	3:O:2945[B]:VAL:O	2.01	0.60
3:O:2964[B]:PRO:HG3	3:O:3040[B]:VAL:HG11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3218[B]:LEU:O	3:O:3219[B]:LEU:HD13	2.01	0.60
3:R:3182[A]:GLN:O	3:R:3183[A]:LEU:HD12	2.02	0.60
2:T:2901:LEU:HB2	1:V:1074:ILE:HB	1.84	0.60
3:U:2971[B]:ASP:N	3:d:3090[B]:ASN:HD22	2.00	0.60
3:U:2975[B]:PHE:CZ	3:d:3254[B]:MET:N	2.69	0.60
3:U:2998[B]:ASP:O	3:U:3001[B]:LYS:HB2	2.01	0.60
3:U:3124[A]:ASP:OD2	3:U:3187[A]:TYR:OH	2.15	0.60
3:U:3147[B]:GLU:HG3	3:U:3149[B]:ASN:HD21	1.65	0.60
3:U:3222[A]:ILE:HG13	3:U:3224[A]:GLN:HG2	1.84	0.60
1:V:317:VAL:HG22	1:V:383:VAL:HG22	1.82	0.60
2:W:2394:VAL:H	2:W:2448:THR:HG22	1.67	0.60
3:X:2998[B]:ASP:O	3:X:3001[B]:LYS:HB2	2.01	0.60
3:X:3156[A]:MET:HA	3:X:3157[A]:PRO:C	2.26	0.60
3:X:3194[B]:GLY:O	3:X:3195[B]:MET:HG2	2.01	0.60
3:a:3104[A]:MET:SD	3:a:3110[A]:THR:HG22	2.42	0.60
1:b:736:MET:HG3	1:b:772:ARG:HD2	1.84	0.60
3:d:3135[A]:LYS:HG3	3:d:3141[A]:TYR:CD1	2.33	0.60
3:d:3156[B]:MET:HA	3:d:3157[B]:PRO:C	2.26	0.60
3:d:3276[B]:ASP:HB3	3:d:3278[B]:HIS:HB2	1.83	0.60
3:d:3281[A]:PHE:CE1	3:d:3305[A]:ILE:HG21	2.36	0.60
3:C:3025[B]:VAL:HG22	3:C:3025[B]:VAL:O	2.00	0.60
3:C:3182[B]:GLN:O	3:C:3183[B]:LEU:HD12	2.02	0.60
3:F:2948[B]:ASP:HB3	3:F:2953[B]:GLY:CA	2.24	0.60
3:F:3023[A]:ILE:O	3:F:3024[A]:LEU:C	2.45	0.60
3:F:3104[B]:MET:SD	3:F:3110[B]:THR:HG22	2.42	0.60
3:F:3156[A]:MET:HA	3:F:3157[A]:PRO:C	2.26	0.60
3:F:3169[B]:LYS:HD3	3:a:3148[B]:ILE:C	2.24	0.60
3:F:3200[A]:LEU:HD22	3:F:3204[A]:LEU:HD13	1.83	0.60
3:F:3284[A]:LYS:CD	3:F:3285[A]:VAL:H	2.09	0.60
3:F:3298[A]:ASN:ND2	3:F:3301[A]:PRO:C	2.60	0.60
1:G:448:SER:O	1:G:450:LYS:NZ	2.35	0.60
1:G:1414:THR:HG23	1:G:1477:LEU:HD13	1.84	0.60
2:H:2373:MET:HB3	2:H:2381:LEU:HD11	1.84	0.60
3:I:2945[B]:VAL:HG22	3:I:2945[B]:VAL:O	2.01	0.60
3:I:3134[A]:GLN:O	3:I:3135[A]:LYS:C	2.44	0.60
3:I:3134[B]:GLN:O	3:I:3135[B]:LYS:C	2.44	0.60
3:I:3218[A]:LEU:O	3:I:3219[A]:LEU:HD13	2.01	0.60
3:L:3023[B]:ILE:O	3:L:3024[B]:LEU:C	2.45	0.60
3:L:3288[A]:MET:CG	3:L:3295[A]:LEU:HD21	2.32	0.60
3:L:3298[A]:ASN:ND2	3:L:3301[A]:PRO:C	2.60	0.60
3:L:3298[B]:ASN:ND2	3:L:3301[B]:PRO:C	2.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2939[B]:ARG:HH11	3:O:2939[B]:ARG:HG3	1.66	0.60
3:O:3135[B]:LYS:CB	3:O:3141[B]:TYR:CD1	2.85	0.60
3:O:3147[B]:GLU:HG3	3:O:3149[B]:ASN:HD21	1.65	0.60
3:O:3197[B]:ILE:HD12	1:P:1617:LYS:O	2.02	0.60
3:O:3212[A]:ARG:HH11	3:O:3212[A]:ARG:CG	2.12	0.60
3:O:3222[A]:ILE:HG13	3:O:3224[A]:GLN:HG2	1.84	0.60
1:P:149:GLU:OE1	1:P:152:LYS:NZ	2.28	0.60
2:Q:2722:GLN:NE2	2:Q:2769:PHE:O	2.31	0.60
1:S:1074:ILE:HB	2:W:2901:LEU:HB2	1.83	0.60
3:U:3104[B]:MET:SD	3:U:3110[B]:THR:HG22	2.42	0.60
3:U:3139[B]:LEU:HD22	3:U:3139[B]:LEU:N	2.16	0.60
3:U:3307[A]:PHE:HE1	3:U:3309[A]:PRO:CG	2.08	0.60
2:W:2506:ARG:NE	2:W:2578:GLU:OE2	2.29	0.60
2:W:2603:PRO:HG2	2:W:2606:LEU:HD12	1.84	0.60
3:X:2942[B]:LEU:CD1	3:X:3033[B]:PHE:CE1	2.85	0.60
3:X:3200[A]:LEU:HD22	3:X:3204[A]:LEU:HD13	1.83	0.60
3:X:3288[A]:MET:CG	3:X:3295[A]:LEU:HD21	2.32	0.60
3:X:3298[A]:ASN:CB	3:X:3300[A]:LEU:N	2.60	0.60
1:Y:1063:ARG:HB3	1:Y:1065:LYS:HD2	1.84	0.60
3:a:2939[B]:ARG:HG3	3:a:2939[B]:ARG:HH11	1.66	0.60
3:a:2942[B]:LEU:CD1	3:a:3033[B]:PHE:CE1	2.85	0.60
3:a:3023[A]:ILE:O	3:a:3024[A]:LEU:C	2.45	0.60
3:a:3120[B]:HIS:C	3:a:3122[B]:ASN:N	2.55	0.60
3:a:3173[B]:THR:HG22	3:a:3174[B]:GLY:H	1.67	0.60
3:d:2942[A]:LEU:CD1	3:d:3033[A]:PHE:CE1	2.85	0.60
3:d:2965[A]:LEU:CD1	3:d:2975[A]:PHE:H	2.08	0.60
3:d:2998[A]:ASP:O	3:d:3001[A]:LYS:HB2	2.01	0.60
3:d:3014[B]:TRP:CE3	3:d:3092[B]:ILE:HD12	2.37	0.60
3:d:3025[B]:VAL:HG22	3:d:3025[B]:VAL:O	2.00	0.60
3:d:3104[A]:MET:SD	3:d:3110[A]:THR:HG22	2.42	0.60
3:d:3182[A]:GLN:O	3:d:3183[A]:LEU:HD12	2.02	0.60
3:d:3222[A]:ILE:HG13	3:d:3224[A]:GLN:HG2	1.84	0.60
3:d:3274[B]:ARG:HA	3:d:3274[B]:ARG:NE	2.16	0.60
3:C:3014[A]:TRP:CE3	3:C:3092[A]:ILE:HD12	2.37	0.60
3:C:3104[B]:MET:SD	3:C:3110[B]:THR:HG22	2.42	0.60
3:C:3135[A]:LYS:CB	3:C:3141[A]:TYR:CD1	2.85	0.60
3:C:3191[A]:ASN:ND2	3:C:3191[A]:ASN:H	1.99	0.60
3:C:3274[A]:ARG:HA	3:C:3274[A]:ARG:NE	2.16	0.60
2:E:2564:PRO:HA	2:E:2673:GLU:HG3	1.84	0.60
3:F:3090[B]:ASN:HB3	3:a:2972[B]:GLY:CA	2.31	0.60
3:F:3104[A]:MET:SD	3:F:3110[A]:THR:HG22	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3194[B]:GLY:O	3:F:3195[B]:MET:HG2	2.01	0.60
3:I:2942[B]:LEU:CD1	3:I:3033[B]:PHE:CE1	2.85	0.60
3:I:3014[B]:TRP:CE3	3:I:3092[B]:ILE:HD12	2.37	0.60
3:I:3071[B]:PHE:O	3:I:3074[B]:GLU:HB2	2.02	0.60
3:I:3104[B]:MET:SD	3:I:3110[B]:THR:HG22	2.42	0.60
3:I:3196[A]:THR:OG1	1:J:416:ASN:ND2	2.34	0.60
3:L:2957[A]:ILE:HA	3:L:2960[A]:PHE:HE1	1.64	0.60
1:P:1442:MET:HE1	1:P:1454:PHE:HA	1.82	0.60
3:R:2942[B]:LEU:CD1	3:R:3033[B]:PHE:CE1	2.85	0.60
3:R:3096[A]:VAL:HG11	3:R:3115[A]:LEU:HD13	1.81	0.60
3:R:3281[A]:PHE:CE1	3:R:3305[A]:ILE:HG21	2.36	0.60
3:R:3298[B]:ASN:CB	3:R:3300[B]:LEU:N	2.60	0.60
1:S:212:ASN:OD1	1:S:215:ARG:NH1	2.35	0.60
1:S:832:LYS:HB2	1:S:834:ASP:OD1	2.02	0.60
3:U:2932[A]:PRO:CA	3:U:2935[A]:ILE:HD12	2.31	0.60
3:U:2969[A]:TYR:CD2	3:U:2970[A]:PRO:CD	2.85	0.60
3:U:3023[A]:ILE:O	3:U:3024[A]:LEU:C	2.45	0.60
3:U:3135[A]:LYS:CB	3:U:3141[A]:TYR:CD1	2.85	0.60
3:U:3182[A]:GLN:O	3:U:3183[A]:LEU:HD12	2.02	0.60
3:U:3222[B]:ILE:HG13	3:U:3224[B]:GLN:HG2	1.84	0.60
3:U:3254[B]:MET:C	3:d:2975[B]:PHE:CE1	2.79	0.60
3:X:2930[A]:LEU:HD22	3:X:2930[A]:LEU:N	2.02	0.60
3:X:2942[A]:LEU:CD1	3:X:3033[A]:PHE:CE1	2.85	0.60
3:X:3014[A]:TRP:CE3	3:X:3092[A]:ILE:HD12	2.37	0.60
3:X:3139[B]:LEU:N	3:X:3139[B]:LEU:HD22	2.16	0.60
3:X:3162[B]:ASP:OD1	3:X:3162[B]:ASP:N	2.31	0.60
3:X:3284[A]:LYS:HE2	3:X:3284[A]:LYS:CA	2.30	0.60
3:a:3014[B]:TRP:CE3	3:a:3092[B]:ILE:HD12	2.37	0.60
3:a:3023[B]:ILE:O	3:a:3024[B]:LEU:C	2.45	0.60
3:a:3134[A]:GLN:O	3:a:3135[A]:LYS:C	2.44	0.60
3:a:3182[B]:GLN:O	3:a:3183[B]:LEU:HD12	2.02	0.60
3:a:3298[B]:ASN:CB	3:a:3300[B]:LEU:N	2.60	0.60
3:d:2964[A]:PRO:HG3	3:d:3040[A]:VAL:HG11	1.82	0.60
3:d:2964[B]:PRO:HG3	3:d:3040[B]:VAL:HG11	1.82	0.60
3:d:3156[A]:MET:HA	3:d:3157[A]:PRO:C	2.26	0.60
3:d:3173[A]:THR:HG22	3:d:3174[A]:GLY:H	1.67	0.60
3:d:3191[B]:ASN:ND2	3:d:3191[B]:ASN:H	1.99	0.60
3:d:3288[A]:MET:CG	3:d:3295[A]:LEU:HD21	2.32	0.60
3:d:3298[A]:ASN:ND2	3:d:3301[A]:PRO:C	2.60	0.60
3:d:3298[B]:ASN:ND2	3:d:3301[B]:PRO:C	2.60	0.60
1:A:7:VAL:HG13	1:A:104:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:GLY:HA3	1:A:771:TRP:CE3	2.37	0.59
3:C:3155[B]:MET:HE2	3:L:3153[B]:LYS:CD	2.32	0.59
3:C:3218[B]:LEU:O	3:C:3219[B]:LEU:HD13	2.01	0.59
3:C:3298[A]:ASN:ND2	3:C:3301[A]:PRO:C	2.60	0.59
3:C:3298[B]:ASN:ND2	3:C:3301[B]:PRO:C	2.60	0.59
1:D:81:VAL:HA	1:D:85:SER:HB3	1.84	0.59
1:D:321:LEU:HB2	1:D:338:ALA:HB2	1.83	0.59
3:F:2942[A]:LEU:CD1	3:F:3033[A]:PHE:CE1	2.85	0.59
3:F:2998[B]:ASP:O	3:F:3001[B]:LYS:HB2	2.01	0.59
3:F:3134[A]:GLN:O	3:F:3135[A]:LYS:C	2.44	0.59
3:F:3150[B]:LYS:HE2	3:a:3157[B]:PRO:HB2	1.84	0.59
1:G:128:ILE:HG22	1:G:202:TYR:CG	2.37	0.59
1:G:567:LEU:HD22	1:G:568:PHE:H	1.67	0.59
3:I:2932[B]:PRO:CA	3:I:2935[B]:ILE:HD12	2.30	0.59
3:I:3014[A]:TRP:CE3	3:I:3092[A]:ILE:HD12	2.37	0.59
3:I:3023[A]:ILE:O	3:I:3024[A]:LEU:C	2.45	0.59
3:I:3038[A]:ILE:HG12	3:I:3112[A]:TYR:CE2	2.35	0.59
3:I:3071[A]:PHE:O	3:I:3074[A]:GLU:HB2	2.02	0.59
3:I:3096[B]:VAL:HG11	3:I:3115[B]:LEU:HD13	1.81	0.59
3:I:3172[B]:SER:HB3	3:R:3150[B]:LYS:HA	1.82	0.59
1:J:450:LYS:NZ	1:J:505:ARG:HH21	2.00	0.59
2:K:2545:SER:HB3	2:K:2547:MET:N	2.17	0.59
3:L:3173[A]:THR:HB	3:L:3176[A]:LYS:HG2	1.81	0.59
3:L:3276[B]:ASP:HB3	3:L:3278[B]:HIS:HB2	1.83	0.59
3:L:3281[B]:PHE:CE1	3:L:3305[B]:ILE:HG21	2.36	0.59
3:L:3293[B]:LYS:CB	3:L:3294[B]:SER:CB	2.54	0.59
3:O:2965[B]:LEU:CD2	3:X:3156[B]:MET:HE3	2.32	0.59
3:O:3135[A]:LYS:CB	3:O:3141[A]:TYR:CD1	2.85	0.59
3:O:3200[A]:LEU:HD22	3:O:3204[A]:LEU:HD13	1.83	0.59
3:O:3200[B]:LEU:HD22	3:O:3204[B]:LEU:HD13	1.83	0.59
3:O:3222[B]:ILE:HG13	3:O:3224[B]:GLN:HG2	1.84	0.59
1:P:1372:ILE:HD11	1:S:1392:ASP:HB2	1.84	0.59
3:R:2998[B]:ASP:O	3:R:3001[B]:LYS:HB2	2.02	0.59
3:R:3162[A]:ASP:OD1	3:R:3162[A]:ASP:N	2.31	0.59
3:R:3288[A]:MET:CG	3:R:3295[A]:LEU:HD21	2.32	0.59
2:T:2889:ALA:N	2:T:2890:VAL:HA	2.16	0.59
3:U:3071[B]:PHE:O	3:U:3074[B]:GLU:HB2	2.02	0.59
3:U:3147[A]:GLU:HG3	3:U:3149[A]:ASN:HD21	1.65	0.59
3:U:3153[B]:LYS:CG	3:d:2979[B]:GLN:NE2	2.65	0.59
3:U:3182[B]:GLN:O	3:U:3183[B]:LEU:HD12	2.02	0.59
3:U:3254[B]:MET:HG2	3:d:3255[B]:PRO:HD2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:567:LEU:HA	1:V:571:PRO:HD2	1.84	0.59
2:W:2344:LEU:HA	2:W:2345:ASN:C	2.26	0.59
3:X:3182[A]:GLN:O	3:X:3183[A]:LEU:HD12	2.02	0.59
1:Y:462:HIS:HA	1:Y:490:TRP:HH2	1.67	0.59
1:Y:1348:TRP:CD1	1:Y:1403:LEU:HD13	2.37	0.59
3:a:2945[B]:VAL:HG22	3:a:2945[B]:VAL:O	2.01	0.59
3:a:3135[B]:LYS:CB	3:a:3141[B]:TYR:CD1	2.85	0.59
3:a:3274[B]:ARG:HA	3:a:3274[B]:ARG:NE	2.16	0.59
3:a:3288[B]:MET:CG	3:a:3295[B]:LEU:HD21	2.32	0.59
3:a:3293[B]:LYS:CB	3:a:3294[B]:SER:CB	2.54	0.59
1:b:330:GLN:O	1:b:332:ASP:N	2.31	0.59
2:c:2800:LYS:O	3:d:3023[A]:ILE:HD13	2.00	0.59
3:d:2939[B]:ARG:HH11	3:d:2939[B]:ARG:HG3	1.66	0.59
3:d:3104[B]:MET:SD	3:d:3110[B]:THR:HG22	2.42	0.59
3:d:3183[B]:LEU:N	3:d:3184[B]:ASN:HA	2.11	0.59
3:d:3200[B]:LEU:HD22	3:d:3204[B]:LEU:HD13	1.82	0.59
1:A:69:HIS:NE2	9:A:5001:CUO:O1	2.35	0.59
1:A:1210:LYS:HG3	2:E:2743:ALA:HB3	1.84	0.59
3:C:3071[A]:PHE:O	3:C:3074[A]:GLU:HB2	2.02	0.59
3:C:3222[B]:ILE:HG13	3:C:3224[B]:GLN:HG2	1.84	0.59
3:C:3293[A]:LYS:CB	3:C:3294[A]:SER:CB	2.54	0.59
3:F:2975[B]:PHE:CZ	3:a:2961[B]:HIS:CA	2.73	0.59
3:F:3014[B]:TRP:CE3	3:F:3092[B]:ILE:HD12	2.37	0.59
3:F:3182[A]:GLN:O	3:F:3183[A]:LEU:HD12	2.02	0.59
3:I:2942[A]:LEU:CD1	3:I:3033[A]:PHE:CE1	2.85	0.59
3:I:3038[B]:ILE:HG22	3:I:3041[B]:ALA:H	1.65	0.59
3:I:3156[B]:MET:HA	3:I:3157[B]:PRO:C	2.26	0.59
3:I:3276[B]:ASP:HB3	3:I:3278[B]:HIS:HB2	1.83	0.59
2:K:2545:SER:HA	2:K:2546:LEU:CG	2.31	0.59
3:L:2939[B]:ARG:HH11	3:L:2939[B]:ARG:HG3	1.66	0.59
3:L:3014[B]:TRP:CE3	3:L:3092[B]:ILE:HD12	2.37	0.59
3:L:3023[A]:ILE:O	3:L:3024[A]:LEU:C	2.45	0.59
3:L:3135[B]:LYS:CB	3:L:3141[B]:TYR:CD1	2.85	0.59
2:N:2644:LEU:HD22	2:N:2687:ILE:HG22	1.82	0.59
3:O:2949[A]:LYS:HZ2	3:O:2950[A]:THR:HA	1.67	0.59
3:R:3274[A]:ARG:HA	3:R:3274[A]:ARG:NE	2.16	0.59
3:R:3298[A]:ASN:ND2	3:R:3301[A]:PRO:C	2.60	0.59
3:R:3298[A]:ASN:CA	3:R:3300[A]:LEU:HD23	2.31	0.59
3:R:3298[B]:ASN:CA	3:R:3300[B]:LEU:HD23	2.31	0.59
3:U:3096[A]:VAL:HG11	3:U:3115[A]:LEU:HD13	1.81	0.59
3:U:3254[B]:MET:HG3	3:d:2975[B]:PHE:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3298[B]:ASN:CA	3:U:3300[B]:LEU:HD23	2.31	0.59
3:X:2939[A]:ARG:HH11	3:X:2939[A]:ARG:HG3	1.67	0.59
3:X:3071[B]:PHE:O	3:X:3074[B]:GLU:HB2	2.02	0.59
1:Y:416:ASN:ND2	3:d:3196[A]:THR:HG21	2.16	0.59
3:a:2969[A]:TYR:CD2	3:a:2970[A]:PRO:CD	2.85	0.59
1:b:447:MET:HA	1:b:455:TYR:CB	2.32	0.59
3:d:2930[B]:LEU:H	3:d:2930[B]:LEU:CD2	1.98	0.59
3:d:3134[A]:GLN:O	3:d:3135[A]:LYS:C	2.44	0.59
3:d:3194[B]:GLY:O	3:d:3195[B]:MET:HG2	2.01	0.59
2:B:2722:GLN:NE2	2:B:2769:PHE:O	2.32	0.59
3:C:2969[B]:TYR:CZ	3:L:3120[B]:HIS:CD2	2.71	0.59
3:C:3173[B]:THR:HG22	3:C:3174[B]:GLY:H	1.67	0.59
3:C:3249[B]:GLY:HA2	3:L:2974[B]:ALA:O	1.90	0.59
1:D:942:VAL:HG21	1:D:1041:ILE:HD11	1.84	0.59
3:F:2980[B]:HIS:N	3:a:2968[B]:GLN:O	2.33	0.59
3:F:3132[B]:ALA:CB	3:F:3197[B]:ILE:HD13	2.33	0.59
3:F:3135[A]:LYS:CB	3:F:3141[A]:TYR:CD1	2.85	0.59
3:F:3135[B]:LYS:CB	3:F:3141[B]:TYR:CD1	2.85	0.59
3:F:3155[B]:MET:SD	3:a:3154[B]:PRO:CG	2.88	0.59
3:F:3160[B]:SER:CB	3:a:3150[B]:LYS:HZ2	1.91	0.59
3:F:3274[B]:ARG:HA	3:F:3274[B]:ARG:NE	2.16	0.59
3:F:3298[B]:ASN:CA	3:F:3300[B]:LEU:HD23	2.31	0.59
3:I:2972[B]:GLY:C	3:R:3090[B]:ASN:HB3	2.26	0.59
3:I:2989[B]:HIS:CE1	3:R:2970[B]:PRO:CD	2.84	0.59
3:I:3135[A]:LYS:CB	3:I:3141[A]:TYR:CD1	2.85	0.59
3:I:3153[B]:LYS:C	3:R:3155[B]:MET:CB	2.74	0.59
3:I:3153[B]:LYS:HB3	3:R:3155[B]:MET:C	2.27	0.59
3:I:3169[B]:LYS:CD	3:R:3148[B]:ILE:C	2.64	0.59
3:I:3191[B]:ASN:ND2	3:I:3191[B]:ASN:H	1.99	0.59
3:I:3222[B]:ILE:HG13	3:I:3224[B]:GLN:HG2	1.84	0.59
3:I:3251[B]:ASP:HB2	3:R:3251[B]:ASP:CB	2.09	0.59
1:J:602:THR:O	1:J:605:SER:OG	2.20	0.59
3:L:2949[A]:LYS:HZ2	3:L:2950[A]:THR:HA	1.66	0.59
3:L:3104[B]:MET:SD	3:L:3110[B]:THR:HG22	2.42	0.59
3:L:3139[B]:LEU:N	3:L:3139[B]:LEU:HD22	2.16	0.59
3:L:3217[B]:PHE:HE1	3:L:3230[B]:PHE:HZ	0.80	0.59
3:L:3298[A]:ASN:CB	3:L:3300[A]:LEU:N	2.60	0.59
3:O:2970[B]:PRO:O	3:X:2989[B]:HIS:CA	2.35	0.59
3:O:3156[A]:MET:HA	3:O:3157[A]:PRO:C	2.26	0.59
3:O:3157[B]:PRO:HA	3:X:3152[B]:LYS:N	2.16	0.59
3:R:2969[A]:TYR:CD2	3:R:2970[A]:PRO:CD	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3071[A]:PHE:O	3:R:3074[A]:GLU:HB2	2.02	0.59
3:R:3156[A]:MET:HA	3:R:3157[A]:PRO:C	2.26	0.59
3:R:3188[A]:ASP:N	3:R:3188[A]:ASP:OD2	2.36	0.59
3:R:3217[B]:PHE:HE1	3:R:3230[B]:PHE:HZ	0.80	0.59
3:R:3276[A]:ASP:HB3	3:R:3278[A]:HIS:HB2	1.83	0.59
3:U:2970[B]:PRO:HB3	3:d:2985[B]:PHE:CD2	2.37	0.59
3:U:3276[B]:ASP:HB3	3:U:3278[B]:HIS:HB2	1.83	0.59
1:V:760:ILE:HG21	1:V:777:TYR:HE2	1.67	0.59
1:V:830:ASN:OD1	1:V:830:ASN:N	2.34	0.59
3:X:2928[A]:ASN:N	3:X:2930[A]:LEU:HD21	2.18	0.59
3:X:3024[B]:LEU:O	3:X:3031[B]:ASN:ND2	2.36	0.59
3:X:3104[B]:MET:SD	3:X:3110[B]:THR:HG22	2.42	0.59
3:X:3134[A]:GLN:O	3:X:3135[A]:LYS:C	2.44	0.59
3:X:3218[B]:LEU:O	3:X:3219[B]:LEU:HD13	2.01	0.59
2:Z:2806:ALA:HB2	2:Z:2856:ILE:HD11	1.84	0.59
3:a:2964[A]:PRO:HG3	3:a:3040[A]:VAL:HG11	1.82	0.59
3:a:3014[A]:TRP:CE3	3:a:3092[A]:ILE:HD12	2.37	0.59
3:a:3276[A]:ASP:HB3	3:a:3278[A]:HIS:HB2	1.83	0.59
3:d:2945[B]:VAL:HG22	3:d:2945[B]:VAL:O	2.01	0.59
3:d:2969[A]:TYR:CD2	3:d:2970[A]:PRO:HG2	2.38	0.59
3:d:2998[B]:ASP:O	3:d:3001[B]:LYS:HB2	2.01	0.59
3:d:3071[B]:PHE:O	3:d:3074[B]:GLU:HB2	2.02	0.59
1:A:558:HIS:ND1	1:A:558:HIS:O	2.35	0.59
3:C:3071[B]:PHE:O	3:C:3074[B]:GLU:HB2	2.02	0.59
3:C:3104[A]:MET:SD	3:C:3110[A]:THR:HG22	2.42	0.59
3:C:3135[B]:LYS:CB	3:C:3141[B]:TYR:CD1	2.85	0.59
3:C:3152[B]:LYS:CG	3:L:3169[B]:LYS:O	2.40	0.59
3:C:3174[B]:GLY:N	3:L:3154[B]:PRO:CD	2.62	0.59
3:C:3191[B]:ASN:ND2	3:C:3191[B]:ASN:H	1.99	0.59
3:F:2928[A]:ASN:N	3:F:2930[A]:LEU:HD21	2.18	0.59
3:F:2969[A]:TYR:CD2	3:F:2970[A]:PRO:CD	2.85	0.59
3:F:2983[B]:VAL:CB	3:a:3160[B]:SER:HA	2.33	0.59
1:G:330:GLN:O	1:G:332:ASP:N	2.35	0.59
1:G:898:GLY:N	1:G:899:MET:HA	2.18	0.59
3:I:2985[B]:PHE:CE2	3:R:2968[B]:GLN:O	2.54	0.59
3:I:3024[A]:LEU:O	3:I:3031[A]:ASN:ND2	2.36	0.59
3:I:3155[B]:MET:C	3:R:3153[B]:LYS:HD2	2.26	0.59
3:I:3218[B]:LEU:O	3:I:3219[B]:LEU:HD13	2.01	0.59
3:I:3255[B]:PRO:HB2	3:R:2959[B]:SER:HB3	1.74	0.59
3:I:3255[B]:PRO:CG	3:R:2959[B]:SER:CA	2.80	0.59
3:L:3134[A]:GLN:O	3:L:3135[A]:LYS:C	2.44	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3222[B]:ILE:HG13	3:L:3224[B]:GLN:HG2	1.84	0.59
3:L:3276[A]:ASP:HB3	3:L:3278[A]:HIS:HB2	1.83	0.59
1:M:67:MET:HE1	1:M:233:PRO:HG2	1.84	0.59
2:N:2556:TYR:CE1	2:N:2845:PRO:HD2	2.30	0.59
3:O:2928[B]:ASN:N	3:O:2930[B]:LEU:HD21	2.17	0.59
3:O:2945[A]:VAL:HG22	3:O:2945[A]:VAL:O	2.01	0.59
3:O:3024[A]:LEU:O	3:O:3031[A]:ASN:ND2	2.36	0.59
3:O:3071[A]:PHE:O	3:O:3074[A]:GLU:HB2	2.02	0.59
3:O:3182[A]:GLN:O	3:O:3183[A]:LEU:HD12	2.02	0.59
3:O:3281[A]:PHE:CE1	3:O:3305[A]:ILE:HG21	2.36	0.59
3:R:2935[A]:ILE:HD13	3:R:2935[A]:ILE:N	2.18	0.59
3:R:2945[A]:VAL:HG22	3:R:2945[A]:VAL:O	2.01	0.59
3:R:2945[B]:VAL:HG22	3:R:2945[B]:VAL:O	2.01	0.59
3:R:3024[A]:LEU:O	3:R:3031[A]:ASN:ND2	2.36	0.59
3:R:3104[A]:MET:SD	3:R:3110[A]:THR:HG22	2.42	0.59
3:R:3284[B]:LYS:CD	3:R:3285[B]:VAL:H	2.10	0.59
1:S:1358:LEU:HD23	1:S:1456:LEU:HD21	1.83	0.59
2:T:2094:ARG:HH21	2:W:2094:ARG:HH21	1.49	0.59
3:U:2968[B]:GLN:N	3:d:3256[B]:TRP:CB	2.46	0.59
3:U:3134[A]:GLN:O	3:U:3135[A]:LYS:C	2.44	0.59
3:U:3154[B]:PRO:HD2	3:d:2984[B]:THR:HG21	1.81	0.59
3:U:3162[B]:ASP:CB	3:d:3260[B]:ARG:CZ	2.81	0.59
3:U:3188[B]:ASP:N	3:U:3188[B]:ASP:OD2	2.36	0.59
3:U:3191[A]:ASN:ND2	3:U:3191[A]:ASN:H	1.99	0.59
3:U:3298[B]:ASN:ND2	3:U:3301[B]:PRO:C	2.60	0.59
3:X:3001[A]:LYS:HE3	3:X:3002[A]:ALA:HB2	1.85	0.59
3:X:3157[A]:PRO:O	3:X:3160[A]:SER:N	2.30	0.59
3:X:3222[A]:ILE:HG13	3:X:3224[A]:GLN:HG2	1.84	0.59
3:X:3222[B]:ILE:HG13	3:X:3224[B]:GLN:HG2	1.84	0.59
3:X:3281[A]:PHE:CE1	3:X:3305[A]:ILE:HG21	2.36	0.59
3:a:2928[A]:ASN:N	3:a:2930[A]:LEU:HD21	2.17	0.59
3:a:3001[A]:LYS:HE3	3:a:3002[A]:ALA:HB2	1.85	0.59
3:a:3222[B]:ILE:HG13	3:a:3224[B]:GLN:HG2	1.84	0.59
3:a:3298[A]:ASN:ND2	3:a:3301[A]:PRO:C	2.60	0.59
3:a:3298[A]:ASN:HD21	3:a:3301[A]:PRO:HA	1.60	0.59
3:d:2961[A]:HIS:CE1	3:d:2980[A]:HIS:NE2	2.57	0.59
2:B:2571:ARG:NH1	2:B:2771:TYR:HB3	2.18	0.59
3:C:2939[A]:ARG:HG3	3:C:2939[A]:ARG:HH11	1.66	0.59
3:C:3182[A]:GLN:O	3:C:3183[A]:LEU:HD12	2.02	0.59
3:C:3255[B]:PRO:HB3	3:L:2964[B]:PRO:C	2.25	0.59
1:D:142:ARG:NH1	1:D:340:GLN:HE22	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:899:MET:HE2	1:D:1012:GLU:CD	2.26	0.59
2:E:2218:SER:HB3	2:E:2221:THR:HG23	1.84	0.59
3:F:3096[A]:VAL:HG11	3:F:3115[A]:LEU:HD13	1.81	0.59
3:F:3147[B]:GLU:HG3	3:F:3149[B]:ASN:HD21	1.65	0.59
3:F:3149[B]:ASN:ND2	3:a:3163[B]:ASN:ND2	2.49	0.59
3:F:3156[B]:MET:HB3	3:a:2982[B]:MET:CG	2.31	0.59
1:G:1207:TYR:O	1:G:1211:TYR:OH	2.16	0.59
3:I:2928[A]:ASN:N	3:I:2930[A]:LEU:HD21	2.17	0.59
3:I:3182[B]:GLN:O	3:I:3183[B]:LEU:HD12	2.02	0.59
3:I:3274[B]:ARG:HA	3:I:3274[B]:ARG:NE	2.16	0.59
2:K:2252:GLU:O	2:K:2389:ARG:NH2	2.35	0.59
3:L:2945[B]:VAL:HG22	3:L:2945[B]:VAL:O	2.01	0.59
3:L:2998[A]:ASP:O	3:L:3001[A]:LYS:HB2	2.01	0.59
3:L:3182[B]:GLN:O	3:L:3183[B]:LEU:HD12	2.02	0.59
3:L:3191[B]:ASN:ND2	3:L:3191[B]:ASN:H	2.00	0.59
1:M:492:ARG:HD2	1:M:692:VAL:HG13	1.85	0.59
3:O:3134[B]:GLN:O	3:O:3135[B]:LYS:C	2.44	0.59
3:O:3135[B]:LYS:HG3	3:O:3141[B]:TYR:CD1	2.33	0.59
3:O:3279[B]:ASP:OD1	3:O:3279[B]:ASP:N	2.25	0.59
3:R:2942[A]:LEU:CD1	3:R:3033[A]:PHE:CE1	2.85	0.59
3:U:2935[A]:ILE:HD13	3:U:2935[A]:ILE:N	2.18	0.59
3:U:3257[B]:ALA:HB2	3:d:2974[B]:ALA:N	2.17	0.59
1:V:402:THR:HG23	1:V:659:CYS:HA	1.84	0.59
1:V:673:PHE:HB3	1:V:677:LEU:HB2	1.84	0.59
2:W:2856:ILE:HG22	2:W:2859:VAL:HB	1.85	0.59
3:X:2969[A]:TYR:CD2	3:X:2970[A]:PRO:CD	2.85	0.59
1:Y:898:GLY:N	1:Y:899:MET:HA	2.16	0.59
1:Y:1286:ARG:NH2	1:Y:1333:GLU:OE2	2.35	0.59
3:a:2948[A]:ASP:CB	3:a:2949[A]:LYS:HA	2.16	0.59
3:a:2969[A]:TYR:CD2	3:a:2970[A]:PRO:HG2	2.38	0.59
1:b:1492:PRO:HB2	1:b:1497:SER:HB3	1.83	0.59
2:c:2124:SER:HB2	2:c:2129:PRO:HG2	1.83	0.59
2:c:2141:HIS:ND1	2:c:2141:HIS:O	2.35	0.59
3:d:3023[B]:ILE:O	3:d:3024[B]:LEU:C	2.45	0.59
3:d:3288[B]:MET:CG	3:d:3295[B]:LEU:HD21	2.32	0.59
3:C:2964[B]:PRO:HG3	3:C:3040[B]:VAL:HG11	1.82	0.59
3:C:3038[A]:ILE:HG12	3:C:3112[A]:TYR:CE2	2.35	0.59
3:C:3120[A]:HIS:C	3:C:3122[A]:ASN:N	2.55	0.59
3:F:2945[B]:VAL:HG22	3:F:2945[B]:VAL:O	2.01	0.59
3:F:2949[B]:LYS:HZ2	3:F:2950[B]:THR:HA	1.67	0.59
3:F:3024[A]:LEU:O	3:F:3031[A]:ASN:ND2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3139[A]:LEU:N	3:F:3139[A]:LEU:HD22	2.16	0.59
3:F:3155[B]:MET:CG	3:a:3154[B]:PRO:CD	2.78	0.59
3:F:3155[B]:MET:HE3	3:a:3156[B]:MET:HG2	1.84	0.59
3:F:3157[B]:PRO:N	3:a:2982[B]:MET:SD	2.74	0.59
3:F:3160[B]:SER:HA	3:a:2983[B]:VAL:N	2.09	0.59
3:F:3160[B]:SER:O	3:a:3147[B]:GLU:HG3	2.01	0.59
3:F:3284[A]:LYS:HE2	3:F:3284[A]:LYS:CA	2.30	0.59
3:F:3307[A]:PHE:HE1	3:F:3309[A]:PRO:CG	2.08	0.59
3:I:2969[A]:TYR:CD2	3:I:2970[A]:PRO:HG2	2.38	0.59
3:I:2998[A]:ASP:O	3:I:3001[A]:LYS:HB2	2.02	0.59
3:I:3023[B]:ILE:O	3:I:3024[B]:LEU:C	2.45	0.59
3:I:3147[B]:GLU:H	3:R:3161[B]:GLU:HA	1.66	0.59
3:I:3150[B]:LYS:O	3:R:3159[B]:SER:CB	2.48	0.59
3:I:3169[B]:LYS:HG2	3:R:3151[B]:LEU:N	2.06	0.59
3:I:3255[B]:PRO:CG	3:R:2959[B]:SER:HA	2.31	0.59
3:I:3274[A]:ARG:NE	3:I:3274[A]:ARG:HA	2.16	0.59
3:I:3288[B]:MET:CG	3:I:3295[B]:LEU:HD21	2.32	0.59
3:I:3298[A]:ASN:CA	3:I:3300[A]:LEU:HD23	2.31	0.59
2:K:2509:ILE:HD11	2:K:2605:LEU:HD23	1.84	0.59
3:L:3024[A]:LEU:O	3:L:3031[A]:ASN:ND2	2.36	0.59
3:L:3071[A]:PHE:O	3:L:3074[A]:GLU:HB2	2.02	0.59
3:L:3071[B]:PHE:O	3:L:3074[B]:GLU:HB2	2.02	0.59
3:O:3104[B]:MET:SD	3:O:3110[B]:THR:HG22	2.42	0.59
3:R:2928[A]:ASN:N	3:R:2930[A]:LEU:HD21	2.17	0.59
3:R:3001[A]:LYS:HE3	3:R:3002[A]:ALA:HB2	1.85	0.59
3:R:3024[B]:LEU:O	3:R:3031[B]:ASN:ND2	2.36	0.59
3:R:3135[A]:LYS:CB	3:R:3141[A]:TYR:CD1	2.85	0.59
3:R:3218[B]:LEU:O	3:R:3219[B]:LEU:HD13	2.01	0.59
3:R:3222[A]:ILE:HG13	3:R:3224[A]:GLN:HG2	1.84	0.59
1:S:1324:ARG:NH1	1:S:1516:VAL:O	2.35	0.59
3:U:3071[A]:PHE:O	3:U:3074[A]:GLU:HB2	2.02	0.59
3:U:3120[B]:HIS:C	3:U:3122[B]:ASN:N	2.55	0.59
3:U:3156[A]:MET:HA	3:U:3157[A]:PRO:C	2.26	0.59
2:W:2252:GLU:HG2	2:W:2385:ILE:HG23	1.83	0.59
3:X:2932[A]:PRO:CA	3:X:2935[A]:ILE:HD12	2.30	0.59
3:X:2945[A]:VAL:HG22	3:X:2945[A]:VAL:O	2.01	0.59
1:Y:553:LEU:HB2	1:Y:557:VAL:HG11	1.84	0.59
2:Z:2851:ASN:OD1	2:Z:2851:ASN:N	2.32	0.59
3:a:2935[A]:ILE:HD13	3:a:2935[A]:ILE:N	2.18	0.59
3:a:3071[B]:PHE:O	3:a:3074[B]:GLU:HB2	2.03	0.59
3:a:3182[A]:GLN:O	3:a:3183[A]:LEU:HD12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3191[B]:ASN:ND2	3:a:3191[B]:ASN:H	1.99	0.59
1:b:355:ALA:HB1	1:b:776:VAL:HB	1.85	0.59
1:b:673:PHE:HB3	1:b:677:LEU:HB2	1.83	0.59
3:d:2935[B]:ILE:HD13	3:d:2935[B]:ILE:N	2.18	0.59
3:d:3132[B]:ALA:CB	3:d:3197[B]:ILE:HD13	2.33	0.59
3:d:3134[B]:GLN:O	3:d:3135[B]:LYS:C	2.44	0.59
3:d:3135[A]:LYS:CB	3:d:3141[A]:TYR:CD1	2.85	0.59
3:d:3135[B]:LYS:CB	3:d:3141[B]:TYR:CD1	2.85	0.59
2:B:2141:HIS:ND1	2:B:2141:HIS:O	2.36	0.59
3:C:2981[B]:GLY:O	3:L:2966[B]:SER:O	2.21	0.59
3:C:3023[A]:ILE:O	3:C:3024[A]:LEU:C	2.45	0.59
3:C:3132[B]:ALA:CB	3:C:3197[B]:ILE:HD13	2.33	0.59
1:D:240:PHE:HA	1:D:263:ALA:HB3	1.83	0.59
3:F:2928[B]:ASN:N	3:F:2930[B]:LEU:HD21	2.18	0.59
3:F:2935[A]:ILE:HD13	3:F:2935[A]:ILE:N	2.18	0.59
3:F:2979[B]:GLN:NE2	3:a:3156[B]:MET:CG	2.52	0.59
3:F:3014[A]:TRP:CE3	3:F:3092[A]:ILE:HD12	2.37	0.59
3:F:3156[B]:MET:HA	3:F:3157[B]:PRO:C	2.26	0.59
1:G:105:VAL:HG12	1:G:123:PHE:HB3	1.85	0.59
1:G:957:ASN:HB3	1:G:960:PHE:H	1.67	0.59
2:H:2090:LYS:NZ	2:H:2099:GLU:OE2	2.34	0.59
2:H:2868:GLU:OE2	3:I:2933[A]:SER:N	2.32	0.59
3:I:2935[A]:ILE:HD13	3:I:2935[A]:ILE:N	2.18	0.59
3:I:2939[B]:ARG:HH11	3:I:2939[B]:ARG:HG3	1.67	0.59
3:I:2961[B]:HIS:ND1	3:R:2975[B]:PHE:HE1	1.98	0.59
3:I:3276[A]:ASP:HB3	3:I:3278[A]:HIS:HB2	1.83	0.59
2:K:2731:PRO:HB3	2:K:2734:LYS:HG3	1.82	0.59
3:L:2942[B]:LEU:CD1	3:L:3033[B]:PHE:CE1	2.85	0.59
3:L:3014[A]:TRP:CD2	3:L:3092[A]:ILE:HD12	2.38	0.59
3:L:3281[A]:PHE:CE1	3:L:3305[A]:ILE:HG21	2.36	0.59
3:O:2974[B]:ALA:HA	3:X:2979[B]:GLN:CD	2.27	0.59
3:O:2987[B]:HIS:NE2	3:O:3178[B]:PHE:HE1	1.95	0.59
3:O:3071[B]:PHE:O	3:O:3074[B]:GLU:HB2	2.02	0.59
3:U:3024[A]:LEU:O	3:U:3031[A]:ASN:ND2	2.36	0.59
3:U:3104[A]:MET:SD	3:U:3110[A]:THR:HG22	2.42	0.59
3:U:3120[A]:HIS:C	3:U:3122[A]:ASN:N	2.55	0.59
3:U:3134[B]:GLN:O	3:U:3135[B]:LYS:C	2.44	0.59
3:X:3014[B]:TRP:CE3	3:X:3092[B]:ILE:HD12	2.37	0.59
3:a:3212[B]:ARG:HH11	3:a:3212[B]:ARG:CG	2.12	0.59
1:b:710:GLY:O	1:b:841:LYS:NZ	2.33	0.59
1:b:1348:TRP:HD1	1:b:1403:LEU:HD13	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:1441:SER:OG	1:b:1442:MET:N	2.34	0.59
3:d:2969[B]:TYR:CD2	3:d:2970[B]:PRO:HG2	2.38	0.59
3:d:3132[A]:ALA:CB	3:d:3197[A]:ILE:HD13	2.33	0.59
2:B:2550:THR:H	2:B:2553:ALA:HB3	1.66	0.59
3:C:2945[A]:VAL:HG22	3:C:2945[A]:VAL:O	2.01	0.59
3:C:2961[B]:HIS:CE1	3:C:2980[B]:HIS:NE2	2.57	0.59
3:C:3093[B]:HIS:ND1	3:L:2971[B]:ASP:CB	2.25	0.59
3:C:3253[B]:GLU:OE1	3:L:2974[B]:ALA:C	2.46	0.59
3:F:2969[A]:TYR:CD2	3:F:2970[A]:PRO:HG2	2.38	0.59
3:F:3071[B]:PHE:O	3:F:3074[B]:GLU:HB2	2.02	0.59
3:F:3274[A]:ARG:NE	3:F:3274[A]:ARG:HA	2.16	0.59
3:I:3152[B]:LYS:CB	3:R:3171[B]:HIS:CA	2.81	0.59
3:I:3298[A]:ASN:ND2	3:I:3301[A]:PRO:C	2.60	0.59
2:K:2497:GLU:HB2	2:K:2498:VAL:HA	1.84	0.59
2:K:2507:ARG:HA	2:K:2779:ASP:HB2	1.85	0.59
3:L:3000[B]:LEU:N	3:L:3000[B]:LEU:HD23	2.18	0.59
3:O:2942[A]:LEU:CD1	3:O:3033[A]:PHE:CE1	2.85	0.59
3:O:3038[B]:ILE:HG23	3:X:2969[B]:TYR:OH	2.02	0.59
3:O:3104[A]:MET:SD	3:O:3110[A]:THR:HG22	2.42	0.59
3:O:3191[A]:ASN:ND2	3:O:3191[A]:ASN:H	1.99	0.59
1:P:871:GLN:NE2	1:P:964:ILE:O	2.33	0.59
1:P:898:GLY:N	1:P:899:MET:HA	2.17	0.59
2:Q:2128:LEU:HD23	2:Q:2216:PHE:HZ	1.68	0.59
2:Q:2133:PRO:HG2	2:Q:2140:ARG:HA	1.83	0.59
3:R:3288[B]:MET:CG	3:R:3295[B]:LEU:HD21	2.32	0.59
1:S:804:ASP:OD1	1:S:805:VAL:N	2.36	0.59
2:T:2386:ARG:HB3	2:T:2496:LEU:HD21	1.82	0.59
3:U:2928[B]:ASN:N	3:U:2930[B]:LEU:HD21	2.17	0.59
3:U:2942[B]:LEU:CD1	3:U:3033[B]:PHE:CE1	2.85	0.59
3:U:2967[B]:CYS:SG	3:d:3257[B]:ALA:O	2.61	0.59
3:U:3014[B]:TRP:CE3	3:U:3092[B]:ILE:HD12	2.37	0.59
3:U:3132[B]:ALA:CB	3:U:3197[B]:ILE:HD13	2.33	0.59
3:X:2948[B]:ASP:CB	3:X:2949[B]:LYS:CA	2.78	0.59
3:X:3014[B]:TRP:CD2	3:X:3092[B]:ILE:HD12	2.38	0.59
3:X:3071[A]:PHE:O	3:X:3074[A]:GLU:HB2	2.03	0.59
3:X:3135[A]:LYS:CB	3:X:3141[A]:TYR:CD1	2.85	0.59
3:X:3135[B]:LYS:CB	3:X:3141[B]:TYR:CD1	2.85	0.59
3:X:3288[B]:MET:CG	3:X:3295[B]:LEU:HD21	2.32	0.59
3:X:3298[A]:ASN:ND2	3:X:3301[A]:PRO:C	2.60	0.59
3:X:3298[B]:ASN:CB	3:X:3300[B]:LEU:N	2.60	0.59
1:Y:1323:HIS:CD2	9:Y:2105:CUO:O2	2.54	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:2939[A]:ARG:HH11	3:a:2939[A]:ARG:HG3	1.66	0.59
3:d:2928[A]:ASN:N	3:d:2930[A]:LEU:HD21	2.17	0.59
3:d:2928[B]:ASN:N	3:d:2930[B]:LEU:HD21	2.17	0.59
3:d:3071[A]:PHE:O	3:d:3074[A]:GLU:HB2	2.02	0.59
3:d:3298[A]:ASN:CA	3:d:3300[A]:LEU:HD23	2.31	0.59
2:B:2128:LEU:HD13	2:B:2286:HIS:CG	2.38	0.59
3:C:2942[A]:LEU:CD1	3:C:3033[A]:PHE:CE1	2.85	0.59
3:C:2942[B]:LEU:CD1	3:C:3033[B]:PHE:CE1	2.85	0.59
3:C:2969[A]:TYR:CD2	3:C:2970[A]:PRO:HG2	2.38	0.59
3:C:2987[A]:HIS:NE2	3:C:3178[A]:PHE:HE1	1.95	0.59
3:C:3014[B]:TRP:CE3	3:C:3092[B]:ILE:HD12	2.37	0.59
2:E:2816:SER:HB2	2:E:2886:VAL:HG21	1.85	0.59
3:F:2942[B]:LEU:CD1	3:F:3033[B]:PHE:CE1	2.85	0.59
3:F:2949[A]:LYS:HZ2	3:F:2950[A]:THR:HA	1.68	0.59
3:F:2966[B]:SER:OG	3:a:3255[B]:PRO:C	2.45	0.59
3:F:2966[B]:SER:HB3	3:a:2982[B]:MET:HE2	1.84	0.59
3:F:3000[B]:LEU:HD23	3:F:3000[B]:LEU:N	2.18	0.59
3:F:3134[B]:GLN:O	3:F:3135[B]:LYS:C	2.44	0.59
3:F:3153[B]:LYS:CD	3:a:3155[B]:MET:C	2.74	0.59
3:I:3001[A]:LYS:HE3	3:I:3002[A]:ALA:HB2	1.85	0.59
1:J:109:LEU:HD12	1:J:119:LYS:HB3	1.84	0.59
1:J:546:PHE:O	1:J:561:ARG:NH1	2.29	0.59
3:L:2965[B]:LEU:HD11	3:L:2974[B]:ALA:C	2.28	0.59
3:L:2969[A]:TYR:CD2	3:L:2970[A]:PRO:CD	2.85	0.59
3:L:3104[A]:MET:SD	3:L:3110[A]:THR:HG22	2.42	0.59
3:L:3156[A]:MET:HA	3:L:3157[A]:PRO:C	2.26	0.59
1:M:1492:PRO:HB2	1:M:1497:SER:HB3	1.85	0.59
2:N:2856:ILE:HG22	2:N:2859:VAL:HB	1.83	0.59
3:O:2935[B]:ILE:HD13	3:O:2935[B]:ILE:N	2.18	0.59
3:O:2969[B]:TYR:CB	3:X:3158[B]:PHE:CD1	2.78	0.59
3:O:3014[B]:TRP:CE3	3:O:3092[B]:ILE:HD12	2.37	0.59
3:O:3288[A]:MET:CG	3:O:3295[A]:LEU:HD21	2.32	0.59
2:Q:2128:LEU:HD13	2:Q:2286:HIS:CG	2.38	0.59
3:R:3014[A]:TRP:CE3	3:R:3092[A]:ILE:HD12	2.37	0.59
3:R:3071[B]:PHE:O	3:R:3074[B]:GLU:HB2	2.02	0.59
3:R:3157[A]:PRO:O	3:R:3160[A]:SER:N	2.30	0.59
3:R:3220[A]:ARG:HH11	3:R:3220[A]:ARG:CG	2.12	0.59
3:R:3284[A]:LYS:HE2	3:R:3284[A]:LYS:CA	2.30	0.59
1:S:1627:ARG:NH2	1:S:1629:GLU:OE1	2.35	0.59
3:U:2939[B]:ARG:HG3	3:U:2939[B]:ARG:HH11	1.67	0.59
3:U:2945[A]:VAL:HG22	3:U:2945[A]:VAL:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2969[B]:TYR:CD2	3:U:2970[B]:PRO:CD	2.86	0.59
3:U:2969[B]:TYR:CD2	3:U:2970[B]:PRO:HG2	2.38	0.59
3:U:2998[A]:ASP:O	3:U:3001[A]:LYS:HB2	2.01	0.59
3:U:3023[B]:ILE:O	3:U:3024[B]:LEU:C	2.45	0.59
3:U:3113[B]:ASP:O	3:U:3115[B]:LEU:N	2.36	0.59
3:U:3161[B]:GLU:C	3:d:3260[B]:ARG:HH12	2.07	0.59
3:U:3191[B]:ASN:ND2	3:U:3191[B]:ASN:H	1.99	0.59
3:U:3288[A]:MET:CG	3:U:3295[A]:LEU:HD21	2.32	0.59
1:V:1000:GLU:OE1	1:V:1141:ARG:NH2	2.36	0.59
1:V:1505:ARG:O	1:V:1509:THR:OG1	2.21	0.59
3:X:3000[B]:LEU:HD23	3:X:3000[B]:LEU:N	2.18	0.59
3:X:3134[B]:GLN:O	3:X:3135[B]:LYS:C	2.44	0.59
3:X:3274[A]:ARG:HA	3:X:3274[A]:ARG:NE	2.16	0.59
3:a:3000[B]:LEU:HD23	3:a:3000[B]:LEU:N	2.18	0.59
3:a:3156[A]:MET:HA	3:a:3157[A]:PRO:C	2.26	0.59
3:a:3222[A]:ILE:HG13	3:a:3224[A]:GLN:HG2	1.84	0.59
3:d:2942[B]:LEU:CD1	3:d:3033[B]:PHE:CE1	2.85	0.59
3:d:3001[A]:LYS:HE3	3:d:3002[A]:ALA:HB2	1.85	0.59
3:d:3023[A]:ILE:O	3:d:3024[A]:LEU:C	2.45	0.59
3:d:3284[B]:LYS:HE2	3:d:3284[B]:LYS:CA	2.30	0.59
1:A:1210:LYS:HD3	2:E:2744:PHE:CE1	2.37	0.59
2:B:2541:GLY:O	2:B:2545:SER:OG	2.13	0.59
3:C:2935[A]:ILE:HD13	3:C:2935[A]:ILE:N	2.18	0.59
3:C:2965[B]:LEU:HD11	3:C:2974[B]:ALA:C	2.28	0.59
3:C:3000[B]:LEU:N	3:C:3000[B]:LEU:HD23	2.18	0.59
3:C:3113[B]:ASP:O	3:C:3115[B]:LEU:N	2.36	0.59
3:C:3146[B]:CYS:O	3:L:3161[B]:GLU:HG3	2.03	0.59
3:C:3288[B]:MET:CG	3:C:3295[B]:LEU:HD21	2.32	0.59
1:D:490:TRP:CZ3	1:D:494:VAL:HG21	2.38	0.59
1:D:896:HIS:HB2	1:D:905:TRP:CD1	2.38	0.59
2:E:2833:GLY:HA3	2:E:2854:MET:HE1	1.84	0.59
3:F:2991[B]:LEU:O	3:F:2994[B]:LYS:HB3	2.03	0.59
3:F:3023[B]:ILE:O	3:F:3024[B]:LEU:C	2.45	0.59
3:F:3103[A]:GLY:O	3:F:3106[A]:THR:HG22	2.03	0.59
3:F:3155[B]:MET:CE	3:a:3156[B]:MET:HG2	2.32	0.59
3:F:3158[B]:PHE:HB2	3:a:3153[B]:LYS:HB2	1.84	0.59
3:F:3222[A]:ILE:HG13	3:F:3224[A]:GLN:HG2	1.84	0.59
1:G:898:GLY:N	1:G:899:MET:SD	2.68	0.59
3:I:2930[B]:LEU:H	3:I:2930[B]:LEU:CD2	1.98	0.59
3:I:2969[A]:TYR:CD2	3:I:2970[A]:PRO:CD	2.85	0.59
3:I:3153[B]:LYS:HD3	3:R:2988[B]:TRP:HD1	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3156[B]:MET:HG2	3:R:3155[B]:MET:HE1	1.83	0.59
3:I:3288[A]:MET:CG	3:I:3295[A]:LEU:HD21	2.32	0.59
1:J:1302:SER:HB2	1:J:1303:GLU:HB2	1.85	0.59
3:L:3014[B]:TRP:CD2	3:L:3092[B]:ILE:HD12	2.38	0.59
1:M:1013:ILE:HD11	1:M:1175:PHE:CD2	2.37	0.59
3:O:2942[B]:LEU:CD1	3:O:3033[B]:PHE:CE1	2.85	0.59
3:O:2969[A]:TYR:CD2	3:O:2970[A]:PRO:CD	2.86	0.59
3:O:3288[B]:MET:CG	3:O:3295[B]:LEU:HD21	2.32	0.59
3:R:3014[A]:TRP:CD2	3:R:3092[A]:ILE:HD12	2.38	0.59
3:R:3298[B]:ASN:ND2	3:R:3301[B]:PRO:C	2.60	0.59
2:T:2166:LEU:HA	2:T:2169:HIS:HB2	1.83	0.59
3:U:2945[B]:VAL:HG22	3:U:2945[B]:VAL:O	2.02	0.59
3:U:2995[B]:GLN:HG2	3:U:3168[B]:THR:HG21	1.85	0.59
3:U:3161[B]:GLU:CA	3:d:3146[B]:CYS:HB2	2.27	0.59
3:U:3176[B]:LYS:HD3	3:d:3152[B]:LYS:CD	2.32	0.59
1:V:79:ALA:O	1:V:83:HIS:ND1	2.27	0.59
1:V:566:ARG:HB2	1:V:609:TRP:NE1	2.18	0.59
1:V:864:ASP:HB3	1:V:869:GLY:HA3	1.85	0.59
3:X:3000[A]:LEU:N	3:X:3000[A]:LEU:HD23	2.18	0.59
3:X:3038[A]:ILE:HG12	3:X:3112[A]:TYR:CE2	2.35	0.59
3:X:3113[A]:ASP:O	3:X:3115[A]:LEU:N	2.36	0.59
3:X:3113[B]:ASP:O	3:X:3115[B]:LEU:N	2.36	0.59
3:X:3147[A]:GLU:HG3	3:X:3149[A]:ASN:HD21	1.65	0.59
3:a:2935[B]:ILE:HD13	3:a:2935[B]:ILE:N	2.18	0.59
3:a:2948[A]:ASP:CB	3:a:2949[A]:LYS:CA	2.78	0.59
3:a:3135[A]:LYS:CB	3:a:3141[A]:TYR:CD1	2.85	0.59
3:a:3274[A]:ARG:NE	3:a:3274[A]:ARG:HA	2.16	0.59
3:a:3288[A]:MET:CG	3:a:3295[A]:LEU:HD21	2.32	0.59
3:d:2969[A]:TYR:CD2	3:d:2970[A]:PRO:CD	2.85	0.59
3:d:3000[B]:LEU:HD23	3:d:3000[B]:LEU:N	2.18	0.59
3:d:3014[B]:TRP:CD2	3:d:3092[B]:ILE:HD12	2.38	0.59
3:d:3024[A]:LEU:O	3:d:3031[A]:ASN:ND2	2.36	0.59
3:d:3113[B]:ASP:O	3:d:3115[B]:LEU:N	2.36	0.59
3:d:3191[A]:ASN:ND2	3:d:3191[A]:ASN:H	1.99	0.59
2:B:2361:LYS:HD2	2:B:2362:GLN:HG3	1.84	0.58
3:C:2928[B]:ASN:N	3:C:2930[B]:LEU:HD21	2.17	0.58
3:C:2939[B]:ARG:HH11	3:C:2939[B]:ARG:HG3	1.66	0.58
3:C:3001[B]:LYS:HE3	3:C:3002[B]:ALA:HB2	1.85	0.58
3:C:3014[A]:TRP:CD2	3:C:3092[A]:ILE:HD12	2.38	0.58
3:C:3132[A]:ALA:CB	3:C:3197[A]:ILE:HD13	2.33	0.58
3:C:3293[B]:LYS:CB	3:C:3294[B]:SER:CB	2.54	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2986[A]:PRO:HB3	3:F:3127[A]:TRP:CE3	2.38	0.58
3:I:2968[B]:GLN:HG2	3:R:2981[B]:GLY:H	1.67	0.58
3:I:2981[B]:GLY:HA3	3:R:2966[B]:SER:O	2.02	0.58
3:I:3014[B]:TRP:CD2	3:I:3092[B]:ILE:HD12	2.38	0.58
3:I:3024[B]:LEU:O	3:I:3031[B]:ASN:ND2	2.36	0.58
3:I:3104[A]:MET:SD	3:I:3110[A]:THR:HG22	2.42	0.58
1:J:11:THR:HG22	1:J:13:ASP:H	1.68	0.58
2:K:2179:ASP:HA	2:K:2300:ASN:ND2	2.17	0.58
3:L:2928[A]:ASN:N	3:L:2930[A]:LEU:HD21	2.18	0.58
3:L:2935[B]:ILE:HD13	3:L:2935[B]:ILE:N	2.18	0.58
3:L:2942[A]:LEU:CD1	3:L:3033[A]:PHE:CE1	2.85	0.58
3:L:2991[A]:LEU:O	3:L:2994[A]:LYS:HB3	2.03	0.58
3:L:3000[A]:LEU:N	3:L:3000[A]:LEU:HD23	2.18	0.58
3:L:3001[B]:LYS:HE3	3:L:3002[B]:ALA:HB2	1.85	0.58
3:L:3113[A]:ASP:O	3:L:3115[A]:LEU:N	2.36	0.58
3:L:3156[B]:MET:HA	3:L:3157[B]:PRO:C	2.26	0.58
3:L:3182[A]:GLN:O	3:L:3183[A]:LEU:HD12	2.02	0.58
2:N:2265:ILE:HD12	2:N:2443:TYR:CD1	2.38	0.58
2:N:2303:ARG:NH2	2:N:2372:GLU:O	2.36	0.58
3:O:2998[A]:ASP:O	3:O:3001[A]:LYS:HB2	2.02	0.58
3:O:3014[A]:TRP:CE3	3:O:3092[A]:ILE:HD12	2.37	0.58
3:R:3113[B]:ASP:O	3:R:3115[B]:LEU:N	2.36	0.58
3:R:3132[B]:ALA:CB	3:R:3197[B]:ILE:HD13	2.33	0.58
1:S:51:ASP:OD2	1:S:813:THR:OG1	2.21	0.58
2:T:2625:LEU:HA	2:T:2638:ARG:HH22	1.65	0.58
3:U:2942[A]:LEU:CD1	3:U:3033[A]:PHE:CE1	2.85	0.58
3:U:2987[A]:HIS:NE2	3:U:3178[A]:PHE:HE1	1.95	0.58
3:U:3161[B]:GLU:HB2	3:d:3260[B]:ARG:HH11	1.67	0.58
3:U:3212[B]:ARG:HH11	3:U:3212[B]:ARG:CG	2.12	0.58
3:U:3298[B]:ASN:CB	3:U:3300[B]:LEU:N	2.60	0.58
2:W:2254:THR:HG23	2:W:2317:LEU:HD13	1.85	0.58
2:W:2830:GLN:HG2	2:W:2863:ARG:NE	2.18	0.58
3:X:2948[B]:ASP:HB3	3:X:2953[B]:GLY:CA	2.24	0.58
3:X:2986[A]:PRO:HB3	3:X:3127[A]:TRP:CE3	2.38	0.58
3:X:3001[B]:LYS:HE3	3:X:3002[B]:ALA:HB2	1.85	0.58
3:a:2945[A]:VAL:HG22	3:a:2945[A]:VAL:O	2.02	0.58
3:a:3113[A]:ASP:O	3:a:3115[A]:LEU:N	2.36	0.58
3:a:3113[B]:ASP:O	3:a:3115[B]:LEU:N	2.36	0.58
2:c:2849:ASP:HB3	2:c:2850:ARG:NE	2.18	0.58
3:d:2945[A]:VAL:HG22	3:d:2945[A]:VAL:O	2.02	0.58
3:d:3014[A]:TRP:CE3	3:d:3092[A]:ILE:HD12	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3103[A]:GLY:O	3:d:3106[A]:THR:HG22	2.03	0.58
3:d:3120[A]:HIS:C	3:d:3122[A]:ASN:N	2.55	0.58
3:d:3176[B]:LYS:HB3	3:d:3176[B]:LYS:HZ2	1.68	0.58
1:A:71:LEU:HD21	1:A:261:SER:HA	1.84	0.58
1:A:619:SER:HB2	1:A:805:VAL:HG11	1.85	0.58
1:A:1148:LEU:HB2	1:A:1188:PHE:HD2	1.67	0.58
3:C:2960[B]:PHE:O	3:L:3255[B]:PRO:HD2	2.03	0.58
3:C:2969[A]:TYR:CD2	3:C:2970[A]:PRO:CD	2.86	0.58
3:C:3156[A]:MET:HA	3:C:3157[A]:PRO:C	2.26	0.58
3:F:2962[B]:GLY:C	3:a:3255[B]:PRO:CG	2.76	0.58
3:F:3001[B]:LYS:HE3	3:F:3002[B]:ALA:HB2	1.85	0.58
3:F:3014[A]:TRP:CD2	3:F:3092[A]:ILE:HD12	2.38	0.58
3:F:3183[B]:LEU:N	3:F:3184[B]:ASN:HA	2.11	0.58
3:F:3188[A]:ASP:N	3:F:3188[A]:ASP:OD2	2.36	0.58
3:F:3251[B]:ASP:OD1	3:a:3108[B]:HIS:HE1	1.83	0.58
2:H:2109:ARG:NH1	2:H:2169:HIS:O	2.36	0.58
3:I:2928[B]:ASN:N	3:I:2930[B]:LEU:HD21	2.18	0.58
3:I:3154[B]:PRO:HD3	3:R:3173[B]:THR:C	2.28	0.58
3:I:3173[A]:THR:HB	3:I:3176[A]:LYS:HG2	1.81	0.58
3:I:3182[A]:GLN:O	3:I:3183[A]:LEU:HD12	2.02	0.58
3:I:3258[B]:PHE:HA	3:R:3162[B]:ASP:OD2	2.02	0.58
1:J:285:THR:HB	1:J:288:GLU:H	1.68	0.58
3:L:2995[A]:GLN:HG2	3:L:3168[A]:THR:HG21	1.85	0.58
3:L:3024[B]:LEU:O	3:L:3031[B]:ASN:ND2	2.36	0.58
3:L:3273[B]:LEU:CB	3:L:3275[B]:LEU:HD13	2.28	0.58
3:L:3298[B]:ASN:CA	3:L:3300[B]:LEU:HD23	2.31	0.58
3:O:2968[B]:GLN:HE22	3:X:2985[B]:PHE:HA	1.51	0.58
3:O:2995[B]:GLN:HG2	3:O:3168[B]:THR:HG21	1.85	0.58
3:O:3096[A]:VAL:HG11	3:O:3115[A]:LEU:HD13	1.81	0.58
3:O:3096[B]:VAL:HG11	3:O:3115[B]:LEU:HD13	1.81	0.58
3:O:3182[B]:GLN:O	3:O:3183[B]:LEU:HD12	2.02	0.58
3:O:3298[B]:ASN:CA	3:O:3300[B]:LEU:HD23	2.31	0.58
3:R:3014[B]:TRP:CE3	3:R:3092[B]:ILE:HD12	2.37	0.58
3:R:3183[A]:LEU:N	3:R:3184[A]:ASN:HA	2.12	0.58
1:S:984:ASP:OD1	1:S:985:PHE:N	2.29	0.58
1:S:1348:TRP:CG	1:S:1430:ILE:HD11	2.38	0.58
3:U:2935[B]:ILE:HD13	3:U:2935[B]:ILE:N	2.18	0.58
3:U:2969[A]:TYR:CD2	3:U:2970[A]:PRO:HG2	2.38	0.58
3:U:2969[B]:TYR:CE1	3:d:2980[B]:HIS:CE1	2.91	0.58
3:U:3113[A]:ASP:O	3:U:3115[A]:LEU:N	2.36	0.58
3:U:3132[A]:ALA:CB	3:U:3197[A]:ILE:HD13	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3156[B]:MET:HA	3:U:3157[B]:PRO:C	2.26	0.58
1:V:121:ASN:HD21	1:V:124:TYR:CB	2.17	0.58
3:X:2991[B]:LEU:O	3:X:2994[B]:LYS:HB3	2.03	0.58
3:X:3191[B]:ASN:ND2	3:X:3191[B]:ASN:H	1.99	0.58
1:Y:166:GLU:OE2	1:Y:297:ARG:NH1	2.37	0.58
1:Y:1302:SER:OG	1:Y:1494:ARG:NH1	2.31	0.58
3:a:2948[B]:ASP:HB3	3:a:2953[B]:GLY:CA	2.24	0.58
3:a:3024[B]:LEU:O	3:a:3031[B]:ASN:ND2	2.36	0.58
3:a:3103[B]:GLY:O	3:a:3106[B]:THR:HG22	2.03	0.58
3:a:3132[B]:ALA:CB	3:a:3197[B]:ILE:HD13	2.33	0.58
1:b:905:TRP:HE1	1:b:1083:PRO:HD2	1.68	0.58
3:d:2935[A]:ILE:HD13	3:d:2935[A]:ILE:N	2.18	0.58
3:d:3222[B]:ILE:HG13	3:d:3224[B]:GLN:HG2	1.84	0.58
3:C:3023[B]:ILE:O	3:C:3024[B]:LEU:C	2.45	0.58
3:C:3108[B]:HIS:CE1	3:L:3251[B]:ASP:OD1	2.47	0.58
3:C:3288[A]:MET:CG	3:C:3295[A]:LEU:HD21	2.32	0.58
2:E:2866:PRO:HB2	2:E:2868:GLU:OE1	2.02	0.58
3:F:2998[A]:ASP:O	3:F:3001[A]:LYS:HB2	2.02	0.58
3:F:3014[B]:TRP:CD2	3:F:3092[B]:ILE:HD12	2.38	0.58
3:F:3024[B]:LEU:O	3:F:3031[B]:ASN:ND2	2.36	0.58
3:F:3113[A]:ASP:O	3:F:3115[A]:LEU:N	2.36	0.58
3:F:3113[B]:ASP:O	3:F:3115[B]:LEU:N	2.36	0.58
3:F:3152[B]:LYS:CG	3:a:3172[B]:SER:OG	2.28	0.58
1:G:573:LYS:HB3	1:G:574:GLY:HA2	1.85	0.58
3:I:2969[B]:TYR:HE2	3:R:3120[B]:HIS:CD2	2.21	0.58
3:I:3000[A]:LEU:N	3:I:3000[A]:LEU:HD23	2.18	0.58
3:I:3103[A]:GLY:O	3:I:3106[A]:THR:HG22	2.03	0.58
3:I:3113[A]:ASP:O	3:I:3115[A]:LEU:N	2.36	0.58
3:I:3132[B]:ALA:CB	3:I:3197[B]:ILE:HD13	2.33	0.58
3:I:3156[B]:MET:HG2	3:R:3155[B]:MET:CE	2.32	0.58
3:I:3279[A]:ASP:OD1	3:I:3279[A]:ASP:N	2.25	0.58
1:J:567:LEU:HD23	1:J:571:PRO:HG2	1.85	0.58
3:L:2969[A]:TYR:CD2	3:L:2970[A]:PRO:HG2	2.38	0.58
3:L:3001[A]:LYS:HE3	3:L:3002[A]:ALA:HB2	1.85	0.58
3:L:3096[A]:VAL:HG11	3:L:3115[A]:LEU:HD13	1.81	0.58
3:L:3132[B]:ALA:CB	3:L:3197[B]:ILE:HD13	2.33	0.58
3:L:3135[A]:LYS:CB	3:L:3141[A]:TYR:CD1	2.85	0.58
3:L:3218[A]:LEU:O	3:L:3219[A]:LEU:HD13	2.01	0.58
1:M:361:GLU:HG2	1:M:363:THR:HG22	1.84	0.58
1:M:527:LEU:O	1:M:561:ARG:NH1	2.36	0.58
1:M:1321:HIS:HD2	1:M:1465:TRP:CH2	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2928[A]:ASN:N	3:O:2930[A]:LEU:HD21	2.17	0.58
3:O:2969[A]:TYR:CD2	3:O:2970[A]:PRO:HG2	2.38	0.58
3:O:3014[A]:TRP:CD2	3:O:3092[A]:ILE:HD12	2.38	0.58
3:O:3023[A]:ILE:O	3:O:3024[A]:LEU:C	2.45	0.58
3:O:3191[B]:ASN:ND2	3:O:3191[B]:ASN:H	1.99	0.58
1:P:110:PHE:N	1:P:119:LYS:O	2.35	0.58
1:P:972:SER:HA	1:P:1028:VAL:HG22	1.84	0.58
3:R:2935[B]:ILE:HD13	3:R:2935[B]:ILE:N	2.18	0.58
3:R:2952[A]:ALA:H	3:R:2953[A]:GLY:CA	2.04	0.58
3:R:3176[B]:LYS:HB3	3:R:3176[B]:LYS:HZ2	1.66	0.58
1:S:1407:THR:HG22	1:S:1426:LEU:HD21	1.86	0.58
3:U:2991[B]:LEU:O	3:U:2994[B]:LYS:HB3	2.03	0.58
3:U:3014[A]:TRP:CD2	3:U:3092[A]:ILE:HD12	2.38	0.58
3:U:3014[B]:TRP:CD2	3:U:3092[B]:ILE:HD12	2.38	0.58
3:U:3103[A]:GLY:O	3:U:3106[A]:THR:HG22	2.03	0.58
1:V:527:LEU:HD23	1:V:632:LEU:HD12	1.86	0.58
1:V:941:LEU:HD22	1:V:941:LEU:H	1.69	0.58
3:X:2965[B]:LEU:HD11	3:X:2974[B]:ALA:C	2.28	0.58
3:X:3188[B]:ASP:N	3:X:3188[B]:ASP:OD2	2.36	0.58
1:Y:456:GLN:NE2	1:Y:549:PRO:O	2.30	0.58
3:a:3293[A]:LYS:CB	3:a:3294[A]:SER:CB	2.54	0.58
1:b:705:THR:HG22	1:b:1118:THR:HG23	1.85	0.58
3:d:2995[B]:GLN:HG2	3:d:3168[B]:THR:HG21	1.85	0.58
3:d:3182[B]:GLN:O	3:d:3183[B]:LEU:HD12	2.02	0.58
1:A:573:LYS:HB3	1:A:574:GLY:HA2	1.86	0.58
3:C:2928[A]:ASN:N	3:C:2930[A]:LEU:HD21	2.18	0.58
3:C:2966[B]:SER:CB	3:L:2982[B]:MET:HE2	2.31	0.58
3:C:3129[B]:ILE:HD13	3:C:3190[B]:LEU:O	2.04	0.58
2:E:2890:VAL:N	2:E:2891:LEU:HA	2.19	0.58
3:F:2945[A]:VAL:HG22	3:F:2945[A]:VAL:O	2.01	0.58
3:F:3298[B]:ASN:CB	3:F:3300[B]:LEU:CD2	2.61	0.58
1:G:1078:ARG:NH2	2:K:2876:LYS:O	2.36	0.58
1:G:1199:VAL:O	1:G:1203:MET:HG2	2.03	0.58
3:I:2949[A]:LYS:HZ2	3:I:2950[A]:THR:HA	1.67	0.58
3:I:2995[A]:GLN:HG2	3:I:3168[A]:THR:HG21	1.85	0.58
3:I:3001[B]:LYS:HE3	3:I:3002[B]:ALA:HB2	1.85	0.58
3:I:3129[B]:ILE:HD13	3:I:3190[B]:LEU:O	2.04	0.58
1:J:167:ASP:OD1	1:J:168:PHE:N	2.37	0.58
3:L:3298[B]:ASN:CB	3:L:3300[B]:LEU:N	2.60	0.58
3:O:2948[A]:ASP:CB	3:O:2949[A]:LYS:CA	2.78	0.58
3:O:2978[B]:CYS:O	3:X:3154[B]:PRO:HG3	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3113[A]:ASP:O	3:O:3115[A]:LEU:N	2.36	0.58
3:O:3132[A]:ALA:CB	3:O:3197[A]:ILE:HD13	2.33	0.58
3:O:3298[A]:ASN:CB	3:O:3300[A]:LEU:N	2.60	0.58
2:Q:2107:LEU:HD23	2:Q:2208:PRO:HB2	1.85	0.58
1:S:128:ILE:HG22	1:S:130:PHE:O	2.02	0.58
1:S:997:SER:O	1:S:1001:GLN:NE2	2.34	0.58
2:T:2800:LYS:C	3:U:3023[A]:ILE:HD11	2.29	0.58
3:U:2957[A]:ILE:HA	3:U:2960[A]:PHE:HE1	1.64	0.58
3:U:2966[A]:SER:HB3	3:U:2977[A]:CYS:HB2	1.78	0.58
3:U:3103[B]:GLY:O	3:U:3106[B]:THR:HG22	2.03	0.58
3:U:3288[B]:MET:CG	3:U:3295[B]:LEU:HD21	2.32	0.58
3:X:3014[A]:TRP:CD2	3:X:3092[A]:ILE:HD12	2.38	0.58
3:X:3182[B]:GLN:O	3:X:3183[B]:LEU:HD12	2.02	0.58
3:X:3211[A]:ASP:OD1	3:X:3211[A]:ASP:N	2.27	0.58
1:Y:899:MET:HE2	1:Y:1186:TRP:CD2	2.38	0.58
1:Y:1304:ASP:N	1:Y:1305:GLY:HA2	2.19	0.58
3:a:2942[A]:LEU:CD1	3:a:3033[A]:PHE:CE1	2.85	0.58
3:a:2949[B]:LYS:HZ2	3:a:2950[B]:THR:HA	1.67	0.58
1:b:684:ARG:O	1:b:687:SER:OG	2.20	0.58
1:b:750:ALA:HA	1:b:796:TYR:HB3	1.85	0.58
1:b:1138:ALA:HA	1:b:1240:ILE:HG22	1.86	0.58
3:d:3113[A]:ASP:O	3:d:3115[A]:LEU:N	2.36	0.58
6:GA:1:NAG:O3	6:GA:2:NAG:C7	2.51	0.58
3:C:2991[A]:LEU:O	3:C:2994[A]:LYS:HB3	2.03	0.58
3:C:2995[B]:GLN:HG2	3:C:3168[B]:THR:HG21	1.85	0.58
3:C:3024[A]:LEU:O	3:C:3031[A]:ASN:ND2	2.36	0.58
3:C:3113[A]:ASP:O	3:C:3115[A]:LEU:N	2.36	0.58
1:D:105:VAL:HG12	1:D:123:PHE:HB3	1.86	0.58
2:E:2680:HIS:NE2	2:E:2684:HIS:CD2	2.70	0.58
3:F:2965[B]:LEU:HD13	3:a:3256[B]:TRP:NE1	2.06	0.58
3:F:2966[B]:SER:HA	3:a:3255[B]:PRO:O	2.02	0.58
3:F:2986[B]:PRO:HB3	3:F:3127[B]:TRP:CE3	2.38	0.58
3:F:3129[B]:ILE:HD13	3:F:3190[B]:LEU:O	2.04	0.58
3:F:3153[B]:LYS:NZ	3:a:3158[B]:PHE:H	2.00	0.58
3:F:3188[B]:ASP:N	3:F:3188[B]:ASP:OD2	2.36	0.58
3:F:3225[A]:SER:OG	3:F:3290[A]:ILE:HD13	2.04	0.58
3:F:3255[B]:PRO:O	3:a:2966[B]:SER:CA	2.52	0.58
2:H:2252:GLU:HG3	2:H:2389:ARG:HE	1.69	0.58
3:I:2967[B]:CYS:CB	3:R:2979[B]:GLN:C	2.65	0.58
3:I:3173[B]:THR:CA	3:R:3154[B]:PRO:N	2.67	0.58
1:J:61:GLY:HA2	1:J:354:PHE:HE1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:474:LEU:H	1:J:474:LEU:HD13	1.68	0.58
3:L:2965[A]:LEU:HD11	3:L:2974[A]:ALA:C	2.28	0.58
3:L:3188[B]:ASP:N	3:L:3188[B]:ASP:OD2	2.36	0.58
3:L:3191[A]:ASN:ND2	3:L:3191[A]:ASN:H	1.99	0.58
3:O:2932[B]:PRO:CA	3:O:2935[B]:ILE:HD12	2.30	0.58
3:O:2948[B]:ASP:HB3	3:O:2953[B]:GLY:CA	2.24	0.58
3:O:2969[B]:TYR:CG	3:X:3158[B]:PHE:CD1	2.70	0.58
3:O:2974[B]:ALA:HB3	3:X:2977[B]:CYS:O	2.02	0.58
3:O:2991[A]:LEU:O	3:O:2994[A]:LYS:HB3	2.03	0.58
3:O:3108[B]:HIS:HE2	3:X:2967[B]:CYS:HB3	1.67	0.58
3:O:3134[A]:GLN:O	3:O:3135[A]:LYS:C	2.44	0.58
3:O:3188[A]:ASP:N	3:O:3188[A]:ASP:OD2	2.36	0.58
1:P:472:ASP:HB3	1:S:1638:SER:HB2	1.85	0.58
3:R:3014[B]:TRP:CD2	3:R:3092[B]:ILE:HD12	2.38	0.58
3:R:3104[B]:MET:SD	3:R:3110[B]:THR:HG22	2.42	0.58
3:R:3188[B]:ASP:OD2	3:R:3188[B]:ASP:N	2.36	0.58
2:T:2598:PRO:HD3	2:T:2651:GLN:HB3	1.85	0.58
2:T:2643:GLU:O	2:T:2647:LEU:N	2.37	0.58
3:U:2928[A]:ASN:N	3:U:2930[A]:LEU:HD21	2.18	0.58
3:U:3135[B]:LYS:CB	3:U:3141[B]:TYR:CD1	2.85	0.58
1:V:444:GLU:HG3	1:V:544:PRO:HG3	1.85	0.58
1:V:754:GLU:OE2	1:V:799:ARG:NH2	2.33	0.58
3:X:3103[B]:GLY:O	3:X:3106[B]:THR:HG22	2.03	0.58
3:X:3132[A]:ALA:CB	3:X:3197[A]:ILE:HD13	2.33	0.58
3:X:3132[B]:ALA:CB	3:X:3197[B]:ILE:HD13	2.33	0.58
3:X:3176[A]:LYS:HB3	3:X:3176[A]:LYS:HZ2	1.68	0.58
3:X:3191[A]:ASN:ND2	3:X:3191[A]:ASN:H	1.99	0.58
1:Y:456:GLN:HG2	1:Y:551:GLU:HB2	1.83	0.58
3:a:3071[A]:PHE:O	3:a:3074[A]:GLU:HB2	2.03	0.58
3:a:3103[A]:GLY:O	3:a:3106[A]:THR:HG22	2.03	0.58
3:a:3225[A]:SER:OG	3:a:3290[A]:ILE:HD13	2.04	0.58
1:b:545:PHE:O	1:b:561:ARG:NH2	2.37	0.58
3:d:2939[A]:ARG:HH11	3:d:2939[A]:ARG:HG3	1.66	0.58
3:d:2986[B]:PRO:HB3	3:d:3127[B]:TRP:CE3	2.39	0.58
3:d:3129[A]:ILE:HD13	3:d:3190[A]:LEU:O	2.04	0.58
3:d:3225[A]:SER:OG	3:d:3290[A]:ILE:HD13	2.04	0.58
3:C:2960[A]:PHE:CD1	3:C:2960[A]:PHE:N	2.72	0.58
3:C:2986[A]:PRO:HB3	3:C:3127[A]:TRP:CE3	2.38	0.58
3:C:2987[B]:HIS:NE2	3:C:3178[B]:PHE:HE1	1.95	0.58
3:C:3103[B]:GLY:O	3:C:3106[B]:THR:HG22	2.03	0.58
3:C:3253[B]:GLU:OE1	3:L:2975[B]:PHE:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3298[A]:ASN:CB	3:C:3300[A]:LEU:N	2.60	0.58
1:D:946:GLU:HG2	1:D:955:LYS:HB3	1.85	0.58
3:F:2930[B]:LEU:HD22	3:F:2930[B]:LEU:N	2.02	0.58
3:F:2935[B]:ILE:HD13	3:F:2935[B]:ILE:N	2.18	0.58
3:F:2961[A]:HIS:HB3	3:F:3111[A]:SER:HG	1.65	0.58
3:F:2965[B]:LEU:HD11	3:F:2974[B]:ALA:C	2.28	0.58
3:F:3120[A]:HIS:C	3:F:3122[A]:ASN:N	2.55	0.58
3:F:3132[A]:ALA:CB	3:F:3197[A]:ILE:HD13	2.33	0.58
3:F:3222[B]:ILE:HG13	3:F:3224[B]:GLN:HG2	1.84	0.58
1:G:105:VAL:HB	1:G:137:ARG:HH12	1.68	0.58
2:H:2309:GLN:HE21	2:H:2320:TYR:HD1	1.52	0.58
3:I:2961[B]:HIS:O	3:R:2975[B]:PHE:CE1	2.57	0.58
3:I:2983[B]:VAL:CA	3:R:3160[B]:SER:HA	2.26	0.58
3:I:2986[A]:PRO:HB3	3:I:3127[A]:TRP:CE3	2.38	0.58
3:I:3158[B]:PHE:CB	3:R:3153[B]:LYS:HB2	2.32	0.58
3:I:3173[B]:THR:CB	3:R:3173[B]:THR:HG23	2.28	0.58
1:J:806:ASN:ND2	4:u:1:NAG:H82	2.18	0.58
2:K:2426:PHE:HB3	2:K:2445:MET:HE1	1.86	0.58
3:L:2935[A]:ILE:HD13	3:L:2935[A]:ILE:N	2.18	0.58
3:L:2986[B]:PRO:HB3	3:L:3127[B]:TRP:CE3	2.38	0.58
3:L:3103[A]:GLY:O	3:L:3106[A]:THR:HG22	2.03	0.58
3:L:3129[A]:ILE:HD13	3:L:3190[A]:LEU:O	2.04	0.58
3:L:3132[A]:ALA:CB	3:L:3197[A]:ILE:HD13	2.33	0.58
1:M:931:TRP:CD1	1:M:1048:ASN:HD22	2.22	0.58
3:O:3001[B]:LYS:HE3	3:O:3002[B]:ALA:HB2	1.85	0.58
3:O:3129[A]:ILE:HD13	3:O:3190[A]:LEU:O	2.04	0.58
3:O:3132[B]:ALA:CB	3:O:3197[B]:ILE:HD13	2.33	0.58
3:O:3293[B]:LYS:CB	3:O:3294[B]:SER:CB	2.54	0.58
1:P:1472:GLN:OE1	1:P:1475:ARG:NH1	2.36	0.58
2:Q:2128:LEU:HD23	2:Q:2216:PHE:CZ	2.39	0.58
2:Q:2825:ILE:HG23	2:Q:2826:GLU:H	1.67	0.58
3:R:2986[B]:PRO:HB3	3:R:3127[B]:TRP:CE3	2.38	0.58
3:R:3135[B]:LYS:CB	3:R:3141[B]:TYR:CD1	2.85	0.58
2:T:2533:ASP:HB3	2:T:2755:PRO:HG3	1.84	0.58
3:U:2986[B]:PRO:HB3	3:U:3127[B]:TRP:CE3	2.38	0.58
3:U:2995[A]:GLN:HG2	3:U:3168[A]:THR:HG21	1.85	0.58
3:U:3258[B]:PHE:O	3:d:2968[B]:GLN:NE2	2.37	0.58
1:V:105:VAL:HB	1:V:137:ARG:NH2	2.18	0.58
3:X:2928[B]:ASN:N	3:X:2930[B]:LEU:HD21	2.18	0.58
3:X:2995[A]:GLN:HG2	3:X:3168[A]:THR:HG21	1.85	0.58
3:X:3225[A]:SER:OG	3:X:3290[A]:ILE:HD13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3273[A]:LEU:CB	3:X:3275[A]:LEU:HD13	2.28	0.58
1:Y:588:GLU:OE2	1:Y:728:ARG:NH2	2.33	0.58
3:a:3024[A]:LEU:O	3:a:3031[A]:ASN:ND2	2.36	0.58
3:a:3191[A]:ASN:ND2	3:a:3191[A]:ASN:H	1.99	0.58
3:d:2948[A]:ASP:CB	3:d:2949[A]:LYS:CA	2.78	0.58
3:d:3024[B]:LEU:O	3:d:3031[B]:ASN:ND2	2.36	0.58
1:A:140:ASP:OD2	1:A:142:ARG:NE	2.27	0.58
1:A:219:LEU:HG	1:A:279:LEU:O	2.04	0.58
3:C:2991[B]:LEU:O	3:C:2994[B]:LYS:HB3	2.03	0.58
3:C:2995[A]:GLN:HG2	3:C:3168[A]:THR:HG21	1.85	0.58
3:C:3001[A]:LYS:HE3	3:C:3002[A]:ALA:HB2	1.85	0.58
3:C:3156[B]:MET:C	3:L:2982[B]:MET:SD	2.87	0.58
1:D:10:LEU:HD12	1:D:104:LEU:HD21	1.86	0.58
1:D:499:GLU:HG3	1:D:511:VAL:HG12	1.85	0.58
3:F:3155[B]:MET:SD	3:a:3154[B]:PRO:HD2	2.43	0.58
3:F:3248[B]:LEU:C	3:a:2974[B]:ALA:H	2.10	0.58
3:F:3288[A]:MET:CG	3:F:3295[A]:LEU:HD21	2.32	0.58
3:I:2935[B]:ILE:HD13	3:I:2935[B]:ILE:N	2.18	0.58
3:I:2939[A]:ARG:HH11	3:I:2939[A]:ARG:HG3	1.66	0.58
3:I:3113[B]:ASP:O	3:I:3115[B]:LEU:N	2.36	0.58
3:I:3135[B]:LYS:CB	3:I:3141[B]:TYR:CD1	2.85	0.58
3:I:3160[B]:SER:CB	3:R:2982[B]:MET:HA	2.33	0.58
3:I:3217[A]:PHE:HE1	3:I:3230[A]:PHE:HZ	0.80	0.58
3:I:3225[B]:SER:OG	3:I:3290[B]:ILE:HD13	2.04	0.58
1:J:714:ARG:NH1	1:J:1115:GLU:OE1	2.37	0.58
1:J:907:ARG:NH2	1:J:1057:GLN:OE1	2.37	0.58
3:L:2995[B]:GLN:HG2	3:L:3168[B]:THR:HG21	1.85	0.58
3:L:3188[A]:ASP:N	3:L:3188[A]:ASP:OD2	2.36	0.58
2:N:2667:GLU:HB3	2:N:2730:LEU:HD22	1.85	0.58
3:O:3000[B]:LEU:N	3:O:3000[B]:LEU:HD23	2.18	0.58
3:R:2965[A]:LEU:HD11	3:R:2974[A]:ALA:C	2.28	0.58
3:R:3000[A]:LEU:HD23	3:R:3000[A]:LEU:N	2.18	0.58
3:R:3103[B]:GLY:O	3:R:3106[B]:THR:HG22	2.03	0.58
1:S:854:LEU:HD23	1:S:941:LEU:HD21	1.85	0.58
1:S:1152:LYS:HB3	1:S:1181:GLU:HA	1.85	0.58
3:U:3024[B]:LEU:O	3:U:3031[B]:ASN:ND2	2.36	0.58
3:U:3170[B]:ALA:C	3:d:3148[B]:ILE:HG21	2.28	0.58
3:U:3217[B]:PHE:HE1	3:U:3230[B]:PHE:HZ	0.80	0.58
1:V:488:PRO:HB2	1:V:641:TRP:CE3	2.39	0.58
2:W:2802:ASP:OD2	3:X:2932[A]:PRO:HD3	2.03	0.58
3:X:2935[A]:ILE:HD13	3:X:2935[A]:ILE:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3023[B]:ILE:O	3:X:3024[B]:LEU:C	2.45	0.58
2:Z:2560:LEU:HD23	2:Z:2565:THR:HB	1.85	0.58
2:Z:2690:HIS:HA	2:Z:2886:VAL:O	2.03	0.58
3:a:2928[B]:ASN:N	3:a:2930[B]:LEU:HD21	2.18	0.58
3:a:2960[A]:PHE:CD1	3:a:2960[A]:PHE:N	2.72	0.58
3:a:2965[A]:LEU:HD11	3:a:2974[A]:ALA:C	2.28	0.58
3:a:2986[B]:PRO:HB3	3:a:3127[B]:TRP:CE3	2.38	0.58
3:a:3014[B]:TRP:CD2	3:a:3092[B]:ILE:HD12	2.38	0.58
3:a:3132[A]:ALA:CB	3:a:3197[A]:ILE:HD13	2.33	0.58
3:a:3225[B]:SER:OG	3:a:3290[B]:ILE:HD13	2.04	0.58
1:b:931:TRP:CG	1:b:1018:ILE:HD11	2.38	0.58
3:d:2995[A]:GLN:HG2	3:d:3168[A]:THR:HG21	1.85	0.58
3:d:3293[B]:LYS:CB	3:d:3294[B]:SER:CB	2.54	0.58
1:A:942:VAL:HG11	1:A:1041:ILE:HD11	1.85	0.58
3:C:2968[B]:GLN:NE2	3:L:3086[B]:GLU:CG	2.66	0.58
3:C:3103[A]:GLY:O	3:C:3106[A]:THR:HG22	2.03	0.58
3:C:3225[B]:SER:OG	3:C:3290[B]:ILE:HD13	2.04	0.58
1:D:1154:SER:HB2	1:D:1220:MET:HE2	1.86	0.58
1:D:1397:LEU:HB2	1:D:1433:TRP:HB3	1.86	0.58
1:D:1472:GLN:OE1	1:D:1475:ARG:NH1	2.37	0.58
3:F:2982[B]:MET:HE2	3:a:2966[B]:SER:C	2.28	0.58
3:F:3000[A]:LEU:N	3:F:3000[A]:LEU:HD23	2.18	0.58
3:F:3071[A]:PHE:O	3:F:3074[A]:GLU:HB2	2.02	0.58
3:F:3191[B]:ASN:ND2	3:F:3191[B]:ASN:H	1.99	0.58
3:I:2976[B]:ALA:H	3:R:2976[B]:ALA:HB3	1.67	0.58
3:I:2991[B]:LEU:O	3:I:2994[B]:LYS:HB3	2.03	0.58
1:J:1138:ALA:HA	1:J:1240:ILE:HG22	1.84	0.58
3:L:2928[B]:ASN:N	3:L:2930[B]:LEU:HD21	2.18	0.58
3:L:2991[A]:LEU:O	3:L:2994[A]:LYS:N	2.37	0.58
2:N:2711:HIS:HA	2:N:2714:VAL:HG22	1.86	0.58
2:N:2803:ARG:HH21	2:N:2805:PHE:HZ	1.52	0.58
3:O:2935[A]:ILE:HD13	3:O:2935[A]:ILE:N	2.18	0.58
3:O:2965[A]:LEU:HD11	3:O:2974[A]:ALA:C	2.28	0.58
3:O:3103[B]:GLY:O	3:O:3106[B]:THR:HG22	2.03	0.58
1:P:935:ILE:HD11	1:P:980:TYR:CE2	2.39	0.58
3:R:2960[B]:PHE:CD1	3:R:2960[B]:PHE:N	2.72	0.58
3:R:2995[B]:GLN:HG2	3:R:3168[B]:THR:HG21	1.85	0.58
3:U:2932[B]:PRO:CA	3:U:2935[B]:ILE:HD12	2.30	0.58
3:U:3014[A]:TRP:CE3	3:U:3092[A]:ILE:HD12	2.37	0.58
3:U:3298[A]:ASN:CB	3:U:3300[A]:LEU:N	2.60	0.58
3:X:2986[B]:PRO:HB3	3:X:3127[B]:TRP:CE3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2991[A]:LEU:O	3:X:2994[A]:LYS:HB3	2.03	0.58
3:a:3298[A]:ASN:CB	3:a:3300[A]:LEU:N	2.60	0.58
1:b:1632:LEU:HB3	1:b:1641:THR:HB	1.86	0.58
2:c:2890:VAL:N	2:c:2891:LEU:HA	2.18	0.58
3:C:2935[B]:ILE:HD13	3:C:2935[B]:ILE:N	2.18	0.58
3:C:3024[B]:LEU:O	3:C:3031[B]:ASN:ND2	2.36	0.58
3:C:3129[A]:ILE:HD13	3:C:3190[A]:LEU:O	2.04	0.58
3:C:3156[B]:MET:C	3:L:3153[B]:LYS:HZ2	2.04	0.58
3:C:3293[A]:LYS:CD	3:C:3294[A]:SER:N	2.63	0.58
1:D:104:LEU:HD23	1:D:123:PHE:HE2	1.69	0.58
1:D:317:VAL:HG22	1:D:383:VAL:HG22	1.85	0.58
1:D:462:HIS:HA	1:D:490:TRP:HH2	1.68	0.58
1:D:1315:GLY:HA3	1:D:1601:TRP:HB2	1.85	0.58
1:D:1397:LEU:HA	1:D:1433:TRP:HD1	1.68	0.58
3:F:2970[B]:PRO:HA	3:a:2985[B]:PHE:CE2	2.37	0.58
3:F:2995[B]:GLN:HG2	3:F:3168[B]:THR:HG21	1.85	0.58
1:G:1162:ALA:HB1	1:G:1167:ASP:OD2	2.04	0.58
3:I:2991[A]:LEU:O	3:I:2994[A]:LYS:HB3	2.03	0.58
3:I:2991[A]:LEU:O	3:I:2994[A]:LYS:N	2.37	0.58
3:I:3000[B]:LEU:HD23	3:I:3000[B]:LEU:N	2.18	0.58
3:I:3014[A]:TRP:CD2	3:I:3092[A]:ILE:HD12	2.38	0.58
3:I:3129[A]:ILE:HD13	3:I:3190[A]:LEU:O	2.04	0.58
3:L:2932[A]:PRO:CA	3:L:2935[A]:ILE:HD12	2.30	0.58
3:L:3113[B]:ASP:O	3:L:3115[B]:LEU:N	2.36	0.58
3:L:3225[A]:SER:OG	3:L:3290[A]:ILE:HD13	2.04	0.58
1:M:105:VAL:HG12	1:M:123:PHE:HB3	1.84	0.58
3:O:3129[B]:ILE:HD13	3:O:3190[B]:LEU:O	2.04	0.58
3:O:3293[A]:LYS:CD	3:O:3294[A]:SER:N	2.64	0.58
1:P:1421:VAL:HG23	1:P:1422:HIS:HD1	1.68	0.58
3:R:2928[B]:ASN:N	3:R:2930[B]:LEU:HD21	2.17	0.58
3:R:2965[B]:LEU:HD11	3:R:2974[B]:ALA:C	2.28	0.58
3:R:2969[A]:TYR:CD2	3:R:2970[A]:PRO:HG2	2.38	0.58
3:R:2995[A]:GLN:HG2	3:R:3168[A]:THR:HG21	1.85	0.58
3:R:3113[A]:ASP:O	3:R:3115[A]:LEU:N	2.36	0.58
3:R:3132[A]:ALA:CB	3:R:3197[A]:ILE:HD13	2.33	0.58
3:R:3225[A]:SER:OG	3:R:3290[A]:ILE:HD13	2.04	0.58
1:S:574:GLY:C	1:S:576:HIS:HA	2.28	0.58
1:S:1018:ILE:HA	1:S:1021:LEU:HG	1.85	0.58
3:U:2965[A]:LEU:HD11	3:U:2974[A]:ALA:C	2.28	0.58
3:U:3129[B]:ILE:HD13	3:U:3190[B]:LEU:O	2.04	0.58
1:V:472:ASP:OD1	1:V:472:ASP:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:2089:ARG:HD2	2:W:2175:VAL:O	2.04	0.58
3:X:2945[B]:VAL:HG22	3:X:2945[B]:VAL:O	2.01	0.58
3:a:3129[B]:ILE:HD13	3:a:3190[B]:LEU:O	2.04	0.58
3:a:3188[A]:ASP:N	3:a:3188[A]:ASP:OD2	2.36	0.58
3:d:2991[B]:LEU:O	3:d:2994[B]:LYS:HB3	2.03	0.58
1:A:781:ILE:HG23	1:A:784:ALA:HB3	1.85	0.58
1:A:1372:ILE:HD13	1:b:1390:ASP:HB3	1.84	0.58
1:A:1642:GLN:NE2	1:A:1642:GLN:O	2.36	0.58
3:C:3014[B]:TRP:CD2	3:C:3092[B]:ILE:HD12	2.38	0.58
3:C:3135[A]:LYS:HG3	3:C:3141[A]:TYR:CD1	2.33	0.58
1:D:744:VAL:HG12	1:D:802:ILE:HG23	1.85	0.58
1:D:1029:SER:OG	1:D:1030:MET:N	2.34	0.58
3:F:2991[A]:LEU:O	3:F:2994[A]:LYS:HB3	2.03	0.58
3:F:3019[B]:HIS:CD2	3:F:3019[B]:HIS:H	2.22	0.58
3:F:3103[B]:GLY:O	3:F:3106[B]:THR:HG22	2.03	0.58
1:G:949:ASP:OD1	1:G:950:ALA:N	2.37	0.58
1:G:1467:ILE:HD13	1:G:1532:PHE:HB2	1.85	0.58
2:H:2181:THR:HB	2:H:2374:ASN:H	1.69	0.58
2:H:2851:ASN:OD1	2:H:2851:ASN:N	2.36	0.58
3:I:2960[B]:PHE:CD2	3:I:3157[B]:PRO:CG	2.74	0.58
3:I:2965[B]:LEU:HG	3:R:3249[B]:GLY:CA	2.33	0.58
3:I:3154[B]:PRO:HB3	3:R:3174[B]:GLY:H	1.60	0.58
3:I:3255[B]:PRO:CG	3:R:2964[B]:PRO:N	2.65	0.58
3:I:3293[B]:LYS:CD	3:I:3294[B]:SER:N	2.64	0.58
3:L:2986[A]:PRO:HB3	3:L:3127[A]:TRP:CE3	2.38	0.58
3:O:3019[B]:HIS:H	3:O:3019[B]:HIS:CD2	2.22	0.58
3:O:3024[B]:LEU:O	3:O:3031[B]:ASN:ND2	2.36	0.58
3:O:3169[B]:LYS:HZ1	3:X:3148[B]:ILE:H	1.51	0.58
1:P:1171:LYS:NZ	1:P:1174:GLU:OE2	2.29	0.58
3:R:3001[B]:LYS:HE3	3:R:3002[B]:ALA:HB2	1.85	0.58
3:R:3293[B]:LYS:CD	3:R:3294[B]:SER:N	2.64	0.58
1:S:979:LEU:HB2	1:S:980:TYR:CD2	2.38	0.58
2:T:2687:ILE:HD11	2:T:2695:MET:HG2	1.84	0.58
3:U:3001[A]:LYS:HE3	3:U:3002[A]:ALA:HB2	1.85	0.58
1:V:1013:ILE:HD11	1:V:1148:LEU:HD11	1.85	0.58
3:X:2991[B]:LEU:O	3:X:2994[B]:LYS:N	2.37	0.58
3:X:3225[B]:SER:OG	3:X:3290[B]:ILE:HD13	2.04	0.58
2:Z:2544:GLY:HA3	2:Z:2699:MET:O	2.04	0.58
3:a:2995[A]:GLN:HG2	3:a:3168[A]:THR:HG21	1.85	0.58
3:a:3014[A]:TRP:CD2	3:a:3092[A]:ILE:HD12	2.38	0.58
1:b:308:LEU:O	1:b:772:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:2638:ARG:HH11	2:c:2706:ILE:HG13	1.68	0.58
3:d:2991[A]:LEU:O	3:d:2994[A]:LYS:HB3	2.03	0.58
1:A:926:LEU:HD11	1:A:1043:MET:HB3	1.85	0.57
1:D:639:ARG:NH2	1:D:707:PHE:O	2.37	0.57
1:D:900:ALA:HB3	1:D:1076:ILE:HD12	1.85	0.57
3:F:3157[B]:PRO:HD2	3:a:3153[B]:LYS:NZ	2.18	0.57
3:I:3019[B]:HIS:CD2	3:I:3019[B]:HIS:H	2.22	0.57
3:I:3103[B]:GLY:O	3:I:3106[B]:THR:HG22	2.03	0.57
3:I:3132[A]:ALA:CB	3:I:3197[A]:ILE:HD13	2.33	0.57
3:I:3293[A]:LYS:CB	3:I:3294[A]:SER:CB	2.54	0.57
1:J:425:ARG:NE	1:J:499:GLU:OE2	2.35	0.57
1:J:460:GLU:HB3	1:J:465:PRO:HG2	1.85	0.57
1:J:1492:PRO:HB2	1:J:1497:SER:HB3	1.86	0.57
2:K:2601:ASN:OD1	2:K:2601:ASN:N	2.36	0.57
2:K:2606:LEU:HD13	2:K:2706:ILE:HG13	1.85	0.57
3:L:3284[B]:LYS:CD	3:L:3285[B]:VAL:H	2.10	0.57
2:N:2722:GLN:NE2	2:N:2769:PHE:O	2.34	0.57
3:O:2991[A]:LEU:O	3:O:2994[A]:LYS:N	2.37	0.57
3:O:2991[B]:LEU:O	3:O:2994[B]:LYS:N	2.37	0.57
3:O:3113[B]:ASP:O	3:O:3115[B]:LEU:N	2.36	0.57
3:O:3176[B]:LYS:HB3	3:O:3176[B]:LYS:HZ2	1.68	0.57
1:P:567:LEU:HD13	1:P:571:PRO:HA	1.86	0.57
2:Q:2117:ASP:OD2	2:Q:2168:ARG:NH1	2.36	0.57
2:Q:2142:ALA:HB1	2:Q:2143:CYS:HB2	1.86	0.57
3:R:2960[B]:PHE:CD2	3:R:3157[B]:PRO:CG	2.74	0.57
3:R:2991[A]:LEU:O	3:R:2994[A]:LYS:HB3	2.03	0.57
1:S:187:GLY:HA3	1:S:195:SER:HB3	1.85	0.57
1:S:565:GLU:HG3	1:S:566:ARG:H	1.69	0.57
3:U:2965[B]:LEU:HD23	3:d:3220[B]:ARG:HH11	1.67	0.57
3:U:2969[B]:TYR:C	3:d:3086[B]:GLU:OE1	2.47	0.57
3:U:2991[B]:LEU:O	3:U:2994[B]:LYS:N	2.37	0.57
3:U:3001[B]:LYS:HE3	3:U:3002[B]:ALA:HB2	1.85	0.57
3:U:3129[A]:ILE:HD13	3:U:3190[A]:LEU:O	2.04	0.57
3:U:3225[B]:SER:OG	3:U:3290[B]:ILE:HD13	2.04	0.57
1:V:984:ASP:OD1	1:V:984:ASP:N	2.36	0.57
3:X:3023[A]:ILE:O	3:X:3024[A]:LEU:C	2.45	0.57
1:Y:372:ALA:O	1:Y:375:SER:OG	2.21	0.57
1:Y:1348:TRP:CG	1:Y:1430:ILE:HD11	2.39	0.57
3:a:2960[B]:PHE:CD1	3:a:2960[B]:PHE:N	2.72	0.57
3:a:2965[B]:LEU:HD11	3:a:2974[B]:ALA:C	2.28	0.57
3:a:2986[A]:PRO:HB3	3:a:3127[A]:TRP:CE3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:980:TYR:CE2	1:b:1021:LEU:HD13	2.39	0.57
2:c:2265:ILE:HD12	2:c:2443:TYR:CG	2.39	0.57
3:d:2986[A]:PRO:HB3	3:d:3127[A]:TRP:CE3	2.39	0.57
3:d:2991[B]:LEU:O	3:d:2994[B]:LYS:N	2.37	0.57
1:A:124:TYR:O	1:A:137:ARG:NH2	2.37	0.57
1:A:979:LEU:HD22	1:A:979:LEU:H	1.69	0.57
1:A:1144:VAL:HG22	1:A:1196:ILE:HD12	1.86	0.57
2:B:2544:GLY:HA3	2:B:2699:MET:O	2.05	0.57
3:C:2948[A]:ASP:HB3	3:C:2953[A]:GLY:CA	2.24	0.57
3:C:2991[A]:LEU:O	3:C:2994[A]:LYS:N	2.37	0.57
3:C:3135[B]:LYS:HG3	3:C:3141[B]:TYR:CD1	2.33	0.57
3:C:3225[A]:SER:OG	3:C:3290[A]:ILE:HD13	2.04	0.57
3:C:3298[B]:ASN:CA	3:C:3300[B]:LEU:HD23	2.31	0.57
3:F:2965[A]:LEU:HD11	3:F:2974[A]:ALA:C	2.28	0.57
3:F:2967[B]:CYS:CB	3:a:2980[B]:HIS:N	2.66	0.57
3:F:3163[B]:ASN:HD21	3:a:3149[B]:ASN:CB	2.05	0.57
1:G:1018:ILE:HB	1:G:1045:HIS:CD2	2.39	0.57
2:H:2756:ASN:HD21	2:H:2759:THR:HG23	1.69	0.57
3:I:3130[B]:TRP:CE2	3:I:3134[B]:GLN:NE2	2.72	0.57
3:I:3160[B]:SER:HB2	3:R:2982[B]:MET:CB	2.28	0.57
3:I:3169[B]:LYS:HE3	3:R:3150[B]:LYS:HB2	1.86	0.57
2:K:2394:VAL:HG11	2:K:2451:LEU:HD12	1.85	0.57
1:M:704:ASP:OD1	1:M:704:ASP:N	2.37	0.57
2:N:2506:ARG:NE	2:N:2578:GLU:OE2	2.27	0.57
3:O:3130[B]:TRP:CE2	3:O:3134[B]:GLN:NE2	2.72	0.57
3:R:2932[A]:PRO:CA	3:R:2935[A]:ILE:HD12	2.31	0.57
3:R:2952[B]:ALA:N	3:R:2953[B]:GLY:HA2	2.06	0.57
3:R:3023[A]:ILE:O	3:R:3024[A]:LEU:C	2.45	0.57
3:U:2967[B]:CYS:CB	3:d:3256[B]:TRP:CA	2.79	0.57
3:U:2991[A]:LEU:O	3:U:2994[A]:LYS:N	2.37	0.57
3:U:3019[A]:HIS:CD2	3:U:3019[A]:HIS:H	2.22	0.57
3:U:3255[B]:PRO:C	3:d:2975[B]:PHE:HA	2.28	0.57
1:V:157:GLU:OE2	1:V:296:ARG:NH2	2.37	0.57
1:V:262:LYS:NZ	1:V:795:GLU:OE1	2.37	0.57
3:X:2995[B]:GLN:HG2	3:X:3168[B]:THR:HG21	1.85	0.57
3:X:3024[A]:LEU:O	3:X:3031[A]:ASN:ND2	2.36	0.57
3:X:3103[A]:GLY:O	3:X:3106[A]:THR:HG22	2.03	0.57
1:Y:1550:ARG:HE	3:d:3008[B]:GLY:C	2.11	0.57
1:Y:1616:LYS:NZ	3:d:3188[B]:ASP:HA	2.19	0.57
1:Y:1656:ASP:H	3:d:3006[B]:LYS:CB	2.15	0.57
3:a:2991[B]:LEU:O	3:a:2994[B]:LYS:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:2995[B]:GLN:HG2	3:a:3168[B]:THR:HG21	1.85	0.57
3:a:3001[B]:LYS:HE3	3:a:3002[B]:ALA:HB2	1.85	0.57
1:b:105:VAL:HB	1:b:137:ARG:HH22	1.67	0.57
1:b:977:GLU:HG3	1:b:978:ALA:H	1.69	0.57
3:d:3103[B]:GLY:O	3:d:3106[B]:THR:HG22	2.03	0.57
1:A:447:MET:HA	1:A:455:TYR:HB2	1.86	0.57
2:B:2179:ASP:HA	2:B:2300:ASN:ND2	2.18	0.57
2:B:2226:GLU:OE2	2:B:2278:GLU:N	2.37	0.57
2:B:2830:GLN:HB2	2:B:2863:ARG:HH22	1.69	0.57
2:B:2833:GLY:HA3	2:B:2854:MET:HE1	1.86	0.57
3:C:2985[B]:PHE:HD2	3:L:2968[B]:GLN:O	1.87	0.57
3:C:3019[A]:HIS:CD2	3:C:3019[A]:HIS:H	2.22	0.57
3:C:3130[A]:TRP:CE2	3:C:3134[A]:GLN:NE2	2.72	0.57
1:D:518:LYS:HD2	1:D:519:PRO:HD2	1.86	0.57
1:D:757:VAL:HG21	1:D:781:ILE:HG13	1.86	0.57
1:D:1627:ARG:NH2	1:D:1629:GLU:OE1	2.37	0.57
2:E:2242:TRP:O	2:E:2246:ASN:ND2	2.34	0.57
3:F:2952[B]:ALA:H	3:F:2953[B]:GLY:CA	2.04	0.57
3:F:2956[B]:LYS:HD2	3:a:3257[B]:ALA:HB3	1.85	0.57
3:F:2967[B]:CYS:SG	3:a:2982[B]:MET:SD	3.03	0.57
3:F:2969[B]:TYR:CA	3:a:2989[B]:HIS:NE2	2.68	0.57
3:F:2991[B]:LEU:O	3:F:2994[B]:LYS:N	2.37	0.57
3:F:3001[A]:LYS:HE3	3:F:3002[A]:ALA:HB2	1.85	0.57
1:G:439:LEU:HD23	1:G:509:ILE:HD12	1.86	0.57
1:G:1486:LEU:HB2	2:K:2486:ILE:HB	1.85	0.57
3:I:2981[B]:GLY:N	3:R:2968[B]:GLN:HG2	2.19	0.57
3:I:3188[A]:ASP:N	3:I:3188[A]:ASP:OD2	2.36	0.57
1:J:469:PRO:O	1:J:669:LYS:HD2	2.04	0.57
1:J:1150:GLY:N	1:J:1186:TRP:O	2.36	0.57
1:J:1324:ARG:NE	1:J:1462:ASP:OD1	2.37	0.57
2:K:2090:LYS:NZ	2:K:2099:GLU:OE2	2.32	0.57
3:L:2991[B]:LEU:O	3:L:2994[B]:LYS:HB3	2.03	0.57
3:L:2991[B]:LEU:O	3:L:2994[B]:LYS:N	2.37	0.57
3:L:3019[A]:HIS:CD2	3:L:3019[A]:HIS:H	2.22	0.57
3:L:3120[A]:HIS:HA	3:L:3123[A]:THR:HG1	1.68	0.57
3:L:3129[B]:ILE:HD13	3:L:3190[B]:LEU:O	2.04	0.57
3:O:2960[B]:PHE:CD1	3:O:2960[B]:PHE:N	2.72	0.57
3:O:2986[A]:PRO:HB3	3:O:3127[A]:TRP:CE3	2.38	0.57
3:O:3284[A]:LYS:HE2	3:O:3284[A]:LYS:CA	2.29	0.57
1:P:1171:LYS:HG2	1:P:1173:GLY:H	1.69	0.57
3:R:3000[B]:LEU:HD23	3:R:3000[B]:LEU:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3103[A]:GLY:O	3:R:3106[A]:THR:HG22	2.03	0.57
3:R:3284[B]:LYS:HE2	3:R:3284[B]:LYS:CA	2.30	0.57
3:U:2948[B]:ASP:CB	3:U:2949[B]:LYS:CA	2.78	0.57
3:U:2972[B]:GLY:CA	3:d:3247[B]:VAL:HG13	2.34	0.57
3:U:3225[A]:SER:OG	3:U:3290[A]:ILE:HD13	2.04	0.57
3:U:3256[B]:TRP:CB	3:d:2969[B]:TYR:H	2.12	0.57
1:V:545:PHE:O	1:V:561:ARG:NH2	2.36	0.57
3:X:3129[B]:ILE:HD13	3:X:3190[B]:LEU:O	2.04	0.57
3:X:3307[A]:PHE:HE1	3:X:3309[A]:PRO:CG	2.08	0.57
3:a:3293[A]:LYS:CD	3:a:3294[A]:SER:N	2.64	0.57
1:b:227:ARG:CZ	1:b:227:ARG:HA	2.34	0.57
1:b:583:LEU:HG	1:b:602:THR:HG21	1.85	0.57
1:b:1493:MET:HG2	1:b:1511:SER:O	2.04	0.57
3:d:2965[A]:LEU:HD11	3:d:2974[A]:ALA:C	2.28	0.57
3:d:3014[A]:TRP:CD2	3:d:3092[A]:ILE:HD12	2.38	0.57
3:d:3019[A]:HIS:H	3:d:3019[A]:HIS:CD2	2.22	0.57
1:A:460:GLU:CD	1:A:1368:ARG:HH22	2.12	0.57
1:A:801:ASP:N	1:A:801:ASP:OD1	2.35	0.57
2:B:2345:ASN:N	2:E:2515:ARG:HD3	2.16	0.57
2:B:2515:ARG:HD3	2:E:2345:ASN:H	1.70	0.57
3:C:3000[A]:LEU:HD23	3:C:3000[A]:LEU:N	2.18	0.57
3:C:3079[B]:CYS:HB3	3:L:3161[B]:GLU:CG	2.30	0.57
3:C:3120[B]:HIS:C	3:C:3122[B]:ASN:N	2.55	0.57
3:C:3156[B]:MET:HE2	3:L:2979[B]:GLN:HG3	0.78	0.57
1:D:329:ARG:HB2	1:G:1583:CYS:N	2.18	0.57
3:F:3172[B]:SER:HB3	3:a:3150[B]:LYS:CA	2.34	0.57
2:H:2158:TYR:O	2:H:2161:GLN:HB3	2.04	0.57
3:I:2965[A]:LEU:HD11	3:I:2974[A]:ALA:C	2.28	0.57
3:I:2966[B]:SER:CB	3:R:3254[B]:MET:CB	2.81	0.57
3:I:3225[A]:SER:OG	3:I:3290[A]:ILE:HD13	2.04	0.57
1:J:979:LEU:HB3	1:J:980:TYR:CD1	2.39	0.57
3:L:2987[B]:HIS:NE2	3:L:3178[B]:PHE:HE1	1.95	0.57
3:L:3130[A]:TRP:CE2	3:L:3134[A]:GLN:NE2	2.72	0.57
3:L:3225[B]:SER:OG	3:L:3290[B]:ILE:HD13	2.04	0.57
3:O:3014[B]:TRP:CD2	3:O:3092[B]:ILE:HD12	2.38	0.57
3:O:3225[A]:SER:OG	3:O:3290[A]:ILE:HD13	2.04	0.57
1:P:1458:HIS:HA	1:P:1461:VAL:HB	1.86	0.57
2:Q:2180:TRP:HB3	2:Q:2184:MET:HE2	1.85	0.57
3:R:3130[B]:TRP:CE2	3:R:3134[B]:GLN:NE2	2.73	0.57
3:R:3135[B]:LYS:HG3	3:R:3141[B]:TYR:HE1	1.29	0.57
1:S:618:MET:HE1	1:S:633:HIS:HD2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3162[B]:ASP:HB3	3:d:3260[B]:ARG:CZ	2.35	0.57
3:U:3252[B]:TYR:CD2	3:d:3222[B]:ILE:HA	2.40	0.57
1:V:51:ASP:CG	1:V:52:GLY:HA2	2.29	0.57
1:V:450:LYS:NZ	1:V:451:SER:H	2.01	0.57
1:V:899:MET:HE2	1:V:1012:GLU:OE2	2.05	0.57
1:V:949:ASP:OD1	1:V:950:ALA:N	2.36	0.57
3:X:2932[B]:PRO:CA	3:X:2935[B]:ILE:HD12	2.30	0.57
1:Y:804:ASP:OD1	1:Y:805:VAL:N	2.37	0.57
1:Y:928:TYR:HB2	1:Y:1048:ASN:HB2	1.86	0.57
1:Y:947:TYR:HE1	1:Y:957:ASN:H	1.51	0.57
1:Y:1137:LYS:HA	1:Y:1141:ARG:HH12	1.69	0.57
3:a:3176[A]:LYS:H	3:a:3176[A]:LYS:CE	2.17	0.57
2:c:2114:ARG:HH12	2:c:2120:GLU:HG3	1.69	0.57
3:d:3212[B]:ARG:HH11	3:d:3212[B]:ARG:CG	2.12	0.57
1:A:959:PHE:HA	1:A:1040:PRO:HG2	1.86	0.57
3:C:3150[B]:LYS:N	3:L:3169[B]:LYS:HG2	2.10	0.57
3:C:3160[B]:SER:OG	3:L:2983[B]:VAL:HG22	2.00	0.57
1:D:460:GLU:O	1:D:467:LYS:NZ	2.33	0.57
3:F:2948[A]:ASP:CB	3:F:2949[A]:LYS:CA	2.78	0.57
3:F:2995[A]:GLN:HG2	3:F:3168[A]:THR:HG21	1.86	0.57
3:F:3158[B]:PHE:N	3:a:3153[B]:LYS:CE	2.62	0.57
3:F:3160[B]:SER:CB	3:a:3150[B]:LYS:CE	2.78	0.57
3:F:3174[B]:GLY:N	3:a:3154[B]:PRO:CA	2.65	0.57
3:F:3255[B]:PRO:HG2	3:a:2964[B]:PRO:HD2	1.85	0.57
3:F:3283[A]:ILE:CB	3:F:3305[A]:ILE:HD11	2.35	0.57
3:F:3298[A]:ASN:CA	3:F:3300[A]:LEU:HD23	2.31	0.57
1:G:493:LEU:HD12	1:G:668:MET:HG3	1.86	0.57
1:G:1361:GLU:HG3	1:G:1363:THR:H	1.69	0.57
3:I:2965[B]:LEU:HD11	3:I:2974[B]:ALA:C	2.29	0.57
3:I:2965[B]:LEU:HD13	3:R:3256[B]:TRP:HE1	1.66	0.57
3:I:2989[B]:HIS:ND1	3:R:2970[B]:PRO:HD3	2.08	0.57
3:L:2960[A]:PHE:CD2	3:L:3157[A]:PRO:CG	2.74	0.57
3:L:3019[B]:HIS:CD2	3:L:3019[B]:HIS:H	2.22	0.57
3:L:3103[B]:GLY:O	3:L:3106[B]:THR:HG22	2.03	0.57
3:L:3176[A]:LYS:HB3	3:L:3176[A]:LYS:HZ2	1.68	0.57
3:O:2965[B]:LEU:HD11	3:O:2974[B]:ALA:C	2.28	0.57
3:O:2968[B]:GLN:CG	3:X:2984[B]:THR:CB	2.79	0.57
3:O:2969[B]:TYR:N	3:X:2988[B]:TRP:CB	2.55	0.57
3:O:2975[B]:PHE:C	3:X:3155[B]:MET:HA	2.09	0.57
3:O:3001[A]:LYS:HE3	3:O:3002[A]:ALA:HB2	1.85	0.57
3:O:3130[A]:TRP:CE2	3:O:3134[A]:GLN:NE2	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2991[B]:LEU:O	3:R:2994[B]:LYS:N	2.37	0.57
3:R:3089[A]:HIS:CE1	3:R:3119[A]:HIS:CE1	2.81	0.57
2:T:2872:GLU:OE1	2:T:2874:ASP:N	2.36	0.57
3:U:2948[B]:ASP:HB3	3:U:2953[B]:GLY:CA	2.24	0.57
3:U:2991[A]:LEU:O	3:U:2994[A]:LYS:HB3	2.03	0.57
3:U:3130[B]:TRP:CE2	3:U:3134[B]:GLN:NE2	2.72	0.57
3:U:3217[A]:PHE:HE1	3:U:3230[A]:PHE:HZ	0.80	0.57
3:X:2935[B]:ILE:HD13	3:X:2935[B]:ILE:N	2.18	0.57
3:X:3130[A]:TRP:CE2	3:X:3134[A]:GLN:NE2	2.72	0.57
3:X:3130[B]:TRP:CE2	3:X:3134[B]:GLN:NE2	2.72	0.57
3:X:3284[A]:LYS:CD	3:X:3285[A]:VAL:H	2.10	0.57
3:X:3298[A]:ASN:CA	3:X:3300[A]:LEU:HD23	2.31	0.57
1:Y:931:TRP:CD1	1:Y:1048:ASN:HD22	2.23	0.57
3:a:2987[B]:HIS:NE2	3:a:3178[B]:PHE:HE1	1.95	0.57
3:a:2991[B]:LEU:O	3:a:2994[B]:LYS:N	2.37	0.57
1:b:19:GLN:NE2	1:b:121:ASN:OD1	2.37	0.57
1:b:549:PRO:HA	1:b:557:VAL:HB	1.87	0.57
1:b:931:TRP:CD1	1:b:1048:ASN:HD22	2.23	0.57
1:b:975:PRO:HG2	1:b:1024:GLY:HA3	1.86	0.57
3:d:3293[B]:LYS:CD	3:d:3294[B]:SER:N	2.64	0.57
3:C:3130[B]:TRP:CE2	3:C:3134[B]:GLN:NE2	2.72	0.57
3:C:3156[B]:MET:HE2	3:L:2979[B]:GLN:HB3	1.77	0.57
3:C:3169[B]:LYS:HG2	3:L:3150[B]:LYS:H	1.69	0.57
3:C:3298[A]:ASN:CA	3:C:3300[A]:LEU:HD23	2.31	0.57
1:D:488:PRO:HB2	1:D:641:TRP:CE3	2.39	0.57
1:D:1372:ILE:HD11	1:G:1392:ASP:HB2	1.85	0.57
3:F:2960[A]:PHE:CD1	3:F:2960[A]:PHE:N	2.72	0.57
3:F:2961[A]:HIS:CE1	3:F:2980[A]:HIS:NE2	2.57	0.57
3:F:3130[B]:TRP:CZ2	3:F:3134[B]:GLN:NE2	2.73	0.57
1:G:760:ILE:HG21	1:G:777:TYR:HE2	1.68	0.57
1:G:1101:VAL:HG21	2:K:2873:HIS:ND1	2.19	0.57
2:H:2086:ASN:N	2:H:2086:ASN:OD1	2.37	0.57
2:H:2597:MET:HE2	2:H:2598:PRO:HD2	1.86	0.57
3:I:2986[B]:PRO:HB3	3:I:3127[B]:TRP:CE3	2.38	0.57
3:I:2989[B]:HIS:HE1	3:R:2969[B]:TYR:HA	1.56	0.57
3:I:2991[B]:LEU:O	3:I:2994[B]:LYS:N	2.37	0.57
3:I:3130[A]:TRP:CZ2	3:I:3134[A]:GLN:NE2	2.73	0.57
3:I:3162[B]:ASP:CG	3:R:3259[B]:ASP:H	2.12	0.57
3:I:3162[B]:ASP:O	3:R:3150[B]:LYS:NZ	2.36	0.57
3:I:3169[B]:LYS:CB	3:R:3149[B]:ASN:OD1	2.44	0.57
3:I:3256[B]:TRP:CA	3:R:2966[B]:SER:HA	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2795:ILE:O	2:K:2798:GLN:HG2	2.05	0.57
1:M:240:PHE:HA	1:M:263:ALA:HB3	1.87	0.57
3:O:2932[A]:PRO:CA	3:O:2935[A]:ILE:HD12	2.31	0.57
3:O:2948[A]:ASP:HB3	3:O:2953[A]:GLY:CA	2.24	0.57
3:O:2963[B]:MET:CE	3:X:2975[B]:PHE:HB2	2.30	0.57
3:O:3000[A]:LEU:HD23	3:O:3000[A]:LEU:N	2.18	0.57
1:P:1394:GLN:HG2	1:P:1395:PRO:HD2	1.86	0.57
3:R:2961[A]:HIS:NE2	3:R:2980[A]:HIS:CE1	2.73	0.57
3:R:3019[B]:HIS:CD2	3:R:3019[B]:HIS:H	2.22	0.57
3:R:3023[B]:ILE:O	3:R:3024[B]:LEU:C	2.45	0.57
3:R:3129[B]:ILE:HD13	3:R:3190[B]:LEU:O	2.04	0.57
3:R:3130[A]:TRP:CE2	3:R:3134[A]:GLN:NE2	2.72	0.57
3:R:3130[B]:TRP:CZ2	3:R:3134[B]:GLN:NE2	2.73	0.57
1:S:946:GLU:HG2	1:S:955:LYS:HB3	1.85	0.57
1:S:1140:ASN:ND2	1:S:1236:TYR:OH	2.37	0.57
2:T:2833:GLY:HA3	2:T:2854:MET:HE1	1.85	0.57
3:U:2965[B]:LEU:HD11	3:U:2974[B]:ALA:C	2.28	0.57
3:U:2965[B]:LEU:HA	3:d:3220[B]:ARG:HH11	1.59	0.57
3:U:2986[A]:PRO:HB3	3:U:3127[A]:TRP:CE3	2.38	0.57
3:U:3000[B]:LEU:HD23	3:U:3000[B]:LEU:N	2.18	0.57
3:U:3130[B]:TRP:CZ2	3:U:3134[B]:GLN:NE2	2.73	0.57
3:U:3180[A]:TYR:C	3:U:3183[A]:LEU:HD22	2.30	0.57
3:X:3183[A]:LEU:N	3:X:3184[A]:ASN:HA	2.11	0.57
1:Y:688:VAL:HG12	1:Y:690:THR:HG23	1.87	0.57
2:Z:2128:LEU:HD13	2:Z:2286:HIS:CG	2.40	0.57
2:Z:2866:PRO:CG	3:a:2933[A]:SER:HB2	2.34	0.57
1:b:35:GLN:HE21	1:b:129:LYS:HB2	1.69	0.57
1:b:1143:ALA:HA	1:b:1195:ASP:O	2.03	0.57
3:d:2969[B]:TYR:CE2	3:d:2970[B]:PRO:CG	2.86	0.57
3:d:3130[B]:TRP:CZ2	3:d:3134[B]:GLN:NE2	2.73	0.57
3:d:3225[B]:SER:OG	3:d:3290[B]:ILE:HD13	2.04	0.57
2:B:2344:LEU:HA	2:B:2345:ASN:C	2.29	0.57
3:C:2972[B]:GLY:C	3:L:3090[B]:ASN:CG	2.71	0.57
3:C:2991[B]:LEU:O	3:C:2994[B]:LYS:N	2.37	0.57
3:C:3293[B]:LYS:CD	3:C:3294[B]:SER:N	2.63	0.57
3:C:3298[A]:ASN:HD21	3:C:3301[A]:PRO:HA	1.60	0.57
1:D:908:LEU:HD22	1:D:1096:THR:HG23	1.85	0.57
1:G:639:ARG:NH2	1:G:707:PHE:O	2.37	0.57
1:G:943:LEU:HD13	1:G:944:GLU:HG3	1.86	0.57
3:I:3173[B]:THR:C	3:R:3154[B]:PRO:CA	2.77	0.57
3:I:3180[B]:TYR:C	3:I:3183[B]:LEU:HD22	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3220[A]:ARG:HH11	3:I:3220[A]:ARG:CG	2.12	0.57
1:J:572:SER:OG	1:J:573:LYS:N	2.35	0.57
1:J:619:SER:HB2	1:J:805:VAL:HG11	1.86	0.57
1:J:1639:LYS:HD3	6:w:1:NAG:O5	2.04	0.57
3:L:2961[B]:HIS:NE2	3:L:2980[B]:HIS:CE1	2.73	0.57
3:L:3173[A]:THR:HG22	3:L:3174[A]:GLY:H	1.67	0.57
3:O:2986[B]:PRO:HB3	3:O:3127[B]:TRP:CE3	2.38	0.57
3:O:3023[B]:ILE:O	3:O:3024[B]:LEU:C	2.45	0.57
3:O:3103[A]:GLY:O	3:O:3106[A]:THR:HG22	2.03	0.57
3:O:3217[B]:PHE:HE1	3:O:3230[B]:PHE:HZ	0.81	0.57
3:O:3255[B]:PRO:N	3:X:3160[B]:SER:C	2.44	0.57
3:O:3283[B]:ILE:CB	3:O:3305[B]:ILE:HD11	2.35	0.57
1:P:163:LEU:HB3	1:P:293:LEU:HD21	1.86	0.57
3:R:2971[B]:ASP:CG	3:R:2973[B]:THR:HG1	2.10	0.57
3:R:3283[B]:ILE:CB	3:R:3305[B]:ILE:HD11	2.35	0.57
1:S:622:HIS:CE1	1:S:767:LYS:H	2.23	0.57
1:S:879:SER:HB2	1:S:1182:ASN:ND2	2.18	0.57
3:X:2949[B]:LYS:HZ2	3:X:2950[B]:THR:HA	1.69	0.57
3:X:3129[A]:ILE:HD13	3:X:3190[A]:LEU:O	2.04	0.57
1:Y:533:VAL:HG12	1:Y:540:THR:HG22	1.87	0.57
3:a:3180[A]:TYR:C	3:a:3183[A]:LEU:HD22	2.30	0.57
3:a:3180[B]:TYR:C	3:a:3183[B]:LEU:HD22	2.30	0.57
1:b:639:ARG:NH2	1:b:707:PHE:O	2.36	0.57
1:b:961:SER:OG	1:b:972:SER:O	2.17	0.57
3:d:2942[B]:LEU:HD13	3:d:3033[B]:PHE:CZ	2.40	0.57
3:d:3000[A]:LEU:N	3:d:3000[A]:LEU:HD23	2.18	0.57
1:A:1263:LEU:HD11	1:A:1358:LEU:HD22	1.86	0.57
2:B:2879:LEU:HD13	2:B:2901:LEU:HD11	1.85	0.57
3:C:2942[B]:LEU:HD13	3:C:3033[B]:PHE:CZ	2.40	0.57
3:C:2986[B]:PRO:HB3	3:C:3127[B]:TRP:CE3	2.38	0.57
3:C:3130[A]:TRP:CZ2	3:C:3134[A]:GLN:NE2	2.73	0.57
3:C:3152[B]:LYS:HB2	3:L:3172[B]:SER:CA	2.32	0.57
3:C:3180[B]:TYR:C	3:C:3183[B]:LEU:HD22	2.30	0.57
1:D:929:TRP:O	1:D:1048:ASN:ND2	2.37	0.57
1:D:1155:LEU:HD13	1:D:1217:ILE:HG21	1.87	0.57
1:D:1166:THR:HB	1:D:1168:GLN:N	2.20	0.57
3:F:3013[B]:ASP:OD1	3:F:3015[B]:THR:OG1	2.23	0.57
3:F:3093[A]:HIS:CE1	3:F:3119[A]:HIS:CD2	2.92	0.57
2:H:2598:PRO:HG3	2:H:2651:GLN:HB2	1.85	0.57
3:I:2942[B]:LEU:HD13	3:I:3033[B]:PHE:CZ	2.40	0.57
3:I:3130[A]:TRP:CE2	3:I:3134[A]:GLN:NE2	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3293[B]:LYS:CB	3:I:3294[B]:SER:CB	2.54	0.57
1:J:566:ARG:H	1:J:567:LEU:HD13	1.69	0.57
1:J:1462:ASP:OD2	1:J:1525:TYR:OH	2.17	0.57
1:M:11:THR:HG22	1:M:13:ASP:H	1.68	0.57
1:M:1472:GLN:OE1	1:M:1475:ARG:NH1	2.38	0.57
3:O:2969[B]:TYR:CE1	3:X:3168[B]:THR:HG22	2.38	0.57
3:O:3013[B]:ASP:OD1	3:O:3015[B]:THR:OG1	2.23	0.57
1:P:832:LYS:HD3	1:P:833:PHE:H	1.69	0.57
3:R:2952[B]:ALA:HB3	3:R:2954[B]:TYR:N	2.18	0.57
3:R:3225[B]:SER:OG	3:R:3290[B]:ILE:HD13	2.04	0.57
1:S:1493:MET:HG2	1:S:1511:SER:O	2.04	0.57
2:T:2803:ARG:HE	2:T:2805:PHE:HZ	1.53	0.57
3:U:2969[A]:TYR:CE2	3:U:2970[A]:PRO:CG	2.86	0.57
1:V:126:GLY:HA3	1:V:202:TYR:O	2.04	0.57
1:V:897:HIS:HB3	1:V:899:MET:HE1	1.86	0.57
3:X:3019[B]:HIS:CD2	3:X:3019[B]:HIS:H	2.22	0.57
3:X:3220[B]:ARG:HG2	3:X:3221[B]:ALA:H	1.70	0.57
3:X:3283[B]:ILE:CB	3:X:3305[B]:ILE:HD11	2.35	0.57
1:Y:1019:HIS:NE2	1:Y:1046:HIS:CE1	2.73	0.57
3:a:3130[A]:TRP:CE2	3:a:3134[A]:GLN:NE2	2.72	0.57
3:a:3130[B]:TRP:CE2	3:a:3134[B]:GLN:NE2	2.72	0.57
3:a:3284[B]:LYS:CD	3:a:3285[B]:VAL:H	2.09	0.57
3:d:2960[B]:PHE:CD1	3:d:2960[B]:PHE:N	2.72	0.57
3:d:3013[B]:ASP:OD1	3:d:3015[B]:THR:OG1	2.23	0.57
3:d:3129[B]:ILE:HD13	3:d:3190[B]:LEU:O	2.04	0.57
2:B:2500:ILE:HG13	2:B:2501:PRO:HD2	1.87	0.57
3:C:2971[B]:ASP:CB	3:L:3093[B]:HIS:ND1	2.56	0.57
3:C:3019[B]:HIS:H	3:C:3019[B]:HIS:CD2	2.22	0.57
3:C:3130[B]:TRP:CZ2	3:C:3134[B]:GLN:NE2	2.73	0.57
2:E:2687:ILE:HD11	2:E:2695:MET:HG2	1.87	0.57
3:F:2942[B]:LEU:HD13	3:F:3033[B]:PHE:CZ	2.40	0.57
3:F:2971[B]:ASP:C	3:a:3090[B]:ASN:HB3	2.30	0.57
3:F:3129[A]:ILE:HD13	3:F:3190[A]:LEU:O	2.04	0.57
3:F:3288[B]:MET:CG	3:F:3295[B]:LEU:HD21	2.32	0.57
1:G:1427:HIS:CD2	1:G:1457:HIS:HE1	2.23	0.57
3:I:2942[A]:LEU:HD13	3:I:3033[A]:PHE:CZ	2.40	0.57
3:I:2979[B]:GLN:NE2	3:R:3156[B]:MET:H	2.02	0.57
3:I:2995[B]:GLN:HG2	3:I:3168[B]:THR:HG21	1.86	0.57
3:I:3130[B]:TRP:CZ2	3:I:3134[B]:GLN:NE2	2.73	0.57
3:I:3255[B]:PRO:CB	3:R:2964[B]:PRO:CD	2.83	0.57
1:J:179:HIS:HB2	1:J:213:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2942[B]:LEU:HD13	3:L:3033[B]:PHE:CZ	2.40	0.57
3:L:3130[B]:TRP:CE2	3:L:3134[B]:GLN:NE2	2.72	0.57
3:L:3130[B]:TRP:CZ2	3:L:3134[B]:GLN:NE2	2.73	0.57
3:L:3288[B]:MET:CG	3:L:3295[B]:LEU:HD21	2.32	0.57
3:L:3293[A]:LYS:CB	3:L:3294[A]:SER:CB	2.54	0.57
2:N:2133:PRO:HG2	2:N:2140:ARG:HA	1.84	0.57
3:O:2971[A]:ASP:CG	3:O:2973[A]:THR:HG1	2.13	0.57
3:O:2991[B]:LEU:O	3:O:2994[B]:LYS:HB3	2.03	0.57
3:O:3108[B]:HIS:HB2	3:X:2970[B]:PRO:CA	2.33	0.57
3:O:3130[A]:TRP:CZ2	3:O:3134[A]:GLN:NE2	2.73	0.57
3:O:3225[B]:SER:OG	3:O:3290[B]:ILE:HD13	2.04	0.57
3:O:3284[B]:LYS:HE2	3:O:3284[B]:LYS:CA	2.29	0.57
3:R:2942[A]:LEU:HD13	3:R:3033[A]:PHE:CZ	2.40	0.57
3:R:2961[B]:HIS:NE2	3:R:2980[B]:HIS:CE1	2.73	0.57
3:R:3019[A]:HIS:CD2	3:R:3019[A]:HIS:H	2.22	0.57
3:R:3129[A]:ILE:HD13	3:R:3190[A]:LEU:O	2.04	0.57
1:S:124:TYR:O	1:S:137:ARG:NH2	2.38	0.57
1:S:837:HIS:HA	1:S:1113:HIS:O	2.04	0.57
1:S:898:GLY:N	1:S:899:MET:HA	2.20	0.57
2:T:2177:TYR:HB2	2:T:2300:ASN:HB2	1.87	0.57
3:U:3000[A]:LEU:N	3:U:3000[A]:LEU:HD23	2.18	0.57
3:U:3130[A]:TRP:CZ2	3:U:3134[A]:GLN:NE2	2.73	0.57
3:U:3173[B]:THR:CG2	3:d:3152[B]:LYS:O	2.50	0.57
3:U:3253[B]:GLU:N	3:d:3255[B]:PRO:HG3	2.19	0.57
1:V:1358:LEU:HD23	1:V:1456:LEU:HD21	1.86	0.57
3:X:2965[A]:LEU:HD11	3:X:2974[A]:ALA:C	2.28	0.57
1:Y:187:GLY:HA3	1:Y:195:SER:HB3	1.87	0.57
2:Z:2832:ALA:HB1	2:Z:2856:ILE:HG21	1.86	0.57
3:a:2961[A]:HIS:NE2	3:a:2980[A]:HIS:CE1	2.73	0.57
3:a:2991[A]:LEU:O	3:a:2994[A]:LYS:HB3	2.03	0.57
3:a:3220[A]:ARG:HG2	3:a:3221[A]:ALA:H	1.70	0.57
1:b:717:GLN:O	1:b:721:GLU:HG3	2.05	0.57
1:b:977:GLU:HB3	1:b:979:LEU:HD21	1.86	0.57
3:d:3130[A]:TRP:CZ2	3:d:3134[A]:GLN:NE2	2.73	0.57
1:A:904:HIS:O	1:A:907:ARG:HB3	2.05	0.57
1:A:941:LEU:HD11	1:A:959:PHE:CD2	2.40	0.57
2:B:2142:ALA:HB1	2:B:2143:CYS:HB2	1.85	0.57
3:C:2942[A]:LEU:HD13	3:C:3033[A]:PHE:CZ	2.40	0.57
3:C:3147[B]:GLU:CD	3:L:3169[B]:LYS:HZ2	1.91	0.57
3:C:3248[B]:LEU:CB	3:L:2972[B]:GLY:C	2.54	0.57
3:F:3180[B]:TYR:C	3:F:3183[B]:LEU:HD22	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:883:CYS:N	1:G:894:CYS:SG	2.78	0.57
3:I:3150[B]:LYS:CA	3:R:3172[B]:SER:HB3	2.35	0.57
3:I:3180[A]:TYR:C	3:I:3183[A]:LEU:HD22	2.30	0.57
3:I:3284[B]:LYS:HE2	3:I:3284[B]:LYS:CA	2.29	0.57
1:J:1241:GLY:HA2	1:J:1252:PRO:HB3	1.87	0.57
1:M:43:GLU:HG3	1:M:44:PRO:HA	1.87	0.57
1:M:127:GLU:HG3	1:M:135:THR:HG23	1.86	0.57
1:M:589:GLN:HG2	1:M:594:ASP:HB3	1.87	0.57
1:M:602:THR:O	1:M:605:SER:OG	2.19	0.57
3:O:3160[B]:SER:CB	3:X:3151[B]:LEU:HG	2.35	0.57
3:O:3251[B]:ASP:O	3:X:2967[B]:CYS:HB3	2.04	0.57
2:Q:2799:LYS:HA	2:Q:2803:ARG:HH12	1.69	0.57
3:R:2986[A]:PRO:HB3	3:R:3127[A]:TRP:CE3	2.38	0.57
3:R:3251[B]:ASP:HB3	3:R:3252[B]:TYR:CD1	2.40	0.57
1:S:1498:ASN:ND2	1:S:1500:THR:O	2.37	0.57
3:U:3130[A]:TRP:CE2	3:U:3134[A]:GLN:NE2	2.72	0.57
3:U:3161[B]:GLU:HB2	3:d:3260[B]:ARG:HD2	1.85	0.57
3:U:3176[B]:LYS:H	3:U:3176[B]:LYS:CE	2.17	0.57
3:U:3251[A]:ASP:HB3	3:U:3252[A]:TYR:CD1	2.40	0.57
1:V:329:ARG:HA	1:Y:1583:CYS:O	2.04	0.57
3:X:2942[B]:LEU:HD13	3:X:3033[B]:PHE:CZ	2.40	0.57
3:X:3307[B]:PHE:HE1	3:X:3309[B]:PRO:CG	2.08	0.57
1:Y:859:ALA:O	1:Y:863:ALA:N	2.38	0.57
1:Y:1618:LEU:HA	3:d:3190[B]:LEU:HB2	1.87	0.57
3:a:2991[A]:LEU:O	3:a:2994[A]:LYS:N	2.37	0.57
1:b:838:ARG:NH1	1:b:915:ASN:OD1	2.38	0.57
3:d:3251[A]:ASP:HB3	3:d:3252[A]:TYR:CD1	2.40	0.57
2:B:2516:ASP:OD1	2:E:2168:ARG:NH2	2.35	0.56
3:C:3013[B]:ASP:OD1	3:C:3015[B]:THR:OG1	2.23	0.56
3:C:3153[B]:LYS:HD3	3:L:3155[B]:MET:CE	2.30	0.56
3:C:3155[B]:MET:HG2	3:L:3154[B]:PRO:C	2.30	0.56
3:F:2942[A]:LEU:HD13	3:F:3033[A]:PHE:CZ	2.40	0.56
3:F:3130[B]:TRP:CE2	3:F:3134[B]:GLN:NE2	2.72	0.56
3:F:3152[B]:LYS:HB2	3:a:3172[B]:SER:H	0.64	0.56
3:F:3173[A]:THR:HG22	3:F:3174[A]:GLY:H	1.67	0.56
3:F:3284[B]:LYS:HE2	3:F:3284[B]:LYS:CA	2.30	0.56
1:G:262:LYS:NZ	1:G:795:GLU:OE1	2.36	0.56
2:H:2128:LEU:HD13	2:H:2286:HIS:CG	2.40	0.56
3:I:3093[B]:HIS:CE1	3:I:3119[B]:HIS:CD2	2.92	0.56
3:I:3169[B]:LYS:NZ	3:R:3149[B]:ASN:CG	2.62	0.56
1:J:903:PRO:HG2	1:J:904:HIS:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2800:LYS:O	3:L:3023[A]:ILE:CD1	2.53	0.56
3:L:2949[B]:LYS:HZ2	3:L:2950[B]:THR:HA	1.69	0.56
3:L:3220[B]:ARG:HG2	3:L:3221[B]:ALA:H	1.70	0.56
1:M:136:ALA:H	1:M:190:PHE:HE2	1.51	0.56
3:O:2942[B]:LEU:HD13	3:O:3033[B]:PHE:CZ	2.40	0.56
3:O:3153[B]:LYS:HG3	3:X:3176[B]:LYS:HD3	1.76	0.56
3:R:2960[A]:PHE:CD1	3:R:2960[A]:PHE:N	2.72	0.56
3:R:2991[A]:LEU:O	3:R:2994[A]:LYS:N	2.37	0.56
3:R:3251[A]:ASP:HB3	3:R:3252[A]:TYR:CD1	2.40	0.56
3:R:3283[A]:ILE:CB	3:R:3305[A]:ILE:HD11	2.35	0.56
1:S:879:SER:HB2	1:S:1182:ASN:HD22	1.70	0.56
3:U:3150[B]:LYS:CG	3:d:3156[B]:MET:CG	2.83	0.56
2:W:2808:PHE:CZ	2:W:2821:LEU:HD13	2.33	0.56
3:X:2991[A]:LEU:O	3:X:2994[A]:LYS:N	2.37	0.56
3:X:3283[A]:ILE:CB	3:X:3305[A]:ILE:HD11	2.35	0.56
1:Y:151:GLN:N	1:Y:151:GLN:OE1	2.38	0.56
1:Y:1485:ALA:HB3	1:Y:1489:MET:HE2	1.85	0.56
3:a:3130[A]:TRP:CZ2	3:a:3134[A]:GLN:NE2	2.73	0.56
3:a:3130[B]:TRP:CZ2	3:a:3134[B]:GLN:NE2	2.73	0.56
1:b:35:GLN:OE1	1:b:35:GLN:HA	2.05	0.56
3:d:3093[B]:HIS:CE1	3:d:3119[B]:HIS:CD2	2.92	0.56
3:d:3130[B]:TRP:CE2	3:d:3134[B]:GLN:NE2	2.72	0.56
2:B:2627:GLY:HA3	2:B:2703:PHE:O	2.05	0.56
3:F:2987[B]:HIS:NE2	3:F:3178[B]:PHE:HE1	1.95	0.56
3:F:2991[A]:LEU:O	3:F:2994[A]:LYS:N	2.37	0.56
3:F:3120[B]:HIS:C	3:F:3122[B]:ASN:N	2.55	0.56
3:F:3163[B]:ASN:H	3:a:3147[B]:GLU:CD	2.13	0.56
1:G:1543:ILE:HD11	3:L:3272[A]:HIS:CD2	2.40	0.56
2:H:2863:ARG:HB3	2:H:2865:ILE:HG13	1.87	0.56
3:I:2932[A]:PRO:CA	3:I:2935[A]:ILE:HD12	2.30	0.56
3:I:2966[B]:SER:HA	3:R:3256[B]:TRP:CA	2.34	0.56
3:I:3255[B]:PRO:HB3	3:R:2964[B]:PRO:HD2	1.86	0.56
3:I:3293[A]:LYS:CD	3:I:3294[A]:SER:N	2.64	0.56
1:J:361:GLU:HG2	1:J:363:THR:HG22	1.87	0.56
3:L:2942[A]:LEU:HD13	3:L:3033[A]:PHE:CZ	2.40	0.56
3:O:2949[B]:LYS:HZ2	3:O:2950[B]:THR:HA	1.70	0.56
3:O:3130[B]:TRP:CZ2	3:O:3134[B]:GLN:NE2	2.73	0.56
1:P:105:VAL:HB	1:P:137:ARG:NH2	2.20	0.56
3:U:3135[B]:LYS:HG3	3:U:3141[B]:TYR:CD1	2.33	0.56
3:U:3257[B]:ALA:H	3:d:2969[B]:TYR:N	1.96	0.56
3:U:3284[A]:LYS:HE2	3:U:3284[A]:LYS:CA	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2969[A]:TYR:CD2	3:X:2970[A]:PRO:HG2	2.38	0.56
3:X:3180[B]:TYR:C	3:X:3183[B]:LEU:HD22	2.30	0.56
3:X:3251[A]:ASP:HB3	3:X:3252[A]:TYR:CD1	2.40	0.56
3:X:3293[A]:LYS:CD	3:X:3294[A]:SER:N	2.64	0.56
3:a:2942[B]:LEU:HD13	3:a:3033[B]:PHE:CZ	2.40	0.56
3:a:3284[A]:LYS:HE2	3:a:3284[A]:LYS:CA	2.30	0.56
1:b:1013:ILE:HD11	1:b:1175:PHE:CD2	2.40	0.56
3:d:3019[B]:HIS:CD2	3:d:3019[B]:HIS:H	2.22	0.56
3:d:3130[A]:TRP:CE2	3:d:3134[A]:GLN:NE2	2.72	0.56
3:d:3283[B]:ILE:CB	3:d:3305[B]:ILE:HD11	2.35	0.56
1:A:128:ILE:HG22	1:A:130:PHE:O	2.05	0.56
1:A:1195:ASP:HA	1:A:1196:ILE:HG22	1.86	0.56
2:B:2161:GLN:HE22	2:B:2348:THR:HG21	1.71	0.56
2:B:2300:ASN:OD1	2:B:2303:ARG:NH1	2.38	0.56
2:B:2344:LEU:HA	2:B:2345:ASN:O	2.05	0.56
3:C:2983[B]:VAL:HB	3:L:3160[B]:SER:HA	1.86	0.56
3:C:3154[B]:PRO:CB	3:L:3151[B]:LEU:CA	2.79	0.56
3:C:3180[A]:TYR:C	3:C:3183[A]:LEU:HD22	2.30	0.56
3:C:3220[B]:ARG:HG2	3:C:3221[B]:ALA:H	1.70	0.56
3:C:3255[B]:PRO:HG2	3:L:2962[B]:GLY:N	2.05	0.56
3:C:3283[B]:ILE:CB	3:C:3305[B]:ILE:HD11	2.35	0.56
1:D:885:SER:HB3	1:D:886:PRO:HA	1.86	0.56
2:E:2568:HIS:ND1	2:E:2765:PRO:HB3	2.20	0.56
3:F:3130[A]:TRP:CE2	3:F:3134[A]:GLN:NE2	2.72	0.56
3:F:3180[A]:TYR:C	3:F:3183[A]:LEU:HD22	2.30	0.56
3:F:3225[B]:SER:OG	3:F:3290[B]:ILE:HD13	2.04	0.56
3:F:3255[B]:PRO:N	3:a:2966[B]:SER:OG	2.38	0.56
1:G:480:CYS:SG	1:G:621:LEU:HD11	2.45	0.56
2:H:2180:TRP:HD1	2:H:2247:ILE:HD11	1.69	0.56
3:I:2931[B]:THR:HG1	3:I:2934[B]:GLU:CD	2.03	0.56
3:I:2965[B]:LEU:CD1	3:R:3256[B]:TRP:NE1	2.66	0.56
3:I:2965[B]:LEU:HA	3:R:3253[B]:GLU:CD	2.30	0.56
3:I:2973[B]:THR:OG1	3:R:3093[B]:HIS:HD2	1.88	0.56
3:I:2981[B]:GLY:N	3:R:2968[B]:GLN:OE1	2.38	0.56
3:I:3013[A]:ASP:OD1	3:I:3015[A]:THR:OG1	2.23	0.56
3:I:3152[B]:LYS:HB3	3:R:3171[B]:HIS:C	2.28	0.56
3:I:3259[B]:ASP:H	3:R:3162[B]:ASP:CB	2.18	0.56
3:I:3283[B]:ILE:CB	3:I:3305[B]:ILE:HD11	2.35	0.56
1:J:353:ASN:HD22	1:J:772:ARG:HH22	1.51	0.56
1:J:729:VAL:HG12	1:J:782:THR:HG23	1.86	0.56
1:J:836:GLN:HG3	1:J:838:ARG:NH2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:841:LYS:HA	1:J:1117:ASP:HB2	1.86	0.56
1:J:871:GLN:NE2	1:J:966:SER:OG	2.36	0.56
1:J:1013:ILE:HG21	1:J:1192:TYR:CD1	2.40	0.56
1:J:1034:GLU:HB2	1:J:1182:ASN:HD21	1.71	0.56
1:J:1439:VAL:HG22	1:J:1440:HIS:HD2	1.71	0.56
1:J:1587:ALA:HA	1:J:1614:GLU:HG2	1.88	0.56
3:L:2960[A]:PHE:CD1	3:L:2960[A]:PHE:N	2.72	0.56
3:L:3093[A]:HIS:CE1	3:L:3119[A]:HIS:CD2	2.92	0.56
3:L:3180[A]:TYR:C	3:L:3183[A]:LEU:HD22	2.30	0.56
3:L:3298[A]:ASN:HA	3:L:3299[A]:LEU:HB3	1.88	0.56
1:M:479:CYS:HB3	1:M:670:PRO:HD3	1.87	0.56
3:O:2971[B]:ASP:CG	3:O:2973[B]:THR:HG1	2.12	0.56
3:O:2995[A]:GLN:HG2	3:O:3168[A]:THR:HG21	1.85	0.56
3:O:3180[A]:TYR:C	3:O:3183[A]:LEU:HD22	2.30	0.56
3:O:3252[B]:TYR:HA	3:X:3157[B]:PRO:HA	1.86	0.56
3:O:3256[B]:TRP:NE1	3:X:3161[B]:GLU:CG	2.68	0.56
3:O:3256[B]:TRP:NE1	3:X:3161[B]:GLU:HG3	2.21	0.56
3:O:3283[A]:ILE:CB	3:O:3305[A]:ILE:HD11	2.35	0.56
3:O:3293[B]:LYS:CD	3:O:3294[B]:SER:N	2.64	0.56
1:P:931:TRP:CG	1:P:1018:ILE:HD11	2.39	0.56
3:R:2948[B]:ASP:HB3	3:R:2953[B]:GLY:CA	2.24	0.56
3:R:2991[B]:LEU:O	3:R:2994[B]:LYS:HB3	2.03	0.56
3:R:3130[A]:TRP:CZ2	3:R:3134[A]:GLN:NE2	2.73	0.56
3:R:3220[A]:ARG:HG2	3:R:3221[A]:ALA:H	1.70	0.56
3:R:3268[A]:LYS:O	3:R:3271[A]:VAL:HG23	2.06	0.56
3:U:2965[B]:LEU:CG	3:d:3221[B]:ALA:N	2.66	0.56
3:U:2969[B]:TYR:CD1	3:d:3107[B]:LEU:HD13	2.38	0.56
3:U:3151[B]:LEU:C	3:d:3153[B]:LYS:HA	2.31	0.56
3:U:3188[A]:ASP:N	3:U:3188[A]:ASP:OD2	2.36	0.56
3:U:3268[A]:LYS:O	3:U:3271[A]:VAL:HG23	2.06	0.56
3:U:3283[A]:ILE:CB	3:U:3305[A]:ILE:HD11	2.35	0.56
3:U:3283[B]:ILE:CB	3:U:3305[B]:ILE:HD11	2.35	0.56
3:U:3293[B]:LYS:CB	3:U:3294[B]:SER:CB	2.54	0.56
1:V:392:PRO:O	1:V:395:THR:OG1	2.23	0.56
1:V:1296:VAL:HB	1:V:1446:ASP:HB3	1.88	0.56
2:W:2234:GLN:HG3	2:W:2235:PRO:HD2	1.86	0.56
2:W:2235:PRO:HG3	2:W:2240:GLN:NE2	2.20	0.56
3:X:3130[A]:TRP:CZ2	3:X:3134[A]:GLN:NE2	2.73	0.56
3:X:3130[B]:TRP:CZ2	3:X:3134[B]:GLN:NE2	2.73	0.56
1:Y:190:PHE:HB3	1:Y:193:SER:HB2	1.87	0.56
2:Z:2121:THR:HG23	2:c:2615:TRP:CH2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:2542:TYR:HB2	2:Z:2573:TYR:HE1	1.70	0.56
2:Z:2764:THR:HB	2:Z:2767:LYS:HG3	1.87	0.56
3:a:3000[A]:LEU:N	3:a:3000[A]:LEU:HD23	2.18	0.56
3:a:3173[A]:THR:HG22	3:a:3174[A]:GLY:H	1.67	0.56
3:a:3283[B]:ILE:CB	3:a:3305[B]:ILE:HD11	2.35	0.56
1:b:372:ALA:O	1:b:375:SER:OG	2.22	0.56
1:b:517:THR:HG21	1:b:708:PHE:HE1	1.70	0.56
1:b:749:VAL:HB	1:b:754:GLU:HB3	1.87	0.56
3:d:2965[B]:LEU:HD11	3:d:2974[B]:ALA:C	2.28	0.56
3:d:2991[A]:LEU:O	3:d:2994[A]:LYS:N	2.37	0.56
3:d:3220[A]:ARG:HH11	3:d:3220[A]:ARG:CG	2.12	0.56
3:C:3156[B]:MET:HA	3:C:3157[B]:PRO:C	2.26	0.56
3:C:3284[A]:LYS:HE2	3:C:3284[A]:LYS:CA	2.30	0.56
1:D:137:ARG:NH1	1:D:203:ASP:OD1	2.39	0.56
1:D:883:CYS:N	1:D:894:CYS:SG	2.78	0.56
3:F:2975[B]:PHE:CE1	3:a:2961[B]:HIS:O	2.58	0.56
3:F:3298[A]:ASN:HA	3:F:3299[A]:LEU:HB3	1.88	0.56
3:I:3212[A]:ARG:HH11	3:I:3212[A]:ARG:CG	2.12	0.56
3:I:3268[A]:LYS:O	3:I:3271[A]:VAL:HG23	2.06	0.56
3:I:3284[A]:LYS:CD	3:I:3285[A]:VAL:H	2.09	0.56
2:K:2092:VAL:HG11	2:K:2188:PRO:HB3	1.87	0.56
3:L:3180[B]:TYR:C	3:L:3183[B]:LEU:HD22	2.30	0.56
3:L:3183[A]:LEU:N	3:L:3184[A]:ASN:HA	2.12	0.56
3:L:3251[A]:ASP:HB3	3:L:3252[A]:TYR:CD1	2.40	0.56
3:L:3268[A]:LYS:O	3:L:3271[A]:VAL:HG23	2.06	0.56
2:N:2128:LEU:HD23	2:N:2216:PHE:HZ	1.70	0.56
3:O:3157[B]:PRO:CB	3:X:3150[B]:LYS:HA	2.36	0.56
3:O:3162[B]:ASP:N	3:O:3162[B]:ASP:OD1	2.31	0.56
3:O:3281[A]:PHE:HE1	3:O:3305[A]:ILE:HD13	1.71	0.56
1:P:157:GLU:OE2	1:P:296:ARG:NH2	2.39	0.56
2:Q:2596:THR:HG21	2:Q:2783:PHE:HZ	1.71	0.56
3:R:2942[B]:LEU:HD13	3:R:3033[B]:PHE:CZ	2.40	0.56
3:U:2975[B]:PHE:CE1	3:d:3256[B]:TRP:NE1	2.71	0.56
2:Z:2568:HIS:ND1	2:Z:2765:PRO:HB3	2.20	0.56
1:b:864:ASP:HB3	1:b:869:GLY:HA3	1.86	0.56
2:c:2826:GLU:HG2	2:c:2876:LYS:HD3	1.86	0.56
3:d:3251[B]:ASP:HB3	3:d:3252[B]:TYR:CD1	2.40	0.56
1:A:1195:ASP:HA	1:A:1196:ILE:CB	2.36	0.56
3:C:2971[B]:ASP:HB2	3:L:3090[B]:ASN:HA	1.88	0.56
3:C:3255[B]:PRO:CD	3:L:2961[B]:HIS:C	2.78	0.56
1:D:1209:ASP:O	1:D:1211:TYR:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2641:GLN:HB3	2:E:2643:GLU:OE1	2.05	0.56
3:F:3019[A]:HIS:CD2	3:F:3019[A]:HIS:H	2.22	0.56
3:F:3256[B]:TRP:N	3:a:2966[B]:SER:HA	2.20	0.56
3:F:3293[A]:LYS:CB	3:F:3294[A]:SER:CB	2.54	0.56
3:I:3153[B]:LYS:HD2	3:R:3155[B]:MET:C	2.31	0.56
3:I:3255[B]:PRO:HG3	3:R:2964[B]:PRO:CD	2.36	0.56
1:J:533:VAL:HG12	1:J:540:THR:HG22	1.87	0.56
1:J:1028:VAL:HA	1:J:1035:TYR:CD2	2.40	0.56
2:K:2799:LYS:HA	2:K:2803:ARG:HH12	1.70	0.56
3:L:3130[A]:TRP:CZ2	3:L:3134[A]:GLN:NE2	2.73	0.56
3:L:3283[A]:ILE:CB	3:L:3305[A]:ILE:HD11	2.35	0.56
3:L:3283[B]:ILE:CB	3:L:3305[B]:ILE:HD11	2.35	0.56
3:O:3013[A]:ASP:OD1	3:O:3015[A]:THR:OG1	2.23	0.56
2:Q:2830:GLN:O	2:Q:2863:ARG:NH2	2.38	0.56
3:R:3093[B]:HIS:CE1	3:R:3119[B]:HIS:CD2	2.92	0.56
2:T:2799:LYS:HA	2:T:2803:ARG:HH12	1.70	0.56
3:U:2948[A]:ASP:HB3	3:U:2953[A]:GLY:CA	2.24	0.56
3:U:2961[A]:HIS:NE2	3:U:2980[A]:HIS:CE1	2.73	0.56
3:U:3220[A]:ARG:HG2	3:U:3221[A]:ALA:H	1.70	0.56
3:U:3255[B]:PRO:HG3	3:d:3252[B]:TYR:CA	1.99	0.56
1:V:109:LEU:HG	1:V:118:ALA:HB1	1.87	0.56
2:W:2833:GLY:HA3	2:W:2854:MET:HE1	1.88	0.56
3:X:3019[A]:HIS:H	3:X:3019[A]:HIS:CD2	2.22	0.56
3:X:3188[A]:ASP:N	3:X:3188[A]:ASP:OD2	2.36	0.56
1:Y:1075:GLU:HG2	2:c:2900:SER:HA	1.88	0.56
1:Y:1542:ARG:O	3:d:3002[B]:ALA:HB2	2.05	0.56
2:Z:2651:GLN:CD	2:Z:2651:GLN:H	2.13	0.56
3:a:3129[A]:ILE:HD13	3:a:3190[A]:LEU:O	2.04	0.56
3:a:3251[A]:ASP:HB3	3:a:3252[A]:TYR:CD1	2.40	0.56
3:a:3268[A]:LYS:O	3:a:3271[A]:VAL:HG23	2.06	0.56
2:c:2698:LEU:HD12	2:c:2838:LEU:HB3	1.86	0.56
2:c:2879:LEU:HD12	2:c:2899:PRO:HB2	1.88	0.56
3:C:2949[A]:LYS:NZ	3:C:2950[A]:THR:HA	2.21	0.56
3:C:2965[A]:LEU:HD11	3:C:2974[A]:ALA:C	2.28	0.56
3:C:3153[B]:LYS:HA	3:L:3173[B]:THR:C	2.30	0.56
3:C:3255[B]:PRO:HD3	3:L:2961[B]:HIS:O	2.05	0.56
1:D:1242:ASN:ND2	1:D:1479:TYR:OH	2.38	0.56
2:E:2122:ILE:O	2:E:2125:PHE:HB2	2.05	0.56
3:F:2965[B]:LEU:CA	3:a:3255[B]:PRO:HA	2.34	0.56
3:F:3130[A]:TRP:CZ2	3:F:3134[A]:GLN:NE2	2.73	0.56
3:F:3200[B]:LEU:O	3:F:3204[B]:LEU:HD13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2956[B]:LYS:CD	3:R:3257[B]:ALA:HB3	2.22	0.56
3:I:2969[B]:TYR:HA	3:R:2989[B]:HIS:NE2	2.19	0.56
3:I:3093[A]:HIS:CE1	3:I:3119[A]:HIS:CD2	2.92	0.56
3:I:3154[B]:PRO:HA	3:R:3153[B]:LYS:O	2.05	0.56
3:L:2960[B]:PHE:CD1	3:L:2960[B]:PHE:N	2.72	0.56
3:L:3268[B]:LYS:O	3:L:3271[B]:VAL:HG23	2.06	0.56
3:L:3281[B]:PHE:HE1	3:L:3305[B]:ILE:HD13	1.71	0.56
1:M:684:ARG:O	1:M:687:SER:OG	2.23	0.56
1:M:1164:ASP:OD1	1:M:1164:ASP:N	2.37	0.56
1:M:1182:ASN:OD1	1:M:1182:ASN:N	2.34	0.56
1:M:1604:ASP:OD1	1:M:1605:ARG:NH1	2.39	0.56
3:O:2966[B]:SER:HB2	3:O:2977[B]:CYS:CB	2.21	0.56
3:O:2974[B]:ALA:CB	3:X:2977[B]:CYS:HA	2.36	0.56
3:O:3173[B]:THR:HG22	3:O:3174[B]:GLY:H	1.67	0.56
3:O:3200[A]:LEU:O	3:O:3204[A]:LEU:HD13	2.06	0.56
3:O:3220[A]:ARG:HG2	3:O:3221[A]:ALA:H	1.70	0.56
1:P:302:ALA:H	1:P:363:THR:HB	1.70	0.56
2:Q:2426:PHE:HB3	2:Q:2445:MET:HE1	1.88	0.56
3:R:3180[A]:TYR:C	3:R:3183[A]:LEU:HD22	2.30	0.56
3:R:3268[B]:LYS:O	3:R:3271[B]:VAL:HG23	2.06	0.56
2:T:2142:ALA:HB1	2:T:2143:CYS:HB2	1.88	0.56
2:T:2757:PRO:HB3	2:T:2760:ARG:HH21	1.70	0.56
3:U:2942[B]:LEU:HD13	3:U:3033[B]:PHE:CZ	2.40	0.56
3:U:2979[B]:GLN:HE21	3:d:3153[B]:LYS:HE2	1.69	0.56
3:U:3180[B]:TYR:C	3:U:3183[B]:LEU:HD22	2.30	0.56
3:U:3251[B]:ASP:HB3	3:U:3252[B]:TYR:CD1	2.40	0.56
3:U:3257[B]:ALA:N	3:d:2968[B]:GLN:C	2.61	0.56
2:W:2161:GLN:OE1	2:W:2345:ASN:ND2	2.38	0.56
3:X:3220[B]:ARG:HH11	3:X:3220[B]:ARG:CG	2.12	0.56
2:Z:2476:LEU:HD22	4:MA:2:NAG:H82	1.86	0.56
2:Z:2644:LEU:HB2	2:Z:2686:LEU:HB3	1.88	0.56
3:a:2942[A]:LEU:HD13	3:a:3033[A]:PHE:CZ	2.40	0.56
3:a:3200[B]:LEU:O	3:a:3204[B]:LEU:HD13	2.06	0.56
3:a:3281[B]:PHE:HE1	3:a:3305[B]:ILE:HD13	1.71	0.56
3:d:3180[A]:TYR:C	3:d:3183[A]:LEU:HD22	2.30	0.56
3:C:3090[B]:ASN:CG	3:L:2972[B]:GLY:C	2.67	0.56
3:C:3281[A]:PHE:HE1	3:C:3305[A]:ILE:HD13	1.71	0.56
1:D:389:THR:OG1	4:j:1:NAG:O7	2.21	0.56
1:D:830:ASN:N	1:D:830:ASN:OD1	2.30	0.56
3:F:3153[B]:LYS:HD3	3:a:3155[B]:MET:HB3	1.83	0.56
3:F:3155[B]:MET:O	3:a:3153[B]:LYS:CE	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3251[A]:ASP:HB3	3:F:3252[A]:TYR:CD1	2.40	0.56
1:G:460:GLU:OE2	1:G:1368:ARG:NH2	2.38	0.56
1:G:668:MET:HE2	1:G:668:MET:HA	1.86	0.56
1:G:1281:MET:HE1	1:G:1330:VAL:HG23	1.88	0.56
2:H:2179:ASP:HA	2:H:2300:ASN:ND2	2.21	0.56
3:I:3172[B]:SER:HB3	3:R:3150[B]:LYS:O	2.00	0.56
3:I:3220[A]:ARG:HG2	3:I:3221[A]:ALA:H	1.70	0.56
3:I:3255[B]:PRO:O	3:R:2966[B]:SER:OG	2.21	0.56
3:I:3268[B]:LYS:O	3:I:3271[B]:VAL:HG23	2.06	0.56
1:J:873:VAL:CG2	1:J:912:ASN:HB3	2.35	0.56
2:K:2128:LEU:HD13	2:K:2286:HIS:CG	2.41	0.56
2:K:2680:HIS:CE1	2:K:2711:HIS:NE2	2.73	0.56
3:L:3083[B]:ILE:HD12	3:L:3260[B]:ARG:HB2	1.88	0.56
1:M:1553:ILE:HD11	1:M:1622:GLN:HG3	1.88	0.56
2:N:2795:ILE:O	2:N:2799:LYS:HG3	2.06	0.56
3:O:2969[B]:TYR:HE1	3:X:3168[B]:THR:CG2	2.18	0.56
3:O:3251[A]:ASP:HB3	3:O:3252[A]:TYR:CD1	2.40	0.56
3:O:3298[B]:ASN:CB	3:O:3300[B]:LEU:CD2	2.61	0.56
1:P:372:ALA:O	1:P:375:SER:OG	2.21	0.56
1:P:946:GLU:HG2	1:P:955:LYS:HB3	1.88	0.56
2:T:2089:ARG:HD2	2:T:2175:VAL:O	2.06	0.56
2:T:2554:PRO:HA	2:T:2555:GLU:HB2	1.87	0.56
3:U:2961[B]:HIS:NE2	3:U:2980[B]:HIS:CE1	2.73	0.56
3:U:2969[B]:TYR:HB2	3:d:3256[B]:TRP:NE1	2.21	0.56
3:U:3157[B]:PRO:O	3:d:3147[B]:GLU:CD	2.48	0.56
2:W:2218:SER:HG	2:W:2221:THR:HG1	1.53	0.56
1:Y:912:ASN:ND2	1:Y:1091:ASN:OD1	2.38	0.56
3:a:3083[A]:ILE:HD12	3:a:3260[A]:ARG:HB2	1.88	0.56
3:a:3307[B]:PHE:HE1	3:a:3309[B]:PRO:CG	2.08	0.56
1:b:24:ALA:HB3	1:b:83:HIS:HB3	1.87	0.56
3:d:2942[A]:LEU:HD13	3:d:3033[A]:PHE:CZ	2.40	0.56
3:C:2969[B]:TYR:CA	3:L:2985[B]:PHE:CE2	2.61	0.56
3:C:3200[A]:LEU:O	3:C:3204[A]:LEU:HD13	2.06	0.56
3:C:3251[A]:ASP:HB3	3:C:3252[A]:TYR:CD1	2.40	0.56
3:C:3283[A]:ILE:CB	3:C:3305[A]:ILE:HD11	2.35	0.56
2:E:2398:PHE:HE1	2:E:2466:THR:HG21	1.70	0.56
3:F:2961[A]:HIS:NE2	3:F:2980[A]:HIS:CE1	2.73	0.56
3:F:2966[B]:SER:CB	3:a:3255[B]:PRO:C	2.78	0.56
3:F:3093[B]:HIS:CE1	3:F:3119[B]:HIS:CD2	2.92	0.56
1:G:1636:ASN:CB	1:G:1639:LYS:HD3	2.36	0.56
3:I:3154[B]:PRO:CD	3:R:3155[B]:MET:CG	2.67	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3281[A]:PHE:HE1	3:I:3305[A]:ILE:HD13	1.71	0.56
2:K:2133:PRO:HG2	2:K:2140:ARG:HA	1.87	0.56
3:L:3220[A]:ARG:HG2	3:L:3221[A]:ALA:H	1.70	0.56
1:M:148:GLN:C	1:M:150:GLY:H	2.13	0.56
1:M:452:ILE:HG21	1:M:1367:SER:HB2	1.88	0.56
1:M:673:PHE:HB3	1:M:677:LEU:HB2	1.88	0.56
1:M:1328:SER:HB2	1:M:1523:LEU:HD13	1.88	0.56
2:N:2867:PRO:O	2:N:2870:LEU:HB2	2.06	0.56
3:O:2963[B]:MET:HB2	3:X:2970[B]:PRO:HD2	1.88	0.56
3:O:2964[B]:PRO:HA	3:X:2975[B]:PHE:CE2	2.29	0.56
3:O:2977[B]:CYS:CA	3:X:3153[B]:LYS:HG2	2.05	0.56
3:O:3169[B]:LYS:CE	3:X:3148[B]:ILE:N	2.67	0.56
1:P:905:TRP:HE1	1:P:1083:PRO:HD2	1.70	0.56
1:P:1339:SER:CB	1:P:1340:GLY:HA2	2.36	0.56
2:Q:2711:HIS:HA	2:Q:2714:VAL:HG22	1.86	0.56
3:R:3180[B]:TYR:C	3:R:3183[B]:LEU:HD22	2.30	0.56
3:R:3200[B]:LEU:O	3:R:3204[B]:LEU:HD13	2.06	0.56
1:S:516:TRP:HB2	1:S:579:LEU:HD13	1.87	0.56
1:S:564:ASP:OD1	1:S:564:ASP:N	2.39	0.56
3:U:3228[B]:VAL:CG2	3:U:3245[B]:PHE:CE2	2.89	0.56
3:U:3268[B]:LYS:O	3:U:3271[B]:VAL:HG23	2.06	0.56
1:V:492:ARG:HD2	1:V:692:VAL:HG13	1.87	0.56
2:W:2680:HIS:NE2	2:W:2684:HIS:CD2	2.74	0.56
3:X:3013[B]:ASP:OD1	3:X:3015[B]:THR:OG1	2.23	0.56
3:X:3083[B]:ILE:HD12	3:X:3260[B]:ARG:HB2	1.88	0.56
3:X:3135[A]:LYS:HG3	3:X:3141[A]:TYR:CD1	2.33	0.56
1:Y:148:GLN:HG3	1:Y:150:GLY:O	2.06	0.56
1:Y:215:ARG:HE	1:Y:279:LEU:HA	1.70	0.56
3:a:3293[B]:LYS:CD	3:a:3294[B]:SER:N	2.64	0.56
1:b:648:GLN:OE1	1:b:651:ARG:NH1	2.38	0.56
1:b:1209:ASP:OD1	1:b:1209:ASP:N	2.22	0.56
2:c:2373:MET:HB3	2:c:2381:LEU:HD11	1.87	0.56
2:c:2742:MET:HA	2:c:2765:PRO:HB2	1.87	0.56
1:A:326:GLU:CD	1:A:326:GLU:H	2.13	0.56
1:A:516:TRP:CD2	1:A:606:ILE:HD11	2.41	0.56
1:A:1573:CYS:HB2	1:A:1627:ARG:HG2	1.87	0.56
3:C:2969[B]:TYR:CG	3:C:2970[B]:PRO:HD2	2.41	0.56
3:C:3083[A]:ILE:HD12	3:C:3260[A]:ARG:HB2	1.88	0.56
3:C:3173[B]:THR:C	3:L:3154[B]:PRO:HD3	2.30	0.56
2:E:2263:PHE:HE1	2:E:2304:LEU:HB3	1.71	0.56
3:F:2987[A]:HIS:NE2	3:F:3178[A]:PHE:HE1	1.95	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3150[B]:LYS:CG	3:a:3158[B]:PHE:CA	2.50	0.56
3:F:3256[B]:TRP:HE1	3:a:2965[B]:LEU:HD12	1.41	0.56
1:G:906:HIS:CD2	9:G:2104:CUO:O1	2.59	0.56
1:G:1415:ASP:OD1	1:G:1416:PHE:N	2.38	0.56
1:G:1494:ARG:HG3	1:G:1494:ARG:HH11	1.70	0.56
3:I:2948[B]:ASP:CB	3:I:2949[B]:LYS:CA	2.78	0.56
3:I:2961[A]:HIS:NE2	3:I:2980[A]:HIS:CE1	2.73	0.56
3:I:2966[B]:SER:OG	3:R:3255[B]:PRO:O	2.24	0.56
3:I:3078[B]:PHE:CE2	3:R:3161[B]:GLU:OE1	2.58	0.56
1:J:157:GLU:OE2	1:J:296:ARG:NH2	2.39	0.56
2:K:2887:ASP:O	2:K:2890:VAL:N	2.38	0.56
3:L:3176[B]:LYS:H	3:L:3176[B]:LYS:CE	2.17	0.56
3:L:3200[A]:LEU:O	3:L:3204[A]:LEU:HD13	2.06	0.56
1:M:19:GLN:NE2	1:M:121:ASN:OD1	2.39	0.56
1:M:1261:LYS:HG3	1:M:1266:PHE:HE1	1.71	0.56
3:O:2965[B]:LEU:O	3:X:3153[B]:LYS:NZ	2.24	0.56
3:O:2968[B]:GLN:HB3	3:X:2988[B]:TRP:CB	2.16	0.56
3:O:3180[B]:TYR:C	3:O:3183[B]:LEU:HD22	2.30	0.56
3:O:3228[A]:VAL:CG2	3:O:3245[A]:PHE:CE2	2.89	0.56
1:P:494:VAL:HG23	1:P:671:PHE:HZ	1.71	0.56
1:P:1348:TRP:CD1	1:P:1403:LEU:HD13	2.41	0.56
2:Q:2643:GLU:O	2:Q:2647:LEU:N	2.39	0.56
3:R:2969[A]:TYR:CE2	3:R:2970[A]:PRO:CG	2.86	0.56
3:U:3013[A]:ASP:OD1	3:U:3015[A]:THR:OG1	2.23	0.56
3:U:3083[B]:ILE:HD12	3:U:3260[B]:ARG:HB2	1.88	0.56
3:U:3153[B]:LYS:HB2	3:d:3154[B]:PRO:C	2.24	0.56
3:U:3154[B]:PRO:O	3:d:3153[B]:LYS:HE3	2.05	0.56
3:U:3211[A]:ASP:OD1	3:U:3211[A]:ASP:N	2.27	0.56
3:U:3255[B]:PRO:HB2	3:d:2974[B]:ALA:O	2.05	0.56
3:U:3298[B]:ASN:CB	3:U:3300[B]:LEU:CD2	2.61	0.56
1:V:566:ARG:NH1	1:V:745:ASP:OD1	2.39	0.56
3:X:3200[B]:LEU:O	3:X:3204[B]:LEU:HD13	2.06	0.56
3:X:3251[B]:ASP:HB3	3:X:3252[B]:TYR:CD1	2.40	0.56
3:X:3268[A]:LYS:O	3:X:3271[A]:VAL:HG23	2.06	0.56
3:a:3013[A]:ASP:OD1	3:a:3015[A]:THR:OG1	2.23	0.56
2:c:2643:GLU:O	2:c:2647:LEU:N	2.38	0.56
2:c:2760:ARG:O	2:c:2763:SER:OG	2.22	0.56
3:d:3083[B]:ILE:HD12	3:d:3260[B]:ARG:HB2	1.88	0.56
3:d:3200[B]:LEU:O	3:d:3204[B]:LEU:HD13	2.06	0.56
1:A:606:ILE:O	1:A:610:THR:OG1	2.23	0.56
1:A:897:HIS:HB3	1:A:899:MET:SD	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:HIS:O	1:A:992:ALA:N	2.38	0.56
2:B:2406:SER:HB3	2:B:2429:LEU:HA	1.87	0.56
3:C:2969[B]:TYR:OH	3:L:3120[B]:HIS:HD2	1.75	0.56
3:C:3083[B]:ILE:HD12	3:C:3260[B]:ARG:HB2	1.88	0.56
3:C:3154[B]:PRO:O	3:L:3155[B]:MET:SD	2.64	0.56
3:C:3200[B]:LEU:O	3:C:3204[B]:LEU:HD13	2.06	0.56
2:E:2823:ILE:HG12	2:E:2832:ALA:HB2	1.86	0.56
3:F:3228[B]:VAL:CG2	3:F:3245[B]:PHE:CE2	2.89	0.56
1:G:1104:ASP:O	1:G:1111:ASN:ND2	2.39	0.56
2:H:2711:HIS:HA	2:H:2714:VAL:HG22	1.88	0.56
3:I:2949[A]:LYS:NZ	3:I:2950[A]:THR:HA	2.21	0.56
3:I:3019[A]:HIS:H	3:I:3019[A]:HIS:CD2	2.22	0.56
3:I:3163[B]:ASN:CG	3:R:3150[B]:LYS:HE3	2.19	0.56
3:I:3200[A]:LEU:O	3:I:3204[A]:LEU:HD13	2.06	0.56
3:I:3200[B]:LEU:O	3:I:3204[B]:LEU:HD13	2.06	0.56
3:I:3250[B]:GLY:HA2	3:R:3252[B]:TYR:CZ	2.41	0.56
1:J:944:GLU:O	1:J:957:ASN:ND2	2.39	0.56
3:L:3033[B]:PHE:HD1	3:L:3114[B]:PRO:HB2	1.72	0.56
3:L:3183[B]:LEU:N	3:L:3184[B]:ASN:HA	2.11	0.56
3:L:3200[B]:LEU:O	3:L:3204[B]:LEU:HD13	2.06	0.56
2:N:2394:VAL:HA	2:N:2488:ARG:HA	1.86	0.56
2:N:2800:LYS:O	3:O:3023[A]:ILE:HD13	2.00	0.56
3:O:2942[A]:LEU:HD13	3:O:3033[A]:PHE:CZ	2.40	0.56
3:O:3019[A]:HIS:CD2	3:O:3019[A]:HIS:H	2.22	0.56
3:O:3093[A]:HIS:CE1	3:O:3119[A]:HIS:CD2	2.92	0.56
3:O:3200[B]:LEU:O	3:O:3204[B]:LEU:HD13	2.06	0.56
1:P:895:CYS:O	1:P:897:HIS:ND1	2.37	0.56
3:R:3083[A]:ILE:HD12	3:R:3260[A]:ARG:HB2	1.88	0.56
2:T:2276:GLY:O	2:T:2283:ASN:ND2	2.39	0.56
3:U:2942[A]:LEU:HD13	3:U:3033[A]:PHE:CZ	2.40	0.56
3:U:2952[A]:ALA:HB3	3:U:2954[A]:TYR:N	2.17	0.56
3:U:3200[B]:LEU:O	3:U:3204[B]:LEU:HD13	2.06	0.56
1:V:1161:ILE:HB	1:V:1203:MET:HE3	1.88	0.56
1:V:1206:HIS:CE1	1:V:1209:ASP:HB2	2.41	0.56
1:V:1414:THR:HG23	1:V:1477:LEU:HD13	1.87	0.56
3:X:2949[B]:LYS:NZ	3:X:2950[B]:THR:HA	2.21	0.56
3:X:2969[A]:TYR:CG	3:X:2970[A]:PRO:HD2	2.41	0.56
3:X:3033[A]:PHE:HD1	3:X:3114[A]:PRO:HB2	1.71	0.56
3:X:3228[B]:VAL:CG2	3:X:3245[B]:PHE:CE2	2.89	0.56
2:Z:2503:ASN:HB3	2:c:2168:ARG:O	2.06	0.56
3:a:3200[A]:LEU:O	3:a:3204[A]:LEU:HD13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:1358:LEU:O	1:b:1375:ASN:ND2	2.36	0.56
2:c:2472:ASN:N	2:c:2473:GLY:HA2	2.21	0.56
2:c:2568:HIS:ND1	2:c:2765:PRO:HB3	2.21	0.56
3:d:3093[A]:HIS:CE1	3:d:3119[A]:HIS:CD2	2.92	0.56
3:d:3120[B]:HIS:C	3:d:3122[B]:ASN:N	2.55	0.56
3:d:3180[B]:TYR:C	3:d:3183[B]:LEU:HD22	2.30	0.56
3:d:3281[A]:PHE:HE1	3:d:3305[A]:ILE:HD13	1.71	0.56
3:C:3220[A]:ARG:HG2	3:C:3221[A]:ALA:H	1.70	0.55
3:C:3268[B]:LYS:O	3:C:3271[B]:VAL:HG23	2.06	0.55
3:C:3307[B]:PHE:HE1	3:C:3309[B]:PRO:CG	2.08	0.55
1:D:215:ARG:HE	1:D:279:LEU:HA	1.71	0.55
2:E:2272:SER:HA	2:E:2283:ASN:HD22	1.71	0.55
3:F:3159[B]:SER:CB	3:a:2984[B]:THR:CB	2.82	0.55
1:G:215:ARG:HE	1:G:279:LEU:HA	1.70	0.55
1:G:490:TRP:HE1	1:G:670:PRO:HD3	1.70	0.55
1:G:893:ALA:HB2	1:G:1182:ASN:HB2	1.88	0.55
1:G:979:LEU:HD12	1:G:980:TYR:HA	1.87	0.55
3:I:3155[B]:MET:HE3	3:R:3156[B]:MET:HG2	1.86	0.55
3:I:3251[A]:ASP:HB3	3:I:3252[A]:TYR:CD1	2.40	0.55
3:I:3251[B]:ASP:OD1	3:R:3108[B]:HIS:HE1	1.83	0.55
3:I:3283[A]:ILE:CB	3:I:3305[A]:ILE:HD11	2.35	0.55
1:J:219:LEU:HG	1:J:279:LEU:O	2.06	0.55
2:K:2554:PRO:HA	2:K:2555:GLU:HB3	1.89	0.55
2:K:2627:GLY:HA3	2:K:2703:PHE:O	2.06	0.55
1:M:238:ASN:OD1	1:M:238:ASN:N	2.36	0.55
3:O:3033[A]:PHE:HD1	3:O:3114[A]:PRO:HB2	1.71	0.55
3:O:3281[B]:PHE:HE1	3:O:3305[B]:ILE:HD13	1.71	0.55
2:Q:2185:THR:HG23	2:Q:2186:GLU:HG2	1.87	0.55
3:R:3033[B]:PHE:HD1	3:R:3114[B]:PRO:HB2	1.72	0.55
1:S:802:ILE:O	1:S:810:LEU:N	2.37	0.55
3:U:2952[A]:ALA:N	3:U:2953[A]:GLY:HA2	2.06	0.55
1:V:866:GLU:C	1:V:868:THR:H	2.13	0.55
1:V:895:CYS:SG	1:V:896:HIS:N	2.80	0.55
3:X:2942[A]:LEU:HD13	3:X:3033[A]:PHE:CZ	2.40	0.55
3:X:3083[A]:ILE:HD12	3:X:3260[A]:ARG:HB2	1.88	0.55
3:X:3212[A]:ARG:HH11	3:X:3212[A]:ARG:CG	2.12	0.55
1:Y:80:LEU:O	1:Y:84:GLY:HA2	2.05	0.55
1:Y:1616:LYS:C	3:d:3187[B]:TYR:N	2.37	0.55
3:a:3183[A]:LEU:N	3:a:3184[A]:ASN:HA	2.12	0.55
1:b:35:GLN:NE2	1:b:129:LYS:HB2	2.21	0.55
1:b:447:MET:HA	1:b:455:TYR:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:1407:THR:HG22	1:b:1426:LEU:HD21	1.88	0.55
3:d:2948[A]:ASP:HB3	3:d:2953[A]:GLY:CA	2.24	0.55
3:d:3200[A]:LEU:O	3:d:3204[A]:LEU:HD13	2.06	0.55
3:d:3283[A]:ILE:CB	3:d:3305[A]:ILE:HD11	2.35	0.55
1:A:1567:ASP:OD1	1:A:1591:SER:OG	2.21	0.55
3:C:2961[B]:HIS:NE2	3:C:2980[B]:HIS:CE1	2.73	0.55
3:C:3268[A]:LYS:O	3:C:3271[A]:VAL:HG23	2.06	0.55
2:E:2107:LEU:O	2:E:2111:GLN:HB2	2.06	0.55
3:F:2969[A]:TYR:CG	3:F:2970[A]:PRO:HD2	2.41	0.55
3:F:3155[B]:MET:SD	3:a:3154[B]:PRO:CD	2.95	0.55
3:F:3268[B]:LYS:O	3:F:3271[B]:VAL:HG23	2.06	0.55
3:F:3281[B]:PHE:HE1	3:F:3305[B]:ILE:HD13	1.71	0.55
3:F:3298[B]:ASN:CB	3:F:3300[B]:LEU:N	2.60	0.55
2:H:2885:SER:OG	2:H:2886:VAL:N	2.37	0.55
3:I:3162[B]:ASP:N	3:R:2983[B]:VAL:CG2	2.65	0.55
3:L:2952[A]:ALA:HB3	3:L:2954[A]:TYR:N	2.18	0.55
3:L:2969[A]:TYR:CG	3:L:2970[A]:PRO:HD2	2.41	0.55
3:L:3083[A]:ILE:HD12	3:L:3260[A]:ARG:HB2	1.88	0.55
1:M:49:ALA:HB3	1:M:55:ILE:HD12	1.88	0.55
2:N:2130:PRO:CB	2:N:2142:ALA:HB3	2.35	0.55
3:O:2971[B]:ASP:CG	3:X:3158[B]:PHE:HZ	2.13	0.55
3:O:3268[A]:LYS:O	3:O:3271[A]:VAL:HG23	2.06	0.55
3:O:3268[B]:LYS:O	3:O:3271[B]:VAL:HG23	2.06	0.55
3:R:2971[A]:ASP:CG	3:R:2973[A]:THR:HG1	2.12	0.55
1:S:931:TRP:CG	1:S:1018:ILE:HD11	2.41	0.55
2:T:2509:ILE:HD11	2:T:2605:LEU:HD23	1.88	0.55
3:U:3019[B]:HIS:CD2	3:U:3019[B]:HIS:H	2.22	0.55
3:U:3158[B]:PHE:CB	3:d:3149[B]:ASN:HB3	2.35	0.55
3:U:3176[B]:LYS:HG3	3:d:3152[B]:LYS:NZ	2.18	0.55
3:U:3281[A]:PHE:HE1	3:U:3305[A]:ILE:HD13	1.71	0.55
3:U:3281[B]:PHE:HE1	3:U:3305[B]:ILE:HD13	1.71	0.55
2:W:2571:ARG:NH1	2:W:2776:TYR:OH	2.33	0.55
2:W:2723:GLU:HG2	2:W:2788:ILE:HD13	1.88	0.55
3:X:3298[B]:ASN:HA	3:X:3299[B]:LEU:HB3	1.88	0.55
1:Y:1136:ARG:O	1:Y:1141:ARG:NH1	2.40	0.55
2:Z:2534:PHE:CD1	2:Z:2755:PRO:HB3	2.41	0.55
3:a:3014[B]:TRP:CZ3	3:a:3119[B]:HIS:CE1	2.94	0.55
3:a:3188[B]:ASP:N	3:a:3188[B]:ASP:OD2	2.36	0.55
1:b:327:ASP:OD1	1:b:328:LYS:N	2.39	0.55
1:b:527:LEU:HD22	1:b:629:MET:HG3	1.89	0.55
1:b:893:ALA:HB2	1:b:1182:ASN:HD22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:965:ASP:OD1	1:b:965:ASP:N	2.36	0.55
3:d:2949[B]:LYS:NZ	3:d:2950[B]:THR:HA	2.21	0.55
3:d:2961[A]:HIS:NE2	3:d:2980[A]:HIS:CE1	2.73	0.55
3:d:3220[A]:ARG:HG2	3:d:3221[A]:ALA:H	1.70	0.55
1:A:195:SER:HB2	1:A:386:ILE:HG13	1.89	0.55
1:A:270:GLU:N	1:A:270:GLU:OE1	2.35	0.55
2:B:2715:ASP:O	2:B:2718:TRP:HB3	2.07	0.55
3:C:3153[B]:LYS:CA	3:L:3173[B]:THR:C	2.78	0.55
3:C:3253[B]:GLU:HG2	3:L:3252[B]:TYR:HB2	1.89	0.55
3:F:2949[A]:LYS:NZ	3:F:2950[A]:THR:HA	2.21	0.55
3:F:3014[A]:TRP:CZ3	3:F:3119[A]:HIS:CE1	2.95	0.55
3:F:3083[B]:ILE:HD12	3:F:3260[B]:ARG:HB2	1.88	0.55
3:F:3156[B]:MET:HG3	3:a:2979[B]:GLN:OE1	1.60	0.55
3:F:3281[A]:PHE:HE1	3:F:3305[A]:ILE:HD13	1.71	0.55
3:F:3283[B]:ILE:CB	3:F:3305[B]:ILE:HD11	2.35	0.55
1:G:792:MET:O	1:G:796:TYR:OH	2.25	0.55
1:G:931:TRP:CD2	1:G:1018:ILE:HD11	2.41	0.55
2:H:2294:PHE:O	2:H:2297:HIS:HB3	2.05	0.55
3:I:3156[B]:MET:HB2	3:R:2982[B]:MET:SD	2.45	0.55
1:J:516:TRP:HH2	1:J:637:VAL:HG22	1.71	0.55
1:J:1017:HIS:O	1:J:1021:LEU:HG	2.06	0.55
2:K:2153:GLN:NE2	2:K:2329:MET:HE1	2.20	0.55
2:K:2562:GLY:H	2:K:2846:TRP:HB2	1.71	0.55
2:K:2885:SER:OG	2:K:2886:VAL:N	2.32	0.55
1:M:494:VAL:HG23	1:M:671:PHE:HZ	1.71	0.55
3:O:2969[A]:TYR:CG	3:O:2970[A]:PRO:HD2	2.42	0.55
3:O:2974[B]:ALA:CB	3:X:2977[B]:CYS:O	2.53	0.55
3:O:3157[B]:PRO:HA	3:X:3153[B]:LYS:H	1.70	0.55
1:S:549:PRO:HA	1:S:557:VAL:HG12	1.87	0.55
2:T:2218:SER:O	2:T:2221:THR:OG1	2.21	0.55
2:T:2849:ASP:OD2	2:T:2850:ARG:NH2	2.39	0.55
3:U:2952[B]:ALA:N	3:U:2953[B]:GLY:HA2	2.06	0.55
3:U:3156[B]:MET:SD	3:d:2982[B]:MET:CA	2.93	0.55
1:V:473:ALA:HB3	1:V:476:ARG:HB3	1.88	0.55
1:V:1019:HIS:NE2	1:V:1046:HIS:CE1	2.74	0.55
1:V:1397:LEU:HB2	1:V:1433:TRP:HB3	1.88	0.55
2:W:2823:ILE:CG1	2:W:2830:GLN:HE22	2.16	0.55
3:X:3014[A]:TRP:CZ3	3:X:3119[A]:HIS:CE1	2.95	0.55
2:Z:2470:ALA:HB2	2:Z:2476:LEU:HD11	1.87	0.55
1:b:729:VAL:HG11	1:b:785:LEU:HD12	1.86	0.55
3:d:2961[B]:HIS:NE2	3:d:2980[B]:HIS:CE1	2.73	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3014[A]:TRP:CZ3	3:d:3119[A]:HIS:CE1	2.95	0.55
3:d:3176[A]:LYS:H	3:d:3176[A]:LYS:CE	2.17	0.55
3:d:3298[B]:ASN:HA	3:d:3299[B]:LEU:HB3	1.88	0.55
1:A:357:PRO:HB3	1:A:774:ASP:HB2	1.88	0.55
1:A:439:LEU:HD23	1:A:509:ILE:HD12	1.88	0.55
2:B:2553:ALA:N	2:B:2554:PRO:HD3	2.21	0.55
3:C:2965[B]:LEU:HA	3:L:3255[B]:PRO:HA	1.89	0.55
3:C:3013[A]:ASP:OD1	3:C:3015[A]:THR:OG1	2.23	0.55
3:C:3155[B]:MET:CE	3:L:3153[B]:LYS:HD3	2.33	0.55
3:C:3156[B]:MET:HB3	3:L:2982[B]:MET:HB2	1.86	0.55
3:C:3176[A]:LYS:H	3:C:3176[A]:LYS:CE	2.17	0.55
1:D:926:LEU:HD12	1:D:927:PRO:HD2	1.88	0.55
1:D:1324:ARG:NH1	1:D:1519:TYR:HB3	2.22	0.55
2:E:2180:TRP:HD1	2:E:2247:ILE:HD11	1.71	0.55
3:F:2932[A]:PRO:CA	3:F:2935[A]:ILE:HD12	2.30	0.55
3:F:2985[B]:PHE:HZ	3:a:2970[B]:PRO:CA	2.11	0.55
3:F:3254[B]:MET:HB2	3:a:2966[B]:SER:CB	2.36	0.55
3:F:3298[B]:ASN:HA	3:F:3299[B]:LEU:HB3	1.88	0.55
1:G:418:ASP:OD1	1:G:419:THR:N	2.40	0.55
1:G:904:HIS:HB3	1:G:1105:VAL:HG21	1.88	0.55
1:G:944:GLU:O	1:G:957:ASN:ND2	2.40	0.55
3:I:2961[B]:HIS:NE2	3:I:2980[B]:HIS:CE1	2.73	0.55
3:I:2969[A]:TYR:CG	3:I:2970[A]:PRO:HD2	2.41	0.55
3:I:3033[B]:PHE:HD1	3:I:3114[B]:PRO:HB2	1.71	0.55
1:J:462:HIS:HA	1:J:490:TRP:HH2	1.71	0.55
1:J:566:ARG:HH22	1:J:803:LYS:HZ1	1.53	0.55
2:K:2180:TRP:HB3	2:K:2184:MET:HE2	1.87	0.55
2:K:2346:PRO:O	2:K:2349:THR:OG1	2.20	0.55
3:L:2949[A]:LYS:NZ	3:L:2950[A]:THR:HA	2.21	0.55
3:L:3013[A]:ASP:OD1	3:L:3015[A]:THR:OG1	2.23	0.55
1:M:488:PRO:HB2	1:M:641:TRP:CE3	2.42	0.55
2:N:2548:CYS:O	2:N:2556:TYR:HB3	2.06	0.55
3:O:2947[A]:ALA:HA	3:O:2949[A]:LYS:HB3	1.89	0.55
3:O:3083[A]:ILE:HD12	3:O:3260[A]:ARG:HB2	1.88	0.55
3:O:3160[B]:SER:OG	3:X:3151[B]:LEU:N	2.39	0.55
3:O:3251[B]:ASP:CG	3:X:2968[B]:GLN:OE1	2.49	0.55
3:U:2969[B]:TYR:CZ	3:d:3107[B]:LEU:HD11	2.05	0.55
3:U:2969[B]:TYR:CG	3:U:2970[B]:PRO:HD2	2.41	0.55
1:V:1125:SER:O	1:V:1129:LEU:HB2	2.06	0.55
1:Y:565:GLU:C	1:Y:567:LEU:HA	2.32	0.55
3:a:2932[B]:PRO:CA	3:a:2935[B]:ILE:HD12	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2947[B]:ALA:HA	3:d:2949[B]:LYS:HB3	1.89	0.55
3:d:3151[B]:LEU:HB2	3:d:3175[B]:TYR:HE2	1.67	0.55
3:d:3268[A]:LYS:O	3:d:3271[A]:VAL:HG23	2.06	0.55
1:A:142:ARG:O	1:A:145:GLN:NE2	2.40	0.55
1:A:1166:THR:N	1:A:1167:ASP:HA	2.22	0.55
3:C:2947[B]:ALA:HA	3:C:2949[B]:LYS:HB3	1.89	0.55
3:C:2982[B]:MET:N	3:L:2967[B]:CYS:CB	2.67	0.55
3:C:3153[B]:LYS:CB	3:L:3155[B]:MET:H	2.13	0.55
3:C:3188[B]:ASP:N	3:C:3188[B]:ASP:OD2	2.36	0.55
3:C:3228[B]:VAL:CG2	3:C:3245[B]:PHE:CE2	2.89	0.55
3:F:2949[B]:LYS:NZ	3:F:2950[B]:THR:HA	2.21	0.55
3:F:3183[A]:LEU:N	3:F:3184[A]:ASN:HA	2.11	0.55
3:F:3255[B]:PRO:HB3	3:a:2964[B]:PRO:CD	2.36	0.55
1:G:164:GLU:O	1:G:297:ARG:NH2	2.39	0.55
2:H:2890:VAL:N	2:H:2891:LEU:HA	2.22	0.55
1:J:447:MET:HA	1:J:455:TYR:HB2	1.88	0.55
1:J:494:VAL:HG13	1:J:631:TRP:HZ3	1.72	0.55
3:L:3014[A]:TRP:CZ3	3:L:3119[A]:HIS:CE1	2.94	0.55
3:L:3033[A]:PHE:HD1	3:L:3114[A]:PRO:HB2	1.72	0.55
3:O:3083[B]:ILE:HD12	3:O:3260[B]:ARG:HB2	1.88	0.55
1:P:1493:MET:HG2	1:P:1511:SER:O	2.06	0.55
2:Q:2851:ASN:OD1	2:Q:2851:ASN:N	2.38	0.55
3:R:3281[B]:PHE:HE1	3:R:3305[B]:ILE:HD13	1.71	0.55
2:T:2680:HIS:NE2	2:T:2684:HIS:CD2	2.74	0.55
3:U:2947[A]:ALA:HA	3:U:2949[A]:LYS:HB3	1.89	0.55
3:U:3033[A]:PHE:HD1	3:U:3114[A]:PRO:HB2	1.72	0.55
3:U:3159[B]:SER:HB3	3:d:3147[B]:GLU:HG3	1.88	0.55
3:U:3273[A]:LEU:HB2	3:U:3275[A]:LEU:CD1	2.34	0.55
1:V:17:ASN:HD21	1:V:86:THR:H	1.55	0.55
2:W:2562:GLY:H	2:W:2846:TRP:CB	2.19	0.55
3:X:2969[A]:TYR:CE2	3:X:2970[A]:PRO:CG	2.86	0.55
3:X:3293[B]:LYS:CB	3:X:3294[B]:SER:CB	2.54	0.55
3:a:2969[A]:TYR:CE2	3:a:2970[A]:PRO:CG	2.86	0.55
3:a:3014[A]:TRP:CZ3	3:a:3119[A]:HIS:CE1	2.94	0.55
3:a:3083[B]:ILE:HD12	3:a:3260[B]:ARG:HB2	1.88	0.55
3:a:3268[B]:LYS:O	3:a:3271[B]:VAL:HG23	2.06	0.55
1:b:1573:CYS:HB2	1:b:1627:ARG:HG2	1.89	0.55
3:d:3228[B]:VAL:CG2	3:d:3245[B]:PHE:CE2	2.89	0.55
1:A:723:ALA:O	1:A:728:ARG:NH1	2.40	0.55
1:A:1493:MET:HG2	1:A:1511:SER:O	2.06	0.55
3:C:2949[A]:LYS:HZ2	3:C:2950[A]:THR:HA	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2963[B]:MET:C	3:L:3255[B]:PRO:HB3	2.32	0.55
3:C:2969[A]:TYR:CG	3:C:2970[A]:PRO:HD2	2.42	0.55
3:C:3014[A]:TRP:CZ3	3:C:3119[A]:HIS:CE1	2.94	0.55
3:C:3014[B]:TRP:CZ3	3:C:3119[B]:HIS:CE1	2.94	0.55
3:F:2960[B]:PHE:CD1	3:F:2960[B]:PHE:N	2.72	0.55
3:F:2983[B]:VAL:HG23	3:a:3160[B]:SER:C	2.27	0.55
1:G:559:THR:HG21	1:G:627:ASP:HA	1.88	0.55
1:G:664:VAL:HG12	1:G:690:THR:HG22	1.89	0.55
1:G:1576:THR:H	1:G:1581:GLU:HB3	1.71	0.55
3:I:3281[B]:PHE:HE1	3:I:3305[B]:ILE:HD13	1.71	0.55
1:J:307:ARG:NH1	1:J:772:ARG:O	2.40	0.55
3:L:3014[B]:TRP:CZ3	3:L:3119[B]:HIS:CE1	2.94	0.55
3:L:3284[A]:LYS:HE2	3:L:3284[A]:LYS:CA	2.30	0.55
1:M:883:CYS:N	1:M:894:CYS:SG	2.80	0.55
2:N:2128:LEU:HD23	2:N:2216:PHE:CZ	2.42	0.55
3:O:2949[B]:LYS:NZ	3:O:2950[B]:THR:HA	2.21	0.55
3:O:3014[A]:TRP:CZ3	3:O:3119[A]:HIS:CE1	2.95	0.55
3:O:3154[B]:PRO:HD2	3:X:3176[B]:LYS:HZ1	1.66	0.55
3:O:3254[B]:MET:HE3	3:X:3172[B]:SER:HB2	1.87	0.55
1:P:1002:GLU:HB2	1:P:1065:LYS:HD3	1.87	0.55
3:R:3120[B]:HIS:HA	3:R:3123[B]:THR:HG1	1.71	0.55
3:R:3220[B]:ARG:HG2	3:R:3221[B]:ALA:H	1.70	0.55
3:R:3281[A]:PHE:HE1	3:R:3305[A]:ILE:HD13	1.71	0.55
3:U:2952[B]:ALA:HB3	3:U:2954[B]:TYR:N	2.17	0.55
3:U:3013[B]:ASP:OD1	3:U:3015[B]:THR:OG1	2.23	0.55
3:U:3014[A]:TRP:CZ3	3:U:3119[A]:HIS:CE1	2.95	0.55
3:U:3014[B]:TRP:CZ3	3:U:3119[B]:HIS:CE1	2.95	0.55
3:U:3033[B]:PHE:HD1	3:U:3114[B]:PRO:HB2	1.72	0.55
3:U:3093[B]:HIS:CE1	3:U:3119[B]:HIS:CD2	2.92	0.55
1:V:741:SER:HB2	1:V:764:GLY:H	1.71	0.55
1:V:1271:MET:HE1	1:V:1357:ARG:HH11	1.72	0.55
1:V:1301:PRO:HB3	1:V:1308:VAL:HG12	1.88	0.55
3:X:3176[B]:LYS:CE	3:X:3176[B]:LYS:H	2.17	0.55
3:X:3180[A]:TYR:C	3:X:3183[A]:LEU:HD22	2.30	0.55
3:X:3268[B]:LYS:O	3:X:3271[B]:VAL:HG23	2.06	0.55
1:Y:164:GLU:HG3	1:Y:297:ARG:HE	1.72	0.55
2:Z:2480:LEU:HD22	4:MA:2:NAG:H81	1.87	0.55
3:a:3019[A]:HIS:CD2	3:a:3019[A]:HIS:H	2.22	0.55
3:a:3228[B]:VAL:CG2	3:a:3245[B]:PHE:CE2	2.89	0.55
3:a:3283[A]:ILE:CB	3:a:3305[A]:ILE:HD11	2.35	0.55
3:d:2969[A]:TYR:CG	3:d:2970[A]:PRO:HD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3151[A]:LEU:HB2	3:d:3175[A]:TYR:HE2	1.67	0.55
3:d:3281[B]:PHE:HE1	3:d:3305[B]:ILE:HD13	1.71	0.55
1:A:2:LEU:HD21	1:A:81:VAL:HG21	1.87	0.55
1:A:573:LYS:HD3	1:A:757:VAL:O	2.06	0.55
1:A:1160:PHE:CD1	1:A:1169:LYS:HD3	2.41	0.55
1:A:1296:VAL:HB	1:A:1446:ASP:HB3	1.87	0.55
1:A:1358:LEU:HD23	1:A:1456:LEU:HD21	1.89	0.55
3:C:3253[B]:GLU:HA	3:L:3253[B]:GLU:CA	2.33	0.55
3:F:2983[B]:VAL:HG21	3:a:3161[B]:GLU:HB2	1.85	0.55
3:F:3014[B]:TRP:CZ3	3:F:3119[B]:HIS:CE1	2.95	0.55
3:I:3033[A]:PHE:HD1	3:I:3114[A]:PRO:HB2	1.72	0.55
1:J:630:PHE:O	1:J:633:HIS:HB3	2.07	0.55
3:L:2948[B]:ASP:HB3	3:L:2953[B]:GLY:CA	2.24	0.55
1:M:77:GLU:O	1:M:81:VAL:HG23	2.07	0.55
1:M:954:ALA:O	1:M:956:PRO:HD3	2.07	0.55
1:M:1074:ILE:HB	2:Q:2901:LEU:HB2	1.88	0.55
2:N:2265:ILE:HD12	2:N:2443:TYR:CG	2.42	0.55
3:O:2961[B]:HIS:NE2	3:O:2980[B]:HIS:CE1	2.73	0.55
3:O:3135[A]:LYS:HG3	3:O:3141[A]:TYR:CD1	2.33	0.55
3:O:3251[B]:ASP:HB3	3:O:3252[B]:TYR:CD1	2.40	0.55
3:R:2949[B]:LYS:NZ	3:R:2950[B]:THR:HA	2.21	0.55
3:R:2949[B]:LYS:C	3:R:2949[B]:LYS:HZ3	2.10	0.55
3:R:3176[A]:LYS:H	3:R:3176[A]:LYS:CE	2.17	0.55
3:R:3183[B]:LEU:N	3:R:3184[B]:ASN:HA	2.12	0.55
3:R:3200[A]:LEU:O	3:R:3204[A]:LEU:HD13	2.06	0.55
1:S:1315:GLY:HA3	1:S:1601:TRP:CB	2.37	0.55
2:T:2114:ARG:HG3	2:W:2526:ARG:HE	1.72	0.55
2:T:2115:SER:OG	2:T:2116:SER:N	2.39	0.55
2:T:2237:LEU:H	2:T:2237:LEU:HD13	1.71	0.55
3:U:3093[A]:HIS:CE1	3:U:3119[A]:HIS:CD2	2.92	0.55
3:U:3169[B]:LYS:HD3	3:d:3146[B]:CYS:HA	1.88	0.55
1:V:1136:ARG:O	1:V:1141:ARG:NH1	2.39	0.55
3:X:2960[B]:PHE:CD1	3:X:2960[B]:PHE:N	2.72	0.55
1:Y:11:THR:HG22	1:Y:13:ASP:H	1.71	0.55
3:a:3019[A]:HIS:CD2	3:a:3019[A]:HIS:N	2.75	0.55
3:d:2949[B]:LYS:HZ2	3:d:2950[B]:THR:HA	1.71	0.55
1:A:875:ALA:C	1:A:877:HIS:H	2.15	0.55
3:C:3153[B]:LYS:HD3	3:L:3155[B]:MET:HE2	1.87	0.55
1:D:140:ASP:OD2	1:D:142:ARG:NE	2.40	0.55
1:D:1206:HIS:N	1:D:1206:HIS:ND1	2.54	0.55
3:F:2947[B]:ALA:HA	3:F:2949[B]:LYS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2952[A]:ALA:HB3	3:F:2954[A]:TYR:N	2.17	0.55
3:F:3156[B]:MET:H	3:a:2979[B]:GLN:NE2	2.04	0.55
3:F:3200[A]:LEU:O	3:F:3204[A]:LEU:HD13	2.06	0.55
1:G:21:SER:HB2	1:G:83:HIS:O	2.07	0.55
3:I:2947[B]:ALA:HA	3:I:2949[B]:LYS:HB3	1.89	0.55
3:I:2966[B]:SER:HA	3:R:3256[B]:TRP:N	2.22	0.55
3:I:3259[B]:ASP:HB3	3:R:3162[B]:ASP:HA	1.87	0.55
2:K:2786:MET:HE1	2:K:2794:LEU:HB2	1.89	0.55
3:L:2932[B]:PRO:CA	3:L:2935[B]:ILE:HD12	2.30	0.55
3:O:3220[B]:ARG:HG2	3:O:3221[B]:ALA:H	1.70	0.55
3:R:2969[A]:TYR:CG	3:R:2970[A]:PRO:HD2	2.41	0.55
3:R:3273[B]:LEU:HB2	3:R:3275[B]:LEU:CD1	2.34	0.55
1:S:902:PHE:CE2	1:S:1012:GLU:HB2	2.41	0.55
3:U:3096[B]:VAL:HG11	3:U:3115[B]:LEU:HD12	1.89	0.55
1:V:714:ARG:HH11	1:V:837:HIS:CD2	2.24	0.55
3:X:2960[B]:PHE:CD2	3:X:3157[B]:PRO:CG	2.74	0.55
3:X:3013[A]:ASP:OD1	3:X:3015[A]:THR:OG1	2.23	0.55
3:X:3093[A]:HIS:CE1	3:X:3119[A]:HIS:CD2	2.92	0.55
3:X:3220[A]:ARG:HG2	3:X:3221[A]:ALA:H	1.70	0.55
3:X:3228[A]:VAL:CG2	3:X:3245[A]:PHE:CE2	2.89	0.55
1:Y:905:TRP:HZ2	1:Y:1083:PRO:HG2	1.70	0.55
1:Y:1618:LEU:CA	3:d:3190[B]:LEU:HB2	2.36	0.55
3:a:2969[A]:TYR:CG	3:a:2970[A]:PRO:HD2	2.41	0.55
3:a:3014[A]:TRP:C	3:a:3014[A]:TRP:CD1	2.85	0.55
3:a:3298[B]:ASN:HA	3:a:3299[B]:LEU:HB3	1.88	0.55
1:b:1180:SER:H	1:b:1183:GLU:HG2	1.72	0.55
1:b:1564:ALA:HB1	4:QA:1:NAG:H83	1.89	0.55
2:c:2811:HIS:HB3	2:c:2847:HIS:CD2	2.42	0.55
3:d:2932[B]:PRO:CA	3:d:2935[B]:ILE:HD12	2.30	0.55
3:d:2957[B]:ILE:HA	3:d:2960[B]:PHE:HE1	1.64	0.55
3:d:3033[B]:PHE:HD1	3:d:3114[B]:PRO:HB2	1.72	0.55
1:A:71:LEU:HD22	1:A:266:LEU:HD21	1.88	0.55
1:A:877:HIS:HD2	1:A:1033:LEU:HD13	1.72	0.55
1:A:979:LEU:CB	1:A:980:TYR:HA	2.36	0.55
1:A:1135:ARG:O	1:A:1139:LYS:NZ	2.31	0.55
2:B:2606:LEU:HD22	2:B:2706:ILE:HG12	1.87	0.55
2:B:2635:TYR:HB2	1:b:109:LEU:HD21	1.89	0.55
3:C:2985[B]:PHE:CE2	3:L:2969[B]:TYR:O	2.59	0.55
1:D:1304:ASP:H	1:D:1305:GLY:HA2	1.72	0.55
2:E:2089:ARG:HD2	2:E:2175:VAL:O	2.07	0.55
3:F:2983[B]:VAL:CG2	3:a:3160[B]:SER:CA	2.82	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2983[B]:VAL:CG2	3:a:3160[B]:SER:OG	2.46	0.55
3:F:3014[A]:TRP:C	3:F:3014[A]:TRP:CD1	2.85	0.55
3:F:3019[B]:HIS:CD2	3:F:3019[B]:HIS:N	2.75	0.55
3:F:3033[B]:PHE:HD1	3:F:3114[B]:PRO:HB2	1.72	0.55
3:F:3157[B]:PRO:C	3:a:3150[B]:LYS:HD3	2.17	0.55
3:F:3162[B]:ASP:HA	3:a:3147[B]:GLU:OE1	2.07	0.55
3:F:3255[B]:PRO:HB2	3:a:2959[B]:SER:C	2.32	0.55
1:G:1576:THR:H	1:G:1581:GLU:HG2	1.72	0.55
2:H:2698:LEU:HD12	2:H:2838:LEU:HB3	1.89	0.55
3:I:3083[B]:ILE:HD12	3:I:3260[B]:ARG:HB2	1.88	0.55
3:I:3150[B]:LYS:CG	3:R:3158[B]:PHE:HA	2.20	0.55
3:I:3220[B]:ARG:HG2	3:I:3221[B]:ALA:H	1.70	0.55
1:J:328:LYS:NZ	1:M:1631:GLU:OE1	2.30	0.55
3:L:3135[A]:LYS:HG3	3:L:3141[A]:TYR:CD1	2.33	0.55
1:M:1471:LEU:HD23	1:M:1541:GLU:HG2	1.89	0.55
1:M:1650:ILE:H	2:Q:2327:GLU:HG2	1.72	0.55
2:N:2795:ILE:O	2:N:2798:GLN:HG2	2.07	0.55
3:O:3157[B]:PRO:HD3	3:X:3153[B]:LYS:CA	2.37	0.55
1:P:957:ASN:N	1:P:958:PRO:HA	2.22	0.55
1:P:1627:ARG:NH2	1:P:1629:GLU:OE1	2.38	0.55
1:P:1639:LYS:NZ	1:S:471:PRO:O	2.32	0.55
3:R:2949[A]:LYS:NZ	3:R:2950[A]:THR:HA	2.21	0.55
3:R:3019[A]:HIS:CD2	3:R:3019[A]:HIS:N	2.75	0.55
1:S:81:VAL:HA	1:S:85:SER:HB3	1.88	0.55
3:U:2949[B]:LYS:NZ	3:U:2950[B]:THR:HA	2.21	0.55
3:U:2974[B]:ALA:HB1	3:d:3220[B]:ARG:HD3	1.89	0.55
3:U:2980[B]:HIS:HB2	3:d:2969[B]:TYR:CZ	2.42	0.55
3:U:3082[B]:GLU:CD	3:d:2970[B]:PRO:CB	2.77	0.55
3:U:3155[B]:MET:CE	3:d:3153[B]:LYS:HE2	2.29	0.55
3:U:3258[B]:PHE:CA	3:d:2969[B]:TYR:O	2.54	0.55
3:U:3284[B]:LYS:HE2	3:U:3284[B]:LYS:CA	2.30	0.55
2:W:2472:ASN:N	2:W:2473:GLY:HA2	2.21	0.55
3:X:2949[A]:LYS:NZ	3:X:2950[A]:THR:HA	2.21	0.55
3:X:2961[A]:HIS:NE2	3:X:2980[A]:HIS:CE1	2.73	0.55
3:X:3135[B]:LYS:HG3	3:X:3141[B]:TYR:CD1	2.33	0.55
3:X:3200[A]:LEU:O	3:X:3204[A]:LEU:HD13	2.06	0.55
3:X:3284[A]:LYS:HD3	3:X:3284[A]:LYS:C	2.32	0.55
2:Z:2132:CYS:O	2:Z:2334:LYS:HD3	2.07	0.55
3:a:2947[A]:ALA:HA	3:a:2949[A]:LYS:HB3	1.89	0.55
3:a:2949[B]:LYS:NZ	3:a:2950[B]:THR:HA	2.21	0.55
3:a:3019[B]:HIS:CD2	3:a:3019[B]:HIS:N	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:163:LEU:HB3	1:b:293:LEU:HD21	1.89	0.55
2:c:2476:LEU:HD12	2:c:2480:LEU:HD21	1.89	0.55
3:d:2949[A]:LYS:NZ	3:d:2950[A]:THR:HA	2.21	0.55
3:d:3019[B]:HIS:CD2	3:d:3019[B]:HIS:N	2.75	0.55
1:A:931:TRP:CZ3	1:A:995:ILE:HD11	2.42	0.55
1:A:983:PRO:HB3	1:A:989:THR:HG22	1.88	0.55
2:B:2870:LEU:HD21	2:B:2901:LEU:HD23	1.89	0.55
3:C:2947[A]:ALA:HA	3:C:2949[A]:LYS:HB3	1.89	0.55
3:C:2961[B]:HIS:O	3:L:3255[B]:PRO:HD3	2.07	0.55
3:C:2965[B]:LEU:CD2	3:L:3253[B]:GLU:OE2	2.14	0.55
3:C:2972[B]:GLY:C	3:L:3090[B]:ASN:CB	2.80	0.55
3:C:3298[A]:ASN:HA	3:C:3299[A]:LEU:HB3	1.88	0.55
1:D:105:VAL:HB	1:D:137:ARG:HH22	1.72	0.55
2:E:2265:ILE:HD12	2:E:2443:TYR:CG	2.42	0.55
2:E:2606:LEU:HD21	2:E:2709:VAL:HG21	1.88	0.55
2:E:2635:TYR:HB2	1:G:109:LEU:HD21	1.88	0.55
3:F:2932[B]:PRO:CA	3:F:2935[B]:ILE:HD12	2.30	0.55
3:F:2966[B]:SER:CA	3:a:3256[B]:TRP:N	2.61	0.55
3:F:3082[B]:GLU:OE2	3:F:3086[B]:GLU:HB2	2.07	0.55
3:F:3176[B]:LYS:H	3:F:3176[B]:LYS:CE	2.17	0.55
3:F:3228[A]:VAL:CG2	3:F:3245[A]:PHE:CE2	2.89	0.55
3:F:3256[B]:TRP:CD1	3:a:2965[B]:LEU:HD13	2.41	0.55
3:F:3307[B]:PHE:HE1	3:F:3309[B]:PRO:CG	2.08	0.55
3:F:3307[B]:PHE:C	3:F:3307[B]:PHE:CD1	2.85	0.55
1:G:235:CYS:HA	1:G:820:VAL:O	2.07	0.55
2:H:2107:LEU:HD23	2:H:2208:PRO:HB2	1.88	0.55
3:I:2947[A]:ALA:HA	3:I:2949[A]:LYS:HB3	1.89	0.55
3:I:2949[B]:LYS:NZ	3:I:2950[B]:THR:HA	2.21	0.55
3:I:2979[B]:GLN:C	3:R:2967[B]:CYS:HB2	2.10	0.55
3:I:3293[A]:LYS:CG	3:I:3294[A]:SER:HB2	2.36	0.55
1:J:928:TYR:HB3	1:J:1047:SER:HB3	1.89	0.55
2:K:2132:CYS:O	2:K:2334:LYS:HD3	2.07	0.55
2:K:2550:THR:O	2:K:2553:ALA:N	2.28	0.55
3:L:2960[B]:PHE:CD2	3:L:3157[B]:PRO:CG	2.74	0.55
3:L:3082[B]:GLU:OE2	3:L:3086[B]:GLU:HB2	2.07	0.55
3:L:3307[A]:PHE:HE1	3:L:3309[A]:PRO:CG	2.08	0.55
2:N:2094:ARG:HH21	2:Q:2094:ARG:HH21	1.53	0.55
3:O:2969[A]:TYR:CE2	3:O:2970[A]:PRO:CG	2.86	0.55
3:O:3033[B]:PHE:HD1	3:O:3114[B]:PRO:HB2	1.72	0.55
3:O:3307[A]:PHE:C	3:O:3307[A]:PHE:CD1	2.85	0.55
1:P:1441:SER:OG	1:P:1442:MET:N	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2932[B]:PRO:CA	3:R:2935[B]:ILE:HD12	2.30	0.55
3:R:3307[B]:PHE:C	3:R:3307[B]:PHE:CD1	2.85	0.55
1:S:1195:ASP:HA	1:S:1196:ILE:CB	2.37	0.55
3:U:2969[A]:TYR:CG	3:U:2970[A]:PRO:HD2	2.41	0.55
3:U:3284[B]:LYS:HD3	3:U:3284[B]:LYS:C	2.31	0.55
1:V:979:LEU:HB3	1:V:980:TYR:CD2	2.42	0.55
2:W:2890:VAL:H	2:W:2891:LEU:HA	1.70	0.55
3:X:3281[A]:PHE:HE1	3:X:3305[A]:ILE:HD13	1.71	0.55
1:Y:416:ASN:OD1	3:d:3196[A]:THR:HG21	2.08	0.55
1:Y:747:PHE:HB2	1:Y:799:ARG:HB3	1.89	0.55
3:a:2932[A]:PRO:CA	3:a:2935[A]:ILE:HD12	2.30	0.55
3:a:2969[B]:TYR:CE2	3:a:2970[B]:PRO:CG	2.86	0.55
3:d:2947[A]:ALA:HA	3:d:2949[A]:LYS:HB3	1.89	0.55
3:d:3211[A]:ASP:OD1	3:d:3211[A]:ASP:N	2.28	0.55
3:d:3268[B]:LYS:O	3:d:3271[B]:VAL:HG23	2.06	0.55
1:A:1257:SER:O	1:A:1525:TYR:HA	2.07	0.54
3:C:2933[B]:SER:C	3:C:2936[B]:GLU:H	2.16	0.54
3:C:3033[B]:PHE:HD1	3:C:3114[B]:PRO:HB2	1.71	0.54
3:C:3185[B]:TYR:C	3:C:3185[B]:TYR:CD2	2.86	0.54
2:E:2294:PHE:O	2:E:2297:HIS:HB3	2.06	0.54
3:F:2937[B]:ASN:CB	3:F:3006[B]:LYS:CD	2.86	0.54
1:G:10:LEU:HD12	1:G:104:LEU:HD21	1.88	0.54
3:I:2981[B]:GLY:H	3:R:2968[B]:GLN:CG	2.19	0.54
3:I:3013[B]:ASP:OD1	3:I:3015[B]:THR:OG1	2.23	0.54
3:I:3083[A]:ILE:HD12	3:I:3260[A]:ARG:HB2	1.88	0.54
3:I:3096[B]:VAL:HG11	3:I:3115[B]:LEU:HD12	1.89	0.54
3:I:3172[B]:SER:OG	3:R:3151[B]:LEU:N	2.41	0.54
3:I:3173[B]:THR:HG22	3:I:3174[B]:GLY:H	1.68	0.54
3:I:3176[B]:LYS:H	3:I:3176[B]:LYS:CE	2.17	0.54
3:I:3251[B]:ASP:C	3:R:3251[B]:ASP:HB3	2.32	0.54
3:I:3284[A]:LYS:HE2	3:I:3284[A]:LYS:CA	2.30	0.54
1:J:415:VAL:HG21	1:J:697:ALA:CB	2.36	0.54
1:J:899:MET:HB3	1:J:1012:GLU:OE1	2.07	0.54
1:J:1328:SER:HB2	1:J:1523:LEU:HD13	1.88	0.54
3:L:2933[A]:SER:C	3:L:2936[A]:GLU:H	2.15	0.54
3:L:2969[B]:TYR:CG	3:L:2970[B]:PRO:HD2	2.41	0.54
3:L:3273[A]:LEU:CB	3:L:3275[A]:LEU:CD1	2.85	0.54
1:M:1296:VAL:HB	1:M:1446:ASP:HB3	1.89	0.54
3:O:3173[A]:THR:HG22	3:O:3174[A]:GLY:H	1.67	0.54
1:P:329:ARG:HA	1:S:1583:CYS:O	2.06	0.54
3:R:3013[B]:ASP:OD1	3:R:3015[B]:THR:OG1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3014[A]:TRP:CZ3	3:R:3119[A]:HIS:CE1	2.94	0.54
3:R:3014[B]:TRP:CZ3	3:R:3119[B]:HIS:CE1	2.94	0.54
3:R:3096[B]:VAL:HG11	3:R:3115[B]:LEU:HD12	1.89	0.54
3:R:3132[A]:ALA:HB1	3:R:3197[A]:ILE:HD13	1.89	0.54
3:R:3293[A]:LYS:CG	3:R:3294[A]:SER:HB2	2.36	0.54
3:U:2933[B]:SER:HA	3:U:2935[B]:ILE:CD1	2.38	0.54
3:U:2970[B]:PRO:C	3:d:3090[B]:ASN:HD22	2.14	0.54
3:U:2973[B]:THR:HA	3:d:3247[B]:VAL:HG11	1.89	0.54
3:U:3132[B]:ALA:HB1	3:U:3197[B]:ILE:HD13	1.89	0.54
3:U:3255[B]:PRO:HG2	3:d:3252[B]:TYR:HB3	1.89	0.54
1:V:1470:GLU:HB3	1:V:1537:ILE:HD13	1.89	0.54
3:X:2933[A]:SER:HA	3:X:2935[A]:ILE:CD1	2.38	0.54
3:X:2952[B]:ALA:HB3	3:X:2954[B]:TYR:N	2.17	0.54
3:X:3033[B]:PHE:HD1	3:X:3114[B]:PRO:HB2	1.71	0.54
3:X:3211[B]:ASP:OD1	3:X:3211[B]:ASP:N	2.28	0.54
3:X:3293[B]:LYS:CG	3:X:3294[B]:SER:HB2	2.36	0.54
3:a:3014[B]:TRP:C	3:a:3014[B]:TRP:CD1	2.85	0.54
3:a:3019[B]:HIS:CD2	3:a:3019[B]:HIS:H	2.22	0.54
3:a:3082[B]:GLU:OE2	3:a:3086[B]:GLU:HB2	2.07	0.54
3:a:3307[A]:PHE:CD1	3:a:3307[A]:PHE:C	2.85	0.54
1:b:7:VAL:HG13	1:b:104:LEU:HD12	1.89	0.54
1:b:597:VAL:O	1:b:601:VAL:HG12	2.07	0.54
1:b:926:LEU:HD11	1:b:1043:MET:HB3	1.88	0.54
1:b:1627:ARG:NH2	1:b:1629:GLU:OE1	2.38	0.54
3:d:2969[B]:TYR:CD2	3:d:2970[B]:PRO:CD	2.86	0.54
1:A:483:GLY:HA3	1:A:771:TRP:HE3	1.73	0.54
3:C:2949[B]:LYS:NZ	3:C:2950[B]:THR:HA	2.21	0.54
3:C:3079[B]:CYS:HA	3:L:3161[B]:GLU:OE1	2.07	0.54
3:C:3157[B]:PRO:CA	3:L:2982[B]:MET:SD	2.94	0.54
1:D:132:ASN:OD1	1:D:132:ASN:N	2.34	0.54
1:D:449:ASP:HB2	1:D:1280:GLN:NE2	2.22	0.54
1:D:1034:GLU:HG3	1:D:1182:ASN:HD21	1.72	0.54
1:D:1310:THR:HG23	1:D:1597:THR:HG23	1.89	0.54
3:F:2933[A]:SER:HA	3:F:2935[A]:ILE:CD1	2.37	0.54
3:F:2952[B]:ALA:HB3	3:F:2954[B]:TYR:N	2.17	0.54
3:F:3185[A]:TYR:C	3:F:3185[A]:TYR:CD2	2.86	0.54
3:F:3220[B]:ARG:HG2	3:F:3221[B]:ALA:H	1.70	0.54
3:F:3252[B]:TYR:C	3:a:3252[B]:TYR:C	2.75	0.54
3:I:2937[A]:ASN:CB	3:I:3006[A]:LYS:CD	2.86	0.54
3:I:2983[B]:VAL:CG2	3:R:3160[B]:SER:OG	2.52	0.54
3:I:3014[A]:TRP:CZ3	3:I:3119[A]:HIS:CE1	2.94	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1203:MET:HB2	1:J:1205:LEU:HB2	1.90	0.54
3:L:3196[A]:THR:OG1	3:L:3199[A]:GLN:CB	2.56	0.54
3:L:3307[B]:PHE:CD1	3:L:3307[B]:PHE:C	2.85	0.54
2:N:2180:TRP:CD1	2:N:2247:ILE:HD11	2.43	0.54
3:O:2933[B]:SER:HA	3:O:2935[B]:ILE:CD1	2.37	0.54
3:O:2969[B]:TYR:H	3:X:2988[B]:TRP:CG	2.24	0.54
3:O:3014[B]:TRP:CZ3	3:O:3119[B]:HIS:CE1	2.95	0.54
3:O:3019[A]:HIS:CD2	3:O:3019[A]:HIS:N	2.75	0.54
3:O:3093[B]:HIS:CE1	3:O:3119[B]:HIS:CD2	2.92	0.54
3:O:3183[A]:LEU:N	3:O:3184[A]:ASN:HA	2.12	0.54
3:R:3014[B]:TRP:C	3:R:3014[B]:TRP:CD1	2.85	0.54
3:R:3019[B]:HIS:CD2	3:R:3019[B]:HIS:N	2.75	0.54
3:R:3082[B]:GLU:OE2	3:R:3086[B]:GLU:HB2	2.07	0.54
1:S:873:VAL:HA	1:S:876:PHE:CD2	2.42	0.54
1:S:1260:ARG:HD3	1:S:1331:GLU:OE1	2.07	0.54
2:T:2506:ARG:NE	2:T:2578:GLU:OE2	2.27	0.54
3:U:3083[A]:ILE:HD12	3:U:3260[A]:ARG:HB2	1.88	0.54
3:U:3089[A]:HIS:CE1	3:U:3119[A]:HIS:CE1	2.81	0.54
3:U:3298[B]:ASN:HA	3:U:3299[B]:LEU:HB3	1.88	0.54
1:V:51:ASP:OD1	1:V:51:ASP:N	2.37	0.54
2:W:2556:TYR:CE1	2:W:2845:PRO:HD2	2.35	0.54
3:X:2960[A]:PHE:CD1	3:X:2960[A]:PHE:N	2.72	0.54
3:X:3082[A]:GLU:OE2	3:X:3086[A]:GLU:HB2	2.08	0.54
1:Y:402:THR:HG23	1:Y:659:CYS:HA	1.87	0.54
1:Y:1070:ALA:HB3	1:Y:1077:LEU:HD21	1.90	0.54
2:Z:2446:GLU:HG2	2:Z:2448:THR:HG22	1.89	0.54
3:a:2933[A]:SER:HA	3:a:2935[A]:ILE:CD1	2.38	0.54
3:a:3033[B]:PHE:HD1	3:a:3114[B]:PRO:HB2	1.71	0.54
3:a:3211[A]:ASP:OD1	3:a:3211[A]:ASP:N	2.28	0.54
3:a:3281[A]:PHE:HE1	3:a:3305[A]:ILE:HD13	1.71	0.54
3:a:3298[A]:ASN:HA	3:a:3299[A]:LEU:HB3	1.88	0.54
1:b:103:GLU:OE2	1:b:106:GLN:NE2	2.40	0.54
3:d:2937[A]:ASN:CB	3:d:3006[A]:LYS:CD	2.86	0.54
3:d:3014[B]:TRP:CZ3	3:d:3119[B]:HIS:CE1	2.95	0.54
2:B:2313:LYS:HD3	2:B:2320:TYR:HE2	1.72	0.54
3:C:2933[A]:SER:HA	3:C:2935[A]:ILE:CD1	2.37	0.54
3:C:2960[B]:PHE:CD2	3:C:3157[B]:PRO:CG	2.74	0.54
3:C:2988[B]:TRP:CD1	3:L:3153[B]:LYS:CD	2.81	0.54
3:C:3014[A]:TRP:C	3:C:3014[A]:TRP:CD1	2.85	0.54
3:C:3149[B]:ASN:HB2	3:L:3163[B]:ASN:HD21	1.54	0.54
3:C:3169[B]:LYS:CG	3:L:3150[B]:LYS:N	2.64	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3252[B]:TYR:CG	3:L:3223[B]:GLY:O	2.60	0.54
3:C:3273[A]:LEU:CB	3:C:3275[A]:LEU:CD1	2.86	0.54
1:D:983:PRO:HB3	1:D:989:THR:OG1	2.08	0.54
1:D:1315:GLY:HA3	1:D:1601:TRP:CB	2.37	0.54
2:E:2768:LEU:HD23	2:E:2774:LEU:HD21	1.88	0.54
3:F:2952[B]:ALA:N	3:F:2953[B]:GLY:HA2	2.06	0.54
3:F:2969[B]:TYR:CE2	3:a:3120[B]:HIS:CD2	2.95	0.54
3:F:2976[B]:ALA:O	3:a:2976[B]:ALA:O	2.26	0.54
3:F:3154[B]:PRO:HD2	3:a:3155[B]:MET:CG	2.21	0.54
3:I:3014[B]:TRP:C	3:I:3014[B]:TRP:CD1	2.85	0.54
3:I:3153[B]:LYS:HG2	3:R:3155[B]:MET:CB	2.32	0.54
3:I:3196[A]:THR:OG1	3:I:3199[A]:GLN:CB	2.56	0.54
3:I:3253[B]:GLU:HG3	3:R:2965[B]:LEU:HA	1.89	0.54
3:I:3273[B]:LEU:HB2	3:I:3275[B]:LEU:CD1	2.34	0.54
3:I:3307[B]:PHE:CD1	3:I:3307[B]:PHE:C	2.85	0.54
1:J:673:PHE:HB3	1:J:677:LEU:HB2	1.89	0.54
3:L:2937[A]:ASN:CB	3:L:3006[A]:LYS:CD	2.85	0.54
3:L:3013[B]:ASP:OD1	3:L:3015[B]:THR:OG1	2.23	0.54
3:L:3082[A]:GLU:OE2	3:L:3086[A]:GLU:HB2	2.08	0.54
3:L:3240[A]:THR:CG2	3:L:3241[A]:PHE:N	2.71	0.54
1:M:744:VAL:HG22	1:M:760:ILE:HG12	1.89	0.54
1:M:1438:ASP:HB3	1:M:1441:SER:HB2	1.88	0.54
3:O:2968[B]:GLN:CB	3:X:2979[B]:GLN:HG2	2.36	0.54
3:O:3162[B]:ASP:OD2	3:X:3150[B]:LYS:NZ	2.39	0.54
3:O:3196[B]:THR:OG1	3:O:3199[B]:GLN:CB	2.56	0.54
3:R:2933[B]:SER:HA	3:R:2935[B]:ILE:CD1	2.37	0.54
3:R:2949[B]:LYS:HZ2	3:R:2950[B]:THR:HA	1.71	0.54
3:R:3082[A]:GLU:OE2	3:R:3086[A]:GLU:HB2	2.08	0.54
3:U:3019[B]:HIS:CD2	3:U:3019[B]:HIS:N	2.75	0.54
3:U:3151[A]:LEU:HB2	3:U:3175[A]:TYR:HE2	1.68	0.54
3:U:3151[B]:LEU:HB2	3:U:3175[B]:TYR:HE2	1.68	0.54
3:U:3151[B]:LEU:O	3:d:3153[B]:LYS:HA	2.08	0.54
3:U:3200[A]:LEU:O	3:U:3204[A]:LEU:HD13	2.06	0.54
1:V:664:VAL:O	1:V:689:PRO:HD2	2.06	0.54
3:X:2947[A]:ALA:HA	3:X:2949[A]:LYS:HB3	1.89	0.54
3:X:3196[B]:THR:OG1	3:X:3199[B]:GLN:CB	2.56	0.54
1:Y:1170:MET:HB2	1:Y:1203:MET:HE2	1.88	0.54
3:a:3093[B]:HIS:CE1	3:a:3119[B]:HIS:CD2	2.92	0.54
3:a:3185[B]:TYR:C	3:a:3185[B]:TYR:CD2	2.86	0.54
3:a:3273[B]:LEU:CB	3:a:3275[B]:LEU:CD1	2.86	0.54
3:a:3284[B]:LYS:HD3	3:a:3284[B]:LYS:C	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:806:ASN:N	1:b:807:GLY:HA2	2.22	0.54
2:c:2780:HIS:HD2	2:c:2782:ASN:OD1	1.90	0.54
2:c:2883:ILE:HD12	2:c:2894:ASN:HA	1.89	0.54
1:A:864:ASP:HB3	1:A:869:GLY:HA3	1.89	0.54
1:A:1641:THR:HG21	6:h:2:NAG:H81	1.88	0.54
3:C:2969[A]:TYR:CE2	3:C:2970[A]:PRO:CG	2.86	0.54
3:C:3042[A]:ASP:N	3:C:3042[A]:ASP:OD2	2.41	0.54
3:C:3273[B]:LEU:CB	3:C:3275[B]:LEU:CD1	2.86	0.54
3:C:3307[B]:PHE:C	3:C:3307[B]:PHE:CD1	2.85	0.54
1:D:1638:SER:O	1:G:472:ASP:HB3	2.08	0.54
2:E:2573:TYR:HE2	2:E:2707:PHE:HE2	1.54	0.54
2:E:2863:ARG:HB2	2:E:2865:ILE:HG13	1.90	0.54
3:F:2947[A]:ALA:HA	3:F:2949[A]:LYS:HB3	1.89	0.54
3:F:3196[B]:THR:OG1	3:F:3199[B]:GLN:CB	2.56	0.54
3:F:3252[B]:TYR:O	3:a:3253[B]:GLU:CA	2.56	0.54
1:G:898:GLY:HA2	1:G:1186:TRP:HB2	1.90	0.54
2:H:2406:SER:HG	2:H:2430:GLY:H	1.53	0.54
3:I:2933[A]:SER:HA	3:I:2935[A]:ILE:CD1	2.38	0.54
3:I:3014[B]:TRP:CZ3	3:I:3119[B]:HIS:CE1	2.95	0.54
3:I:3082[B]:GLU:OE2	3:I:3086[B]:GLU:HB2	2.07	0.54
1:J:145:GLN:HG2	1:J:151:GLN:CD	2.31	0.54
1:J:402:THR:HG23	1:J:659:CYS:HA	1.88	0.54
2:K:2569:TRP:O	2:K:2572:VAL:HG23	2.08	0.54
2:K:2828:ASP:HB2	2:K:2830:GLN:OE1	2.07	0.54
3:L:3014[B]:TRP:CD1	3:L:3014[B]:TRP:C	2.85	0.54
1:M:499:GLU:HG3	1:M:511:VAL:H	1.72	0.54
1:M:1209:ASP:O	1:M:1211:TYR:HB2	2.06	0.54
3:O:2937[B]:ASN:CB	3:O:3006[B]:LYS:CD	2.86	0.54
3:O:2949[A]:LYS:NZ	3:O:2950[A]:THR:HA	2.21	0.54
3:O:3185[B]:TYR:C	3:O:3185[B]:TYR:CD2	2.86	0.54
3:O:3228[B]:VAL:CG2	3:O:3245[B]:PHE:CE2	2.89	0.54
3:O:3256[B]:TRP:CE2	3:X:3161[B]:GLU:CG	2.90	0.54
1:P:22:LEU:HD12	1:P:25:MET:HG2	1.90	0.54
2:Q:2179:ASP:HA	2:Q:2300:ASN:ND2	2.23	0.54
3:R:3013[A]:ASP:OD1	3:R:3015[A]:THR:OG1	2.23	0.54
3:R:3196[B]:THR:OG1	3:R:3199[B]:GLN:CB	2.56	0.54
1:S:105:VAL:HG12	1:S:123:PHE:HB3	1.89	0.54
1:S:484:MET:HE3	1:S:663:GLU:HG3	1.90	0.54
2:T:2570:HIS:CD2	9:T:3002:CUO:O1	2.60	0.54
3:U:2937[A]:ASN:CB	3:U:3006[A]:LYS:CD	2.86	0.54
3:U:2947[B]:ALA:HA	3:U:2949[B]:LYS:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3240[B]:THR:CG2	3:U:3241[B]:PHE:N	2.71	0.54
3:U:3273[B]:LEU:CB	3:U:3275[B]:LEU:CD1	2.85	0.54
1:V:1390:ASP:CB	1:Y:1372:ILE:HD11	2.36	0.54
3:X:3281[B]:PHE:HE1	3:X:3305[B]:ILE:HD13	1.71	0.54
3:X:3293[A]:LYS:CG	3:X:3294[A]:SER:HB2	2.36	0.54
3:a:2933[B]:SER:C	3:a:2936[B]:GLU:H	2.15	0.54
3:a:3093[A]:HIS:CE1	3:a:3119[A]:HIS:CD2	2.92	0.54
1:b:524:PRO:HD2	1:b:527:LEU:HD11	1.89	0.54
3:d:3014[A]:TRP:CD1	3:d:3014[A]:TRP:C	2.85	0.54
3:d:3083[A]:ILE:HD12	3:d:3260[A]:ARG:HB2	1.88	0.54
1:A:1328:SER:HB2	1:A:1523:LEU:HD13	1.89	0.54
2:B:2122:ILE:O	2:B:2125:PHE:HB2	2.07	0.54
3:C:3033[A]:PHE:HD1	3:C:3114[A]:PRO:HB2	1.72	0.54
3:C:3082[A]:GLU:OE2	3:C:3086[A]:GLU:HB2	2.08	0.54
3:C:3188[A]:ASP:N	3:C:3188[A]:ASP:OD2	2.36	0.54
1:D:105:VAL:HB	1:D:137:ARG:NH2	2.22	0.54
1:D:899:MET:HE2	1:D:1012:GLU:OE2	2.07	0.54
2:E:2275:GLY:HA3	2:E:2283:ASN:HB2	1.90	0.54
3:F:2933[A]:SER:C	3:F:2936[A]:GLU:H	2.16	0.54
3:F:3013[B]:ASP:OD1	3:F:3015[B]:THR:HG23	2.08	0.54
3:F:3083[A]:ILE:HD12	3:F:3260[A]:ARG:HB2	1.88	0.54
3:F:3268[A]:LYS:O	3:F:3271[A]:VAL:HG23	2.06	0.54
1:G:740:THR:OG1	1:G:741:SER:N	2.39	0.54
1:G:1034:GLU:HB2	1:G:1182:ASN:HD21	1.72	0.54
2:H:2446:GLU:HG2	2:H:2448:THR:HG22	1.90	0.54
3:I:2975[B]:PHE:CD1	3:R:3107[B]:LEU:HD21	2.42	0.54
3:I:3132[B]:ALA:HB1	3:I:3197[B]:ILE:HD13	1.89	0.54
3:I:3172[B]:SER:OG	3:R:3150[B]:LYS:C	2.49	0.54
3:I:3185[A]:TYR:C	3:I:3185[A]:TYR:CD2	2.85	0.54
3:I:3307[A]:PHE:HE1	3:I:3309[A]:PRO:CG	2.08	0.54
3:L:2933[B]:SER:C	3:L:2936[B]:GLU:H	2.16	0.54
3:L:2949[B]:LYS:NZ	3:L:2950[B]:THR:HA	2.21	0.54
3:L:3014[A]:TRP:C	3:L:3014[A]:TRP:CD1	2.85	0.54
3:L:3196[B]:THR:OG1	3:L:3199[B]:GLN:CB	2.56	0.54
3:L:3240[B]:THR:CG2	3:L:3241[B]:PHE:N	2.71	0.54
3:L:3281[A]:PHE:HE1	3:L:3305[A]:ILE:HD13	1.71	0.54
3:L:3293[B]:LYS:CD	3:L:3294[B]:SER:N	2.64	0.54
1:M:633:HIS:C	1:M:633:HIS:HD1	2.15	0.54
1:M:1210:LYS:HA	1:M:1211:TYR:HB3	1.89	0.54
2:N:2768:LEU:HA	2:N:2774:LEU:HD11	1.89	0.54
3:O:3014[A]:TRP:C	3:O:3014[A]:TRP:CD1	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3163[B]:ASN:ND2	3:X:3148[B]:ILE:HG22	2.22	0.54
3:O:3185[A]:TYR:C	3:O:3185[A]:TYR:CD2	2.86	0.54
1:P:128:ILE:HG22	1:P:130:PHE:O	2.07	0.54
3:R:2937[A]:ASN:CB	3:R:3006[A]:LYS:CD	2.86	0.54
3:R:2937[B]:ASN:CB	3:R:3006[B]:LYS:CD	2.86	0.54
3:R:3093[A]:HIS:CE1	3:R:3119[A]:HIS:CD2	2.92	0.54
3:R:3196[A]:THR:OG1	3:R:3199[A]:GLN:CB	2.56	0.54
1:S:1549:GLY:HA2	1:S:1656:ASP:HB3	1.89	0.54
3:U:2960[A]:PHE:CD1	3:U:2960[A]:PHE:N	2.72	0.54
3:U:2967[B]:CYS:CB	3:d:3257[B]:ALA:O	2.49	0.54
3:U:3170[B]:ALA:O	3:d:3148[B]:ILE:CG2	2.56	0.54
1:V:419:THR:HG22	1:V:1062:PHE:HA	1.89	0.54
1:V:525:SER:HA	1:V:528:ALA:HB3	1.88	0.54
2:W:2180:TRP:HD1	2:W:2247:ILE:HD11	1.71	0.54
2:W:2757:PRO:HA	2:W:2760:ARG:HE	1.73	0.54
3:X:3240[A]:THR:CG2	3:X:3241[A]:PHE:N	2.71	0.54
3:X:3307[B]:PHE:CD1	3:X:3307[B]:PHE:C	2.85	0.54
2:Z:2179:ASP:HA	2:Z:2300:ASN:ND2	2.22	0.54
3:a:2933[B]:SER:HA	3:a:2935[B]:ILE:CD1	2.37	0.54
3:a:3033[A]:PHE:HD1	3:a:3114[A]:PRO:HB2	1.72	0.54
3:a:3196[A]:THR:OG1	3:a:3199[A]:GLN:CB	2.56	0.54
1:b:450:LYS:HD3	1:b:1338:GLY:O	2.07	0.54
1:b:956:PRO:HB2	1:b:957:ASN:C	2.32	0.54
3:d:2933[B]:SER:HA	3:d:2935[B]:ILE:CD1	2.38	0.54
3:d:2969[A]:TYR:CE2	3:d:2970[A]:PRO:CG	2.86	0.54
3:d:3019[A]:HIS:CD2	3:d:3019[A]:HIS:N	2.75	0.54
3:d:3033[A]:PHE:HD1	3:d:3114[A]:PRO:HB2	1.72	0.54
3:d:3082[B]:GLU:OE2	3:d:3086[B]:GLU:HB2	2.07	0.54
2:B:2271:HIS:O	2:B:2283:ASN:HB3	2.08	0.54
3:C:2932[A]:PRO:CA	3:C:2935[A]:ILE:HD12	2.30	0.54
3:C:3086[B]:GLU:CB	3:L:2968[B]:GLN:HE21	2.21	0.54
3:C:3153[B]:LYS:CE	3:L:3158[B]:PHE:CG	2.79	0.54
3:C:3255[B]:PRO:CD	3:L:2960[B]:PHE:O	2.46	0.54
3:C:3284[B]:LYS:HE2	3:C:3284[B]:LYS:CA	2.29	0.54
1:D:210:HIS:HA	1:D:213:VAL:HG22	1.90	0.54
3:F:3170[B]:ALA:C	3:a:3152[B]:LYS:HB2	2.31	0.54
3:F:3220[A]:ARG:HG2	3:F:3221[A]:ALA:H	1.70	0.54
3:F:3240[B]:THR:CG2	3:F:3241[B]:PHE:N	2.71	0.54
3:I:3150[B]:LYS:HB2	3:R:3159[B]:SER:C	2.23	0.54
3:I:3155[B]:MET:HG3	3:R:3154[B]:PRO:CD	2.33	0.54
1:J:840:ARG:NH2	1:J:914:GLU:OE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1108:TYR:HB2	1:J:1114:TYR:CE1	2.43	0.54
1:J:1470:GLU:HB3	1:J:1537:ILE:HD11	1.90	0.54
3:O:2968[B]:GLN:CG	3:X:2984[B]:THR:OG1	2.55	0.54
3:O:3096[A]:VAL:HG11	3:O:3115[A]:LEU:HD12	1.89	0.54
3:O:3254[B]:MET:SD	3:X:3154[B]:PRO:CB	2.96	0.54
1:P:567:LEU:N	1:P:571:PRO:HB3	2.23	0.54
1:P:1396:GLU:OE2	1:P:1569:ARG:NH2	2.41	0.54
1:P:1639:LYS:HD2	1:S:472:ASP:HA	1.88	0.54
2:Q:2252:GLU:CD	2:Q:2393:ARG:HH12	2.16	0.54
3:R:3220[B]:ARG:HH11	3:R:3220[B]:ARG:CG	2.12	0.54
3:U:2949[A]:LYS:NZ	3:U:2950[A]:THR:HA	2.21	0.54
3:U:2969[B]:TYR:CE2	3:U:2970[B]:PRO:CG	2.86	0.54
3:U:3156[B]:MET:HE3	3:d:2982[B]:MET:CE	2.26	0.54
3:U:3293[A]:LYS:CD	3:U:3294[A]:SER:N	2.64	0.54
2:W:2179:ASP:HA	2:W:2300:ASN:ND2	2.22	0.54
2:W:2336:PHE:O	2:W:2343:ASN:ND2	2.40	0.54
3:X:2931[A]:THR:HG1	3:X:2934[A]:GLU:CD	2.00	0.54
3:X:3042[A]:ASP:N	3:X:3042[A]:ASP:OD2	2.41	0.54
3:X:3047[B]:ARG:HH21	3:X:3113[B]:ASP:CG	2.16	0.54
3:X:3093[B]:HIS:CE1	3:X:3119[B]:HIS:CD2	2.92	0.54
3:X:3284[B]:LYS:HE2	3:X:3284[B]:LYS:CA	2.30	0.54
1:Y:712:SER:O	1:Y:716:LEU:N	2.35	0.54
3:a:3173[B]:THR:HG22	3:a:3175[B]:TYR:H	1.73	0.54
3:a:3240[B]:THR:CG2	3:a:3241[B]:PHE:N	2.71	0.54
3:a:3273[B]:LEU:HB2	3:a:3275[B]:LEU:CD1	2.34	0.54
1:b:150:GLY:HA2	1:b:151:GLN:C	2.33	0.54
1:b:287:GLU:N	1:b:287:GLU:OE1	2.40	0.54
1:b:325:THR:N	1:b:332:ASP:OD1	2.40	0.54
1:b:452:ILE:HD12	1:b:1367:SER:HB2	1.90	0.54
1:b:1258:ARG:NH2	1:b:1332:ASP:OD1	2.41	0.54
1:b:1470:GLU:HG3	1:b:1530:LEU:HD12	1.88	0.54
2:c:2606:LEU:HD22	2:c:2706:ILE:HG12	1.90	0.54
3:d:3013[B]:ASP:OD1	3:d:3015[B]:THR:HG23	2.08	0.54
3:d:3014[B]:TRP:C	3:d:3014[B]:TRP:CD1	2.85	0.54
3:d:3240[A]:THR:CG2	3:d:3241[A]:PHE:N	2.71	0.54
1:A:494:VAL:HG23	1:A:671:PHE:HZ	1.72	0.54
1:A:915:ASN:ND2	1:A:1093:ASP:OD2	2.38	0.54
1:A:1028:VAL:HA	1:A:1035:TYR:CE2	2.43	0.54
3:C:2952[A]:ALA:HB3	3:C:2954[A]:TYR:N	2.18	0.54
3:C:3013[A]:ASP:OD1	3:C:3015[A]:THR:HG23	2.08	0.54
3:C:3079[B]:CYS:CB	3:L:3161[B]:GLU:CB	2.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3293[A]:LYS:CG	3:C:3294[A]:SER:HB2	2.36	0.54
1:D:241:HIS:CE1	1:D:795:GLU:HA	2.43	0.54
1:D:277:ASP:OD1	1:D:278:ASP:N	2.41	0.54
1:D:1414:THR:HG23	1:D:1477:LEU:HD13	1.89	0.54
3:F:3019[A]:HIS:CD2	3:F:3019[A]:HIS:N	2.75	0.54
3:F:3154[B]:PRO:CD	3:a:3173[B]:THR:C	2.78	0.54
1:G:567:LEU:HD13	1:G:569:LYS:H	1.73	0.54
3:I:2933[B]:SER:C	3:I:2936[B]:GLU:H	2.16	0.54
3:I:2989[B]:HIS:CB	3:R:2970[B]:PRO:HD3	2.24	0.54
3:I:3132[A]:ALA:HB1	3:I:3197[A]:ILE:HD13	1.89	0.54
3:I:3185[B]:TYR:C	3:I:3185[B]:TYR:CD2	2.86	0.54
3:I:3240[A]:THR:CG2	3:I:3241[A]:PHE:N	2.71	0.54
3:I:3240[B]:THR:CG2	3:I:3241[B]:PHE:N	2.71	0.54
3:I:3264[A]:TYR:C	3:I:3264[A]:TYR:HD1	2.16	0.54
3:I:3273[A]:LEU:CB	3:I:3275[A]:LEU:CD1	2.86	0.54
1:J:92:TRP:O	1:J:212:ASN:ND2	2.37	0.54
1:J:675:SER:O	1:J:679:ASN:ND2	2.41	0.54
1:J:1490:ASN:O	1:J:1512:ARG:NE	2.41	0.54
1:J:1604:ASP:OD1	1:J:1605:ARG:NH1	2.40	0.54
3:L:2947[B]:ALA:HA	3:L:2949[B]:LYS:HB3	1.89	0.54
3:L:3013[B]:ASP:OD1	3:L:3015[B]:THR:HG23	2.08	0.54
3:L:3185[B]:TYR:C	3:L:3185[B]:TYR:CD2	2.85	0.54
2:N:2336:PHE:HB3	2:N:2348:THR:HG22	1.89	0.54
3:O:2952[B]:ALA:HB3	3:O:2954[B]:TYR:N	2.18	0.54
3:O:3082[A]:GLU:OE2	3:O:3086[A]:GLU:HB2	2.07	0.54
3:O:3153[B]:LYS:HG3	3:X:3176[B]:LYS:HZ2	1.73	0.54
3:O:3173[A]:THR:HG22	3:O:3175[A]:TYR:H	1.73	0.54
1:P:84:GLY:HA2	1:P:85:SER:HB3	1.88	0.54
1:P:705:THR:HG22	1:P:1118:THR:HG23	1.90	0.54
1:P:1317:PRO:HA	1:P:1420:GLU:HG3	1.88	0.54
3:R:3185[A]:TYR:C	3:R:3185[A]:TYR:CD2	2.86	0.54
3:R:3273[A]:LEU:HB2	3:R:3275[A]:LEU:CD1	2.34	0.54
1:S:84:GLY:HA2	1:S:85:SER:HB3	1.90	0.54
2:T:2823:ILE:HG22	2:T:2879:LEU:HD22	1.90	0.54
3:U:2970[B]:PRO:C	3:d:3090[B]:ASN:ND2	2.62	0.54
3:U:3014[B]:TRP:C	3:U:3014[B]:TRP:CD1	2.85	0.54
3:U:3019[A]:HIS:CD2	3:U:3019[A]:HIS:N	2.75	0.54
3:U:3082[B]:GLU:OE2	3:U:3086[B]:GLU:HB2	2.08	0.54
3:U:3173[A]:THR:HG22	3:U:3175[A]:TYR:H	1.73	0.54
3:U:3254[B]:MET:CA	3:d:3254[B]:MET:CA	2.54	0.54
3:X:2933[B]:SER:HA	3:X:2935[B]:ILE:CD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2937[A]:ASN:CB	3:X:3006[A]:LYS:CD	2.86	0.54
3:X:3014[B]:TRP:CZ3	3:X:3119[B]:HIS:CE1	2.95	0.54
1:Y:1556:GLY:HA3	1:Y:1606:LEU:HD13	1.90	0.54
2:Z:2528:LYS:NZ	2:Z:2626:ARG:O	2.40	0.54
3:a:2933[A]:SER:C	3:a:2936[A]:GLU:H	2.16	0.54
3:a:2937[A]:ASN:CB	3:a:3006[A]:LYS:CD	2.86	0.54
3:a:3047[A]:ARG:HH21	3:a:3113[A]:ASP:CG	2.16	0.54
3:a:3176[B]:LYS:H	3:a:3176[B]:LYS:CE	2.17	0.54
1:b:1271:MET:HG2	1:b:1358:LEU:HD13	1.90	0.54
3:d:3284[A]:LYS:HD3	3:d:3284[A]:LYS:C	2.31	0.54
3:d:3307[A]:PHE:C	3:d:3307[A]:PHE:CD1	2.85	0.54
1:A:838:ARG:NH1	1:A:914:GLU:OE2	2.41	0.54
2:B:2883:ILE:HG22	2:B:2894:ASN:HD22	1.72	0.54
3:C:2978[B]:CYS:CA	3:L:3254[B]:MET:HB3	2.26	0.54
3:C:3170[B]:ALA:HA	3:L:3148[B]:ILE:HG22	1.90	0.54
3:C:3196[B]:THR:OG1	3:C:3199[B]:GLN:CB	2.56	0.54
1:D:17:ASN:ND2	1:D:86:THR:H	2.06	0.54
2:E:2320:TYR:HA	2:E:2358:PHE:HB3	1.90	0.54
3:F:3307[A]:PHE:CD1	3:F:3307[A]:PHE:C	2.85	0.54
1:G:287:GLU:OE1	1:G:287:GLU:N	2.37	0.54
2:H:2651:GLN:HG2	2:H:2652:LYS:HD2	1.90	0.54
3:I:2937[B]:ASN:CB	3:I:3006[B]:LYS:CD	2.86	0.54
3:I:3196[B]:THR:OG1	3:I:3199[B]:GLN:CB	2.56	0.54
3:I:3259[B]:ASP:CG	3:R:3162[B]:ASP:HB3	2.30	0.54
3:I:3264[B]:TYR:C	3:I:3264[B]:TYR:HD1	2.16	0.54
1:J:491:HIS:CD2	9:J:5002:CUO:O1	2.59	0.54
3:L:3019[B]:HIS:CD2	3:L:3019[B]:HIS:N	2.75	0.54
3:L:3273[B]:LEU:CB	3:L:3275[B]:LEU:CD1	2.86	0.54
3:L:3307[A]:PHE:C	3:L:3307[A]:PHE:CD1	2.85	0.54
1:M:603:HIS:NE2	1:M:607:HIS:CD2	2.76	0.54
2:N:2526:ARG:HE	2:Q:2114:ARG:HG3	1.73	0.54
3:O:2961[A]:HIS:NE2	3:O:2980[A]:HIS:CE1	2.73	0.54
3:O:3159[B]:SER:O	3:X:3151[B]:LEU:HD12	2.08	0.54
3:O:3293[B]:LYS:CG	3:O:3294[B]:SER:HB2	2.36	0.54
1:P:1011:TYR:OH	1:P:1049:VAL:O	2.22	0.54
3:R:2947[A]:ALA:HA	3:R:2949[A]:LYS:HB3	1.89	0.54
3:R:2960[A]:PHE:CD2	3:R:3157[A]:PRO:CG	2.74	0.54
3:R:3185[B]:TYR:C	3:R:3185[B]:TYR:CD2	2.86	0.54
3:R:3264[A]:TYR:C	3:R:3264[A]:TYR:HD1	2.16	0.54
2:T:2419:ASP:N	2:T:2419:ASP:OD1	2.41	0.54
2:T:2476:LEU:HD13	6:CA:2:NAG:H81	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:2723:GLU:HG2	2:T:2788:ILE:HD12	1.89	0.54
3:U:2933[A]:SER:HA	3:U:2935[A]:ILE:CD1	2.38	0.54
3:U:3173[B]:THR:HG22	3:U:3174[B]:GLY:H	1.67	0.54
3:U:3220[B]:ARG:CG	3:d:2973[B]:THR:CG2	2.82	0.54
3:U:3307[A]:PHE:C	3:U:3307[A]:PHE:CD1	2.85	0.54
1:V:1055:THR:HA	1:V:1119:LEU:HD13	1.89	0.54
3:X:2952[B]:ALA:CA	3:X:2956[B]:LYS:HB3	2.38	0.54
3:X:2954[B]:TYR:CD2	3:X:2954[B]:TYR:C	2.86	0.54
3:X:2961[B]:HIS:NE2	3:X:2980[B]:HIS:CE1	2.73	0.54
3:X:3273[A]:LEU:CB	3:X:3275[A]:LEU:CD1	2.86	0.54
3:X:3307[A]:PHE:C	3:X:3307[A]:PHE:CD1	2.85	0.54
1:Y:949:ASP:HB3	1:Y:955:LYS:HE3	1.89	0.54
3:a:2949[A]:LYS:NZ	3:a:2950[A]:THR:HA	2.21	0.54
3:a:3096[B]:VAL:HG11	3:a:3115[B]:LEU:HD12	1.89	0.54
3:a:3220[B]:ARG:HG2	3:a:3221[B]:ALA:H	1.70	0.54
3:a:3264[B]:TYR:HD1	3:a:3264[B]:TYR:C	2.16	0.54
2:c:2394:VAL:HG11	2:c:2451:LEU:HD12	1.88	0.54
2:c:2570:HIS:CD2	2:c:2711:HIS:CE1	2.93	0.54
3:d:2948[B]:ASP:CB	3:d:2949[B]:LYS:CA	2.78	0.54
3:d:3264[B]:TYR:C	3:d:3264[B]:TYR:HD1	2.16	0.54
3:d:3273[B]:LEU:CB	3:d:3275[B]:LEU:CD1	2.86	0.54
3:d:3307[B]:PHE:CD1	3:d:3307[B]:PHE:C	2.85	0.54
6:5:2:NAG:H61	6:5:3:BMA:H2	1.90	0.54
1:A:1206:HIS:CE1	1:A:1209:ASP:HB2	2.43	0.54
1:A:1206:HIS:HE1	1:A:1209:ASP:HB2	1.72	0.54
2:B:2180:TRP:HB3	2:B:2184:MET:HE2	1.90	0.54
2:B:2506:ARG:NE	2:B:2578:GLU:OE2	2.27	0.54
2:B:2690:HIS:ND1	2:B:2886:VAL:O	2.41	0.54
3:C:2937[B]:ASN:CB	3:C:3006[B]:LYS:CD	2.86	0.54
3:C:3013[B]:ASP:OD1	3:C:3015[B]:THR:HG23	2.08	0.54
3:C:3014[B]:TRP:CD1	3:C:3014[B]:TRP:C	2.85	0.54
3:C:3082[B]:GLU:OE2	3:C:3086[B]:GLU:HB2	2.07	0.54
3:C:3173[B]:THR:HG22	3:C:3175[B]:TYR:H	1.73	0.54
3:C:3185[A]:TYR:C	3:C:3185[A]:TYR:CD2	2.86	0.54
3:C:3264[A]:TYR:C	3:C:3264[A]:TYR:HD1	2.16	0.54
1:D:673:PHE:HB3	1:D:677:LEU:HB2	1.87	0.54
1:D:1492:PRO:HB2	1:D:1497:SER:HB3	1.90	0.54
3:F:2983[B]:VAL:H	3:a:3160[B]:SER:HA	1.73	0.54
3:F:3253[B]:GLU:CB	3:a:2976[B]:ALA:N	2.70	0.54
3:F:3264[B]:TYR:CD1	3:F:3264[B]:TYR:C	2.86	0.54
1:G:1016:ASN:HD22	1:G:1177:VAL:HA	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3082[A]:GLU:OE2	3:I:3086[A]:GLU:HB2	2.08	0.54
3:I:3157[B]:PRO:CD	3:R:2982[B]:MET:HE1	2.37	0.54
1:J:1195:ASP:OD1	1:J:1196:ILE:N	2.40	0.54
2:K:2635:TYR:HB2	1:M:109:LEU:HD21	1.89	0.54
3:L:2933[A]:SER:HA	3:L:2935[A]:ILE:CD1	2.38	0.54
3:L:3173[B]:THR:HG22	3:L:3174[B]:GLY:H	1.67	0.54
1:M:489:HIS:HB3	1:M:689:PRO:HB3	1.88	0.54
3:O:2933[A]:SER:C	3:O:2936[A]:GLU:H	2.16	0.54
3:O:2933[A]:SER:HA	3:O:2935[A]:ILE:CD1	2.38	0.54
3:O:2937[A]:ASN:CB	3:O:3006[A]:LYS:CD	2.86	0.54
3:O:3196[A]:THR:OG1	3:O:3199[A]:GLN:CB	2.56	0.54
3:O:3264[B]:TYR:C	3:O:3264[B]:TYR:HD1	2.16	0.54
3:O:3273[A]:LEU:CB	3:O:3275[A]:LEU:CD1	2.86	0.54
3:O:3307[B]:PHE:C	3:O:3307[B]:PHE:CD1	2.85	0.54
3:R:3273[B]:LEU:CB	3:R:3275[B]:LEU:CD1	2.85	0.54
1:S:843:VAL:HG13	1:S:927:PRO:HB2	1.90	0.54
1:S:1089:ASP:N	1:S:1089:ASP:OD1	2.40	0.54
2:T:2243:LEU:HD11	2:T:2273:TRP:HZ3	1.72	0.54
2:T:2359:ASN:OD1	2:T:2359:ASN:N	2.39	0.54
3:U:2979[B]:GLN:HE21	3:d:3153[B]:LYS:CE	2.20	0.54
3:X:2933[B]:SER:C	3:X:2936[B]:GLU:H	2.15	0.54
3:X:3014[B]:TRP:C	3:X:3014[B]:TRP:CD1	2.85	0.54
3:X:3082[B]:GLU:OE2	3:X:3086[B]:GLU:HB2	2.08	0.54
3:X:3284[B]:LYS:HD3	3:X:3284[B]:LYS:C	2.32	0.54
2:Z:2265:ILE:HD12	2:Z:2443:TYR:CD1	2.42	0.54
2:Z:2867:PRO:HD2	3:a:2932[A]:PRO:CB	2.38	0.54
3:a:3264[A]:TYR:C	3:a:3264[A]:TYR:CD1	2.86	0.54
3:a:3264[A]:TYR:C	3:a:3264[A]:TYR:HD1	2.16	0.54
2:c:2625:LEU:HB2	2:c:2638:ARG:HH22	1.72	0.54
3:d:3047[A]:ARG:HH21	3:d:3113[A]:ASP:CG	2.16	0.54
3:d:3132[B]:ALA:CB	3:d:3197[B]:ILE:CD1	2.86	0.54
3:d:3240[B]:THR:CG2	3:d:3241[B]:PHE:N	2.71	0.54
3:d:3273[A]:LEU:CB	3:d:3275[A]:LEU:CD1	2.85	0.54
1:A:448:SER:OG	1:A:450:LYS:NZ	2.41	0.54
2:B:2603:PRO:HG2	2:B:2606:LEU:HD12	1.90	0.54
3:C:3132[A]:ALA:CB	3:C:3197[A]:ILE:CD1	2.86	0.54
3:C:3157[B]:PRO:HD2	3:L:3153[B]:LYS:HZ1	1.72	0.54
3:C:3240[A]:THR:CG2	3:C:3241[A]:PHE:N	2.71	0.54
1:D:1394:GLN:HG2	1:D:1395:PRO:HD2	1.89	0.54
2:E:2115:SER:OG	2:E:2116:SER:N	2.41	0.54
3:F:2930[B]:LEU:H	3:F:2930[B]:LEU:CD2	1.98	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2933[B]:SER:HA	3:F:2935[B]:ILE:CD1	2.38	0.54
3:F:2954[B]:TYR:CD2	3:F:2954[B]:TYR:C	2.86	0.54
3:F:2962[B]:GLY:C	3:a:3255[B]:PRO:HG3	2.32	0.54
3:F:2975[B]:PHE:CZ	3:a:2961[B]:HIS:O	2.61	0.54
3:F:3042[B]:ASP:N	3:F:3042[B]:ASP:OD2	2.41	0.54
3:F:3047[A]:ARG:HH21	3:F:3113[A]:ASP:CG	2.16	0.54
3:F:3150[B]:LYS:CE	3:a:3160[B]:SER:CB	2.75	0.54
3:F:3173[B]:THR:HG22	3:F:3175[B]:TYR:H	1.73	0.54
3:F:3196[A]:THR:OG1	3:F:3199[A]:GLN:CB	2.56	0.54
3:F:3273[B]:LEU:CB	3:F:3275[B]:LEU:CD1	2.86	0.54
1:G:1273:SER:HB3	1:G:1340:GLY:H	1.72	0.54
3:I:3307[A]:PHE:C	3:I:3307[A]:PHE:CD1	2.85	0.54
1:J:325:THR:HG21	1:J:329:ARG:O	2.08	0.54
3:L:2961[A]:HIS:NE2	3:L:2980[A]:HIS:CE1	2.73	0.54
3:L:3104[B]:MET:HA	3:L:3110[B]:THR:CG2	2.17	0.54
3:L:3228[A]:VAL:CG2	3:L:3245[A]:PHE:CE2	2.89	0.54
3:L:3228[B]:VAL:CG2	3:L:3245[B]:PHE:CE2	2.89	0.54
3:L:3284[B]:LYS:HD3	3:L:3284[B]:LYS:C	2.32	0.54
1:M:1582:ASN:HB3	1:M:1583:CYS:CB	2.33	0.54
3:O:2933[B]:SER:C	3:O:2936[B]:GLU:H	2.15	0.54
3:O:3153[B]:LYS:CD	3:X:3176[B]:LYS:HD2	2.07	0.54
3:O:3284[B]:LYS:HD3	3:O:3284[B]:LYS:C	2.31	0.54
1:P:1163:ALA:HA	1:P:1211:TYR:H	1.73	0.54
2:Q:2300:ASN:OD1	2:Q:2303:ARG:NH1	2.41	0.54
3:R:3264[B]:TYR:HD1	3:R:3264[B]:TYR:C	2.16	0.54
1:S:1328:SER:HB2	1:S:1523:LEU:HD13	1.90	0.54
1:S:1352:PHE:O	1:S:1398:PHE:HB3	2.08	0.54
3:U:2933[A]:SER:C	3:U:2936[A]:GLU:H	2.16	0.54
3:U:3042[B]:ASP:OD2	3:U:3042[B]:ASP:N	2.41	0.54
3:U:3120[A]:HIS:HA	3:U:3123[A]:THR:HG1	1.72	0.54
3:U:3135[A]:LYS:HG3	3:U:3141[A]:TYR:CD1	2.33	0.54
3:U:3240[A]:THR:CG2	3:U:3241[A]:PHE:N	2.71	0.54
3:U:3264[B]:TYR:CD1	3:U:3264[B]:TYR:C	2.86	0.54
3:U:3273[A]:LEU:CB	3:U:3275[A]:LEU:CD1	2.86	0.54
1:V:426:LYS:NZ	1:V:1123:GLY:O	2.21	0.54
3:X:3014[A]:TRP:CD1	3:X:3014[A]:TRP:C	2.85	0.54
3:X:3132[A]:ALA:CB	3:X:3197[A]:ILE:CD1	2.87	0.54
3:X:3176[A]:LYS:H	3:X:3176[A]:LYS:CE	2.17	0.54
2:Z:2825:ILE:HA	2:Z:2877:ILE:HG22	1.90	0.54
3:a:3120[A]:HIS:HA	3:a:3123[A]:THR:HG1	1.73	0.54
1:b:1400:ASN:HD22	1:b:1403:LEU:HG	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2952[B]:ALA:CA	3:d:2956[B]:LYS:HB3	2.38	0.54
1:A:238:ASN:HD21	1:A:820:VAL:HG23	1.72	0.53
3:C:2933[B]:SER:HA	3:C:2935[B]:ILE:CD1	2.38	0.53
3:C:3093[A]:HIS:CE1	3:C:3119[A]:HIS:CD2	2.92	0.53
3:C:3307[A]:PHE:CD1	3:C:3307[A]:PHE:C	2.85	0.53
3:F:2969[B]:TYR:CD2	3:a:3093[B]:HIS:NE2	2.77	0.53
3:F:3033[A]:PHE:HD1	3:F:3114[A]:PRO:HB2	1.72	0.53
3:F:3185[B]:TYR:C	3:F:3185[B]:TYR:CD2	2.86	0.53
3:F:3255[B]:PRO:HA	3:a:2965[B]:LEU:C	2.33	0.53
2:H:2884:LYS:HB2	2:H:2889:ALA:O	2.09	0.53
3:I:2975[B]:PHE:CD1	3:R:3107[B]:LEU:CD2	2.91	0.53
1:J:450:LYS:HZ3	1:J:505:ARG:HH21	1.56	0.53
1:J:873:VAL:HG21	1:J:912:ASN:HB3	1.90	0.53
1:J:1093:ASP:OD1	1:J:1096:THR:OG1	2.20	0.53
3:L:2954[A]:TYR:CD2	3:L:2954[A]:TYR:C	2.86	0.53
3:L:3042[B]:ASP:N	3:L:3042[B]:ASP:OD2	2.41	0.53
1:M:135:THR:HB	1:M:192:HIS:O	2.07	0.53
1:M:613:SER:HA	1:M:805:VAL:HG12	1.90	0.53
1:M:1019:HIS:HE2	1:M:1046:HIS:CE1	2.26	0.53
3:O:3014[B]:TRP:CD1	3:O:3014[B]:TRP:C	2.85	0.53
3:O:3273[B]:LEU:CB	3:O:3275[B]:LEU:CD1	2.86	0.53
1:P:1573:CYS:HB2	1:P:1627:ARG:HG2	1.90	0.53
2:Q:2824:CYS:SG	2:Q:2878:ARG:NH1	2.81	0.53
2:Q:2849:ASP:OD2	2:Q:2850:ARG:NH1	2.40	0.53
3:R:2954[B]:TYR:CD2	3:R:2954[B]:TYR:C	2.86	0.53
3:R:3240[B]:THR:CG2	3:R:3241[B]:PHE:N	2.71	0.53
3:R:3273[A]:LEU:CB	3:R:3275[A]:LEU:CD1	2.85	0.53
1:S:1348:TRP:HD1	1:S:1403:LEU:HD13	1.73	0.53
2:T:2545:SER:CA	2:T:2546:LEU:HB2	2.35	0.53
3:U:2933[B]:SER:C	3:U:2936[B]:GLU:H	2.15	0.53
3:U:2954[B]:TYR:CD2	3:U:2954[B]:TYR:C	2.86	0.53
3:U:3013[B]:ASP:OD1	3:U:3015[B]:THR:HG23	2.08	0.53
3:U:3047[B]:ARG:HH21	3:U:3113[B]:ASP:CG	2.16	0.53
3:U:3162[B]:ASP:CG	3:d:3260[B]:ARG:CZ	2.81	0.53
3:U:3196[B]:THR:OG1	3:U:3199[B]:GLN:CB	2.56	0.53
3:X:3019[A]:HIS:CD2	3:X:3019[A]:HIS:N	2.75	0.53
3:X:3019[B]:HIS:CD2	3:X:3019[B]:HIS:N	2.75	0.53
3:X:3185[A]:TYR:C	3:X:3185[A]:TYR:CD2	2.86	0.53
1:Y:28:ASP:OD2	1:Y:83:HIS:NE2	2.34	0.53
3:a:3132[B]:ALA:CB	3:a:3197[B]:ILE:CD1	2.86	0.53
1:b:778:LYS:HG2	1:b:821:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:1427:HIS:CD2	1:b:1457:HIS:HE1	2.26	0.53
2:c:2650:GLY:N	2:c:2651:GLN:HA	2.22	0.53
3:d:2933[B]:SER:C	3:d:2936[B]:GLU:H	2.15	0.53
3:d:3185[A]:TYR:C	3:d:3185[A]:TYR:CD2	2.86	0.53
3:d:3273[A]:LEU:HB2	3:d:3275[A]:LEU:CD1	2.34	0.53
3:C:2937[A]:ASN:CB	3:C:3006[A]:LYS:CD	2.86	0.53
3:C:3281[B]:PHE:HE1	3:C:3305[B]:ILE:HD13	1.71	0.53
1:D:1595:GLY:O	1:D:1598:GLU:HG2	2.08	0.53
3:F:2933[B]:SER:C	3:F:2936[B]:GLU:H	2.16	0.53
3:F:2975[B]:PHE:HA	3:a:3107[B]:LEU:HD22	1.88	0.53
3:F:3082[A]:GLU:OE2	3:F:3086[A]:GLU:HB2	2.08	0.53
3:F:3132[B]:ALA:CB	3:F:3197[B]:ILE:CD1	2.86	0.53
3:F:3173[A]:THR:HG22	3:F:3175[A]:TYR:H	1.73	0.53
1:G:142:ARG:NH1	1:G:340:GLN:OE1	2.41	0.53
2:H:2739:LEU:HD13	1:J:1207:TYR:HD2	1.73	0.53
2:H:2856:ILE:HG22	2:H:2859:VAL:HB	1.90	0.53
3:I:2933[A]:SER:C	3:I:2936[A]:GLU:H	2.16	0.53
3:I:3132[B]:ALA:CB	3:I:3197[B]:ILE:CD1	2.86	0.53
3:I:3151[A]:LEU:HB2	3:I:3175[A]:TYR:HE2	1.68	0.53
3:I:3153[B]:LYS:NZ	3:R:3158[B]:PHE:H	2.05	0.53
1:M:741:SER:HB3	1:M:764:GLY:H	1.73	0.53
1:M:1348:TRP:HD1	1:M:1403:LEU:HD13	1.74	0.53
2:N:2132:CYS:O	2:N:2334:LYS:HD3	2.07	0.53
2:N:2738:ALA:HB1	2:N:2741:GLN:HB2	1.90	0.53
3:O:2975[B]:PHE:CD1	3:X:3156[B]:MET:CA	2.89	0.53
3:O:3082[B]:GLU:OE2	3:O:3086[B]:GLU:HB2	2.08	0.53
3:O:3240[B]:THR:CG2	3:O:3241[B]:PHE:N	2.71	0.53
3:O:3264[A]:TYR:C	3:O:3264[A]:TYR:HD1	2.16	0.53
3:O:3293[A]:LYS:CB	3:O:3294[A]:SER:CB	2.54	0.53
1:P:931:TRP:CD1	1:P:1048:ASN:HD22	2.26	0.53
2:Q:2578:GLU:HG3	2:Q:2590:VAL:HG23	1.90	0.53
2:Q:2724:LEU:HA	2:Q:2788:ILE:HD11	1.89	0.53
3:R:3173[A]:THR:HG22	3:R:3175[A]:TYR:H	1.73	0.53
3:U:3082[A]:GLU:OE2	3:U:3086[A]:GLU:HB2	2.08	0.53
3:U:3173[B]:THR:HG22	3:U:3175[B]:TYR:H	1.73	0.53
3:U:3185[B]:TYR:C	3:U:3185[B]:TYR:CD2	2.86	0.53
3:U:3220[B]:ARG:NH1	3:d:2974[B]:ALA:HB2	2.24	0.53
3:U:3255[B]:PRO:HD3	3:d:3253[B]:GLU:CA	2.36	0.53
1:V:563:ILE:O	1:V:612:GLY:HA3	2.08	0.53
1:V:1102:PRO:HA	1:V:1105:VAL:HG22	1.91	0.53
3:X:3013[A]:ASP:OD1	3:X:3015[A]:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3185[B]:TYR:C	3:X:3185[B]:TYR:CD2	2.86	0.53
3:a:2948[B]:ASP:CB	3:a:2949[B]:LYS:CA	2.78	0.53
3:a:2952[A]:ALA:HB3	3:a:2954[A]:TYR:N	2.17	0.53
3:a:2954[B]:TYR:CD2	3:a:2954[B]:TYR:C	2.86	0.53
3:a:3013[A]:ASP:OD1	3:a:3015[A]:THR:HG23	2.08	0.53
3:a:3196[B]:THR:OG1	3:a:3199[B]:GLN:CB	2.56	0.53
3:a:3273[A]:LEU:CB	3:a:3275[A]:LEU:CD1	2.86	0.53
1:b:664:VAL:O	1:b:689:PRO:HD2	2.08	0.53
3:d:2960[B]:PHE:CD2	3:d:3157[B]:PRO:CG	2.74	0.53
3:d:3013[A]:ASP:OD1	3:d:3015[A]:THR:HG23	2.08	0.53
3:d:3082[A]:GLU:OE2	3:d:3086[A]:GLU:HB2	2.07	0.53
1:A:416:ASN:ND2	3:F:3196[A]:THR:HG21	2.23	0.53
2:B:2090:LYS:NZ	2:B:2099:GLU:OE2	2.37	0.53
2:B:2212:GLY:HA3	2:B:2290:TYR:O	2.08	0.53
2:B:2509:ILE:HD11	2:B:2605:LEU:HD23	1.89	0.53
2:B:2859:VAL:O	2:B:2863:ARG:HG2	2.07	0.53
3:C:3047[B]:ARG:HH21	3:C:3113[B]:ASP:CG	2.16	0.53
3:C:3153[B]:LYS:HE3	3:L:3155[B]:MET:O	2.09	0.53
3:C:3264[B]:TYR:C	3:C:3264[B]:TYR:HD1	2.16	0.53
1:D:451:SER:OG	1:D:452:ILE:N	2.40	0.53
3:F:2933[B]:SER:CB	3:F:2936[B]:GLU:CB	2.85	0.53
3:F:3155[B]:MET:O	3:a:3153[B]:LYS:CD	2.56	0.53
3:F:3273[B]:LEU:HB2	3:F:3275[B]:LEU:CD1	2.34	0.53
1:G:704:ASP:HB2	1:G:1118:THR:HG21	1.90	0.53
1:G:931:TRP:NE1	1:G:1048:ASN:HD22	2.06	0.53
2:H:2504:ARG:HD3	2:H:2775:GLY:O	2.08	0.53
3:I:2954[B]:TYR:CD2	3:I:2954[B]:TYR:C	2.86	0.53
3:I:3014[A]:TRP:CD1	3:I:3014[A]:TRP:C	2.85	0.53
3:I:3042[A]:ASP:N	3:I:3042[A]:ASP:OD2	2.41	0.53
3:I:3163[B]:ASN:O	3:R:3147[B]:GLU:CD	2.52	0.53
3:I:3264[B]:TYR:C	3:I:3264[B]:TYR:CD1	2.86	0.53
3:I:3273[B]:LEU:CB	3:I:3275[B]:LEU:CD1	2.85	0.53
3:I:3307[B]:PHE:HE1	3:I:3309[B]:PRO:CG	2.08	0.53
1:J:372:ALA:O	1:J:375:SER:OG	2.23	0.53
1:J:566:ARG:HH12	1:J:803:LYS:HZ3	1.57	0.53
2:K:2567:MET:HE3	2:K:2718:TRP:HB2	1.89	0.53
3:L:3093[B]:HIS:CE1	3:L:3119[B]:HIS:CD2	2.92	0.53
1:M:843:VAL:HG13	1:M:927:PRO:HB2	1.90	0.53
3:O:2975[B]:PHE:H	3:X:2979[B]:GLN:NE2	2.07	0.53
3:O:3240[A]:THR:CG2	3:O:3241[A]:PHE:N	2.71	0.53
3:O:3284[A]:LYS:CE	3:O:3284[A]:LYS:CA	2.85	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3013[B]:ASP:OD1	3:R:3015[B]:THR:HG23	2.08	0.53
3:R:3014[A]:TRP:C	3:R:3014[A]:TRP:CD1	2.85	0.53
3:R:3042[A]:ASP:N	3:R:3042[A]:ASP:OD2	2.41	0.53
3:R:3083[B]:ILE:HD12	3:R:3260[B]:ARG:HB2	1.88	0.53
3:R:3228[A]:VAL:CG2	3:R:3245[A]:PHE:CE2	2.89	0.53
3:R:3240[A]:THR:CG2	3:R:3241[A]:PHE:N	2.71	0.53
3:R:3307[A]:PHE:CD1	3:R:3307[A]:PHE:C	2.85	0.53
1:S:1161:ILE:HB	1:S:1203:MET:HE1	1.89	0.53
1:S:1166:THR:OG1	1:S:1168:GLN:OE1	2.25	0.53
2:T:2265:ILE:HD12	2:T:2443:TYR:CG	2.43	0.53
3:U:3185[A]:TYR:C	3:U:3185[A]:TYR:CD2	2.86	0.53
3:U:3264[A]:TYR:C	3:U:3264[A]:TYR:HD1	2.16	0.53
2:W:2344:LEU:HA	2:W:2345:ASN:O	2.08	0.53
2:W:2470:ALA:HB2	2:W:2476:LEU:HD11	1.91	0.53
2:W:2571:ARG:HG3	2:W:2715:ASP:OD1	2.08	0.53
3:X:2952[A]:ALA:HB3	3:X:2954[A]:TYR:N	2.17	0.53
3:X:3047[A]:ARG:HH21	3:X:3113[A]:ASP:CG	2.16	0.53
3:X:3264[A]:TYR:C	3:X:3264[A]:TYR:HD1	2.16	0.53
1:Y:210:HIS:HA	1:Y:213:VAL:HG22	1.89	0.53
2:Z:2419:ASP:OD1	2:Z:2419:ASP:N	2.41	0.53
3:a:2937[B]:ASN:CB	3:a:3006[B]:LYS:CD	2.86	0.53
3:a:3042[B]:ASP:N	3:a:3042[B]:ASP:OD2	2.41	0.53
3:a:3135[B]:LYS:HG3	3:a:3141[B]:TYR:CD1	2.33	0.53
3:a:3228[A]:VAL:CG2	3:a:3245[A]:PHE:CE2	2.89	0.53
2:c:2235:PRO:HG3	2:c:2240:GLN:NE2	2.22	0.53
3:d:2937[B]:ASN:CB	3:d:3006[B]:LYS:CD	2.85	0.53
3:d:3173[A]:THR:HG22	3:d:3175[A]:TYR:H	1.73	0.53
3:d:3196[B]:THR:OG1	3:d:3199[B]:GLN:CB	2.56	0.53
3:d:3264[A]:TYR:C	3:d:3264[A]:TYR:HD1	2.16	0.53
3:d:3284[B]:LYS:HD3	3:d:3284[B]:LYS:C	2.31	0.53
3:d:3293[A]:LYS:CD	3:d:3294[A]:SER:N	2.64	0.53
3:C:3047[A]:ARG:HH21	3:C:3113[A]:ASP:CG	2.16	0.53
3:C:3169[B]:LYS:CD	3:L:3149[B]:ASN:OD1	2.56	0.53
1:D:194:MET:HA	1:D:200:THR:HA	1.90	0.53
3:F:2937[A]:ASN:CB	3:F:3006[A]:LYS:CD	2.85	0.53
3:F:3014[B]:TRP:C	3:F:3014[B]:TRP:CD1	2.85	0.53
3:F:3047[B]:ARG:HH21	3:F:3113[B]:ASP:CG	2.16	0.53
3:F:3157[B]:PRO:N	3:a:3153[B]:LYS:NZ	2.56	0.53
3:F:3293[B]:LYS:CB	3:F:3294[B]:SER:CB	2.54	0.53
1:G:59:LEU:HD13	1:G:68:TRP:CD1	2.44	0.53
3:I:2952[B]:ALA:H	3:I:2953[B]:GLY:CA	2.04	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3019[A]:HIS:CD2	3:I:3019[A]:HIS:N	2.75	0.53
3:I:3047[B]:ARG:HH21	3:I:3113[B]:ASP:CG	2.16	0.53
3:I:3173[A]:THR:HG22	3:I:3175[A]:TYR:H	1.73	0.53
1:J:561:ARG:HH11	1:J:561:ARG:HG2	1.74	0.53
1:J:1210:LYS:HA	1:J:1211:TYR:HB3	1.91	0.53
1:J:1470:GLU:HG3	1:J:1530:LEU:HD12	1.91	0.53
3:L:2937[B]:ASN:CB	3:L:3006[B]:LYS:CD	2.86	0.53
3:L:3185[A]:TYR:C	3:L:3185[A]:TYR:CD2	2.86	0.53
1:M:914:GLU:OE1	1:M:926:LEU:N	2.34	0.53
3:O:3132[A]:ALA:HB1	3:O:3197[A]:ILE:HD13	1.89	0.53
3:O:3132[B]:ALA:HB1	3:O:3197[B]:ILE:HD13	1.89	0.53
3:O:3151[B]:LEU:HB2	3:O:3175[B]:TYR:HE2	1.68	0.53
2:Q:2161:GLN:NE2	2:Q:2348:THR:HG21	2.24	0.53
2:Q:2528:LYS:HA	2:Q:2536:PHE:HB3	1.90	0.53
3:R:2933[A]:SER:C	3:R:2936[A]:GLU:H	2.15	0.53
3:R:2933[B]:SER:C	3:R:2936[B]:GLU:H	2.16	0.53
3:R:3132[A]:ALA:CB	3:R:3197[A]:ILE:CD1	2.86	0.53
3:R:3293[A]:LYS:CD	3:R:3294[A]:SER:N	2.64	0.53
1:S:494:VAL:HG23	1:S:671:PHE:CZ	2.43	0.53
1:S:1470:GLU:OE1	1:S:1473:ARG:NH1	2.42	0.53
3:U:2954[A]:TYR:C	3:U:2954[A]:TYR:CD2	2.86	0.53
3:U:3047[A]:ARG:HH21	3:U:3113[A]:ASP:CG	2.16	0.53
3:U:3132[B]:ALA:CB	3:U:3197[B]:ILE:CD1	2.86	0.53
3:U:3264[B]:TYR:C	3:U:3264[B]:TYR:HD1	2.16	0.53
3:U:3293[A]:LYS:CB	3:U:3294[A]:SER:CB	2.54	0.53
3:U:3307[B]:PHE:C	3:U:3307[B]:PHE:CD1	2.85	0.53
1:V:195:SER:HB2	1:V:386:ILE:HD11	1.91	0.53
1:V:294:LYS:HA	1:V:297:ARG:HD2	1.90	0.53
2:W:2121:THR:O	2:W:2124:SER:OG	2.24	0.53
3:X:3173[A]:THR:HG22	3:X:3175[A]:TYR:H	1.73	0.53
1:Y:1482:ALA:HB3	1:Y:1489:MET:HE3	1.90	0.53
1:Y:1655:SER:C	3:d:3006[B]:LYS:CD	2.81	0.53
3:a:2933[A]:SER:CB	3:a:2936[A]:GLU:CB	2.86	0.53
3:a:3042[A]:ASP:N	3:a:3042[A]:ASP:OD2	2.41	0.53
3:a:3307[B]:PHE:C	3:a:3307[B]:PHE:CD1	2.85	0.53
1:b:655:TYR:HE1	1:b:693:TYR:HB3	1.73	0.53
1:b:1304:ASP:H	1:b:1305:GLY:HA2	1.73	0.53
3:d:2954[B]:TYR:CD2	3:d:2954[B]:TYR:C	2.86	0.53
3:d:3013[A]:ASP:OD1	3:d:3015[A]:THR:OG1	2.23	0.53
1:A:906:HIS:HA	1:A:909:ILE:HB	1.91	0.53
1:A:1195:ASP:HA	1:A:1196:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3019[B]:HIS:CD2	3:C:3019[B]:HIS:N	2.75	0.53
3:C:3042[B]:ASP:N	3:C:3042[B]:ASP:OD2	2.41	0.53
3:C:3132[B]:ALA:HB1	3:C:3197[B]:ILE:HD13	1.89	0.53
3:C:3132[B]:ALA:CB	3:C:3197[B]:ILE:CD1	2.86	0.53
3:C:3154[B]:PRO:HG2	3:L:2984[B]:THR:HB	1.90	0.53
3:C:3249[B]:GLY:O	3:L:3252[B]:TYR:CE2	2.60	0.53
3:C:3298[B]:ASN:HA	3:C:3299[B]:LEU:HB3	1.88	0.53
3:F:2988[B]:TRP:CZ2	3:a:2975[B]:PHE:HE2	2.26	0.53
3:F:3240[A]:THR:CG2	3:F:3241[A]:PHE:N	2.71	0.53
3:F:3293[A]:LYS:CD	3:F:3294[A]:SER:N	2.64	0.53
1:G:308:LEU:O	1:G:772:ARG:NH2	2.41	0.53
1:G:1543:ILE:HD11	3:L:3272[A]:HIS:HD2	1.73	0.53
3:I:3014[A]:TRP:CZ3	3:I:3119[A]:HIS:ND1	2.77	0.53
3:I:3147[A]:GLU:CD	3:I:3149[A]:ASN:HD21	2.17	0.53
3:L:3132[B]:ALA:HB1	3:L:3197[B]:ILE:HD13	1.89	0.53
1:M:415:VAL:HB	1:M:697:ALA:HB2	1.90	0.53
1:M:545:PHE:O	1:M:561:ARG:NH2	2.38	0.53
1:M:907:ARG:NH1	1:M:1050:ASP:OD1	2.42	0.53
3:O:3109[B]:TYR:CG	3:X:2969[B]:TYR:C	2.82	0.53
3:O:3255[B]:PRO:HD3	3:X:3158[B]:PHE:C	2.33	0.53
3:O:3284[A]:LYS:HD3	3:O:3284[A]:LYS:C	2.32	0.53
1:P:61:GLY:HA3	1:P:352:TRP:CB	2.37	0.53
1:P:1196:ILE:O	1:P:1199:VAL:HG12	2.09	0.53
2:Q:2795:ILE:O	2:Q:2799:LYS:HG3	2.08	0.53
3:R:2933[A]:SER:HA	3:R:2935[A]:ILE:CD1	2.38	0.53
3:R:2947[B]:ALA:HA	3:R:2949[B]:LYS:HB3	1.89	0.53
3:R:3013[A]:ASP:OD1	3:R:3015[A]:THR:HG23	2.08	0.53
3:R:3033[A]:PHE:HD1	3:R:3114[A]:PRO:HB2	1.72	0.53
3:R:3047[A]:ARG:HH21	3:R:3113[A]:ASP:CG	2.16	0.53
3:R:3132[B]:ALA:HB1	3:R:3197[B]:ILE:HD13	1.89	0.53
3:R:3264[B]:TYR:C	3:R:3264[B]:TYR:CD1	2.86	0.53
1:S:410:LYS:HE2	1:S:652:GLY:HA2	1.90	0.53
1:S:747:PHE:HB2	1:S:799:ARG:HB3	1.91	0.53
1:S:792:MET:O	1:S:796:TYR:OH	2.16	0.53
3:U:2971[B]:ASP:O	3:d:3247[B]:VAL:CB	2.56	0.53
3:U:3293[B]:LYS:CD	3:U:3294[B]:SER:N	2.64	0.53
1:V:474:LEU:HD23	1:V:474:LEU:H	1.74	0.53
3:X:2933[A]:SER:C	3:X:2936[A]:GLU:H	2.16	0.53
3:X:2937[B]:ASN:CB	3:X:3006[B]:LYS:CD	2.86	0.53
3:X:3081[B]:PHE:C	3:X:3081[B]:PHE:CD1	2.87	0.53
3:X:3151[A]:LEU:HB2	3:X:3175[A]:TYR:HE2	1.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3196[A]:THR:OG1	3:X:3199[A]:GLN:CB	2.56	0.53
3:X:3273[B]:LEU:CB	3:X:3275[B]:LEU:CD1	2.86	0.53
1:Y:124:TYR:O	1:Y:137:ARG:NH2	2.41	0.53
1:Y:1576:THR:OG1	1:Y:1581:GLU:HB2	2.09	0.53
3:a:3081[B]:PHE:CD1	3:a:3081[B]:PHE:C	2.87	0.53
3:a:3293[A]:LYS:CG	3:a:3294[A]:SER:HB2	2.36	0.53
1:b:127:GLU:OE1	1:b:202:TYR:HB3	2.09	0.53
1:b:949:ASP:HB2	1:b:953:GLU:CB	2.38	0.53
1:b:1140:ASN:OD1	1:b:1239:GLY:N	2.36	0.53
1:b:1304:ASP:N	1:b:1305:GLY:HA2	2.23	0.53
1:b:1639:LYS:HE2	4:QA:1:NAG:H61	1.91	0.53
2:c:2680:HIS:NE2	2:c:2684:HIS:CD2	2.75	0.53
1:A:1082:SER:OG	1:A:1083:PRO:HD3	2.08	0.53
3:C:2933[B]:SER:CB	3:C:2936[B]:GLU:CB	2.86	0.53
3:C:2954[B]:TYR:CD2	3:C:2954[B]:TYR:C	2.86	0.53
3:C:3153[B]:LYS:HE3	3:L:3158[B]:PHE:HD2	1.52	0.53
3:C:3183[A]:LEU:N	3:C:3184[A]:ASN:HA	2.11	0.53
3:C:3228[A]:VAL:CG2	3:C:3245[A]:PHE:CE2	2.89	0.53
1:D:704:ASP:OD1	1:D:705:THR:N	2.41	0.53
3:F:3013[A]:ASP:OD1	3:F:3015[A]:THR:HG23	2.08	0.53
3:F:3132[A]:ALA:CB	3:F:3197[A]:ILE:CD1	2.86	0.53
1:G:177:VAL:HG11	1:G:358:TYR:CZ	2.44	0.53
3:I:2954[A]:TYR:C	3:I:2954[A]:TYR:CD2	2.86	0.53
3:I:3013[A]:ASP:OD1	3:I:3015[A]:THR:HG23	2.08	0.53
3:I:3019[B]:HIS:CD2	3:I:3019[B]:HIS:N	2.75	0.53
3:I:3107[B]:LEU:CG	3:R:2975[B]:PHE:CD1	2.88	0.53
3:I:3153[B]:LYS:O	3:R:3154[B]:PRO:C	2.45	0.53
1:J:830:ASN:OD1	1:J:831:VAL:N	2.41	0.53
1:J:949:ASP:OD1	1:J:950:ALA:N	2.40	0.53
1:J:993:ASN:OD1	1:J:1136:ARG:NH2	2.42	0.53
3:L:3132[A]:ALA:HB1	3:L:3197[A]:ILE:HD13	1.89	0.53
3:L:3132[B]:ALA:CB	3:L:3197[B]:ILE:CD1	2.86	0.53
3:L:3151[B]:LEU:HB2	3:L:3175[B]:TYR:HE2	1.67	0.53
3:L:3293[A]:LYS:CD	3:L:3294[A]:SER:N	2.64	0.53
1:M:1170:MET:HB3	1:M:1203:MET:HE2	1.91	0.53
1:M:1587:ALA:HA	1:M:1614:GLU:HG2	1.91	0.53
3:O:2947[B]:ALA:HA	3:O:2949[B]:LYS:HB3	1.89	0.53
3:O:2968[B]:GLN:HG2	3:X:2984[B]:THR:OG1	2.07	0.53
3:O:3013[B]:ASP:OD1	3:O:3015[B]:THR:HG23	2.08	0.53
3:O:3264[B]:TYR:C	3:O:3264[B]:TYR:CD1	2.86	0.53
1:P:494:VAL:HG13	1:P:631:TRP:HZ3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3284[A]:LYS:HD3	3:R:3284[A]:LYS:C	2.31	0.53
2:T:2795:ILE:O	2:T:2798:GLN:HG2	2.08	0.53
3:U:3162[B]:ASP:OD1	3:d:3260[B]:ARG:CZ	2.55	0.53
3:U:3255[B]:PRO:HD3	3:d:3253[B]:GLU:N	2.23	0.53
3:U:3257[B]:ALA:N	3:d:2968[B]:GLN:CA	2.16	0.53
3:U:3269[A]:SER:O	3:U:3272[A]:HIS:HB2	2.09	0.53
1:V:449:ASP:OD1	1:V:1280:GLN:NE2	2.42	0.53
1:V:483:GLY:HA2	1:V:773:PHE:CZ	2.44	0.53
1:V:732:GLY:N	1:V:819:ILE:O	2.30	0.53
3:X:3013[B]:ASP:OD1	3:X:3015[B]:THR:HG23	2.08	0.53
3:X:3173[B]:THR:HG22	3:X:3175[B]:TYR:H	1.73	0.53
1:Y:17:ASN:OD1	1:Y:85:SER:HB3	2.09	0.53
1:Y:1472:GLN:OE1	1:Y:1475:ARG:NH1	2.42	0.53
3:a:2947[B]:ALA:HA	3:a:2949[B]:LYS:HB3	1.89	0.53
3:a:3132[B]:ALA:HB1	3:a:3197[B]:ILE:HD13	1.89	0.53
3:a:3185[A]:TYR:C	3:a:3185[A]:TYR:CD2	2.86	0.53
3:a:3240[A]:THR:CG2	3:a:3241[A]:PHE:N	2.71	0.53
3:a:3269[B]:SER:O	3:a:3272[B]:HIS:HB2	2.09	0.53
1:b:127:GLU:CD	1:b:128:ILE:HA	2.33	0.53
1:b:262:LYS:NZ	1:b:795:GLU:OE1	2.42	0.53
3:d:2932[A]:PRO:CA	3:d:2935[A]:ILE:HD12	2.30	0.53
3:d:2933[A]:SER:HA	3:d:2935[A]:ILE:CD1	2.38	0.53
3:d:3176[B]:LYS:H	3:d:3176[B]:LYS:CE	2.17	0.53
1:A:1171:LYS:HG2	1:A:1173:GLY:H	1.73	0.53
3:C:2952[B]:ALA:HB3	3:C:2954[B]:TYR:N	2.17	0.53
3:C:2954[A]:TYR:CD2	3:C:2954[A]:TYR:C	2.86	0.53
3:C:3014[B]:TRP:CZ3	3:C:3119[B]:HIS:ND1	2.77	0.53
3:C:3196[A]:THR:OG1	3:C:3199[A]:GLN:CB	2.56	0.53
3:C:3273[B]:LEU:HB2	3:C:3275[B]:LEU:CD1	2.34	0.53
1:D:535:PRO:HG3	1:D:985:PHE:CZ	2.44	0.53
1:D:603:HIS:O	1:D:606:ILE:HG22	2.08	0.53
2:E:2746:MET:HE2	2:E:2765:PRO:HG3	1.91	0.53
3:F:3264[A]:TYR:C	3:F:3264[A]:TYR:HD1	2.16	0.53
3:I:3135[A]:LYS:HG3	3:I:3141[A]:TYR:CD1	2.33	0.53
3:I:3173[B]:THR:HG23	3:R:3173[B]:THR:CB	2.37	0.53
3:L:3014[B]:TRP:CZ3	3:L:3119[B]:HIS:ND1	2.77	0.53
3:L:3047[A]:ARG:HH21	3:L:3113[A]:ASP:CG	2.16	0.53
1:M:308:LEU:O	1:M:772:ARG:NH2	2.42	0.53
1:P:956:PRO:HB2	1:P:957:ASN:C	2.34	0.53
1:P:1315:GLY:HA3	1:P:1601:TRP:CB	2.39	0.53
1:S:831:VAL:HG12	1:S:832:LYS:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1638:SER:OG	1:S:1639:LYS:N	2.41	0.53
2:T:2571:ARG:NH1	2:T:2776:TYR:OH	2.39	0.53
3:U:3014[A]:TRP:CD1	3:U:3014[A]:TRP:C	2.85	0.53
3:U:3014[B]:TRP:CZ3	3:U:3119[B]:HIS:ND1	2.77	0.53
3:U:3269[B]:SER:O	3:U:3272[B]:HIS:HB2	2.09	0.53
1:V:568:PHE:N	1:V:568:PHE:HD1	2.07	0.53
1:V:570:GLN:HB3	1:V:571:PRO:HD3	1.91	0.53
1:V:1166:THR:N	1:V:1167:ASP:HA	2.24	0.53
2:W:2635:TYR:HB2	1:Y:109:LEU:HD21	1.89	0.53
3:X:3081[A]:PHE:CD1	3:X:3081[A]:PHE:C	2.87	0.53
3:X:3132[B]:ALA:HB1	3:X:3197[B]:ILE:HD13	1.89	0.53
3:X:3132[B]:ALA:CB	3:X:3197[B]:ILE:CD1	2.86	0.53
3:X:3147[A]:GLU:CD	3:X:3149[A]:ASN:HD21	2.17	0.53
3:X:3240[B]:THR:CG2	3:X:3241[B]:PHE:N	2.71	0.53
1:Y:1013:ILE:HD11	1:Y:1175:PHE:CD2	2.44	0.53
2:Z:2822:LYS:HG2	2:Z:2831:GLU:HA	1.90	0.53
2:Z:2877:ILE:H	1:b:1078:ARG:NH2	2.07	0.53
3:a:2952[B]:ALA:HB3	3:a:2954[B]:TYR:N	2.18	0.53
3:a:3269[A]:SER:O	3:a:3272[A]:HIS:HB2	2.09	0.53
3:d:3081[B]:PHE:C	3:d:3081[B]:PHE:CD1	2.87	0.53
1:A:398:ARG:HH21	1:A:663:GLU:CD	2.16	0.53
2:B:2553:ALA:H	2:B:2554:PRO:HD3	1.74	0.53
2:B:2624:PHE:O	2:B:2638:ARG:NH2	2.34	0.53
3:C:2933[A]:SER:C	3:C:2936[A]:GLU:H	2.16	0.53
3:C:2945[B]:VAL:HG22	3:C:2954[B]:TYR:HB2	1.91	0.53
3:C:3081[B]:PHE:CD1	3:C:3081[B]:PHE:C	2.87	0.53
3:C:3149[B]:ASN:CB	3:L:3163[B]:ASN:HD22	2.01	0.53
3:C:3253[B]:GLU:HB3	3:L:3252[B]:TYR:HB3	1.91	0.53
2:E:2545:SER:CA	2:E:2546:LEU:HB2	2.34	0.53
3:F:2949[B]:LYS:C	3:F:2953[B]:GLY:H	2.17	0.53
3:F:3081[B]:PHE:CD1	3:F:3081[B]:PHE:C	2.87	0.53
3:F:3155[B]:MET:C	3:a:3153[B]:LYS:HB3	2.33	0.53
1:G:1171:LYS:HG2	1:G:1173:GLY:H	1.73	0.53
2:H:2394:VAL:HG11	2:H:2451:LEU:HD12	1.90	0.53
2:H:2506:ARG:NE	2:H:2578:GLU:OE2	2.39	0.53
3:I:3252[B]:TYR:O	3:R:2976[B]:ALA:HB3	2.08	0.53
1:J:93:ASP:HA	1:J:212:ASN:HD21	1.73	0.53
1:J:929:TRP:O	1:J:1048:ASN:ND2	2.41	0.53
2:K:2568:HIS:HD2	2:K:2718:TRP:HH2	1.56	0.53
3:L:2933[B]:SER:HA	3:L:2935[B]:ILE:CD1	2.38	0.53
3:L:3042[A]:ASP:N	3:L:3042[A]:ASP:OD2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3173[A]:THR:HG22	3:L:3175[A]:TYR:H	1.73	0.53
3:L:3264[A]:TYR:HD1	3:L:3264[A]:TYR:C	2.16	0.53
1:M:245:GLU:HG2	1:M:249:ARG:HH11	1.73	0.53
1:M:372:ALA:O	1:M:375:SER:OG	2.26	0.53
1:M:956:PRO:HB2	1:M:958:PRO:HD3	1.91	0.53
3:R:2951[A]:ASP:O	3:R:2956[A]:LYS:HE2	2.09	0.53
3:R:3173[A]:THR:HG22	3:R:3174[A]:GLY:H	1.67	0.53
3:R:3176[B]:LYS:H	3:R:3176[B]:LYS:CE	2.17	0.53
3:R:3284[B]:LYS:CE	3:R:3284[B]:LYS:CA	2.85	0.53
1:S:119:LYS:HD3	1:S:120:LYS:HD3	1.91	0.53
3:U:3081[A]:PHE:C	3:U:3081[A]:PHE:CD1	2.87	0.53
3:U:3230[B]:PHE:H	3:U:3243[B]:GLY:CA	2.22	0.53
2:W:2107:LEU:O	2:W:2111:GLN:HB2	2.09	0.53
2:W:2570:HIS:CD2	9:W:3002:CUO:O1	2.62	0.53
3:X:2947[B]:ALA:HA	3:X:2949[B]:LYS:HB3	1.89	0.53
3:X:2949[A]:LYS:C	3:X:2953[A]:GLY:H	2.17	0.53
3:X:3120[B]:HIS:HA	3:X:3123[B]:THR:HG1	1.72	0.53
3:X:3264[A]:TYR:C	3:X:3264[A]:TYR:CD1	2.86	0.53
3:X:3298[A]:ASN:HA	3:X:3299[A]:LEU:HB3	1.88	0.53
3:a:3081[A]:PHE:C	3:a:3081[A]:PHE:CD1	2.87	0.53
3:a:3082[A]:GLU:OE2	3:a:3086[A]:GLU:HB2	2.07	0.53
3:a:3284[A]:LYS:HD3	3:a:3284[A]:LYS:C	2.32	0.53
2:c:2602:LEU:HG	2:c:2603:PRO:HD2	1.91	0.53
3:d:2945[A]:VAL:HG22	3:d:2954[A]:TYR:HB2	1.91	0.53
3:d:2949[B]:LYS:C	3:d:2953[B]:GLY:H	2.17	0.53
3:d:3185[B]:TYR:C	3:d:3185[B]:TYR:CD2	2.86	0.53
3:d:3196[A]:THR:OG1	3:d:3199[A]:GLN:CB	2.56	0.53
1:A:892:TYR:CE2	1:A:1184:MET:HG3	2.44	0.53
2:B:2326:ILE:HG13	1:D:1650:ILE:HG23	1.91	0.53
3:C:2961[A]:HIS:NE2	3:C:2980[A]:HIS:CE1	2.73	0.53
3:C:3132[A]:ALA:HB1	3:C:3197[A]:ILE:HD13	1.89	0.53
3:C:3150[B]:LYS:H	3:L:3169[B]:LYS:CG	2.12	0.53
3:C:3248[B]:LEU:CD2	3:L:2971[B]:ASP:OD2	2.54	0.53
1:D:301:ARG:HD2	1:D:361:GLU:OE2	2.09	0.53
1:D:589:GLN:O	1:D:651:ARG:NH1	2.42	0.53
1:D:675:SER:O	1:D:679:ASN:ND2	2.42	0.53
1:D:1470:GLU:HG3	1:D:1530:LEU:HD12	1.91	0.53
3:F:3160[B]:SER:HB2	3:a:2982[B]:MET:HB3	1.90	0.53
3:F:3264[B]:TYR:C	3:F:3264[B]:TYR:HD1	2.16	0.53
3:F:3269[A]:SER:O	3:F:3272[A]:HIS:HB2	2.09	0.53
3:F:3273[A]:LEU:CB	3:F:3275[A]:LEU:CD1	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:ASP:OD1	1:G:168:PHE:N	2.42	0.53
1:G:1315:GLY:HA3	1:G:1601:TRP:CB	2.39	0.53
3:I:2951[B]:ASP:O	3:I:2956[B]:LYS:HE2	2.09	0.53
3:I:3013[B]:ASP:OD1	3:I:3015[B]:THR:HG23	2.08	0.53
3:I:3230[B]:PHE:H	3:I:3243[B]:GLY:CA	2.22	0.53
1:J:465:PRO:HG2	1:J:467:LYS:HE2	1.89	0.53
1:J:926:LEU:HD12	1:J:927:PRO:HD2	1.91	0.53
2:K:2157:LEU:O	2:K:2160:VAL:HG22	2.09	0.53
3:L:2945[B]:VAL:HG22	3:L:2954[B]:TYR:HB2	1.91	0.53
3:L:3013[A]:ASP:OD1	3:L:3015[A]:THR:HG23	2.08	0.53
3:L:3264[B]:TYR:C	3:L:3264[B]:TYR:HD1	2.16	0.53
1:M:1075:GLU:HG2	2:Q:2900:SER:HA	1.90	0.53
1:M:1215:LEU:HD23	1:M:1231:VAL:HG11	1.91	0.53
3:O:2960[A]:PHE:CD2	3:O:3157[A]:PRO:CG	2.74	0.53
3:O:3264[A]:TYR:C	3:O:3264[A]:TYR:CD1	2.86	0.53
1:P:804:ASP:OD1	1:P:805:VAL:N	2.42	0.53
3:R:3147[A]:GLU:CD	3:R:3149[A]:ASN:HD21	2.17	0.53
1:S:686:HIS:CE1	1:S:698:GLU:HB3	2.44	0.53
3:U:2945[A]:VAL:HG22	3:U:2954[A]:TYR:HB2	1.91	0.53
3:U:3013[A]:ASP:OD1	3:U:3015[A]:THR:HG23	2.08	0.53
3:U:3014[A]:TRP:CZ3	3:U:3119[A]:HIS:ND1	2.77	0.53
3:U:3132[A]:ALA:CB	3:U:3197[A]:ILE:CD1	2.86	0.53
3:U:3196[A]:THR:OG1	3:U:3199[A]:GLN:CB	2.56	0.53
1:V:579:LEU:H	1:V:579:LEU:HD12	1.74	0.53
2:W:2115:SER:OG	2:W:2116:SER:N	2.42	0.53
3:X:2945[A]:VAL:HG22	3:X:2954[A]:TYR:HB2	1.91	0.53
3:X:3230[A]:PHE:H	3:X:3243[A]:GLY:CA	2.22	0.53
2:Z:2382:GLU:O	2:Z:2386:ARG:HG3	2.09	0.53
3:a:2945[B]:VAL:HG22	3:a:2954[B]:TYR:HB2	1.91	0.53
3:a:3013[B]:ASP:OD1	3:a:3015[B]:THR:HG23	2.08	0.53
3:a:3147[A]:GLU:CD	3:a:3149[A]:ASN:HD21	2.17	0.53
3:a:3230[B]:PHE:H	3:a:3243[B]:GLY:CA	2.22	0.53
1:b:570:GLN:HB3	1:b:571:PRO:HA	1.91	0.53
3:d:2949[A]:LYS:C	3:d:2953[A]:GLY:H	2.17	0.53
3:d:3176[B]:LYS:C	3:d:3177[B]:SER:HG	2.07	0.53
3:d:3264[A]:TYR:C	3:d:3264[A]:TYR:CD1	2.86	0.53
1:A:304:ALA:HB3	1:A:360:HIS:HB3	1.91	0.53
1:A:1138:ALA:HA	1:A:1240:ILE:HG22	1.91	0.53
3:C:3019[A]:HIS:CD2	3:C:3019[A]:HIS:N	2.75	0.53
3:C:3081[A]:PHE:C	3:C:3081[A]:PHE:CD1	2.87	0.53
3:C:3169[B]:LYS:CG	3:L:3150[B]:LYS:H	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3264[A]:TYR:C	3:C:3264[A]:TYR:CD1	2.86	0.53
3:F:2945[A]:VAL:HG22	3:F:2954[A]:TYR:HB2	1.91	0.53
3:F:2945[B]:VAL:HG22	3:F:2954[B]:TYR:HB2	1.91	0.53
3:F:3013[A]:ASP:OD1	3:F:3015[A]:THR:OG1	2.23	0.53
3:F:3014[B]:TRP:CZ3	3:F:3119[B]:HIS:ND1	2.77	0.53
3:F:3081[A]:PHE:C	3:F:3081[A]:PHE:CD1	2.87	0.53
3:F:3132[A]:ALA:HB1	3:F:3197[A]:ILE:HD13	1.89	0.53
1:G:1498:ASN:ND2	1:G:1500:THR:O	2.42	0.53
2:H:2094:ARG:HH21	2:K:2094:ARG:HH21	1.57	0.53
3:I:3042[B]:ASP:N	3:I:3042[B]:ASP:OD2	2.41	0.53
3:I:3173[B]:THR:HG22	3:I:3175[B]:TYR:H	1.73	0.53
3:I:3298[A]:ASN:HA	3:I:3299[A]:LEU:HB3	1.88	0.53
1:J:902:PHE:CD2	1:J:1012:GLU:HG3	2.44	0.53
1:J:956:PRO:HB2	1:J:957:ASN:C	2.33	0.53
2:K:2643:GLU:O	2:K:2647:LEU:HB2	2.09	0.53
3:L:2954[B]:TYR:C	3:L:2954[B]:TYR:CD2	2.86	0.53
3:L:3147[B]:GLU:CD	3:L:3149[B]:ASN:HD21	2.17	0.53
1:M:664:VAL:O	1:M:689:PRO:HD2	2.09	0.53
3:O:2945[B]:VAL:HG22	3:O:2954[B]:TYR:HB2	1.91	0.53
3:O:2949[B]:LYS:C	3:O:2953[B]:GLY:H	2.17	0.53
3:O:3013[A]:ASP:OD1	3:O:3015[A]:THR:HG23	2.08	0.53
1:P:483:GLY:HA3	1:P:771:TRP:CE3	2.44	0.53
1:P:1152:LYS:NZ	1:P:1183:GLU:HG2	2.23	0.53
1:P:1348:TRP:HD1	1:P:1403:LEU:HD13	1.72	0.53
3:R:3047[B]:ARG:HH21	3:R:3113[B]:ASP:CG	2.16	0.53
3:R:3173[B]:THR:HG22	3:R:3175[B]:TYR:H	1.73	0.53
3:R:3230[A]:PHE:H	3:R:3243[A]:GLY:CA	2.22	0.53
3:R:3287[B]:ILE:O	3:R:3287[B]:ILE:HG23	2.09	0.53
3:U:2937[B]:ASN:CB	3:U:3006[B]:LYS:CD	2.86	0.53
3:U:3150[B]:LYS:HG2	3:d:3156[B]:MET:CG	2.38	0.53
3:U:3230[A]:PHE:H	3:U:3243[A]:GLY:CA	2.22	0.53
3:U:3255[B]:PRO:C	3:d:2974[B]:ALA:O	2.52	0.53
3:U:3293[B]:LYS:CG	3:U:3294[B]:SER:HB2	2.36	0.53
1:V:1170:MET:HB3	1:V:1203:MET:HE2	1.90	0.53
3:X:2945[B]:VAL:HG22	3:X:2954[B]:TYR:HB2	1.91	0.53
3:X:3132[A]:ALA:HB1	3:X:3197[A]:ILE:HD13	1.89	0.53
3:X:3264[B]:TYR:C	3:X:3264[B]:TYR:HD1	2.16	0.53
3:X:3269[A]:SER:O	3:X:3272[A]:HIS:HB2	2.09	0.53
3:a:3014[A]:TRP:CZ3	3:a:3119[A]:HIS:ND1	2.77	0.53
1:b:534:ASP:HB2	1:b:541:LYS:HE2	1.91	0.53
1:b:675:SER:HB3	1:b:676:PRO:CD	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:979:LEU:H	1:b:979:LEU:HD13	1.73	0.53
2:c:2851:ASN:OD1	2:c:2851:ASN:N	2.39	0.53
3:d:2954[A]:TYR:C	3:d:2954[A]:TYR:CD2	2.86	0.53
3:d:3042[B]:ASP:N	3:d:3042[B]:ASP:OD2	2.41	0.53
3:d:3047[B]:ARG:HH21	3:d:3113[B]:ASP:CG	2.16	0.53
1:A:121:ASN:HD22	1:A:124:TYR:H	1.57	0.52
1:A:857:ALA:HB1	1:A:920:ASN:O	2.09	0.52
1:A:1086:LEU:HB3	1:A:1090:ILE:CD1	2.39	0.52
3:C:3172[B]:SER:HG	3:L:3149[B]:ASN:C	2.17	0.52
3:C:3176[B]:LYS:H	3:C:3176[B]:LYS:CE	2.17	0.52
3:C:3240[B]:THR:CG2	3:C:3241[B]:PHE:N	2.71	0.52
2:E:2166:LEU:HA	2:E:2169:HIS:HB2	1.91	0.52
2:E:2539:ILE:O	2:E:2573:TYR:OH	2.17	0.52
3:F:2965[B]:LEU:H	3:a:3221[B]:ALA:CB	1.82	0.52
3:F:2975[B]:PHE:CE1	3:a:3107[B]:LEU:CG	2.90	0.52
3:F:3107[B]:LEU:HD12	3:a:2973[B]:THR:C	2.34	0.52
3:F:3157[B]:PRO:HD3	3:a:3254[B]:MET:CE	2.39	0.52
3:F:3230[A]:PHE:H	3:F:3243[A]:GLY:CA	2.22	0.52
3:F:3284[B]:LYS:CE	3:F:3284[B]:LYS:CA	2.85	0.52
1:G:564:ASP:HA	1:G:609:TRP:O	2.09	0.52
2:H:2359:ASN:OD1	2:H:2359:ASN:N	2.42	0.52
3:I:2933[B]:SER:HA	3:I:2935[B]:ILE:CD1	2.38	0.52
3:I:2960[B]:PHE:CD1	3:I:2960[B]:PHE:N	2.72	0.52
3:I:3120[B]:HIS:CD2	3:R:2969[B]:TYR:CZ	2.97	0.52
3:I:3287[B]:ILE:O	3:I:3287[B]:ILE:HG23	2.10	0.52
1:J:43:GLU:HG3	1:J:44:PRO:HA	1.92	0.52
2:K:2539:ILE:O	2:K:2573:TYR:OH	2.11	0.52
3:L:3081[B]:PHE:C	3:L:3081[B]:PHE:CD1	2.87	0.52
1:M:103:GLU:OE2	1:M:106:GLN:NE2	2.42	0.52
1:M:972:SER:HA	1:M:1028:VAL:HG22	1.90	0.52
2:N:2648:ALA:HA	2:N:2654:SER:HB3	1.90	0.52
2:N:2716:ARG:NH2	2:N:2780:HIS:O	2.39	0.52
3:O:3042[A]:ASP:N	3:O:3042[A]:ASP:OD2	2.41	0.52
3:O:3132[B]:ALA:CB	3:O:3197[B]:ILE:CD1	2.87	0.52
3:O:3157[B]:PRO:HA	3:X:3150[B]:LYS:C	2.33	0.52
3:O:3169[B]:LYS:NZ	3:X:3148[B]:ILE:N	2.56	0.52
3:O:3176[A]:LYS:H	3:O:3176[A]:LYS:CE	2.17	0.52
3:O:3273[A]:LEU:HB2	3:O:3275[A]:LEU:CD1	2.34	0.52
2:Q:2403:PHE:CZ	2:Q:2480:LEU:HD11	2.44	0.52
3:R:2945[A]:VAL:HG22	3:R:2954[A]:TYR:HB2	1.91	0.52
3:R:2945[B]:VAL:HG22	3:R:2954[B]:TYR:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2949[A]:LYS:C	3:R:2953[A]:GLY:H	2.17	0.52
3:R:2952[A]:ALA:CA	3:R:2956[A]:LYS:HB3	2.38	0.52
3:R:2954[A]:TYR:CD2	3:R:2954[A]:TYR:C	2.86	0.52
3:R:3014[B]:TRP:CZ3	3:R:3119[B]:HIS:ND1	2.77	0.52
3:R:3269[B]:SER:O	3:R:3272[B]:HIS:HB2	2.09	0.52
3:U:2951[B]:ASP:O	3:U:2956[B]:LYS:HE2	2.09	0.52
3:U:2975[B]:PHE:CB	3:d:3256[B]:TRP:CG	2.70	0.52
3:U:3081[B]:PHE:C	3:U:3081[B]:PHE:CD1	2.87	0.52
3:U:3132[A]:ALA:HB1	3:U:3197[A]:ILE:HD13	1.89	0.52
1:V:980:TYR:HE2	1:V:1021:LEU:HB3	1.73	0.52
2:W:2684:HIS:NE2	2:W:2711:HIS:HE1	2.07	0.52
1:Y:915:ASN:ND2	1:Y:1093:ASP:OD1	2.40	0.52
2:Z:2237:LEU:H	2:Z:2237:LEU:HD22	1.74	0.52
3:a:2931[A]:THR:HG1	3:a:2934[A]:GLU:CD	2.01	0.52
3:a:3115[A]:LEU:O	3:a:3115[A]:LEU:HD22	2.10	0.52
3:a:3132[A]:ALA:CB	3:a:3197[A]:ILE:CD1	2.86	0.52
3:a:3173[A]:THR:HG22	3:a:3175[A]:TYR:H	1.73	0.52
1:b:931:TRP:CZ3	1:b:995:ILE:HD11	2.44	0.52
2:c:2768:LEU:HA	2:c:2774:LEU:HD11	1.91	0.52
2:c:2869:ALA:O	2:c:2875:SER:OG	2.24	0.52
3:d:2933[A]:SER:CB	3:d:2936[A]:GLU:CB	2.85	0.52
3:d:2933[A]:SER:C	3:d:2936[A]:GLU:H	2.15	0.52
3:d:2945[B]:VAL:HG22	3:d:2954[B]:TYR:HB2	1.91	0.52
3:d:3014[B]:TRP:CZ3	3:d:3119[B]:HIS:ND1	2.77	0.52
3:d:3132[A]:ALA:CB	3:d:3197[A]:ILE:CD1	2.86	0.52
3:d:3188[A]:ASP:N	3:d:3188[A]:ASP:OD2	2.36	0.52
3:C:2932[B]:PRO:CA	3:C:2935[B]:ILE:HD12	2.31	0.52
3:C:2933[A]:SER:CB	3:C:2936[A]:GLU:CB	2.86	0.52
3:C:2949[B]:LYS:C	3:C:2953[B]:GLY:H	2.17	0.52
3:C:2969[B]:TYR:HA	3:L:2989[B]:HIS:CE1	2.44	0.52
3:C:3272[A]:HIS:HD2	1:D:1543:ILE:HD11	1.74	0.52
1:D:104:LEU:HD23	1:D:123:PHE:CE2	2.43	0.52
2:E:2795:ILE:O	2:E:2799:LYS:HG3	2.08	0.52
3:F:3269[B]:SER:O	3:F:3272[B]:HIS:HB2	2.09	0.52
1:G:871:GLN:NE2	1:G:964:ILE:HG13	2.24	0.52
1:G:891:LYS:HB2	1:G:892:TYR:CD2	2.44	0.52
1:G:1324:ARG:NH1	1:G:1519:TYR:HB3	2.24	0.52
1:G:1404:TYR:O	1:G:1407:THR:OG1	2.28	0.52
1:G:1528:ASP:N	1:G:1528:ASP:OD1	2.42	0.52
3:I:2975[B]:PHE:CE1	3:R:3107[B]:LEU:HG	2.43	0.52
3:I:3081[A]:PHE:C	3:I:3081[A]:PHE:CD1	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3092[A]:ILE:CG2	3:I:3096[A]:VAL:CG2	2.87	0.52
3:I:3230[A]:PHE:H	3:I:3243[A]:GLY:CA	2.22	0.52
3:I:3293[B]:LYS:CG	3:I:3294[B]:SER:HB2	2.36	0.52
1:J:914:GLU:OE1	1:J:926:LEU:N	2.40	0.52
1:J:1432:SER:OG	1:J:1567:ASP:OD2	2.27	0.52
2:K:2740:ASP:OD1	2:K:2740:ASP:N	2.41	0.52
3:L:3092[B]:ILE:CG2	3:L:3096[B]:VAL:CG2	2.88	0.52
3:L:3173[B]:THR:HG22	3:L:3175[B]:TYR:H	1.73	0.52
3:O:3014[A]:TRP:CZ3	3:O:3119[A]:HIS:ND1	2.77	0.52
3:O:3081[A]:PHE:CD1	3:O:3081[A]:PHE:C	2.87	0.52
3:O:3269[A]:SER:O	3:O:3272[A]:HIS:HB2	2.09	0.52
1:P:566:ARG:N	1:P:567:LEU:HA	2.25	0.52
1:P:597:VAL:HG12	1:P:773:PHE:CD1	2.45	0.52
1:P:899:MET:HE2	1:P:1012:GLU:CD	2.34	0.52
1:P:1339:SER:HB2	1:P:1340:GLY:HA2	1.90	0.52
1:P:1551:ASP:HB3	1:P:1652:PHE:HE1	1.73	0.52
3:R:3092[B]:ILE:CG2	3:R:3096[B]:VAL:CG2	2.88	0.52
3:R:3269[A]:SER:O	3:R:3272[A]:HIS:HB2	2.09	0.52
3:R:3298[A]:ASN:HA	3:R:3299[A]:LEU:HB3	1.88	0.52
1:S:785:LEU:HD13	1:S:792:MET:HA	1.90	0.52
1:S:1301:PRO:HA	1:S:1308:VAL:HA	1.90	0.52
3:U:2933[B]:SER:CB	3:U:2936[B]:GLU:CB	2.85	0.52
3:U:2935[B]:ILE:CD1	3:U:2935[B]:ILE:N	2.73	0.52
3:U:3264[A]:TYR:C	3:U:3264[A]:TYR:CD1	2.86	0.52
1:V:306:PHE:HB3	1:V:308:LEU:HD13	1.91	0.52
1:V:1542:ARG:O	1:V:1546:LYS:HG2	2.09	0.52
2:W:2533:ASP:OD1	2:W:2533:ASP:N	2.41	0.52
3:X:2954[A]:TYR:C	3:X:2954[A]:TYR:CD2	2.86	0.52
3:X:3114[A]:PRO:CD	3:X:3115[A]:LEU:N	2.72	0.52
3:X:3293[B]:LYS:CD	3:X:3294[B]:SER:N	2.64	0.52
1:Y:897:HIS:HB3	1:Y:899:MET:SD	2.50	0.52
3:a:3120[B]:HIS:HA	3:a:3123[B]:THR:HG1	1.71	0.52
3:a:3230[A]:PHE:H	3:a:3243[A]:GLY:CA	2.22	0.52
1:b:1059:LEU:O	1:b:1063:ARG:N	2.40	0.52
3:d:3230[A]:PHE:H	3:d:3243[A]:GLY:CA	2.22	0.52
3:d:3269[B]:SER:O	3:d:3272[B]:HIS:HB2	2.09	0.52
3:d:3298[A]:ASN:CB	3:d:3300[A]:LEU:CD2	2.61	0.52
4:7:1:NAG:C6	4:7:2:NAG:HN2	2.22	0.52
1:A:1075:GLU:HG2	2:E:2900:SER:HA	1.91	0.52
3:C:3066[A]:TYR:CE1	3:C:3193[A]:HIS:CE1	2.98	0.52
3:C:3147[A]:GLU:CD	3:C:3149[A]:ASN:HD21	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3147[B]:GLU:CD	3:C:3149[B]:ASN:HD21	2.17	0.52
3:C:3147[B]:GLU:OE2	3:L:3169[B]:LYS:NZ	2.40	0.52
3:C:3148[B]:ILE:HG22	3:L:3170[B]:ALA:CA	2.38	0.52
1:D:482:HIS:CE1	1:D:621:LEU:HD11	2.44	0.52
2:E:2822:LYS:HG2	2:E:2829:CYS:HB3	1.91	0.52
3:F:2949[A]:LYS:C	3:F:2953[A]:GLY:H	2.17	0.52
3:F:2951[B]:ASP:O	3:F:2956[B]:LYS:HE2	2.09	0.52
3:F:3114[A]:PRO:CD	3:F:3115[A]:LEU:N	2.72	0.52
3:F:3174[B]:GLY:HA2	3:a:3154[B]:PRO:CD	2.37	0.52
3:F:3264[A]:TYR:C	3:F:3264[A]:TYR:CD1	2.86	0.52
3:F:3300[A]:LEU:N	3:F:3300[A]:LEU:CD2	2.73	0.52
1:G:957:ASN:N	1:G:958:PRO:HA	2.24	0.52
2:H:2539:ILE:O	2:H:2573:TYR:OH	2.15	0.52
3:I:2935[A]:ILE:CD1	3:I:2935[A]:ILE:N	2.73	0.52
3:I:2945[A]:VAL:HG22	3:I:2954[A]:TYR:HB2	1.91	0.52
3:I:2973[B]:THR:CG2	3:R:3106[B]:THR:C	2.82	0.52
3:I:3159[B]:SER:CA	3:R:3150[B]:LYS:CA	2.87	0.52
3:I:3228[A]:VAL:CG2	3:I:3245[A]:PHE:CE2	2.89	0.52
3:I:3269[B]:SER:O	3:I:3272[B]:HIS:HB2	2.09	0.52
3:I:3284[B]:LYS:HD3	3:I:3284[B]:LYS:C	2.32	0.52
3:I:3287[A]:ILE:O	3:I:3287[A]:ILE:HG23	2.10	0.52
3:I:3298[B]:ASN:HA	3:I:3299[B]:LEU:HB3	1.88	0.52
2:K:2823:ILE:HG12	2:K:2832:ALA:HB2	1.91	0.52
3:L:2961[A]:HIS:HB3	3:L:3111[A]:SER:HB3	1.92	0.52
3:L:3264[B]:TYR:C	3:L:3264[B]:TYR:CD1	2.86	0.52
3:L:3275[A]:LEU:N	3:L:3275[A]:LEU:CD1	2.73	0.52
3:L:3284[B]:LYS:HE2	3:L:3284[B]:LYS:CA	2.29	0.52
2:N:2252:GLU:HG3	2:N:2385:ILE:HG23	1.91	0.52
2:N:2361:LYS:HD2	2:N:2362:GLN:HG3	1.92	0.52
3:O:2935[A]:ILE:CD1	3:O:2935[A]:ILE:N	2.73	0.52
3:O:2951[A]:ASP:O	3:O:2956[A]:LYS:HE2	2.09	0.52
3:O:3092[A]:ILE:CG2	3:O:3096[A]:VAL:CG2	2.88	0.52
3:O:3230[A]:PHE:H	3:O:3243[A]:GLY:CA	2.22	0.52
3:O:3252[B]:TYR:CG	3:X:2966[B]:SER:O	2.49	0.52
3:O:3300[A]:LEU:N	3:O:3300[A]:LEU:CD2	2.73	0.52
3:R:2949[B]:LYS:C	3:R:2953[B]:GLY:H	2.17	0.52
3:R:3132[B]:ALA:CB	3:R:3197[B]:ILE:CD1	2.86	0.52
3:R:3147[B]:GLU:CD	3:R:3149[B]:ASN:HD21	2.17	0.52
3:R:3230[B]:PHE:H	3:R:3243[B]:GLY:CA	2.22	0.52
1:S:483:GLY:HA2	1:S:773:PHE:CZ	2.45	0.52
1:S:897:HIS:HB3	1:S:899:MET:SD	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:2684:HIS:NE2	2:T:2711:HIS:CE1	2.77	0.52
3:U:2975[B]:PHE:CD1	3:d:3256[B]:TRP:HD1	1.85	0.52
3:U:3254[B]:MET:HG2	3:d:3255[B]:PRO:CD	2.39	0.52
1:V:1081:MET:HG2	1:V:1100:SER:O	2.09	0.52
1:V:1163:ALA:HB2	1:V:1205:LEU:HD21	1.90	0.52
2:W:2373:MET:HG3	2:W:2376:MET:HE3	1.91	0.52
3:X:2935[A]:ILE:CD1	3:X:2936[A]:GLU:N	2.73	0.52
3:X:2951[A]:ASP:O	3:X:2956[A]:LYS:HE2	2.09	0.52
3:X:3139[A]:LEU:CD2	3:X:3139[A]:LEU:N	2.73	0.52
3:X:3230[B]:PHE:H	3:X:3243[B]:GLY:CA	2.22	0.52
3:X:3284[B]:LYS:CE	3:X:3284[B]:LYS:CA	2.85	0.52
1:Y:142:ARG:NH1	1:Y:340:GLN:OE1	2.40	0.52
3:a:2935[A]:ILE:CD1	3:a:2935[A]:ILE:N	2.73	0.52
3:a:2951[B]:ASP:O	3:a:2956[B]:LYS:HE2	2.09	0.52
3:a:2952[B]:ALA:N	3:a:2953[B]:GLY:HA2	2.06	0.52
3:a:3014[B]:TRP:CZ3	3:a:3119[B]:HIS:ND1	2.77	0.52
3:a:3047[B]:ARG:HH21	3:a:3113[B]:ASP:CG	2.16	0.52
1:b:1470:GLU:HB3	1:b:1537:ILE:CD1	2.39	0.52
3:d:2948[A]:ASP:CB	3:d:2949[A]:LYS:HA	2.15	0.52
3:d:3110[B]:THR:O	3:d:3111[B]:SER:C	2.53	0.52
3:d:3230[B]:PHE:H	3:d:3243[B]:GLY:CA	2.22	0.52
3:d:3269[A]:SER:O	3:d:3272[A]:HIS:HB2	2.09	0.52
3:d:3287[A]:ILE:O	3:d:3287[A]:ILE:HG23	2.10	0.52
1:A:164:GLU:OE1	1:A:296:ARG:NH1	2.42	0.52
1:A:905:TRP:HE1	1:A:1083:PRO:CD	2.22	0.52
3:C:2949[A]:LYS:C	3:C:2953[A]:GLY:H	2.17	0.52
3:C:2976[B]:ALA:HB2	3:L:3253[B]:GLU:CG	2.39	0.52
3:C:3269[A]:SER:O	3:C:3272[A]:HIS:HB2	2.09	0.52
1:D:1248:ARG:HG3	1:D:1249:TRP:N	2.24	0.52
1:D:1574:VAL:H	1:G:329:ARG:NH1	2.01	0.52
1:D:1582:ASN:HD21	1:D:1627:ARG:HE	1.57	0.52
2:E:2393:ARG:HH21	2:E:2489:ILE:HD11	1.75	0.52
2:E:2670:CYS:N	2:E:2737:CYS:SG	2.82	0.52
3:F:2951[A]:ASP:O	3:F:2956[A]:LYS:HE2	2.09	0.52
3:F:2960[B]:PHE:CD2	3:F:3157[B]:PRO:CG	2.74	0.52
3:F:3115[B]:LEU:HD22	3:F:3115[B]:LEU:O	2.10	0.52
3:F:3139[A]:LEU:CD2	3:F:3139[A]:LEU:N	2.73	0.52
1:G:1070:ALA:HB3	1:G:1077:LEU:HD21	1.92	0.52
2:H:2554:PRO:HA	2:H:2555:GLU:HB2	1.90	0.52
3:I:3157[B]:PRO:CD	3:R:3153[B]:LYS:NZ	2.73	0.52
3:I:3162[B]:ASP:CA	3:R:3147[B]:GLU:OE1	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3253[B]:GLU:CB	3:R:2976[B]:ALA:N	2.70	0.52
1:J:1631:GLU:OE1	1:M:328:LYS:NZ	2.35	0.52
3:L:2947[A]:ALA:HA	3:L:2949[A]:LYS:HB3	1.89	0.52
3:L:3047[B]:ARG:HH21	3:L:3113[B]:ASP:CG	2.16	0.52
3:L:3081[A]:PHE:CD1	3:L:3081[A]:PHE:C	2.87	0.52
3:L:3230[B]:PHE:H	3:L:3243[B]:GLY:CA	2.22	0.52
1:M:630:PHE:O	1:M:633:HIS:HB3	2.09	0.52
3:O:3014[B]:TRP:CZ3	3:O:3119[B]:HIS:ND1	2.77	0.52
3:O:3047[B]:ARG:HH21	3:O:3113[B]:ASP:CG	2.16	0.52
3:O:3132[A]:ALA:CB	3:O:3197[A]:ILE:CD1	2.86	0.52
3:O:3139[A]:LEU:CD2	3:O:3139[A]:LEU:N	2.73	0.52
3:O:3173[B]:THR:HG22	3:O:3175[B]:TYR:H	1.73	0.52
3:O:3255[B]:PRO:CA	3:X:3161[B]:GLU:CA	2.79	0.52
1:P:1036:SER:OG	1:P:1037:ALA:N	2.41	0.52
3:R:2935[A]:ILE:CD1	3:R:2935[A]:ILE:N	2.73	0.52
3:R:3028[B]:PRO:HG2	3:R:3029[B]:LYS:CG	2.40	0.52
3:R:3092[A]:ILE:CG2	3:R:3096[A]:VAL:CG2	2.88	0.52
3:R:3147[A]:GLU:CB	3:R:3149[A]:ASN:ND2	2.73	0.52
1:S:69:HIS:NE2	9:S:2102:CUO:O2	2.43	0.52
3:U:2951[A]:ASP:O	3:U:2956[A]:LYS:HE2	2.09	0.52
1:V:329:ARG:NH1	1:Y:1582:ASN:O	2.42	0.52
1:V:1260:ARG:HD3	1:V:1331:GLU:OE1	2.10	0.52
3:X:2935[A]:ILE:CD1	3:X:2935[A]:ILE:N	2.73	0.52
3:X:3014[B]:TRP:CZ3	3:X:3119[B]:HIS:ND1	2.77	0.52
1:Y:17:ASN:HA	1:Y:20:VAL:HG12	1.90	0.52
1:Y:1617:LYS:HE2	3:d:3180[B]:TYR:CZ	2.44	0.52
2:Z:2603:PRO:HG2	2:Z:2606:LEU:HD12	1.91	0.52
3:a:3300[A]:LEU:N	3:a:3300[A]:LEU:CD2	2.73	0.52
1:b:132:ASN:HB2	1:b:133:LYS:HG2	1.91	0.52
1:b:957:ASN:N	1:b:958:PRO:HA	2.24	0.52
1:b:1029:SER:OG	1:b:1030:MET:N	2.43	0.52
3:d:3173[B]:THR:HG22	3:d:3175[B]:TYR:H	1.73	0.52
8:0:1:NAG:H62	8:0:2:NAG:N2	2.24	0.52
4:7:1:NAG:H61	4:7:2:NAG:HN2	1.74	0.52
6:CA:1:NAG:H61	6:CA:2:NAG:C8	2.39	0.52
3:C:2952[B]:ALA:CB	3:C:2956[B]:LYS:HB3	2.40	0.52
3:C:2965[B]:LEU:C	3:L:3256[B]:TRP:O	2.45	0.52
3:C:3014[A]:TRP:CZ3	3:C:3119[A]:HIS:ND1	2.77	0.52
1:D:137:ARG:HB2	1:D:186:VAL:O	2.10	0.52
3:F:2961[B]:HIS:HB3	3:F:3111[B]:SER:HB3	1.92	0.52
3:F:3248[B]:LEU:CD1	3:a:2973[B]:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3287[B]:ILE:O	3:F:3287[B]:ILE:HG23	2.10	0.52
1:G:1234:VAL:H	2:K:2738:ALA:HA	1.74	0.52
2:H:2336:PHE:HB3	2:H:2348:THR:HG22	1.92	0.52
3:I:2970[B]:PRO:CD	3:R:2989[B]:HIS:CE1	2.93	0.52
3:I:3300[B]:LEU:N	3:I:3300[B]:LEU:CD2	2.73	0.52
1:J:227:ARG:NH2	1:J:297:ARG:HH22	2.07	0.52
1:J:439:LEU:HD23	1:J:509:ILE:HD12	1.91	0.52
1:J:810:LEU:HD11	4:u:1:NAG:H62	1.90	0.52
1:J:1136:ARG:O	1:J:1141:ARG:NH1	2.43	0.52
3:L:2935[B]:ILE:CD1	3:L:2935[B]:ILE:N	2.73	0.52
3:L:3014[A]:TRP:CZ3	3:L:3119[A]:HIS:ND1	2.77	0.52
3:L:3038[A]:ILE:HG23	3:L:3040[A]:VAL:HG22	1.90	0.52
3:L:3132[A]:ALA:CB	3:L:3197[A]:ILE:CD1	2.87	0.52
3:L:3147[B]:GLU:CB	3:L:3149[B]:ASN:ND2	2.73	0.52
3:L:3151[A]:LEU:HB2	3:L:3175[A]:TYR:HE2	1.68	0.52
3:L:3269[A]:SER:O	3:L:3272[A]:HIS:HB2	2.09	0.52
3:L:3285[A]:VAL:CG2	3:L:3286[A]:THR:N	2.73	0.52
3:O:2977[B]:CYS:H	3:X:3153[B]:LYS:HG2	1.74	0.52
3:O:3115[B]:LEU:HD22	3:O:3115[B]:LEU:O	2.10	0.52
3:O:3230[B]:PHE:H	3:O:3243[B]:GLY:CA	2.22	0.52
3:O:3287[B]:ILE:O	3:O:3287[B]:ILE:HG23	2.10	0.52
3:O:3300[B]:LEU:N	3:O:3300[B]:LEU:CD2	2.73	0.52
1:P:1013:ILE:HD11	1:P:1175:PHE:CD2	2.45	0.52
2:Q:2392:ASP:HB2	2:Q:2491:PRO:HG3	1.90	0.52
2:Q:2821:LEU:HD11	2:Q:2879:LEU:HG	1.92	0.52
3:R:2951[B]:ASP:O	3:R:2956[B]:LYS:HE2	2.09	0.52
3:R:3028[A]:PRO:HG2	3:R:3029[A]:LYS:CG	2.40	0.52
3:R:3285[A]:VAL:CG2	3:R:3286[A]:THR:N	2.73	0.52
3:R:3293[A]:LYS:CB	3:R:3294[A]:SER:CB	2.54	0.52
3:R:3293[B]:LYS:CG	3:R:3294[B]:SER:HB2	2.36	0.52
3:U:3135[A]:LYS:HG3	3:U:3141[A]:TYR:HE1	1.29	0.52
3:U:3147[A]:GLU:CD	3:U:3149[A]:ASN:HD21	2.17	0.52
3:U:3170[B]:ALA:C	3:d:3152[B]:LYS:HZ1	2.17	0.52
1:V:22:LEU:HB3	1:V:122:VAL:HG21	1.92	0.52
1:V:730:PHE:CD1	1:V:780:GLU:HA	2.44	0.52
3:a:2935[B]:ILE:CD1	3:a:2935[B]:ILE:N	2.73	0.52
3:a:2954[A]:TYR:CD2	3:a:2954[A]:TYR:C	2.86	0.52
2:c:2244:PHE:HE2	2:c:2374:ASN:HD22	1.57	0.52
2:c:2849:ASP:HB3	2:c:2850:ARG:HE	1.73	0.52
3:d:2935[A]:ILE:CD1	3:d:2936[A]:GLU:N	2.73	0.52
3:d:2937[A]:ASN:ND2	3:d:3006[A]:LYS:CD	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3092[B]:ILE:CG2	3:d:3096[B]:VAL:CG2	2.88	0.52
3:d:3132[A]:ALA:HB1	3:d:3197[A]:ILE:HD13	1.89	0.52
3:d:3139[A]:LEU:CD2	3:d:3139[A]:LEU:N	2.73	0.52
3:d:3139[B]:LEU:CD2	3:d:3139[B]:LEU:N	2.73	0.52
3:d:3228[A]:VAL:CG2	3:d:3245[A]:PHE:CE2	2.89	0.52
3:d:3287[B]:ILE:O	3:d:3287[B]:ILE:HG23	2.09	0.52
1:A:1144:VAL:HG23	1:A:1194:SER:O	2.09	0.52
1:A:1195:ASP:HA	1:A:1196:ILE:CG2	2.40	0.52
3:C:2961[A]:HIS:HB3	3:C:3111[A]:SER:HB3	1.92	0.52
3:C:3107[B]:LEU:CD1	3:L:2974[B]:ALA:O	2.41	0.52
3:C:3110[A]:THR:O	3:C:3111[A]:SER:C	2.53	0.52
3:C:3173[A]:THR:HG22	3:C:3175[A]:TYR:H	1.73	0.52
3:C:3176[B]:LYS:NZ	3:C:3176[B]:LYS:CB	2.73	0.52
3:C:3293[B]:LYS:CG	3:C:3294[B]:SER:HB2	2.36	0.52
1:D:855:ARG:HD3	1:D:959:PHE:HD2	1.75	0.52
3:F:3115[A]:LEU:O	3:F:3115[A]:LEU:HD22	2.10	0.52
3:F:3139[B]:LEU:CD2	3:F:3139[B]:LEU:N	2.73	0.52
3:F:3147[B]:GLU:CD	3:F:3149[B]:ASN:HD21	2.17	0.52
3:F:3153[B]:LYS:HB2	3:a:3158[B]:PHE:CB	2.27	0.52
3:F:3255[B]:PRO:CB	3:a:2964[B]:PRO:N	2.73	0.52
3:F:3287[A]:ILE:O	3:F:3287[A]:ILE:HG23	2.09	0.52
3:I:2937[B]:ASN:ND2	3:I:3006[B]:LYS:CD	2.73	0.52
3:I:2952[A]:ALA:CA	3:I:2956[A]:LYS:HB3	2.38	0.52
3:I:2952[B]:ALA:CB	3:I:2956[B]:LYS:HB3	2.40	0.52
3:I:2961[B]:HIS:HA	3:R:2975[B]:PHE:CE2	2.33	0.52
3:I:2966[B]:SER:HA	3:R:3255[B]:PRO:C	2.35	0.52
3:I:2970[B]:PRO:HD3	3:R:2989[B]:HIS:CE1	2.45	0.52
3:I:2983[B]:VAL:CG2	3:R:3162[B]:ASP:OD1	2.57	0.52
3:I:3089[A]:HIS:CE1	3:I:3119[A]:HIS:CE1	2.81	0.52
3:I:3115[A]:LEU:HD22	3:I:3115[A]:LEU:O	2.10	0.52
3:I:3135[B]:LYS:HG3	3:I:3141[B]:TYR:CD1	2.33	0.52
3:I:3154[B]:PRO:CD	3:R:3173[B]:THR:C	2.83	0.52
3:I:3255[B]:PRO:HG3	3:R:2962[B]:GLY:O	2.05	0.52
1:J:960:PHE:HD1	1:J:962:GLY:H	1.58	0.52
2:K:2121:THR:O	2:K:2124:SER:OG	2.13	0.52
3:L:3038[B]:ILE:HG23	3:L:3040[B]:VAL:HG22	1.90	0.52
3:L:3110[B]:THR:C	3:L:3112[B]:TYR:N	2.68	0.52
3:L:3115[A]:LEU:HD22	3:L:3115[A]:LEU:O	2.10	0.52
3:L:3300[A]:LEU:N	3:L:3300[A]:LEU:CD2	2.73	0.52
1:M:892:TYR:CE1	1:M:1184:MET:HG3	2.45	0.52
2:N:2270:ILE:HB	2:N:2297:HIS:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2954[B]:TYR:C	3:O:2954[B]:TYR:CD2	2.86	0.52
3:O:3101[B]:PRO:C	3:X:2971[B]:ASP:C	2.78	0.52
3:O:3176[B]:LYS:NZ	3:O:3176[B]:LYS:CB	2.73	0.52
3:O:3183[B]:LEU:N	3:O:3184[B]:ASN:HA	2.11	0.52
2:Q:2822:LYS:HD3	2:Q:2829:CYS:HB2	1.91	0.52
2:Q:2884:LYS:HG2	2:Q:2891:LEU:HD23	1.92	0.52
3:R:2935[B]:ILE:CD1	3:R:2935[B]:ILE:N	2.73	0.52
3:R:3081[A]:PHE:C	3:R:3081[A]:PHE:CD1	2.87	0.52
3:R:3287[A]:ILE:O	3:R:3287[A]:ILE:HG23	2.09	0.52
3:U:3092[A]:ILE:CG2	3:U:3096[A]:VAL:CG2	2.88	0.52
3:U:3139[A]:LEU:CD2	3:U:3139[A]:LEU:N	2.73	0.52
3:U:3147[B]:GLU:CD	3:U:3149[B]:ASN:HD21	2.17	0.52
3:U:3219[A]:LEU:N	3:U:3219[A]:LEU:CD2	2.73	0.52
3:U:3287[A]:ILE:O	3:U:3287[A]:ILE:HG23	2.09	0.52
2:W:2107:LEU:HD23	2:W:2208:PRO:HB2	1.90	0.52
3:X:2951[B]:ASP:O	3:X:2956[B]:LYS:HE2	2.09	0.52
3:X:3273[A]:LEU:HB2	3:X:3275[A]:LEU:CD1	2.34	0.52
3:X:3287[A]:ILE:O	3:X:3287[A]:ILE:HG23	2.10	0.52
1:Y:71:LEU:HD22	1:Y:266:LEU:HD21	1.91	0.52
1:Y:516:TRP:HH2	1:Y:637:VAL:HG22	1.75	0.52
3:a:2945[A]:VAL:HG22	3:a:2954[A]:TYR:HB2	1.91	0.52
3:a:2951[A]:ASP:O	3:a:2956[A]:LYS:HE2	2.09	0.52
3:a:3139[B]:LEU:CD2	3:a:3139[B]:LEU:N	2.73	0.52
3:a:3147[B]:GLU:CD	3:a:3149[B]:ASN:HD21	2.17	0.52
1:b:488:PRO:HB2	1:b:641:TRP:CE3	2.45	0.52
1:b:926:LEU:HD12	1:b:927:PRO:HD2	1.92	0.52
1:b:1228:LEU:HD22	1:b:1229:LYS:HA	1.91	0.52
2:c:2191:LEU:HD13	2:c:2296:LEU:HD22	1.91	0.52
2:c:2476:LEU:HB3	2:c:2480:LEU:CD2	2.39	0.52
3:d:3115[A]:LEU:HD22	3:d:3115[A]:LEU:O	2.10	0.52
3:d:3176[B]:LYS:NZ	3:d:3176[B]:LYS:CB	2.73	0.52
3:d:3183[A]:LEU:N	3:d:3184[A]:ASN:HA	2.12	0.52
3:d:3285[A]:VAL:CG2	3:d:3286[A]:THR:N	2.73	0.52
1:A:1028:VAL:HA	1:A:1035:TYR:CD2	2.43	0.52
2:B:2332:PRO:HB2	2:B:2337:SER:HB2	1.91	0.52
3:C:2937[B]:ASN:ND2	3:C:3006[B]:LYS:CD	2.73	0.52
3:C:2960[B]:PHE:CD1	3:C:2960[B]:PHE:N	2.72	0.52
3:C:2968[B]:GLN:NE2	3:L:3086[B]:GLU:HB3	2.18	0.52
3:C:2972[B]:GLY:CA	3:L:3090[B]:ASN:CB	2.88	0.52
3:C:3264[B]:TYR:C	3:C:3264[B]:TYR:CD1	2.86	0.52
3:C:3273[A]:LEU:HB2	3:C:3275[A]:LEU:CD1	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2344:LEU:HA	2:E:2345:ASN:C	2.34	0.52
3:F:2948[A]:ASP:CB	3:F:2949[A]:LYS:HA	2.16	0.52
3:F:2961[A]:HIS:HB3	3:F:3111[A]:SER:HB3	1.92	0.52
3:F:3014[A]:TRP:CZ3	3:F:3119[A]:HIS:ND1	2.77	0.52
3:F:3092[A]:ILE:CG2	3:F:3096[A]:VAL:CG2	2.87	0.52
3:F:3151[B]:LEU:O	3:a:3154[B]:PRO:HB3	2.09	0.52
3:F:3153[B]:LYS:CB	3:a:3155[B]:MET:CA	2.73	0.52
3:F:3157[B]:PRO:C	3:a:3150[B]:LYS:HE2	2.29	0.52
3:F:3158[B]:PHE:HB2	3:a:3153[B]:LYS:CB	2.39	0.52
3:F:3228[B]:VAL:HG23	3:F:3228[B]:VAL:O	2.10	0.52
1:G:387:ASN:OD1	1:G:387:ASN:N	2.40	0.52
1:G:1286:ARG:HG3	1:G:1337:ARG:NH2	2.25	0.52
2:H:2811:HIS:HB3	2:H:2847:HIS:HD2	1.75	0.52
3:I:3028[A]:PRO:HG2	3:I:3029[A]:LYS:CG	2.40	0.52
3:I:3047[A]:ARG:HH21	3:I:3113[A]:ASP:CG	2.16	0.52
3:I:3110[B]:THR:C	3:I:3112[B]:TYR:N	2.68	0.52
1:J:95:THR:O	1:J:153:ASN:ND2	2.43	0.52
1:J:217:PHE:O	1:J:220:TRP:HB3	2.10	0.52
1:J:695:TYR:H	1:J:695:TYR:HD1	1.56	0.52
1:J:729:VAL:HG11	1:J:785:LEU:HD12	1.92	0.52
1:J:1018:ILE:HA	1:J:1021:LEU:HB2	1.91	0.52
1:J:1182:ASN:O	1:J:1182:ASN:ND2	2.43	0.52
2:K:2413:VAL:O	2:K:2454:MET:HE1	2.09	0.52
2:K:2571:ARG:NH1	2:K:2771:TYR:HB3	2.25	0.52
3:L:2945[A]:VAL:HG22	3:L:2954[A]:TYR:HB2	1.91	0.52
3:L:2949[A]:LYS:C	3:L:2953[A]:GLY:H	2.17	0.52
3:L:2961[B]:HIS:HB3	3:L:3111[B]:SER:HB3	1.91	0.52
3:L:3096[B]:VAL:HG11	3:L:3115[B]:LEU:HD12	1.89	0.52
2:N:2394:VAL:HG11	2:N:2451:LEU:HD12	1.90	0.52
3:O:2945[A]:VAL:HG22	3:O:2954[A]:TYR:HB2	1.91	0.52
3:O:2954[A]:TYR:CD2	3:O:2954[A]:TYR:C	2.86	0.52
3:O:2970[B]:PRO:O	3:X:2989[B]:HIS:HB2	2.10	0.52
3:O:3110[A]:THR:C	3:O:3112[A]:TYR:N	2.68	0.52
3:O:3307[B]:PHE:HE1	3:O:3309[B]:PRO:CG	2.08	0.52
1:P:724:LYS:HA	1:P:728:ARG:NH1	2.25	0.52
1:P:1166:THR:HB	1:P:1167:ASP:C	2.35	0.52
2:Q:2692:LYS:HE2	2:Q:2700:PHE:HE2	1.74	0.52
2:Q:2800:LYS:O	3:R:3023[A]:ILE:HD13	2.02	0.52
3:R:2933[A]:SER:CB	3:R:2936[A]:GLU:CB	2.86	0.52
3:R:3081[B]:PHE:CD1	3:R:3081[B]:PHE:C	2.87	0.52
3:R:3110[B]:THR:O	3:R:3111[B]:SER:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3139[B]:LEU:CD2	3:R:3139[B]:LEU:N	2.73	0.52
3:R:3300[B]:LEU:N	3:R:3300[B]:LEU:CD2	2.73	0.52
1:S:142:ARG:O	1:S:145:GLN:NE2	2.42	0.52
3:U:3066[B]:TYR:CE1	3:U:3193[B]:HIS:CE1	2.98	0.52
3:X:2933[A]:SER:CB	3:X:2936[A]:GLU:CB	2.85	0.52
3:X:3014[A]:TRP:CZ3	3:X:3119[A]:HIS:ND1	2.77	0.52
3:X:3038[A]:ILE:HG23	3:X:3040[A]:VAL:HG22	1.90	0.52
3:X:3110[A]:THR:O	3:X:3111[A]:SER:C	2.53	0.52
3:X:3115[A]:LEU:HD22	3:X:3115[A]:LEU:O	2.10	0.52
3:X:3115[B]:LEU:O	3:X:3115[B]:LEU:HD22	2.10	0.52
1:Y:865:LYS:HG3	1:Y:871:GLN:HG3	1.92	0.52
3:a:2937[B]:ASN:ND2	3:a:3006[B]:LYS:CD	2.73	0.52
3:a:3013[B]:ASP:OD1	3:a:3015[B]:THR:OG1	2.23	0.52
3:a:3115[B]:LEU:HD22	3:a:3115[B]:LEU:O	2.10	0.52
3:a:3135[A]:LYS:HG3	3:a:3141[A]:TYR:CD1	2.33	0.52
3:a:3176[A]:LYS:NZ	3:a:3176[A]:LYS:CB	2.73	0.52
3:a:3287[B]:ILE:O	3:a:3287[B]:ILE:HG23	2.10	0.52
2:c:2496:LEU:HB3	2:c:2498:VAL:HG22	1.91	0.52
3:d:2935[B]:ILE:CD1	3:d:2936[B]:GLU:N	2.73	0.52
3:d:3014[A]:TRP:CZ3	3:d:3119[A]:HIS:ND1	2.77	0.52
3:d:3115[B]:LEU:HD22	3:d:3115[B]:LEU:O	2.10	0.52
3:d:3228[A]:VAL:O	3:d:3228[A]:VAL:HG23	2.10	0.52
1:A:1017:HIS:O	1:A:1021:LEU:HG	2.08	0.52
3:C:2935[A]:ILE:CD1	3:C:2936[A]:GLU:N	2.73	0.52
3:C:2966[B]:SER:O	3:L:2981[B]:GLY:C	2.53	0.52
3:C:3092[B]:ILE:CG2	3:C:3096[B]:VAL:CG2	2.88	0.52
3:C:3139[A]:LEU:CD2	3:C:3139[A]:LEU:N	2.73	0.52
3:C:3230[B]:PHE:H	3:C:3243[B]:GLY:CA	2.22	0.52
3:C:3269[B]:SER:O	3:C:3272[B]:HIS:HB2	2.09	0.52
3:C:3287[B]:ILE:O	3:C:3287[B]:ILE:HG23	2.10	0.52
1:D:109:LEU:HD21	2:H:2635:TYR:HB2	1.91	0.52
1:D:972:SER:HA	1:D:1028:VAL:HG22	1.92	0.52
3:F:2935[B]:ILE:CD1	3:F:2935[B]:ILE:N	2.73	0.52
3:F:2969[A]:TYR:CE2	3:F:2970[A]:PRO:CG	2.86	0.52
1:G:125:SER:OG	1:G:127:GLU:OE2	2.27	0.52
1:G:481:ILE:HD12	1:G:668:MET:HE1	1.92	0.52
1:G:1299:GLN:HB2	1:G:1311:CYS:SG	2.50	0.52
3:I:3115[B]:LEU:HD22	3:I:3115[B]:LEU:O	2.10	0.52
3:I:3132[A]:ALA:CB	3:I:3197[A]:ILE:CD1	2.86	0.52
3:I:3160[B]:SER:CB	3:R:2982[B]:MET:CB	2.88	0.52
3:I:3176[B]:LYS:NZ	3:I:3176[B]:LYS:CB	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3269[A]:SER:O	3:I:3272[A]:HIS:HB2	2.09	0.52
3:I:3275[B]:LEU:N	3:I:3275[B]:LEU:CD1	2.73	0.52
1:J:980:TYR:HE1	1:J:1021:LEU:HD13	1.74	0.52
2:K:2172:ILE:HG13	2:K:2173:VAL:HG13	1.92	0.52
3:L:2949[B]:LYS:C	3:L:2953[B]:GLY:H	2.17	0.52
3:L:2952[A]:ALA:CB	3:L:2956[A]:LYS:HB3	2.40	0.52
3:L:3028[A]:PRO:HG2	3:L:3029[A]:LYS:CG	2.40	0.52
3:L:3028[B]:PRO:HG2	3:L:3029[B]:LYS:CG	2.40	0.52
3:L:3269[B]:SER:O	3:L:3272[B]:HIS:HB2	2.09	0.52
3:L:3293[B]:LYS:CG	3:L:3294[B]:SER:HB2	2.36	0.52
1:M:1583:CYS:SG	1:M:1584:GLY:N	2.80	0.52
3:O:2935[B]:ILE:CD1	3:O:2936[B]:GLU:N	2.73	0.52
3:O:3047[A]:ARG:HH21	3:O:3113[A]:ASP:CG	2.16	0.52
3:O:3081[B]:PHE:C	3:O:3081[B]:PHE:CD1	2.87	0.52
3:O:3113[A]:ASP:O	3:O:3114[A]:PRO:C	2.53	0.52
1:P:468:CYS:SG	1:P:669:LYS:HB3	2.50	0.52
3:R:2937[A]:ASN:ND2	3:R:3006[A]:LYS:CD	2.73	0.52
3:R:3014[A]:TRP:CZ3	3:R:3119[A]:HIS:ND1	2.77	0.52
3:R:3139[A]:LEU:CD2	3:R:3139[A]:LEU:N	2.73	0.52
3:R:3147[B]:GLU:CB	3:R:3149[B]:ASN:ND2	2.73	0.52
3:R:3176[B]:LYS:NZ	3:R:3176[B]:LYS:CB	2.73	0.52
3:R:3228[B]:VAL:CG2	3:R:3245[B]:PHE:CE2	2.89	0.52
3:R:3300[A]:LEU:N	3:R:3300[A]:LEU:CD2	2.73	0.52
2:T:2403:PHE:CZ	2:T:2480:LEU:HD21	2.45	0.52
3:U:2949[A]:LYS:C	3:U:2953[A]:GLY:H	2.17	0.52
3:U:2969[B]:TYR:HB2	3:d:3256[B]:TRP:HE1	1.74	0.52
3:U:3275[A]:LEU:N	3:U:3275[A]:LEU:CD1	2.73	0.52
1:V:563:ILE:HG22	1:V:565:GLU:HG3	1.91	0.52
2:W:2627:GLY:HA3	2:W:2703:PHE:O	2.09	0.52
3:X:2935[B]:ILE:CD1	3:X:2936[B]:GLU:N	2.73	0.52
3:X:2952[A]:ALA:CA	3:X:2956[A]:LYS:HB3	2.38	0.52
3:X:3028[A]:PRO:HG2	3:X:3029[A]:LYS:CG	2.40	0.52
3:X:3096[A]:VAL:HG11	3:X:3115[A]:LEU:HD12	1.89	0.52
3:X:3287[B]:ILE:O	3:X:3287[B]:ILE:HG23	2.10	0.52
3:X:3300[B]:LEU:N	3:X:3300[B]:LEU:CD2	2.73	0.52
1:Y:904:HIS:HB3	1:Y:1105:VAL:HG21	1.91	0.52
1:Y:904:HIS:O	1:Y:907:ARG:HB3	2.10	0.52
1:Y:914:GLU:OE1	1:Y:926:LEU:N	2.39	0.52
1:Y:1000:GLU:HG2	1:Y:1133:ILE:HG23	1.91	0.52
1:Y:1301:PRO:HA	1:Y:1308:VAL:HA	1.92	0.52
2:Z:2595:TRP:HE1	2:Z:2710:HIS:HD2	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:450:LYS:NZ	1:b:1273:SER:OG	2.43	0.52
1:b:745:ASP:OD1	1:b:759:SER:OG	2.25	0.52
1:b:1310:THR:HG23	1:b:1597:THR:HG23	1.90	0.52
3:d:2937[B]:ASN:ND2	3:d:3006[B]:LYS:CD	2.73	0.52
3:d:2952[A]:ALA:HB3	3:d:2954[A]:TYR:N	2.17	0.52
3:d:2952[A]:ALA:CB	3:d:2956[A]:LYS:HB3	2.40	0.52
3:d:3196[B]:THR:CA	3:d:3199[B]:GLN:OE1	2.58	0.52
4:RA:1:NAG:O3	4:RA:2:NAG:O5	2.23	0.52
1:A:198:GLU:OE1	1:A:198:GLU:N	2.36	0.52
1:A:996:ILE:HG23	1:A:1133:ILE:HG22	1.90	0.52
1:A:1414:THR:HG23	1:A:1477:LEU:HD13	1.91	0.52
2:B:2521:MET:HE3	2:B:2605:LEU:HD12	1.91	0.52
3:C:2935[B]:ILE:CD1	3:C:2936[B]:GLU:N	2.73	0.52
3:C:2965[B]:LEU:CD2	3:L:3253[B]:GLU:CG	2.79	0.52
3:C:3028[B]:PRO:HG2	3:C:3029[B]:LYS:CG	2.40	0.52
3:C:3256[B]:TRP:CE2	3:L:2965[B]:LEU:CA	2.93	0.52
3:C:3275[B]:LEU:N	3:C:3275[B]:LEU:CD1	2.73	0.52
3:C:3284[B]:LYS:CE	3:C:3284[B]:LYS:CA	2.85	0.52
3:C:3285[B]:VAL:CG2	3:C:3286[B]:THR:N	2.73	0.52
3:C:3287[A]:ILE:O	3:C:3287[A]:ILE:HG23	2.09	0.52
3:C:3300[A]:LEU:N	3:C:3300[A]:LEU:CD2	2.73	0.52
3:C:3300[B]:LEU:N	3:C:3300[B]:LEU:CD2	2.73	0.52
1:D:439:LEU:HD23	1:D:509:ILE:HD12	1.91	0.52
1:D:1582:ASN:ND2	1:D:1627:ARG:HE	2.07	0.52
2:E:2181:THR:HB	2:E:2374:ASN:H	1.73	0.52
3:F:2952[A]:ALA:CA	3:F:2956[A]:LYS:HB3	2.38	0.52
3:F:3147[A]:GLU:CB	3:F:3149[A]:ASN:ND2	2.73	0.52
3:F:3162[B]:ASP:CB	3:a:3259[B]:ASP:H	2.22	0.52
3:F:3196[A]:THR:CA	3:F:3199[A]:GLN:OE1	2.58	0.52
3:F:3228[A]:VAL:O	3:F:3228[A]:VAL:HG23	2.10	0.52
3:F:3230[B]:PHE:H	3:F:3243[B]:GLY:CA	2.22	0.52
3:F:3253[B]:GLU:N	3:a:3252[B]:TYR:HB2	2.24	0.52
1:G:237:LEU:HB2	1:G:820:VAL:HB	1.92	0.52
3:I:2989[B]:HIS:CD2	3:R:2970[B]:PRO:CB	2.92	0.52
3:I:3081[B]:PHE:C	3:I:3081[B]:PHE:CD1	2.87	0.52
3:I:3110[A]:THR:C	3:I:3112[A]:TYR:N	2.68	0.52
3:I:3139[A]:LEU:CD2	3:I:3139[A]:LEU:N	2.73	0.52
3:I:3147[B]:GLU:CB	3:I:3149[B]:ASN:ND2	2.73	0.52
3:I:3284[A]:LYS:CE	3:I:3284[A]:LYS:CA	2.85	0.52
1:J:121:ASN:HD22	1:J:124:TYR:H	1.57	0.52
1:J:1441:SER:OG	1:J:1442:MET:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3092[A]:ILE:CG2	3:L:3096[A]:VAL:CG2	2.88	0.52
3:L:3114[A]:PRO:CD	3:L:3115[A]:LEU:N	2.72	0.52
3:L:3147[A]:GLU:CD	3:L:3149[A]:ASN:HD21	2.17	0.52
3:L:3219[B]:LEU:N	3:L:3219[B]:LEU:CD2	2.73	0.52
3:L:3228[B]:VAL:O	3:L:3228[B]:VAL:HG23	2.10	0.52
1:M:873:VAL:HA	1:M:876:PHE:CD1	2.45	0.52
1:M:965:ASP:N	1:M:966:SER:HA	2.24	0.52
2:N:2179:ASP:HA	2:N:2300:ASN:ND2	2.24	0.52
2:N:2180:TRP:HB3	2:N:2184:MET:HE2	1.90	0.52
3:O:2933[B]:SER:CB	3:O:2936[B]:GLU:CB	2.85	0.52
3:O:2952[A]:ALA:CB	3:O:2956[A]:LYS:HB3	2.40	0.52
3:O:2961[A]:HIS:HB3	3:O:3111[A]:SER:HB3	1.92	0.52
3:O:3147[A]:GLU:CD	3:O:3149[A]:ASN:HD21	2.17	0.52
3:O:3153[B]:LYS:CG	3:X:3176[B]:LYS:HZ1	2.22	0.52
3:O:3176[A]:LYS:NZ	3:O:3176[A]:LYS:CB	2.73	0.52
3:O:3285[A]:VAL:CG2	3:O:3286[A]:THR:N	2.73	0.52
1:S:110:PHE:N	1:S:119:LYS:O	2.37	0.52
1:S:972:SER:HA	1:S:1028:VAL:HG22	1.92	0.52
1:S:1181:GLU:CD	1:S:1181:GLU:H	2.17	0.52
2:T:2394:VAL:HG11	2:T:2451:LEU:HD12	1.91	0.52
2:T:2825:ILE:HG22	2:T:2863:ARG:NH2	2.24	0.52
3:U:2952[B]:ALA:CB	3:U:2956[B]:LYS:HB3	2.40	0.52
3:U:2961[A]:HIS:HB3	3:U:3111[A]:SER:HB3	1.92	0.52
3:U:3170[B]:ALA:O	3:d:3148[B]:ILE:HG22	2.09	0.52
3:U:3183[B]:LEU:N	3:U:3184[B]:ASN:HA	2.12	0.52
1:V:22:LEU:HD12	1:V:25:MET:HG2	1.92	0.52
1:V:945:ALA:O	1:V:957:ASN:ND2	2.43	0.52
1:V:993:ASN:OD1	1:V:1136:ARG:NH2	2.23	0.52
3:X:2952[B]:ALA:CB	3:X:2956[B]:LYS:HB3	2.40	0.52
1:Y:1470:GLU:OE2	1:Y:1473:ARG:NH1	2.43	0.52
3:a:2961[B]:HIS:HB3	3:a:3111[B]:SER:HB3	1.92	0.52
2:c:2579:GLU:HG2	2:c:2758:THR:HG21	1.91	0.52
3:d:2949[B]:LYS:C	3:d:2949[B]:LYS:HZ3	2.10	0.52
3:d:2951[A]:ASP:O	3:d:2956[A]:LYS:HE2	2.09	0.52
3:d:2957[A]:ILE:HA	3:d:2960[A]:PHE:HE1	1.64	0.52
3:d:3028[A]:PRO:HG2	3:d:3029[A]:LYS:CG	2.40	0.52
3:d:3081[A]:PHE:C	3:d:3081[A]:PHE:CD1	2.87	0.52
3:d:3092[A]:ILE:CG2	3:d:3096[A]:VAL:CG2	2.88	0.52
3:d:3264[B]:TYR:C	3:d:3264[B]:TYR:CD1	2.86	0.52
1:A:885:SER:HB2	1:A:886:PRO:HA	1.91	0.52
1:A:973:ARG:O	1:A:1028:VAL:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2935[A]:ILE:CD1	3:C:2935[A]:ILE:N	2.73	0.52
3:C:3113[B]:ASP:O	3:C:3114[B]:PRO:C	2.53	0.52
3:C:3115[B]:LEU:HD22	3:C:3115[B]:LEU:O	2.10	0.52
3:C:3147[B]:GLU:CB	3:C:3149[B]:ASN:ND2	2.73	0.52
1:D:1470:GLU:HB3	1:D:1537:ILE:CD1	2.40	0.52
1:D:1604:ASP:OD1	1:D:1605:ARG:NH1	2.43	0.52
2:E:2156:ARG:HD2	2:E:2357:VAL:HG12	1.91	0.52
2:E:2509:ILE:HD11	2:E:2605:LEU:HD23	1.92	0.52
2:E:2568:HIS:HD2	2:E:2718:TRP:CH2	2.28	0.52
3:F:3028[A]:PRO:HG2	3:F:3029[A]:LYS:CG	2.40	0.52
3:F:3042[A]:ASP:N	3:F:3042[A]:ASP:OD2	2.41	0.52
3:F:3291[A]:ASP:OD2	3:F:3293[A]:LYS:NZ	2.43	0.52
1:G:564:ASP:HB3	1:G:610:THR:HA	1.92	0.52
3:I:2949[A]:LYS:C	3:I:2953[A]:GLY:H	2.17	0.52
3:I:2952[A]:ALA:HB3	3:I:2954[A]:TYR:N	2.17	0.52
3:I:3014[B]:TRP:CZ3	3:I:3119[B]:HIS:ND1	2.77	0.52
3:I:3028[B]:PRO:HG2	3:I:3029[B]:LYS:CG	2.40	0.52
3:I:3110[B]:THR:O	3:I:3111[B]:SER:C	2.53	0.52
3:I:3254[B]:MET:HE2	3:R:3157[B]:PRO:HD3	1.92	0.52
2:K:2800:LYS:HB3	3:L:3023[A]:ILE:CD1	2.39	0.52
3:L:2952[B]:ALA:N	3:L:2953[B]:GLY:HA2	2.06	0.52
3:L:2952[B]:ALA:CA	3:L:2956[B]:LYS:HB3	2.38	0.52
3:L:3019[A]:HIS:CD2	3:L:3019[A]:HIS:N	2.75	0.52
3:L:3139[A]:LEU:CD2	3:L:3139[A]:LEU:N	2.73	0.52
3:L:3147[A]:GLU:CB	3:L:3149[A]:ASN:ND2	2.73	0.52
1:M:293:LEU:O	1:M:296:ARG:HG2	2.10	0.52
1:M:480:CYS:SG	1:M:621:LEU:HD11	2.49	0.52
1:M:885:SER:HB3	1:M:886:PRO:HA	1.92	0.52
3:O:2935[B]:ILE:CD1	3:O:2935[B]:ILE:N	2.73	0.52
3:O:2952[A]:ALA:HB3	3:O:2954[A]:TYR:N	2.17	0.52
3:O:2975[B]:PHE:CD1	3:X:3158[B]:PHE:N	2.60	0.52
3:O:3102[B]:TYR:HA	3:X:2971[B]:ASP:HA	1.86	0.52
1:P:11:THR:HG22	1:P:13:ASP:H	1.75	0.52
1:P:517:THR:HG21	1:P:708:PHE:HE1	1.74	0.52
3:R:3115[A]:LEU:O	3:R:3115[A]:LEU:HD22	2.10	0.52
3:R:3147[A]:GLU:CG	3:R:3149[A]:ASN:ND2	2.73	0.52
3:R:3307[B]:PHE:HE1	3:R:3309[B]:PRO:CG	2.08	0.52
1:S:954:ALA:O	1:S:956:PRO:HD3	2.09	0.52
2:T:2606:LEU:HD21	2:T:2709:VAL:HG21	1.92	0.52
3:U:3028[A]:PRO:HG2	3:U:3029[A]:LYS:CG	2.40	0.52
3:U:3028[B]:PRO:HG2	3:U:3029[B]:LYS:CG	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3220[B]:ARG:HG3	3:d:2974[B]:ALA:H	1.73	0.52
1:V:929:TRP:O	1:V:1048:ASN:ND2	2.43	0.52
3:X:3176[A]:LYS:N	3:X:3176[A]:LYS:CE	2.73	0.52
3:X:3176[B]:LYS:NZ	3:X:3176[B]:LYS:CB	2.73	0.52
3:X:3219[B]:LEU:N	3:X:3219[B]:LEU:CD2	2.73	0.52
3:X:3269[B]:SER:O	3:X:3272[B]:HIS:HB2	2.09	0.52
1:Y:1621:ASN:HA	3:d:3188[B]:ASP:HB2	1.90	0.52
2:Z:2359:ASN:OD1	2:Z:2359:ASN:N	2.43	0.52
3:a:2952[A]:ALA:CB	3:a:2956[A]:LYS:HB3	2.40	0.52
3:a:3132[A]:ALA:HB1	3:a:3197[A]:ILE:HD13	1.89	0.52
3:a:3220[A]:ARG:HH11	3:a:3220[A]:ARG:CG	2.12	0.52
3:a:3264[B]:TYR:C	3:a:3264[B]:TYR:CD1	2.86	0.52
2:c:2394:VAL:HA	2:c:2488:ARG:HA	1.92	0.52
3:d:2960[A]:PHE:CD2	3:d:3157[A]:PRO:CG	2.74	0.52
3:d:3300[B]:LEU:N	3:d:3300[B]:LEU:CD2	2.73	0.52
1:A:941:LEU:HD11	1:A:959:PHE:HD2	1.75	0.51
3:C:3092[A]:ILE:CG2	3:C:3096[A]:VAL:CG2	2.88	0.51
3:C:3114[B]:PRO:CD	3:C:3115[B]:LEU:N	2.72	0.51
3:C:3147[B]:GLU:OE2	3:L:3163[B]:ASN:O	2.27	0.51
3:C:3154[B]:PRO:N	3:L:3155[B]:MET:HG3	2.17	0.51
2:E:2808:PHE:CE2	2:E:2899:PRO:HG3	2.45	0.51
3:F:2935[A]:ILE:CD1	3:F:2935[A]:ILE:N	2.73	0.51
3:F:2954[A]:TYR:CD2	3:F:2954[A]:TYR:C	2.86	0.51
3:F:2971[B]:ASP:O	3:a:3248[B]:LEU:HD22	2.10	0.51
3:F:3066[B]:TYR:CE1	3:F:3193[B]:HIS:CE1	2.98	0.51
3:F:3147[A]:GLU:CD	3:F:3149[A]:ASN:HD21	2.17	0.51
3:F:3147[B]:GLU:CB	3:F:3149[B]:ASN:ND2	2.73	0.51
3:F:3153[B]:LYS:HZ1	3:a:3158[B]:PHE:H	1.58	0.51
3:F:3162[B]:ASP:HB3	3:a:3259[B]:ASP:H	1.75	0.51
3:F:3176[B]:LYS:N	3:F:3176[B]:LYS:CE	2.73	0.51
3:F:3252[B]:TYR:CE1	3:a:3251[B]:ASP:CG	2.67	0.51
1:G:22:LEU:HD12	1:G:25:MET:HG2	1.92	0.51
1:G:1072:CYS:HA	2:K:2902:ILE:HG22	1.92	0.51
2:H:2161:GLN:NE2	2:H:2345:ASN:OD1	2.43	0.51
3:I:3139[B]:LEU:CD2	3:I:3139[B]:LEU:N	2.73	0.51
3:I:3147[A]:GLU:CB	3:I:3149[A]:ASN:ND2	2.73	0.51
3:I:3147[B]:GLU:CG	3:I:3149[B]:ASN:ND2	2.73	0.51
3:I:3196[A]:THR:HG1	1:J:416:ASN:ND2	2.07	0.51
3:I:3196[B]:THR:CA	3:I:3199[B]:GLN:OE1	2.58	0.51
3:I:3275[A]:LEU:N	3:I:3275[A]:LEU:CD1	2.73	0.51
1:J:61:GLY:HA2	1:J:354:PHE:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:473:ALA:HB3	1:M:1639:LYS:HE3	1.92	0.51
1:J:1046:HIS:HA	1:J:1049:VAL:HB	1.92	0.51
2:K:2512:LEU:HD11	2:K:2591:PRO:HG3	1.91	0.51
2:K:2551:PRO:HD3	2:K:2751:TRP:CH2	2.45	0.51
3:L:2951[B]:ASP:O	3:L:2956[B]:LYS:HE2	2.10	0.51
3:L:2988[B]:TRP:HE3	3:L:2989[B]:HIS:CE1	2.25	0.51
3:L:3101[A]:PRO:HG2	3:L:3102[A]:TYR:CD1	2.46	0.51
3:L:3176[A]:LYS:H	3:L:3176[A]:LYS:CE	2.17	0.51
3:L:3230[A]:PHE:H	3:L:3243[A]:GLY:CA	2.22	0.51
1:M:1262:ASN:OD1	1:M:1263:LEU:N	2.43	0.51
1:M:1315:GLY:HA3	1:M:1601:TRP:CB	2.40	0.51
1:M:1427:HIS:CE1	1:M:1457:HIS:CE1	2.98	0.51
1:M:1458:HIS:NE2	9:M:2105:CUO:O1	2.43	0.51
1:M:1493:MET:HG2	1:M:1511:SER:O	2.10	0.51
2:N:2128:LEU:HD13	2:N:2286:HIS:CG	2.45	0.51
3:O:3092[B]:ILE:CG2	3:O:3096[B]:VAL:CG2	2.88	0.51
3:O:3101[A]:PRO:HG2	3:O:3102[A]:TYR:CD1	2.46	0.51
3:O:3147[B]:GLU:CB	3:O:3149[B]:ASN:ND2	2.73	0.51
1:P:37:ILE:HD13	1:P:75:GLN:HG3	1.91	0.51
3:R:2935[A]:ILE:CD1	3:R:2936[A]:GLU:N	2.73	0.51
3:R:3219[B]:LEU:N	3:R:3219[B]:LEU:CD2	2.73	0.51
1:S:419:THR:O	1:S:1062:PHE:HE1	1.93	0.51
1:S:928:TYR:HB2	1:S:1048:ASN:HB2	1.91	0.51
3:U:2935[B]:ILE:CD1	3:U:2936[B]:GLU:N	2.73	0.51
3:U:2969[B]:TYR:OH	3:d:2980[B]:HIS:CE1	2.63	0.51
3:U:2980[B]:HIS:CB	3:d:2969[B]:TYR:CZ	2.92	0.51
3:U:3254[B]:MET:HE2	3:d:2975[B]:PHE:CE2	2.46	0.51
3:U:3285[A]:VAL:CG2	3:U:3286[A]:THR:N	2.73	0.51
1:V:1411:PHE:O	1:V:1475:ARG:NH2	2.41	0.51
1:V:1421:VAL:HG23	1:V:1422:HIS:HD1	1.75	0.51
2:W:2567:MET:HE3	2:W:2718:TRP:HB2	1.92	0.51
3:X:3101[B]:PRO:HG2	3:X:3102[B]:TYR:CD1	2.46	0.51
3:X:3139[B]:LEU:CD2	3:X:3139[B]:LEU:N	2.73	0.51
1:Y:422:LEU:HD13	1:Y:696:GLN:HG2	1.90	0.51
1:Y:1613:ASP:OD1	3:d:3185[B]:TYR:HA	2.09	0.51
2:Z:2605:LEU:O	2:Z:2622:ASN:ND2	2.40	0.51
3:a:2949[A]:LYS:C	3:a:2953[A]:GLY:H	2.17	0.51
3:a:3028[B]:PRO:HG2	3:a:3029[B]:LYS:CG	2.40	0.51
3:a:3101[A]:PRO:HG2	3:a:3102[A]:TYR:CD1	2.45	0.51
3:a:3287[A]:ILE:O	3:a:3287[A]:ILE:HG23	2.09	0.51
1:b:346:GLY:O	1:b:349:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:1166:THR:HB	1:b:1168:GLN:N	2.25	0.51
4:7:1:NAG:C6	4:7:2:NAG:N2	2.73	0.51
4:MA:1:NAG:C6	4:MA:2:NAG:C1	2.86	0.51
1:A:329:ARG:O	1:b:1583:CYS:N	2.43	0.51
2:B:2168:ARG:NH2	2:E:2515:ARG:HD2	2.26	0.51
3:C:2952[A]:ALA:CB	3:C:2956[A]:LYS:HB3	2.40	0.51
3:C:3096[A]:VAL:HG11	3:C:3115[A]:LEU:HD12	1.89	0.51
2:E:2234:GLN:HG3	2:E:2235:PRO:HD2	1.91	0.51
2:E:2265:ILE:HD11	2:E:2400:LEU:CD1	2.40	0.51
3:F:2937[B]:ASN:ND2	3:F:3006[B]:LYS:CD	2.73	0.51
3:F:3092[B]:ILE:CG2	3:F:3096[B]:VAL:CG2	2.88	0.51
3:F:3159[B]:SER:CB	3:a:2984[B]:THR:OG1	2.58	0.51
3:F:3176[A]:LYS:N	3:F:3176[A]:LYS:CE	2.73	0.51
1:G:979:LEU:HB3	1:G:980:TYR:CD2	2.44	0.51
2:H:2800:LYS:C	3:I:3023[A]:ILE:CD1	2.78	0.51
3:I:2952[A]:ALA:CB	3:I:2956[A]:LYS:HB3	2.40	0.51
3:I:3147[B]:GLU:CD	3:I:3149[B]:ASN:HD21	2.17	0.51
3:I:3150[B]:LYS:HD2	3:R:3160[B]:SER:CB	2.39	0.51
3:I:3188[B]:ASP:N	3:I:3188[B]:ASP:OD2	2.36	0.51
1:J:1171:LYS:HG2	1:J:1173:GLY:H	1.75	0.51
3:L:2935[A]:ILE:CD1	3:L:2935[A]:ILE:N	2.73	0.51
3:L:3176[A]:LYS:NZ	3:L:3176[A]:LYS:CB	2.73	0.51
3:L:3284[A]:LYS:HD3	3:L:3284[A]:LYS:C	2.32	0.51
3:L:3291[B]:ASP:OD2	3:L:3293[B]:LYS:NZ	2.43	0.51
1:M:1335:LEU:HD23	1:M:1339:SER:HA	1.92	0.51
2:N:2094:ARG:CZ	2:Q:2370:MET:HE1	2.40	0.51
2:N:2172:ILE:HG13	2:N:2173:VAL:HG13	1.92	0.51
3:O:2928[B]:ASN:C	3:O:2930[B]:LEU:HD22	2.36	0.51
3:O:2949[A]:LYS:C	3:O:2953[A]:GLY:H	2.17	0.51
3:O:2968[B]:GLN:HB3	3:X:2979[B]:GLN:CB	2.39	0.51
3:O:3019[B]:HIS:CD2	3:O:3019[B]:HIS:N	2.75	0.51
3:O:3101[B]:PRO:HG2	3:O:3102[B]:TYR:CD1	2.45	0.51
3:O:3110[B]:THR:O	3:O:3111[B]:SER:C	2.53	0.51
3:O:3147[B]:GLU:CD	3:O:3149[B]:ASN:HD21	2.17	0.51
3:O:3273[A]:LEU:O	3:O:3275[A]:LEU:HD12	2.11	0.51
3:O:3293[A]:LYS:CG	3:O:3294[A]:SER:HB2	2.36	0.51
1:P:1400:ASN:ND2	1:P:1433:TRP:HZ3	2.07	0.51
3:R:2952[B]:ALA:CA	3:R:2956[B]:LYS:HB3	2.38	0.51
3:R:3120[A]:HIS:HA	3:R:3123[A]:THR:HG1	1.73	0.51
2:T:2622:ASN:HB3	2:T:2625:LEU:HD12	1.93	0.51
3:U:2969[B]:TYR:CE2	3:d:3248[B]:LEU:HD23	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3110[A]:THR:O	3:U:3111[A]:SER:C	2.53	0.51
3:U:3110[A]:THR:C	3:U:3112[A]:TYR:N	2.68	0.51
3:U:3115[A]:LEU:HD22	3:U:3115[A]:LEU:O	2.10	0.51
3:U:3139[B]:LEU:CD2	3:U:3139[B]:LEU:N	2.73	0.51
3:U:3176[A]:LYS:H	3:U:3176[A]:LYS:CE	2.17	0.51
3:U:3228[A]:VAL:CG2	3:U:3245[A]:PHE:CE2	2.89	0.51
3:U:3275[B]:LEU:N	3:U:3275[B]:LEU:CD1	2.73	0.51
3:U:3284[A]:LYS:CE	3:U:3284[A]:LYS:CA	2.85	0.51
3:U:3287[B]:ILE:O	3:U:3287[B]:ILE:HG23	2.09	0.51
3:U:3298[A]:ASN:HA	3:U:3299[A]:LEU:HB3	1.87	0.51
3:U:3300[A]:LEU:N	3:U:3300[A]:LEU:CD2	2.73	0.51
2:W:2476:LEU:HD22	4:HA:2:NAG:H81	1.92	0.51
2:W:2823:ILE:HD13	2:W:2856:ILE:HG21	1.91	0.51
3:X:2949[B]:LYS:C	3:X:2953[B]:GLY:H	2.17	0.51
3:X:3147[A]:GLU:CB	3:X:3149[A]:ASN:ND2	2.73	0.51
3:X:3176[A]:LYS:NZ	3:X:3176[A]:LYS:CB	2.73	0.51
3:X:3273[B]:LEU:O	3:X:3275[B]:LEU:HD12	2.11	0.51
3:X:3300[A]:LEU:N	3:X:3300[A]:LEU:CD2	2.73	0.51
1:Y:7:VAL:HG23	1:Y:91:TYR:O	2.10	0.51
1:Y:1620:LEU:CD1	3:d:3189[B]:ASN:HB2	2.31	0.51
3:a:2949[B]:LYS:C	3:a:2953[B]:GLY:H	2.17	0.51
3:a:3110[A]:THR:C	3:a:3112[A]:TYR:N	2.68	0.51
3:a:3176[B]:LYS:N	3:a:3176[B]:LYS:CE	2.73	0.51
3:a:3275[A]:LEU:N	3:a:3275[A]:LEU:CD1	2.73	0.51
3:a:3293[B]:LYS:CG	3:a:3294[B]:SER:HB2	2.36	0.51
1:b:1195:ASP:OD1	1:b:1196:ILE:N	2.44	0.51
1:A:300:ALA:HB2	1:A:406:PRO:HD3	1.92	0.51
1:A:1245:GLU:OE1	1:A:1246:GLY:N	2.28	0.51
2:B:2569:TRP:O	2:B:2572:VAL:HG23	2.10	0.51
3:C:2945[A]:VAL:HG22	3:C:2954[A]:TYR:HB2	1.91	0.51
3:C:3157[B]:PRO:HA	3:L:2982[B]:MET:SD	2.50	0.51
3:C:3230[A]:PHE:H	3:C:3243[A]:GLY:CA	2.22	0.51
1:D:157:GLU:OE2	1:D:296:ARG:NH2	2.43	0.51
1:D:329:ARG:HD3	1:G:1583:CYS:H	1.76	0.51
1:D:1018:ILE:HD12	1:D:1045:HIS:CD2	2.45	0.51
1:D:1129:LEU:O	1:D:1133:ILE:HG12	2.11	0.51
1:D:1421:VAL:HG23	1:D:1422:HIS:HD1	1.75	0.51
2:E:2179:ASP:HA	2:E:2300:ASN:ND2	2.26	0.51
2:E:2798:GLN:O	2:E:2803:ARG:NH1	2.44	0.51
3:F:2952[B]:ALA:CB	3:F:2956[B]:LYS:HB3	2.40	0.51
3:F:2960[A]:PHE:CD2	3:F:3157[A]:PRO:CG	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2966[B]:SER:C	3:F:2967[B]:CYS:SG	2.94	0.51
3:F:2968[B]:GLN:HG2	3:a:2980[B]:HIS:C	2.32	0.51
3:F:3275[A]:LEU:N	3:F:3275[A]:LEU:CD1	2.73	0.51
3:F:3285[A]:VAL:CG2	3:F:3286[A]:THR:N	2.73	0.51
3:F:3300[B]:LEU:N	3:F:3300[B]:LEU:CD2	2.73	0.51
1:G:1102:PRO:HA	1:G:1105:VAL:HG22	1.91	0.51
1:G:1558:LEU:HD13	2:K:2440:ASP:HA	1.92	0.51
2:H:2275:GLY:HA3	2:H:2283:ASN:HB2	1.93	0.51
2:H:2568:HIS:ND1	2:H:2765:PRO:HB3	2.24	0.51
2:H:2738:ALA:HB2	1:J:1233:SER:HA	1.92	0.51
3:I:2945[B]:VAL:HG22	3:I:2954[B]:TYR:HB2	1.91	0.51
3:I:2961[B]:HIS:HB3	3:I:3111[B]:SER:HB3	1.92	0.51
3:I:2972[B]:GLY:N	3:R:3089[B]:HIS:CD2	2.78	0.51
3:I:2973[B]:THR:OG1	3:R:3093[B]:HIS:CD2	2.64	0.51
3:I:3101[B]:PRO:HG2	3:I:3102[B]:TYR:CD1	2.46	0.51
3:I:3176[A]:LYS:NZ	3:I:3176[A]:LYS:CB	2.73	0.51
3:I:3254[B]:MET:CB	3:R:2966[B]:SER:CB	2.88	0.51
3:I:3285[A]:VAL:CG2	3:I:3286[A]:THR:N	2.73	0.51
1:J:424:PHE:HB2	1:J:1128:GLN:HE22	1.75	0.51
1:J:493:LEU:HD12	1:J:668:MET:HG3	1.92	0.51
1:J:550:ILE:N	1:J:557:VAL:O	2.30	0.51
3:L:3115[B]:LEU:HD22	3:L:3115[B]:LEU:O	2.10	0.51
3:L:3287[B]:ILE:O	3:L:3287[B]:ILE:HG23	2.10	0.51
1:M:1229:LYS:HD2	1:M:1229:LYS:H	1.76	0.51
1:M:1242:ASN:OD1	1:M:1244:GLY:N	2.40	0.51
2:N:2901:LEU:HB2	1:P:1074:ILE:HB	1.91	0.51
3:O:2968[B]:GLN:C	3:X:2988[B]:TRP:HB2	2.35	0.51
3:O:3028[A]:PRO:HG2	3:O:3029[A]:LYS:CG	2.40	0.51
3:O:3269[B]:SER:O	3:O:3272[B]:HIS:HB2	2.09	0.51
2:Q:2411:PHE:HE2	2:Q:2445:MET:HE3	1.75	0.51
2:Q:2830:GLN:HB2	2:Q:2863:ARG:NH1	2.25	0.51
3:R:3264[A]:TYR:C	3:R:3264[A]:TYR:CD1	2.86	0.51
3:U:2933[A]:SER:CB	3:U:2936[A]:GLU:CB	2.86	0.51
3:U:2935[A]:ILE:CD1	3:U:2935[A]:ILE:N	2.73	0.51
3:U:2937[A]:ASN:ND2	3:U:3006[A]:LYS:CD	2.73	0.51
3:U:2937[B]:ASN:ND2	3:U:3006[B]:LYS:CD	2.73	0.51
3:U:2949[B]:LYS:C	3:U:2953[B]:GLY:H	2.17	0.51
3:U:2966[A]:SER:C	3:U:2967[A]:CYS:SG	2.94	0.51
3:U:2971[B]:ASP:O	3:d:3247[B]:VAL:HG12	2.05	0.51
3:U:3114[A]:PRO:CD	3:U:3115[A]:LEU:N	2.72	0.51
3:U:3115[B]:LEU:HD22	3:U:3115[B]:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3293[A]:LYS:CG	3:U:3294[A]:SER:HB2	2.36	0.51
1:V:210:HIS:HA	1:V:213:VAL:HG22	1.92	0.51
1:V:1582:ASN:CB	1:V:1583:CYS:HB2	2.28	0.51
1:Y:639:ARG:HB2	1:Y:703:TYR:CE1	2.46	0.51
2:Z:2415:PRO:HD3	2:Z:2454:MET:HE1	1.90	0.51
3:a:2928[B]:ASN:C	3:a:2930[B]:LEU:HD22	2.36	0.51
3:a:3196[A]:THR:CA	3:a:3199[A]:GLN:OE1	2.58	0.51
3:a:3196[B]:THR:CA	3:a:3199[B]:GLN:OE1	2.58	0.51
1:b:59:LEU:HD13	1:b:68:TRP:CD1	2.45	0.51
1:b:247:PHE:O	1:b:252:ASN:ND2	2.43	0.51
2:c:2506:ARG:NE	2:c:2578:GLU:OE2	2.41	0.51
3:d:2951[B]:ASP:O	3:d:2956[B]:LYS:HE2	2.09	0.51
3:d:2971[A]:ASP:CG	3:d:2973[A]:THR:HG1	2.14	0.51
3:d:3176[A]:LYS:NZ	3:d:3176[A]:LYS:CB	2.73	0.51
3:d:3293[B]:LYS:CG	3:d:3294[B]:SER:HB2	2.36	0.51
1:A:473:ALA:H	1:A:474:LEU:HD23	1.76	0.51
1:A:571:PRO:O	1:A:573:LYS:NZ	2.44	0.51
1:A:946:GLU:HA	1:A:955:LYS:HB3	1.93	0.51
3:C:2975[B]:PHE:CE1	3:L:3107[B]:LEU:HD12	2.39	0.51
3:C:2984[B]:THR:CB	3:L:3154[B]:PRO:HG2	2.40	0.51
3:C:3028[A]:PRO:HG2	3:C:3029[A]:LYS:CG	2.40	0.51
3:C:3110[B]:THR:C	3:C:3112[B]:TYR:N	2.68	0.51
3:C:3273[A]:LEU:O	3:C:3275[A]:LEU:HD12	2.11	0.51
1:D:1055:THR:HG21	1:D:1121:LEU:HD13	1.91	0.51
1:D:1407:THR:HG22	1:D:1426:LEU:HD21	1.93	0.51
2:E:2145:LEU:HD12	2:E:2435:MET:HE1	1.93	0.51
3:F:2935[B]:ILE:CD1	3:F:2936[B]:GLU:N	2.73	0.51
3:F:2952[A]:ALA:CB	3:F:2956[A]:LYS:HB3	2.40	0.51
3:F:2952[B]:ALA:CA	3:F:2956[B]:LYS:HB3	2.38	0.51
3:F:2962[A]:GLY:N	3:F:3111[A]:SER:OG	2.44	0.51
3:F:2978[B]:CYS:O	3:a:2977[B]:CYS:SG	2.68	0.51
3:F:3101[B]:PRO:HG2	3:F:3102[B]:TYR:CD1	2.46	0.51
3:F:3132[B]:ALA:HB1	3:F:3197[B]:ILE:HD13	1.89	0.51
3:F:3273[A]:LEU:O	3:F:3275[A]:LEU:HD12	2.11	0.51
1:G:865:LYS:NZ	1:G:966:SER:OG	2.43	0.51
1:G:1059:LEU:HD13	1:G:1063:ARG:HH21	1.74	0.51
3:I:2966[A]:SER:C	3:I:2967[A]:CYS:SG	2.94	0.51
3:I:2985[B]:PHE:HE2	3:R:2968[B]:GLN:O	1.93	0.51
3:I:3219[B]:LEU:N	3:I:3219[B]:LEU:CD2	2.73	0.51
3:I:3285[B]:VAL:CG2	3:I:3286[B]:THR:N	2.73	0.51
3:I:3291[B]:ASP:OD2	3:I:3293[B]:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3300[A]:LEU:N	3:I:3300[A]:LEU:CD2	2.73	0.51
1:J:566:ARG:HH12	1:J:803:LYS:NZ	2.09	0.51
3:L:2962[A]:GLY:N	3:L:3111[A]:SER:OG	2.44	0.51
3:L:3139[B]:LEU:CD2	3:L:3139[B]:LEU:N	2.73	0.51
3:L:3273[B]:LEU:O	3:L:3275[B]:LEU:HD12	2.11	0.51
1:M:23:ARG:HA	1:M:122:VAL:HG11	1.93	0.51
1:M:911:LEU:HD21	1:M:1095:MET:HE2	1.93	0.51
1:M:980:TYR:CE1	1:M:1021:LEU:HB3	2.45	0.51
3:O:2948[B]:ASP:CB	3:O:2949[B]:LYS:HA	2.16	0.51
3:O:2952[A]:ALA:N	3:O:2953[A]:GLY:HA2	2.06	0.51
3:O:3219[B]:LEU:N	3:O:3219[B]:LEU:CD2	2.73	0.51
3:O:3273[B]:LEU:O	3:O:3275[B]:LEU:HD12	2.11	0.51
3:O:3298[A]:ASN:HA	3:O:3299[A]:LEU:HB3	1.88	0.51
3:O:3298[B]:ASN:HA	3:O:3299[B]:LEU:HB3	1.88	0.51
1:P:1210:LYS:HA	1:P:1211:TYR:HB3	1.93	0.51
3:R:2966[B]:SER:C	3:R:2967[B]:CYS:SG	2.94	0.51
3:R:3104[B]:MET:HA	3:R:3110[B]:THR:CG2	2.17	0.51
3:R:3151[B]:LEU:HB2	3:R:3175[B]:TYR:HE2	1.68	0.51
3:R:3273[B]:LEU:O	3:R:3275[B]:LEU:HD12	2.11	0.51
1:S:1348:TRP:CD1	1:S:1403:LEU:HD13	2.45	0.51
2:T:2625:LEU:HD22	2:T:2626:ARG:HB2	1.92	0.51
3:U:2945[B]:VAL:HG22	3:U:2954[B]:TYR:HB2	1.91	0.51
3:U:3096[A]:VAL:HG11	3:U:3115[A]:LEU:HD12	1.89	0.51
3:U:3110[B]:THR:O	3:U:3111[B]:SER:C	2.53	0.51
3:U:3110[B]:THR:C	3:U:3112[B]:TYR:N	2.68	0.51
1:V:568:PHE:N	1:V:568:PHE:CD1	2.78	0.51
1:V:846:MET:HE1	1:V:854:LEU:HD22	1.93	0.51
2:W:2610:ASP:OD1	2:W:2610:ASP:N	2.44	0.51
3:X:3042[B]:ASP:N	3:X:3042[B]:ASP:OD2	2.41	0.51
3:X:3092[B]:ILE:CG2	3:X:3096[B]:VAL:CG2	2.88	0.51
3:X:3293[A]:LYS:CB	3:X:3294[A]:SER:CB	2.54	0.51
1:Y:148:GLN:C	1:Y:150:GLY:H	2.18	0.51
3:a:2961[A]:HIS:HB3	3:a:3111[A]:SER:HB3	1.92	0.51
3:a:2966[A]:SER:C	3:a:2967[A]:CYS:SG	2.94	0.51
3:a:3092[A]:ILE:CG2	3:a:3096[A]:VAL:CG2	2.88	0.51
3:a:3092[B]:ILE:CG2	3:a:3096[B]:VAL:CG2	2.88	0.51
3:a:3176[A]:LYS:N	3:a:3176[A]:LYS:CE	2.73	0.51
3:a:3183[B]:LEU:N	3:a:3184[B]:ASN:HA	2.12	0.51
3:a:3228[B]:VAL:HG23	3:a:3228[B]:VAL:O	2.10	0.51
1:b:1074:ILE:O	1:b:1078:ARG:HG2	2.09	0.51
2:c:2517:VAL:HG13	2:c:2605:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2952[A]:ALA:N	3:d:2953[A]:GLY:HA2	2.06	0.51
3:d:2961[B]:HIS:HB3	3:d:3111[B]:SER:HB3	1.91	0.51
3:d:3038[B]:ILE:HG23	3:d:3040[B]:VAL:HG22	1.90	0.51
3:d:3101[B]:PRO:HG2	3:d:3102[B]:TYR:CD1	2.46	0.51
3:d:3300[A]:LEU:N	3:d:3300[A]:LEU:CD2	2.73	0.51
1:A:569:LYS:C	1:A:571:PRO:HD3	2.36	0.51
1:A:1158:GLU:CD	1:A:1216:ARG:HE	2.18	0.51
1:A:1302:SER:HB3	1:A:1303:GLU:CA	2.37	0.51
1:A:1348:TRP:CD1	1:A:1403:LEU:HD13	2.45	0.51
2:B:2802:ASP:OD2	2:B:2903:TYR:OH	2.20	0.51
3:C:2961[B]:HIS:HB3	3:C:3111[B]:SER:HB3	1.91	0.51
3:C:3079[B]:CYS:HB3	3:L:3161[B]:GLU:CB	2.41	0.51
3:C:3120[B]:HIS:NE2	3:L:2969[B]:TYR:HE2	1.94	0.51
1:D:573:LYS:HB3	1:D:574:GLY:HA2	1.93	0.51
1:D:806:ASN:ND2	6:k:1:NAG:C8	2.73	0.51
1:D:1082:SER:O	1:D:1086:LEU:HG	2.09	0.51
2:E:2546:LEU:H	2:E:2557:ALA:HA	1.75	0.51
2:E:2728:ARG:HE	2:E:2730:LEU:HD12	1.75	0.51
3:F:2928[B]:ASN:C	3:F:2930[B]:LEU:HD22	2.36	0.51
3:F:2983[B]:VAL:HG22	3:a:3162[B]:ASP:OD1	2.11	0.51
3:F:3108[B]:HIS:HE1	3:a:3251[B]:ASP:CG	2.16	0.51
1:G:203:ASP:O	1:G:206:PHE:HB3	2.11	0.51
2:H:2667:GLU:HB3	2:H:2730:LEU:HD22	1.91	0.51
3:I:2935[A]:ILE:CD1	3:I:2936[A]:GLU:N	2.73	0.51
3:I:3135[B]:LYS:HB2	3:I:3141[B]:TYR:HD1	1.76	0.51
3:I:3155[B]:MET:HB3	3:R:3153[B]:LYS:CD	2.35	0.51
1:J:527:LEU:HD23	1:J:632:LEU:HD12	1.92	0.51
1:J:982:LYS:N	1:J:983:PRO:HD3	2.25	0.51
1:J:1033:LEU:HA	1:J:1036:SER:HB3	1.92	0.51
1:J:1145:THR:HB	1:J:1191:PRO:HB2	1.92	0.51
3:L:3101[B]:PRO:HG2	3:L:3102[B]:TYR:CD1	2.46	0.51
3:L:3176[A]:LYS:N	3:L:3176[A]:LYS:CE	2.73	0.51
3:O:2986[B]:PRO:CB	3:O:3127[B]:TRP:CZ3	2.94	0.51
3:O:3114[B]:PRO:CD	3:O:3115[B]:LEU:N	2.72	0.51
3:O:3176[B]:LYS:N	3:O:3176[B]:LYS:CE	2.73	0.51
3:O:3285[B]:VAL:CG2	3:O:3286[B]:THR:N	2.73	0.51
1:P:132:ASN:HB2	1:P:133:LYS:HA	1.92	0.51
1:P:494:VAL:HG23	1:P:671:PHE:CZ	2.45	0.51
2:Q:2631:TYR:HD1	2:Q:2631:TYR:H	1.58	0.51
3:R:2986[B]:PRO:CB	3:R:3127[B]:TRP:CZ3	2.94	0.51
3:R:3176[A]:LYS:NZ	3:R:3176[A]:LYS:CB	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3273[A]:LEU:O	3:R:3275[A]:LEU:HD12	2.11	0.51
1:S:956:PRO:HB2	1:S:957:ASN:C	2.36	0.51
3:U:2935[A]:ILE:CD1	3:U:2936[A]:GLU:N	2.73	0.51
1:V:43:GLU:HG3	1:V:44:PRO:HA	1.92	0.51
3:X:2935[B]:ILE:CD1	3:X:2935[B]:ILE:N	2.73	0.51
3:X:2961[A]:HIS:HB3	3:X:3111[A]:SER:HB3	1.92	0.51
3:X:2986[A]:PRO:CB	3:X:3127[A]:TRP:CZ3	2.94	0.51
3:X:3092[A]:ILE:CG2	3:X:3096[A]:VAL:CG2	2.88	0.51
3:X:3104[B]:MET:HA	3:X:3110[B]:THR:CG2	2.17	0.51
3:X:3196[A]:THR:CA	3:X:3199[A]:GLN:OE1	2.58	0.51
3:X:3285[A]:VAL:CG2	3:X:3286[A]:THR:N	2.73	0.51
3:X:3291[B]:ASP:OD2	3:X:3293[B]:LYS:NZ	2.44	0.51
2:Z:2128:LEU:HB2	2:Z:2286:HIS:HB3	1.91	0.51
3:a:2952[B]:ALA:CA	3:a:2956[B]:LYS:HB3	2.38	0.51
3:a:2986[B]:PRO:CB	3:a:3127[B]:TRP:CZ3	2.94	0.51
3:a:3139[A]:LEU:CD2	3:a:3139[A]:LEU:N	2.73	0.51
3:a:3176[B]:LYS:NZ	3:a:3176[B]:LYS:CB	2.73	0.51
3:a:3300[B]:LEU:CD2	3:a:3300[B]:LEU:H	2.24	0.51
2:c:2234:GLN:HG3	2:c:2235:PRO:HD2	1.92	0.51
2:c:2562:GLY:H	2:c:2846:TRP:HB2	1.75	0.51
3:d:2952[B]:ALA:CB	3:d:2956[B]:LYS:HB3	2.40	0.51
3:d:3132[B]:ALA:HB1	3:d:3197[B]:ILE:HD13	1.89	0.51
3:d:3275[B]:LEU:N	3:d:3275[B]:LEU:CD1	2.73	0.51
3:d:3293[A]:LYS:CG	3:d:3294[A]:SER:HB2	2.36	0.51
3:d:3298[A]:ASN:HA	3:d:3299[A]:LEU:HB3	1.88	0.51
4:m:1:NAG:C4	4:m:2:NAG:N2	2.73	0.51
3:C:2968[B]:GLN:C	3:L:2985[B]:PHE:CE2	2.89	0.51
3:C:2975[B]:PHE:O	3:L:3254[B]:MET:O	2.29	0.51
3:C:3114[A]:PRO:CD	3:C:3115[A]:LEU:N	2.72	0.51
3:C:3139[B]:LEU:CD2	3:C:3139[B]:LEU:N	2.73	0.51
3:C:3147[B]:GLU:CG	3:C:3149[B]:ASN:ND2	2.73	0.51
3:C:3176[A]:LYS:NZ	3:C:3176[A]:LYS:CB	2.73	0.51
1:D:460:GLU:CD	1:D:1368:ARG:HH21	2.18	0.51
1:D:583:LEU:O	1:D:587:PHE:HD1	1.92	0.51
1:D:1276:ASN:OD1	1:D:1280:GLN:NE2	2.43	0.51
1:D:1321:HIS:CD2	1:D:1321:HIS:H	2.28	0.51
2:E:2180:TRP:HB2	2:E:2243:LEU:HD13	1.93	0.51
3:F:2937[A]:ASN:ND2	3:F:3006[A]:LYS:CD	2.73	0.51
3:F:2982[B]:MET:CE	3:a:2977[B]:CYS:HB3	2.35	0.51
3:F:3110[B]:THR:O	3:F:3111[B]:SER:C	2.53	0.51
3:F:3113[A]:ASP:O	3:F:3114[A]:PRO:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3291[B]:ASP:OD2	3:F:3293[B]:LYS:NZ	2.43	0.51
1:G:140:ASP:CG	1:G:142:ARG:HE	2.19	0.51
3:I:2935[B]:ILE:CD1	3:I:2935[B]:ILE:N	2.73	0.51
3:I:2937[A]:ASN:ND2	3:I:3006[A]:LYS:CD	2.73	0.51
3:I:2982[B]:MET:HB3	3:R:3160[B]:SER:CB	2.40	0.51
3:I:3092[B]:ILE:CG2	3:I:3096[B]:VAL:CG2	2.88	0.51
3:I:3093[B]:HIS:CG	3:R:2971[B]:ASP:O	2.64	0.51
3:I:3249[B]:GLY:N	3:R:2974[B]:ALA:N	2.58	0.51
1:J:320:LYS:NZ	1:J:337:ASP:HB3	2.25	0.51
1:J:598:GLN:HE22	1:J:778:LYS:H	1.58	0.51
1:J:1470:GLU:HB3	1:J:1537:ILE:CD1	2.41	0.51
3:L:2933[A]:SER:CB	3:L:2936[A]:GLU:CB	2.86	0.51
3:L:2937[A]:ASN:ND2	3:L:3006[A]:LYS:CD	2.73	0.51
3:L:2988[A]:TRP:HE3	3:L:2989[A]:HIS:CE1	2.25	0.51
3:L:3211[A]:ASP:OD1	3:L:3211[A]:ASP:N	2.28	0.51
3:L:3273[A]:LEU:HB2	3:L:3275[A]:LEU:CD1	2.34	0.51
3:L:3273[A]:LEU:O	3:L:3275[A]:LEU:HD12	2.11	0.51
1:M:2:LEU:H	1:M:274:TYR:HA	1.76	0.51
1:M:1230:LEU:H	1:M:1230:LEU:HD13	1.76	0.51
2:N:2821:LEU:HD11	2:N:2879:LEU:HD23	1.91	0.51
3:O:2937[A]:ASN:ND2	3:O:3006[A]:LYS:CD	2.73	0.51
3:O:2961[B]:HIS:HB3	3:O:3111[B]:SER:HB3	1.92	0.51
3:O:2962[B]:GLY:N	3:O:3111[B]:SER:OG	2.44	0.51
3:O:2986[A]:PRO:CB	3:O:3127[A]:TRP:CZ3	2.94	0.51
3:O:3219[A]:LEU:N	3:O:3219[A]:LEU:CD2	2.73	0.51
1:P:212:ASN:OD1	1:P:215:ARG:NH1	2.43	0.51
1:P:728:ARG:HE	1:P:730:PHE:HZ	1.58	0.51
1:P:1587:ALA:HA	1:P:1614:GLU:HG2	1.91	0.51
3:R:2933[B]:SER:CB	3:R:2936[B]:GLU:CB	2.85	0.51
3:R:2961[A]:HIS:HB3	3:R:3111[A]:SER:HB3	1.92	0.51
3:R:3101[B]:PRO:HG2	3:R:3102[B]:TYR:CD1	2.46	0.51
3:R:3176[B]:LYS:N	3:R:3176[B]:LYS:CE	2.73	0.51
2:T:2128:LEU:HD13	2:T:2286:HIS:CG	2.46	0.51
3:U:2969[B]:TYR:HE1	3:d:2978[B]:CYS:SG	2.28	0.51
3:U:2986[B]:PRO:CB	3:U:3127[B]:TRP:CZ3	2.94	0.51
3:U:3147[A]:GLU:CG	3:U:3149[A]:ASN:ND2	2.73	0.51
3:U:3176[A]:LYS:N	3:U:3176[A]:LYS:CE	2.73	0.51
3:U:3183[A]:LEU:N	3:U:3184[A]:ASN:HA	2.12	0.51
3:U:3284[A]:LYS:HD3	3:U:3284[A]:LYS:C	2.32	0.51
3:U:3300[B]:LEU:N	3:U:3300[B]:LEU:CD2	2.73	0.51
1:V:1470:GLU:HG3	1:V:1530:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:2650:GLY:H	2:W:2654:SER:HB3	1.76	0.51
3:X:3113[A]:ASP:O	3:X:3114[A]:PRO:C	2.53	0.51
3:X:3151[B]:LEU:HB2	3:X:3175[B]:TYR:HE2	1.67	0.51
3:X:3228[B]:VAL:O	3:X:3228[B]:VAL:HG23	2.10	0.51
1:Y:527:LEU:HD23	1:Y:632:LEU:HD12	1.92	0.51
3:a:2952[A]:ALA:CA	3:a:2956[A]:LYS:HB3	2.38	0.51
3:a:3028[A]:PRO:HG2	3:a:3029[A]:LYS:CG	2.40	0.51
1:b:753:ASN:OD1	1:b:753:ASN:N	2.37	0.51
1:b:1290:ILE:HD13	1:b:1329:LEU:HG	1.93	0.51
1:b:1323:HIS:CD2	9:b:2105:CUO:O1	2.63	0.51
1:b:1467:ILE:HD13	1:b:1532:PHE:HB2	1.93	0.51
3:d:2935[B]:ILE:CD1	3:d:2935[B]:ILE:N	2.73	0.51
3:d:3096[A]:VAL:HG11	3:d:3115[A]:LEU:HD12	1.89	0.51
3:d:3135[A]:LYS:HB2	3:d:3141[A]:TYR:HD1	1.76	0.51
3:d:3273[A]:LEU:O	3:d:3275[A]:LEU:HD12	2.11	0.51
1:A:1013:ILE:HG21	1:A:1192:TYR:CD1	2.45	0.51
3:C:2937[A]:ASN:ND2	3:C:3006[A]:LYS:CD	2.73	0.51
3:C:2951[A]:ASP:O	3:C:2956[A]:LYS:HE2	2.09	0.51
3:C:2951[B]:ASP:O	3:C:2956[B]:LYS:HE2	2.09	0.51
3:C:2966[B]:SER:C	3:C:2967[B]:CYS:SG	2.94	0.51
3:C:2986[A]:PRO:CB	3:C:3127[A]:TRP:CZ3	2.94	0.51
3:C:3153[B]:LYS:HE3	3:L:3155[B]:MET:C	2.36	0.51
2:E:2172:ILE:HG13	2:E:2173:VAL:HG13	1.93	0.51
2:E:2580:SER:O	2:E:2583:ARG:HB3	2.11	0.51
3:F:2961[B]:HIS:CD2	3:F:2988[B]:TRP:CZ3	2.96	0.51
3:F:2971[B]:ASP:OD1	3:a:3248[B]:LEU:HD21	2.11	0.51
3:F:3101[A]:PRO:HG2	3:F:3102[A]:TYR:CD1	2.45	0.51
3:F:3196[B]:THR:O	3:F:3199[B]:GLN:HB2	2.11	0.51
1:G:108:PRO:O	1:G:121:ASN:N	2.42	0.51
1:G:128:ILE:HG13	1:G:130:PHE:O	2.10	0.51
1:G:1060:GLN:HB2	1:G:1067:TYR:HB3	1.92	0.51
1:G:1471:LEU:HD11	1:G:1540:LEU:HD23	1.92	0.51
2:H:2551:PRO:HA	2:H:2554:PRO:HD2	1.91	0.51
3:I:2962[A]:GLY:N	3:I:3111[A]:SER:OG	2.44	0.51
3:I:3104[B]:MET:HA	3:I:3110[B]:THR:CG2	2.17	0.51
1:J:7:VAL:HG13	1:J:104:LEU:HD22	1.93	0.51
1:J:555:ALA:HB3	1:J:558:HIS:CE1	2.46	0.51
3:L:2928[B]:ASN:C	3:L:2930[B]:LEU:HD22	2.36	0.51
3:L:2962[B]:GLY:N	3:L:3111[B]:SER:OG	2.44	0.51
3:L:3113[B]:ASP:O	3:L:3114[B]:PRO:C	2.53	0.51
3:L:3287[A]:ILE:O	3:L:3287[A]:ILE:HG23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3293[A]:LYS:CG	3:L:3294[A]:SER:HB2	2.36	0.51
1:M:402:THR:HG23	1:M:659:CYS:HA	1.92	0.51
1:M:643:ILE:HD13	1:M:708:PHE:HB2	1.91	0.51
2:N:2562:GLY:H	2:N:2846:TRP:HB2	1.76	0.51
3:O:2928[A]:ASN:C	3:O:2930[A]:LEU:HD22	2.36	0.51
3:O:2951[B]:ASP:O	3:O:2956[B]:LYS:HE2	2.09	0.51
3:O:2966[B]:SER:C	3:O:2967[B]:CYS:SG	2.94	0.51
3:O:3096[B]:VAL:HG11	3:O:3115[B]:LEU:HD12	1.89	0.51
3:O:3300[B]:LEU:CD2	3:O:3300[B]:LEU:H	2.24	0.51
3:R:2952[A]:ALA:CB	3:R:2956[A]:LYS:HB3	2.40	0.51
3:R:3023[B]:ILE:O	3:R:3025[B]:VAL:N	2.44	0.51
3:R:3110[A]:THR:O	3:R:3111[A]:SER:C	2.53	0.51
3:R:3114[B]:PRO:CD	3:R:3115[B]:LEU:N	2.73	0.51
1:S:77:GLU:O	1:S:81:VAL:HG23	2.11	0.51
1:S:979:LEU:CB	1:S:980:TYR:HA	2.38	0.51
3:U:2928[B]:ASN:C	3:U:2930[B]:LEU:HD22	2.36	0.51
3:U:2962[A]:GLY:N	3:U:3111[A]:SER:OG	2.44	0.51
3:U:3113[B]:ASP:O	3:U:3114[B]:PRO:C	2.53	0.51
3:U:3291[A]:ASP:OD2	3:U:3293[A]:LYS:NZ	2.43	0.51
1:V:150:GLY:HA2	1:V:151:GLN:C	2.35	0.51
1:V:1315:GLY:HA3	1:V:1601:TRP:HB2	1.91	0.51
2:W:2184:MET:HE3	2:W:2231:LEU:HD11	1.92	0.51
3:X:2952[A]:ALA:CB	3:X:2956[A]:LYS:HB3	2.40	0.51
3:X:2966[A]:SER:C	3:X:2967[A]:CYS:SG	2.94	0.51
3:X:3275[B]:LEU:N	3:X:3275[B]:LEU:CD1	2.73	0.51
1:Y:361:GLU:HG2	1:Y:363:THR:HG22	1.92	0.51
1:Y:1315:GLY:HA3	1:Y:1601:TRP:CG	2.46	0.51
3:a:2962[A]:GLY:N	3:a:3111[A]:SER:OG	2.44	0.51
3:a:2966[B]:SER:C	3:a:2967[B]:CYS:SG	2.94	0.51
3:a:3300[B]:LEU:N	3:a:3300[B]:LEU:CD2	2.73	0.51
3:d:2952[A]:ALA:CA	3:d:2956[A]:LYS:HB3	2.38	0.51
3:d:3028[B]:PRO:HG2	3:d:3029[B]:LYS:CG	2.40	0.51
3:d:3101[A]:PRO:HG2	3:d:3102[A]:TYR:CD1	2.46	0.51
3:d:3273[B]:LEU:O	3:d:3275[B]:LEU:HD12	2.11	0.51
1:A:965:ASP:O	1:A:969:ALA:N	2.44	0.51
1:A:1067:TYR:H	1:A:1067:TYR:HD1	1.58	0.51
2:B:2115:SER:OG	2:B:2116:SER:N	2.41	0.51
2:B:2619:VAL:HG22	1:b:138:ALA:HB2	1.92	0.51
3:C:2935[B]:ILE:CD1	3:C:2935[B]:ILE:N	2.73	0.51
3:C:3023[A]:ILE:O	3:C:3025[A]:VAL:N	2.44	0.51
3:C:3110[A]:THR:C	3:C:3112[A]:TYR:N	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3115[A]:LEU:HD22	3:C:3115[A]:LEU:O	2.10	0.51
3:C:3153[B]:LYS:O	3:L:3153[B]:LYS:O	2.28	0.51
3:C:3196[A]:THR:O	3:C:3199[A]:GLN:HB2	2.11	0.51
3:F:3173[B]:THR:HG21	3:a:3173[B]:THR:OG1	2.11	0.51
3:F:3176[A]:LYS:H	3:F:3176[A]:LYS:CE	2.17	0.51
3:F:3284[B]:LYS:HD3	3:F:3284[B]:LYS:C	2.32	0.51
1:G:1154:SER:HB3	1:G:1220:MET:HE2	1.93	0.51
3:I:2966[B]:SER:C	3:I:2967[B]:CYS:SG	2.94	0.51
3:I:2986[A]:PRO:CB	3:I:3127[A]:TRP:CZ3	2.94	0.51
3:I:3150[B]:LYS:CB	3:R:3159[B]:SER:O	2.51	0.51
3:I:3273[A]:LEU:O	3:I:3275[A]:LEU:HD12	2.11	0.51
1:J:552:PHE:HZ	1:J:623:TYR:HE1	1.58	0.51
1:J:837:HIS:HA	1:J:1113:HIS:O	2.10	0.51
1:J:1155:LEU:HB2	1:J:1177:VAL:CG1	2.41	0.51
2:K:2556:TYR:HD1	2:K:2557:ALA:N	2.08	0.51
3:L:2966[A]:SER:C	3:L:2967[A]:CYS:SG	2.94	0.51
3:L:3151[B]:LEU:CB	3:L:3175[B]:TYR:CD2	2.93	0.51
3:L:3196[B]:THR:O	3:L:3200[B]:LEU:N	2.44	0.51
3:L:3300[B]:LEU:N	3:L:3300[B]:LEU:CD2	2.73	0.51
1:M:563:ILE:O	1:M:612:GLY:HA3	2.11	0.51
1:M:1164:ASP:OD1	1:M:1212:HIS:NE2	2.27	0.51
3:O:2952[B]:ALA:CB	3:O:2956[B]:LYS:HB3	2.40	0.51
3:O:2966[A]:SER:C	3:O:2967[A]:CYS:SG	2.94	0.51
3:O:3023[B]:ILE:O	3:O:3025[B]:VAL:N	2.44	0.51
3:O:3028[B]:PRO:HG2	3:O:3029[B]:LYS:CG	2.40	0.51
3:O:3139[B]:LEU:CD2	3:O:3139[B]:LEU:N	2.73	0.51
3:O:3147[A]:GLU:CB	3:O:3149[A]:ASN:ND2	2.73	0.51
3:O:3287[A]:ILE:O	3:O:3287[A]:ILE:HG23	2.10	0.51
3:R:2928[A]:ASN:C	3:R:2930[A]:LEU:HD22	2.36	0.51
3:R:3101[A]:PRO:HG2	3:R:3102[A]:TYR:CD1	2.46	0.51
3:R:3228[A]:VAL:O	3:R:3228[A]:VAL:HG23	2.10	0.51
3:R:3275[A]:LEU:N	3:R:3275[A]:LEU:CD1	2.73	0.51
1:S:807:GLY:HA2	1:S:808:THR:C	2.36	0.51
3:U:2928[A]:ASN:C	3:U:2930[A]:LEU:HD22	2.36	0.51
3:U:2986[A]:PRO:CB	3:U:3127[A]:TRP:CZ3	2.94	0.51
3:U:3092[B]:ILE:CG2	3:U:3096[B]:VAL:CG2	2.88	0.51
3:U:3147[A]:GLU:CB	3:U:3149[A]:ASN:ND2	2.73	0.51
3:U:3158[B]:PHE:HB2	3:d:3149[B]:ASN:CB	2.40	0.51
3:U:3228[B]:VAL:HG23	3:U:3228[B]:VAL:O	2.10	0.51
2:W:2361:LYS:HD2	2:W:2362:GLN:N	2.26	0.51
2:W:2554:PRO:HA	2:W:2555:GLU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:2816:SER:HB2	2:W:2886:VAL:HG21	1.92	0.51
3:X:2937[A]:ASN:ND2	3:X:3006[A]:LYS:CD	2.73	0.51
3:X:2961[B]:HIS:HB3	3:X:3111[B]:SER:HB3	1.92	0.51
3:X:2969[B]:TYR:CG	3:X:2970[B]:PRO:HD2	2.42	0.51
3:X:3028[B]:PRO:HG2	3:X:3029[B]:LYS:CG	2.40	0.51
3:X:3104[A]:MET:HA	3:X:3110[A]:THR:CG2	2.17	0.51
3:a:3113[B]:ASP:O	3:a:3114[B]:PRO:C	2.53	0.51
3:a:3196[A]:THR:OG1	3:a:3199[A]:GLN:HB2	2.11	0.51
3:a:3219[A]:LEU:N	3:a:3219[A]:LEU:CD2	2.73	0.51
3:a:3273[A]:LEU:O	3:a:3275[A]:LEU:HD12	2.11	0.51
1:b:92:TRP:O	1:b:212:ASN:ND2	2.44	0.51
1:b:521:THR:HA	1:b:568:PHE:HE2	1.76	0.51
3:d:2933[B]:SER:CB	3:d:2936[B]:GLU:CB	2.86	0.51
3:d:2935[A]:ILE:CD1	3:d:2935[A]:ILE:N	2.73	0.51
3:d:2962[A]:GLY:N	3:d:3111[A]:SER:OG	2.44	0.51
3:d:2966[A]:SER:C	3:d:2967[A]:CYS:SG	2.94	0.51
3:d:3023[B]:ILE:O	3:d:3025[B]:VAL:N	2.44	0.51
3:d:3113[B]:ASP:O	3:d:3114[B]:PRO:C	2.53	0.51
3:d:3114[B]:PRO:CD	3:d:3115[B]:LEU:N	2.72	0.51
1:A:931:TRP:CD1	1:A:1048:ASN:HD22	2.29	0.51
1:A:1573:CYS:HA	1:A:1583:CYS:O	2.11	0.51
2:B:2497:GLU:HB2	2:B:2498:VAL:HA	1.91	0.51
3:C:3219[B]:LEU:N	3:C:3219[B]:LEU:CD2	2.73	0.51
3:C:3300[B]:LEU:CD2	3:C:3300[B]:LEU:H	2.24	0.51
1:D:1082:SER:HB3	1:D:1083:PRO:HD3	1.93	0.51
1:D:1358:LEU:O	1:D:1375:ASN:ND2	2.38	0.51
2:E:2554:PRO:HA	2:E:2555:GLU:CB	2.41	0.51
3:F:3023[B]:ILE:O	3:F:3025[B]:VAL:N	2.44	0.51
3:F:3113[B]:ASP:O	3:F:3114[B]:PRO:C	2.53	0.51
3:F:3300[A]:LEU:CD2	3:F:3300[A]:LEU:H	2.24	0.51
3:I:2952[B]:ALA:HB3	3:I:2954[B]:TYR:N	2.17	0.51
3:I:3023[A]:ILE:O	3:I:3025[A]:VAL:N	2.44	0.51
3:I:3150[B]:LYS:O	3:R:3172[B]:SER:CB	2.59	0.51
3:I:3255[B]:PRO:HG3	3:R:2963[B]:MET:N	2.25	0.51
1:J:898:GLY:HA2	1:J:1186:TRP:CB	2.41	0.51
2:K:2795:ILE:O	2:K:2799:LYS:HG3	2.10	0.51
2:K:2816:SER:HB2	2:K:2886:VAL:HG22	1.93	0.51
3:L:2969[A]:TYR:CE2	3:L:2970[A]:PRO:CG	2.86	0.51
1:M:1013:ILE:HG21	1:M:1192:TYR:CD1	2.46	0.51
3:O:2952[A]:ALA:CA	3:O:2956[A]:LYS:HB3	2.38	0.51
3:O:3141[A]:TYR:CD2	3:O:3141[A]:TYR:C	2.86	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3153[B]:LYS:HG2	3:X:3176[B]:LYS:HZ1	1.73	0.51
3:O:3196[B]:THR:O	3:O:3200[B]:LEU:N	2.44	0.51
3:O:3253[B]:GLU:OE2	3:X:3161[B]:GLU:OE1	2.26	0.51
3:O:3300[A]:LEU:CD2	3:O:3300[A]:LEU:H	2.24	0.51
1:P:480:CYS:HA	1:P:490:TRP:CE2	2.45	0.51
1:P:533:VAL:HG12	1:P:540:THR:HG22	1.93	0.51
1:P:883:CYS:HB3	1:P:884:PRO:HD2	1.93	0.51
1:P:1152:LYS:HZ2	1:P:1183:GLU:HG2	1.76	0.51
2:Q:2446:GLU:HG2	2:Q:2448:THR:HG23	1.93	0.51
2:Q:2665:GLU:OE1	2:Q:2798:GLN:NE2	2.39	0.51
3:R:2952[B]:ALA:CB	3:R:2956[B]:LYS:HB3	2.40	0.51
3:R:3201[A]:GLU:O	3:R:3205[A]:LYS:HB2	2.11	0.51
3:R:3275[B]:LEU:N	3:R:3275[B]:LEU:CD1	2.73	0.51
3:U:2952[B]:ALA:CA	3:U:2956[B]:LYS:HB3	2.38	0.51
3:U:3101[B]:PRO:HG2	3:U:3102[B]:TYR:CD1	2.45	0.51
3:U:3228[A]:VAL:O	3:U:3228[A]:VAL:HG23	2.10	0.51
1:V:1195:ASP:OD1	1:V:1196:ILE:N	2.44	0.51
2:W:2394:VAL:HG11	2:W:2451:LEU:HD12	1.93	0.51
3:X:2928[A]:ASN:C	3:X:2930[A]:LEU:HD22	2.36	0.51
3:X:3101[A]:PRO:HG2	3:X:3102[A]:TYR:CD1	2.46	0.51
3:X:3110[B]:THR:C	3:X:3112[B]:TYR:N	2.68	0.51
1:Y:411:ASP:OD1	1:Y:411:ASP:N	2.35	0.51
1:Y:706:LEU:HB2	1:Y:713:ILE:HD11	1.93	0.51
2:Z:2224:THR:HG23	2:Z:2278:GLU:HB3	1.93	0.51
3:a:2937[A]:ASN:ND2	3:a:3006[A]:LYS:CD	2.73	0.51
3:a:2952[B]:ALA:CB	3:a:2956[B]:LYS:HB3	2.40	0.51
3:a:2986[A]:PRO:CB	3:a:3127[A]:TRP:CZ3	2.94	0.51
3:a:3110[B]:THR:O	3:a:3111[B]:SER:C	2.53	0.51
3:a:3147[A]:GLU:CB	3:a:3149[A]:ASN:ND2	2.73	0.51
3:a:3285[A]:VAL:CG2	3:a:3286[A]:THR:N	2.73	0.51
3:d:2928[B]:ASN:C	3:d:2930[B]:LEU:HD22	2.36	0.51
3:d:3004[B]:GLY:O	3:d:3006[B]:LYS:N	2.44	0.51
3:d:3113[A]:ASP:O	3:d:3114[A]:PRO:C	2.53	0.51
3:d:3147[A]:GLU:CD	3:d:3149[A]:ASN:HD21	2.17	0.51
3:d:3196[A]:THR:OG1	3:d:3199[A]:GLN:HB2	2.11	0.51
3:d:3196[B]:THR:O	3:d:3199[B]:GLN:HB2	2.11	0.51
1:A:1046:HIS:HA	1:A:1049:VAL:HB	1.93	0.51
3:C:3093[B]:HIS:CE1	3:C:3119[B]:HIS:CD2	2.92	0.51
3:C:3147[A]:GLU:CB	3:C:3149[A]:ASN:ND2	2.73	0.51
3:C:3176[B]:LYS:N	3:C:3176[B]:LYS:CE	2.73	0.51
3:C:3268[A]:LYS:HG2	1:D:1539:GLN:HE22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3273[B]:LEU:O	3:C:3275[B]:LEU:HD12	2.11	0.51
3:C:3284[B]:LYS:HD3	3:C:3284[B]:LYS:C	2.32	0.51
1:D:135:THR:O	1:D:135:THR:OG1	2.28	0.51
1:D:316:ASN:HD21	1:D:340:GLN:HE21	1.59	0.51
2:E:2802:ASP:OD2	2:E:2903:TYR:OH	2.18	0.51
3:F:2928[A]:ASN:C	3:F:2930[A]:LEU:HD22	2.36	0.51
3:F:3110[A]:THR:C	3:F:3112[A]:TYR:N	2.68	0.51
3:F:3110[B]:THR:C	3:F:3112[B]:TYR:N	2.68	0.51
3:F:3155[B]:MET:H	3:a:3153[B]:LYS:HB3	1.75	0.51
3:F:3155[B]:MET:O	3:a:3153[B]:LYS:CB	2.59	0.51
3:F:3254[B]:MET:CB	3:a:2966[B]:SER:CB	2.89	0.51
3:F:3273[B]:LEU:O	3:F:3275[B]:LEU:HD12	2.11	0.51
2:H:2500:ILE:HG13	2:H:2501:PRO:HD2	1.92	0.51
2:H:2830:GLN:H	2:H:2863:ARG:NH2	2.09	0.51
3:I:2928[B]:ASN:C	3:I:2930[B]:LEU:HD22	2.36	0.51
3:I:3023[B]:ILE:O	3:I:3025[B]:VAL:N	2.44	0.51
3:I:3101[A]:PRO:HG2	3:I:3102[A]:TYR:CD1	2.46	0.51
3:I:3120[B]:HIS:HD2	3:R:2969[B]:TYR:HE2	1.52	0.51
3:I:3196[A]:THR:OG1	3:I:3199[A]:GLN:HB2	2.11	0.51
3:I:3228[B]:VAL:O	3:I:3228[B]:VAL:HG23	2.10	0.51
3:I:3300[A]:LEU:CD2	3:I:3300[A]:LEU:H	2.24	0.51
1:J:483:GLY:HA2	1:J:773:PHE:CZ	2.46	0.51
1:J:1300:CYS:HB3	1:J:1494:ARG:NH1	2.26	0.51
2:K:2547:MET:O	2:K:2751:TRP:HH2	1.94	0.51
2:K:2863:ARG:HB2	2:K:2865:ILE:HG12	1.93	0.51
3:L:2966[B]:SER:C	3:L:2967[B]:CYS:SG	2.94	0.51
3:L:3023[A]:ILE:O	3:L:3025[A]:VAL:N	2.44	0.51
3:O:2952[B]:ALA:CA	3:O:2956[B]:LYS:HB3	2.38	0.51
3:O:2969[B]:TYR:CB	3:X:2988[B]:TRP:O	2.59	0.51
3:O:2976[B]:ALA:CB	3:X:3156[B]:MET:HG2	2.41	0.51
3:O:3023[A]:ILE:O	3:O:3025[A]:VAL:N	2.44	0.51
3:O:3115[A]:LEU:HD22	3:O:3115[A]:LEU:O	2.10	0.51
3:O:3176[A]:LYS:N	3:O:3176[A]:LYS:CE	2.73	0.51
3:O:3196[B]:THR:OG1	3:O:3199[B]:GLN:HB2	2.11	0.51
1:P:59:LEU:HD13	1:P:68:TRP:CD1	2.45	0.51
1:P:1286:ARG:HD2	1:P:1333:GLU:OE1	2.11	0.51
2:Q:2191:LEU:HD13	2:Q:2296:LEU:HD22	1.93	0.51
3:R:3023[A]:ILE:O	3:R:3025[A]:VAL:N	2.44	0.51
3:R:3300[A]:LEU:CD2	3:R:3300[A]:LEU:H	2.24	0.51
1:S:895:CYS:O	1:S:897:HIS:ND1	2.42	0.51
2:T:2856:ILE:HG22	2:T:2859:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2952[A]:ALA:CB	3:U:2956[A]:LYS:HB3	2.40	0.51
3:U:2961[B]:HIS:HB3	3:U:3111[B]:SER:HB3	1.92	0.51
3:U:2962[B]:GLY:N	3:U:3111[B]:SER:OG	2.44	0.51
3:U:3042[A]:ASP:N	3:U:3042[A]:ASP:OD2	2.41	0.51
3:U:3114[B]:PRO:CD	3:U:3115[B]:LEU:N	2.72	0.51
3:U:3147[B]:GLU:CB	3:U:3149[B]:ASN:ND2	2.73	0.51
3:U:3196[A]:THR:O	3:U:3199[A]:GLN:HB2	2.11	0.51
3:U:3201[B]:GLU:O	3:U:3205[B]:LYS:HB2	2.11	0.51
3:U:3300[B]:LEU:CD2	3:U:3300[B]:LEU:H	2.24	0.51
1:V:841:LYS:HA	1:V:1117:ASP:HB2	1.92	0.51
1:V:926:LEU:HD11	1:V:1043:MET:HB3	1.92	0.51
1:V:980:TYR:CE2	1:V:1021:LEU:HB3	2.46	0.51
1:V:1472:GLN:OE1	1:V:1475:ARG:NH1	2.44	0.51
2:W:2415:PRO:HG2	2:W:2417:VAL:O	2.12	0.51
2:W:2497:GLU:HB2	2:W:2498:VAL:HA	1.92	0.51
2:W:2569:TRP:HA	2:W:2746:MET:HE3	1.92	0.51
3:X:3023[A]:ILE:O	3:X:3025[A]:VAL:N	2.44	0.51
3:X:3096[B]:VAL:HG11	3:X:3115[B]:LEU:HD12	1.89	0.51
3:X:3196[B]:THR:O	3:X:3199[B]:GLN:HB2	2.11	0.51
1:Y:905:TRP:CZ2	1:Y:1083:PRO:HG2	2.46	0.51
2:Z:2172:ILE:HG13	2:Z:2173:VAL:HG13	1.93	0.51
3:a:3219[B]:LEU:N	3:a:3219[B]:LEU:CD2	2.73	0.51
1:b:10:LEU:HD12	1:b:104:LEU:HD11	1.93	0.51
1:b:187:GLY:HA3	1:b:195:SER:HB3	1.91	0.51
1:b:548:ALA:O	1:b:559:THR:HG22	2.11	0.51
1:b:1542:ARG:O	1:b:1546:LYS:HG2	2.11	0.51
3:d:3188[B]:ASP:N	3:d:3188[B]:ASP:OD2	2.36	0.51
3:d:3228[B]:VAL:O	3:d:3228[B]:VAL:HG23	2.10	0.51
1:A:1596:GLU:O	1:A:1597:THR:HG22	2.12	0.50
3:C:2975[B]:PHE:HZ	3:L:2961[B]:HIS:CD2	2.28	0.50
3:C:3101[A]:PRO:HG2	3:C:3102[A]:TYR:CD1	2.46	0.50
3:C:3196[B]:THR:OG1	3:C:3199[B]:GLN:HB2	2.11	0.50
3:C:3196[B]:THR:CA	3:C:3199[B]:GLN:OE1	2.58	0.50
3:C:3223[B]:GLY:C	3:L:3252[B]:TYR:CZ	2.88	0.50
3:C:3291[A]:ASP:OD2	3:C:3293[A]:LYS:NZ	2.43	0.50
1:D:468:CYS:HA	1:D:469:PRO:C	2.37	0.50
1:D:490:TRP:HE1	1:D:670:PRO:HD3	1.76	0.50
1:D:1299:GLN:HB2	1:D:1311:CYS:SG	2.52	0.50
2:E:2224:THR:HG23	2:E:2278:GLU:HB3	1.93	0.50
2:E:2795:ILE:O	2:E:2798:GLN:HG2	2.11	0.50
3:F:2935[A]:ILE:CD1	3:F:2936[A]:GLU:N	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3157[B]:PRO:CD	3:a:3153[B]:LYS:NZ	2.74	0.50
3:F:3163[B]:ASN:CG	3:a:3149[B]:ASN:HD22	2.19	0.50
3:F:3196[B]:THR:O	3:F:3200[B]:LEU:N	2.43	0.50
3:F:3201[A]:GLU:O	3:F:3205[A]:LYS:HB2	2.11	0.50
3:F:3255[B]:PRO:HB3	3:a:2964[B]:PRO:N	2.17	0.50
3:F:3293[B]:LYS:CG	3:F:3294[B]:SER:HB2	2.36	0.50
3:I:2949[B]:LYS:C	3:I:2953[B]:GLY:H	2.17	0.50
3:I:3114[A]:PRO:CD	3:I:3115[A]:LEU:N	2.72	0.50
3:I:3254[B]:MET:CE	3:R:3157[B]:PRO:HD3	2.41	0.50
3:I:3300[B]:LEU:CD2	3:I:3300[B]:LEU:H	2.24	0.50
1:J:622:HIS:HE1	1:J:767:LYS:H	1.54	0.50
3:L:2952[A]:ALA:CA	3:L:2956[A]:LYS:HB3	2.38	0.50
3:L:3147[A]:GLU:CG	3:L:3149[A]:ASN:ND2	2.73	0.50
3:L:3217[A]:PHE:CB	3:L:3219[A]:LEU:HD21	2.42	0.50
1:M:447:MET:HA	1:M:455:TYR:HB2	1.93	0.50
1:M:449:ASP:OD2	1:M:1280:GLN:NE2	2.44	0.50
1:M:965:ASP:H	1:M:966:SER:HA	1.76	0.50
1:M:1542:ARG:O	1:M:1546:LYS:HG2	2.11	0.50
2:N:2132:CYS:HB2	2:N:2142:ALA:CB	2.41	0.50
2:N:2556:TYR:CE1	2:N:2844:MET:HG3	2.46	0.50
3:O:2935[A]:ILE:CD1	3:O:2936[A]:GLU:N	2.73	0.50
3:O:2937[B]:ASN:ND2	3:O:3006[B]:LYS:CD	2.73	0.50
3:O:3176[B]:LYS:H	3:O:3176[B]:LYS:CE	2.17	0.50
3:O:3188[B]:ASP:N	3:O:3188[B]:ASP:OD2	2.36	0.50
1:P:928:TYR:HB2	1:P:1048:ASN:HB2	1.92	0.50
2:Q:2361:LYS:HD2	2:Q:2362:GLN:N	2.26	0.50
3:R:2961[B]:HIS:HB3	3:R:3111[B]:SER:HB3	1.92	0.50
3:R:3115[B]:LEU:HD22	3:R:3115[B]:LEU:O	2.10	0.50
3:R:3196[B]:THR:O	3:R:3199[B]:GLN:HB2	2.11	0.50
3:R:3228[B]:VAL:O	3:R:3228[B]:VAL:HG23	2.10	0.50
1:S:516:TRP:CD1	1:S:579:LEU:HB3	2.45	0.50
3:U:3201[A]:GLU:O	3:U:3205[A]:LYS:HB2	2.11	0.50
3:U:3285[B]:VAL:CG2	3:U:3286[B]:THR:N	2.73	0.50
1:V:905:TRP:HE1	1:V:1083:PRO:CD	2.24	0.50
2:W:2180:TRP:HB3	2:W:2184:MET:HE2	1.92	0.50
3:X:2961[A]:HIS:CD2	3:X:2988[A]:TRP:CZ3	2.96	0.50
3:X:2962[B]:GLY:N	3:X:3111[B]:SER:OG	2.44	0.50
3:X:3066[B]:TYR:CE1	3:X:3193[B]:HIS:CE1	2.98	0.50
1:Y:462:HIS:HA	1:Y:490:TRP:CH2	2.45	0.50
2:Z:2610:ASP:HA	2:Z:2621:GLU:HA	1.93	0.50
2:Z:2866:PRO:HG2	3:a:2933[A]:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:2928[A]:ASN:C	3:a:2930[A]:LEU:HD22	2.36	0.50
3:a:3113[A]:ASP:O	3:a:3114[A]:PRO:C	2.53	0.50
3:a:3228[A]:VAL:O	3:a:3228[A]:VAL:HG23	2.10	0.50
3:a:3275[B]:LEU:N	3:a:3275[B]:LEU:CD1	2.73	0.50
1:b:1302:SER:HB3	1:b:1303:GLU:HA	1.91	0.50
2:c:2254:THR:HG23	2:c:2317:LEU:HD13	1.93	0.50
2:c:2560:LEU:HD13	2:c:2569:TRP:CD1	2.47	0.50
3:d:2962[B]:GLY:N	3:d:3111[B]:SER:OG	2.44	0.50
3:d:3110[A]:THR:C	3:d:3112[A]:TYR:N	2.68	0.50
3:d:3147[A]:GLU:CB	3:d:3149[A]:ASN:ND2	2.73	0.50
3:d:3151[B]:LEU:CB	3:d:3175[B]:TYR:CD2	2.93	0.50
3:d:3173[B]:THR:HG22	3:d:3174[B]:GLY:H	1.67	0.50
3:C:2964[B]:PRO:O	3:L:3255[B]:PRO:HA	2.07	0.50
3:C:3101[B]:PRO:HG2	3:C:3102[B]:TYR:CD1	2.46	0.50
3:C:3150[B]:LYS:HZ2	3:L:3160[B]:SER:CA	2.19	0.50
3:C:3154[B]:PRO:HD3	3:L:3173[B]:THR:O	2.10	0.50
3:C:3228[A]:VAL:HG23	3:C:3228[A]:VAL:O	2.10	0.50
3:C:3291[B]:ASP:OD2	3:C:3293[B]:LYS:NZ	2.43	0.50
1:D:957:ASN:N	1:D:958:PRO:HA	2.26	0.50
1:D:1030:MET:HA	1:D:1036:SER:HA	1.93	0.50
3:F:3110[A]:THR:O	3:F:3111[A]:SER:C	2.53	0.50
3:F:3135[A]:LYS:HB2	3:F:3141[A]:TYR:HD1	1.76	0.50
3:F:3155[B]:MET:N	3:a:3153[B]:LYS:HB3	2.27	0.50
3:F:3176[A]:LYS:NZ	3:F:3176[A]:LYS:CB	2.73	0.50
2:H:2134:ASN:OD1	2:H:2137:ALA:N	2.45	0.50
2:H:2833:GLY:HA3	2:H:2854:MET:HE1	1.93	0.50
3:I:2960[A]:PHE:CD2	3:I:3157[A]:PRO:CG	2.74	0.50
3:I:2965[B]:LEU:CA	3:R:3253[B]:GLU:CD	2.68	0.50
3:I:2971[A]:ASP:CG	3:I:2973[A]:THR:HG1	2.12	0.50
3:I:2980[B]:HIS:CA	3:R:2968[B]:GLN:HG2	2.36	0.50
3:I:2986[B]:PRO:CB	3:I:3127[B]:TRP:CZ3	2.94	0.50
3:I:3149[B]:ASN:ND2	3:R:3163[B]:ASN:C	2.67	0.50
3:I:3159[B]:SER:HA	3:R:3150[B]:LYS:CA	2.32	0.50
3:I:3228[B]:VAL:CG2	3:I:3245[B]:PHE:CE2	2.89	0.50
1:J:346:GLY:O	1:J:349:GLU:HB2	2.12	0.50
1:J:982:LYS:H	1:J:983:PRO:HD3	1.76	0.50
1:J:1280:GLN:NE2	1:J:1337:ARG:HB3	2.26	0.50
2:K:2680:HIS:NE2	2:K:2684:HIS:CD2	2.79	0.50
3:L:2948[B]:ASP:CB	3:L:2949[B]:LYS:CA	2.78	0.50
3:L:3113[A]:ASP:O	3:L:3114[A]:PRO:C	2.53	0.50
1:M:387:ASN:OD1	1:M:387:ASN:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:765:GLY:O	1:M:768:GLU:HG2	2.10	0.50
2:N:2571:ARG:NH1	2:N:2715:ASP:OD1	2.44	0.50
3:O:3163[B]:ASN:HD22	3:X:3148[B]:ILE:CG2	2.22	0.50
3:O:3196[A]:THR:O	3:O:3199[A]:GLN:HB2	2.11	0.50
3:O:3254[B]:MET:HG2	3:X:3159[B]:SER:CB	2.40	0.50
1:P:550:ILE:HG13	1:P:558:HIS:H	1.75	0.50
1:P:1438:ASP:OD1	1:P:1439:VAL:N	2.44	0.50
2:Q:2390:GLN:NE2	2:Q:2494:GLN:O	2.44	0.50
3:R:2928[B]:ASN:C	3:R:2930[B]:LEU:HD22	2.36	0.50
3:R:3135[B]:LYS:HB2	3:R:3141[B]:TYR:HD1	1.76	0.50
3:R:3201[B]:GLU:O	3:R:3205[B]:LYS:HB2	2.12	0.50
1:S:166:GLU:OE2	1:S:297:ARG:NH1	2.44	0.50
1:S:517:THR:HG21	1:S:708:PHE:HE1	1.76	0.50
1:S:1565:SER:HB3	1:S:1594:GLY:H	1.75	0.50
1:S:1618:LEU:HD23	3:X:3136[B]:TYR:CE2	2.47	0.50
2:T:2816:SER:HB2	2:T:2886:VAL:HG21	1.93	0.50
3:U:3196[B]:THR:CA	3:U:3199[B]:GLN:OE1	2.58	0.50
1:V:1170:MET:SD	1:V:1199:VAL:HG23	2.51	0.50
1:V:1315:GLY:HA3	1:V:1601:TRP:CB	2.41	0.50
2:W:2799:LYS:HA	2:W:2803:ARG:HH12	1.77	0.50
3:X:2937[B]:ASN:ND2	3:X:3006[B]:LYS:CD	2.73	0.50
3:X:2986[B]:PRO:CB	3:X:3127[B]:TRP:CZ3	2.94	0.50
3:X:3228[A]:VAL:O	3:X:3228[A]:VAL:HG23	2.10	0.50
3:X:3273[A]:LEU:O	3:X:3275[A]:LEU:HD12	2.11	0.50
1:Y:94:TRP:CD1	1:Y:212:ASN:HD22	2.28	0.50
1:Y:643:ILE:HD13	1:Y:708:PHE:HB2	1.93	0.50
1:Y:705:THR:HG22	1:Y:1118:THR:HG23	1.92	0.50
1:Y:906:HIS:HA	1:Y:909:ILE:HB	1.92	0.50
1:Y:1621:ASN:CA	3:d:3188[B]:ASP:HB2	2.42	0.50
3:a:3135[B]:LYS:HB2	3:a:3141[B]:TYR:HD1	1.76	0.50
3:a:3285[B]:VAL:CG2	3:a:3286[B]:THR:N	2.73	0.50
1:b:1348:TRP:CD1	1:b:1403:LEU:HD13	2.45	0.50
3:d:2986[A]:PRO:CB	3:d:3127[A]:TRP:CZ3	2.94	0.50
3:d:2986[B]:PRO:CB	3:d:3127[B]:TRP:CZ3	2.94	0.50
3:d:3042[A]:ASP:N	3:d:3042[A]:ASP:OD2	2.41	0.50
3:d:3201[A]:GLU:O	3:d:3205[A]:LYS:HB2	2.11	0.50
1:A:25:MET:HE2	1:A:34:TYR:HA	1.93	0.50
1:A:704:ASP:OD1	1:A:704:ASP:N	2.41	0.50
1:A:943:LEU:HD13	1:A:944:GLU:N	2.26	0.50
1:A:1299:GLN:O	1:A:1301:PRO:HD3	2.11	0.50
3:C:2962[A]:GLY:N	3:C:3111[A]:SER:OG	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2969[B]:TYR:CD2	3:C:2970[B]:PRO:CD	2.85	0.50
3:C:2973[B]:THR:N	3:L:3090[B]:ASN:HB3	2.26	0.50
3:C:3196[A]:THR:OG1	3:C:3199[A]:GLN:HB2	2.12	0.50
3:C:3201[A]:GLU:O	3:C:3205[A]:LYS:HB2	2.11	0.50
1:D:4:ARG:HD2	1:D:89:ILE:O	2.11	0.50
1:D:395:THR:HG22	1:D:396:ILE:HG13	1.92	0.50
1:D:754:GLU:OE2	1:D:799:ARG:NH2	2.43	0.50
1:D:1206:HIS:CE1	1:D:1209:ASP:HB3	2.47	0.50
2:E:2472:ASN:N	2:E:2473:GLY:HA2	2.26	0.50
3:F:2982[B]:MET:CA	3:a:3160[B]:SER:OG	2.59	0.50
3:F:3004[A]:GLY:O	3:F:3006[A]:LYS:N	2.44	0.50
3:F:3023[A]:ILE:O	3:F:3025[A]:VAL:N	2.44	0.50
3:F:3066[A]:TYR:CE1	3:F:3193[A]:HIS:CE1	2.98	0.50
3:F:3217[B]:PHE:CB	3:F:3219[B]:LEU:HD21	2.42	0.50
3:F:3254[B]:MET:CG	3:a:2966[B]:SER:CB	2.77	0.50
1:G:120:LYS:H	1:G:121:ASN:HA	1.75	0.50
1:G:975:PRO:HG2	1:G:1024:GLY:HA3	1.91	0.50
2:H:2683:ILE:O	2:H:2687:ILE:HG12	2.11	0.50
2:H:2811:HIS:HB3	2:H:2847:HIS:CD2	2.46	0.50
3:I:2928[A]:ASN:C	3:I:2930[A]:LEU:HD22	2.36	0.50
3:I:2962[B]:GLY:N	3:I:3111[B]:SER:OG	2.44	0.50
3:I:2967[B]:CYS:HB3	3:R:2979[B]:GLN:C	2.15	0.50
3:I:2973[B]:THR:O	3:R:3107[B]:LEU:HD12	2.10	0.50
3:I:3159[B]:SER:HA	3:R:3150[B]:LYS:CB	2.30	0.50
3:I:3161[B]:GLU:HA	3:R:3147[B]:GLU:HG2	1.93	0.50
3:I:3196[B]:THR:OG1	3:I:3199[B]:GLN:HB2	2.11	0.50
3:I:3201[A]:GLU:O	3:I:3205[A]:LYS:HB2	2.11	0.50
3:I:3228[A]:VAL:O	3:I:3228[A]:VAL:HG23	2.10	0.50
3:I:3273[B]:LEU:O	3:I:3275[B]:LEU:HD12	2.11	0.50
1:J:480:CYS:SG	1:J:621:LEU:HD11	2.51	0.50
1:J:724:LYS:HA	1:J:728:ARG:HH12	1.77	0.50
2:K:2868:GLU:N	2:K:2868:GLU:OE1	2.45	0.50
3:L:2937[B]:ASN:ND2	3:L:3006[B]:LYS:CD	2.73	0.50
3:L:2957[B]:ILE:HA	3:L:2960[B]:PHE:HE1	1.64	0.50
3:L:3196[B]:THR:OG1	3:L:3199[B]:GLN:HB2	2.11	0.50
3:L:3307[B]:PHE:HE1	3:L:3309[B]:PRO:CG	2.08	0.50
1:M:1348:TRP:HH2	1:M:1461:VAL:HG23	1.77	0.50
2:N:2180:TRP:HD1	2:N:2247:ILE:HD11	1.76	0.50
3:O:3110[A]:THR:O	3:O:3111[A]:SER:C	2.53	0.50
3:O:3220[A]:ARG:HH11	3:O:3220[A]:ARG:CG	2.12	0.50
1:P:597:VAL:O	1:P:601:VAL:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1407:THR:HG22	1:P:1426:LEU:HD21	1.93	0.50
2:Q:2132:CYS:O	2:Q:2334:LYS:HD3	2.11	0.50
3:R:3004[B]:GLY:O	3:R:3006[B]:LYS:N	2.44	0.50
3:R:3135[A]:LYS:HG3	3:R:3141[A]:TYR:CD1	2.33	0.50
3:R:3196[B]:THR:OG1	3:R:3199[B]:GLN:HB2	2.11	0.50
3:U:3196[B]:THR:OG1	3:U:3199[B]:GLN:HB2	2.11	0.50
3:U:3219[B]:LEU:N	3:U:3219[B]:LEU:CD2	2.73	0.50
3:U:3276[A]:ASP:O	3:U:3277[A]:ALA:HB3	2.12	0.50
1:V:1231:VAL:C	1:V:1233:SER:H	2.18	0.50
1:V:1427:HIS:HD2	1:V:1457:HIS:CE1	2.28	0.50
3:X:2952[B]:ALA:CB	3:X:2953[B]:GLY:CA	2.82	0.50
3:X:3110[B]:THR:O	3:X:3111[B]:SER:C	2.53	0.50
3:X:3196[A]:THR:O	3:X:3199[A]:GLN:HB2	2.11	0.50
1:Y:566:ARG:HH11	1:Y:803:LYS:NZ	2.09	0.50
3:a:2933[B]:SER:CB	3:a:2936[B]:GLU:CB	2.85	0.50
1:b:1575:PRO:HA	1:b:1581:GLU:O	2.11	0.50
3:d:2928[A]:ASN:C	3:d:2930[A]:LEU:HD22	2.36	0.50
3:d:2961[A]:HIS:HB3	3:d:3111[A]:SER:HB3	1.92	0.50
3:d:2961[B]:HIS:CD2	3:d:2988[B]:TRP:CZ3	2.96	0.50
3:d:3196[A]:THR:O	3:d:3199[A]:GLN:HB2	2.11	0.50
3:d:3284[A]:LYS:HE2	3:d:3284[A]:LYS:CA	2.30	0.50
3:d:3291[A]:ASP:OD2	3:d:3293[A]:LYS:NZ	2.43	0.50
3:d:3300[A]:LEU:CD2	3:d:3300[A]:LEU:H	2.24	0.50
3:d:3300[B]:LEU:CD2	3:d:3300[B]:LEU:H	2.24	0.50
4:q:1:NAG:C4	4:q:2:NAG:HN2	2.24	0.50
1:A:269:TYR:HA	1:A:272:LEU:HD13	1.91	0.50
1:A:747:PHE:HB2	1:A:799:ARG:HB3	1.93	0.50
1:A:1210:LYS:HA	1:A:1211:TYR:HD2	1.76	0.50
1:A:1631:GLU:OE1	1:b:328:LYS:NZ	2.45	0.50
3:C:2928[A]:ASN:C	3:C:2930[A]:LEU:HD22	2.36	0.50
3:C:3156[B]:MET:CG	3:L:2984[B]:THR:OG1	2.59	0.50
1:D:73:LEU:HD11	1:D:210:HIS:O	2.12	0.50
1:D:1249:TRP:HZ2	1:D:1537:ILE:HD12	1.76	0.50
2:E:2500:ILE:HD11	2:E:2775:GLY:O	2.12	0.50
3:F:2983[B]:VAL:CG2	3:a:3161[B]:GLU:CB	2.86	0.50
3:F:3147[A]:GLU:CG	3:F:3149[A]:ASN:ND2	2.73	0.50
3:F:3176[B]:LYS:NZ	3:F:3176[B]:LYS:CB	2.73	0.50
3:F:3196[A]:THR:O	3:F:3199[A]:GLN:HB2	2.11	0.50
3:F:3276[A]:ASP:O	3:F:3277[A]:ALA:HB3	2.12	0.50
3:F:3284[A]:LYS:HD3	3:F:3284[A]:LYS:C	2.32	0.50
1:G:37:ILE:O	1:G:72:TYR:OH	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1324:ARG:HG2	1:G:1516:VAL:HG12	1.93	0.50
3:I:3110[A]:THR:O	3:I:3111[A]:SER:C	2.53	0.50
3:I:3160[B]:SER:HA	3:R:2983[B]:VAL:HB	1.92	0.50
3:I:3162[B]:ASP:C	3:R:3147[B]:GLU:OE1	2.48	0.50
3:I:3264[A]:TYR:C	3:I:3264[A]:TYR:CD1	2.86	0.50
1:J:110:PHE:N	1:J:119:LYS:O	2.37	0.50
3:L:2951[A]:ASP:O	3:L:2956[A]:LYS:HE2	2.09	0.50
3:L:3196[A]:THR:OG1	3:L:3199[A]:GLN:HB2	2.11	0.50
3:L:3228[A]:VAL:O	3:L:3228[A]:VAL:HG23	2.10	0.50
3:L:3264[A]:TYR:C	3:L:3264[A]:TYR:CD1	2.86	0.50
1:M:979:LEU:HB3	1:M:980:TYR:CA	2.42	0.50
3:O:2962[A]:GLY:N	3:O:3111[A]:SER:OG	2.44	0.50
3:O:3042[B]:ASP:N	3:O:3042[B]:ASP:OD2	2.41	0.50
3:O:3196[A]:THR:OG1	3:O:3199[A]:GLN:HB2	2.11	0.50
3:O:3276[B]:ASP:O	3:O:3277[B]:ALA:HB3	2.12	0.50
3:O:3288[A]:MET:CA	3:O:3295[A]:LEU:HG	2.42	0.50
1:P:566:ARG:HH22	1:P:803:LYS:HD3	1.76	0.50
1:P:1348:TRP:CH2	1:P:1461:VAL:HG23	2.46	0.50
1:P:1631:GLU:OE1	1:S:329:ARG:NH1	2.44	0.50
3:R:2986[A]:PRO:CB	3:R:3127[A]:TRP:CZ3	2.94	0.50
3:R:3183[A]:LEU:H	3:R:3184[A]:ASN:CA	2.22	0.50
3:R:3196[A]:THR:OG1	3:R:3199[A]:GLN:HB2	2.11	0.50
3:R:3196[A]:THR:O	3:R:3199[A]:GLN:HB2	2.11	0.50
3:R:3196[B]:THR:N	3:R:3199[B]:GLN:CB	2.65	0.50
3:R:3276[B]:ASP:O	3:R:3277[B]:ALA:HB3	2.12	0.50
2:T:2630:LYS:C	2:T:2632:GLU:H	2.18	0.50
3:U:3135[B]:LYS:HB2	3:U:3141[B]:TYR:HD1	1.76	0.50
3:U:3273[B]:LEU:O	3:U:3275[B]:LEU:HD12	2.11	0.50
1:V:548:ALA:H	1:V:559:THR:HG22	1.76	0.50
1:V:957:ASN:ND2	1:V:960:PHE:HB2	2.26	0.50
3:X:2962[A]:GLY:N	3:X:3111[A]:SER:OG	2.44	0.50
3:X:3023[B]:ILE:O	3:X:3025[B]:VAL:N	2.44	0.50
3:X:3196[A]:THR:O	3:X:3200[A]:LEU:N	2.44	0.50
1:Y:305:ASN:N	1:Y:400:ILE:O	2.27	0.50
1:Y:1018:ILE:HA	1:Y:1021:LEU:HB2	1.93	0.50
1:Y:1162:ALA:HA	1:Y:1168:GLN:O	2.12	0.50
1:Y:1321:HIS:CD2	1:Y:1465:TRP:HH2	2.30	0.50
2:Z:2265:ILE:HD12	2:Z:2443:TYR:CG	2.46	0.50
3:a:2935[A]:ILE:CD1	3:a:2936[A]:GLU:N	2.73	0.50
3:a:3023[A]:ILE:O	3:a:3025[A]:VAL:N	2.44	0.50
1:b:29:GLU:OE2	1:b:29:GLU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:557:VAL:HG22	1:b:558:HIS:HA	1.93	0.50
1:b:1328:SER:HB2	1:b:1523:LEU:HD13	1.93	0.50
1:b:1636:ASN:C	1:b:1638:SER:H	2.19	0.50
3:d:3096[B]:VAL:HG11	3:d:3115[B]:LEU:HD12	1.89	0.50
3:d:3114[A]:PRO:CD	3:d:3115[A]:LEU:N	2.72	0.50
1:A:716:LEU:O	1:A:720:VAL:HG13	2.11	0.50
1:A:1486:LEU:HD12	2:E:2486:ILE:HG22	1.92	0.50
3:C:2974[B]:ALA:CB	3:L:3253[B]:GLU:OE1	2.58	0.50
3:C:3023[B]:ILE:O	3:C:3025[B]:VAL:N	2.44	0.50
3:C:3038[A]:ILE:HG23	3:C:3040[A]:VAL:HG22	1.90	0.50
3:C:3183[A]:LEU:H	3:C:3184[A]:ASN:CA	2.21	0.50
3:C:3220[B]:ARG:HD3	3:L:2964[B]:PRO:HB3	1.93	0.50
3:C:3256[B]:TRP:CA	3:L:2965[B]:LEU:O	2.56	0.50
1:D:1189:ASP:OD2	1:D:1190:ARG:NH1	2.44	0.50
3:F:2933[A]:SER:CB	3:F:2936[A]:GLU:CB	2.85	0.50
3:F:2986[B]:PRO:CB	3:F:3127[B]:TRP:CZ3	2.94	0.50
3:F:3038[A]:ILE:HG23	3:F:3040[A]:VAL:HG22	1.90	0.50
3:F:3163[B]:ASN:ND2	3:a:3149[B]:ASN:CG	2.70	0.50
3:F:3252[B]:TYR:O	3:a:3252[B]:TYR:O	2.30	0.50
3:F:3285[B]:VAL:CG2	3:F:3286[B]:THR:N	2.73	0.50
1:G:197:LEU:HB3	1:G:344:LEU:HD13	1.94	0.50
1:G:1275:ARG:HH22	1:G:1357:ARG:NH1	2.10	0.50
3:I:2951[A]:ASP:O	3:I:2956[A]:LYS:HE2	2.09	0.50
3:I:2961[A]:HIS:HB3	3:I:3111[A]:SER:HB3	1.92	0.50
3:I:3114[B]:PRO:CD	3:I:3115[B]:LEU:N	2.72	0.50
1:J:488:PRO:HB2	1:J:641:TRP:CE3	2.46	0.50
1:J:854:LEU:HG	1:J:959:PHE:HE2	1.76	0.50
2:K:2687:ILE:HD11	2:K:2695:MET:HG2	1.93	0.50
3:L:2928[A]:ASN:C	3:L:2930[A]:LEU:HD22	2.36	0.50
3:L:3196[A]:THR:O	3:L:3200[A]:LEU:N	2.44	0.50
3:L:3196[B]:THR:O	3:L:3199[B]:GLN:HB2	2.11	0.50
3:L:3201[B]:GLU:O	3:L:3205[B]:LYS:HB2	2.11	0.50
3:L:3276[B]:ASP:O	3:L:3277[B]:ALA:HB3	2.12	0.50
2:N:2849:ASP:OD2	2:N:2850:ARG:NH2	2.45	0.50
3:O:3135[B]:LYS:HB2	3:O:3141[B]:TYR:HD1	1.76	0.50
2:Q:2240:GLN:HG3	2:Q:2241:THR:N	2.26	0.50
3:R:2962[B]:GLY:N	3:R:3111[B]:SER:OG	2.44	0.50
3:R:2965[B]:LEU:CG	3:R:2974[B]:ALA:CB	2.85	0.50
3:R:3217[B]:PHE:CB	3:R:3219[B]:LEU:HD21	2.42	0.50
3:R:3284[B]:LYS:HD3	3:R:3284[B]:LYS:C	2.32	0.50
1:S:432:THR:HG23	1:S:435:GLU:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:551:GLU:OE2	1:S:1368:ARG:NH1	2.44	0.50
3:U:2969[A]:TYR:CD2	3:U:2970[A]:PRO:HD2	2.47	0.50
3:U:3066[A]:TYR:CE1	3:U:3193[A]:HIS:CE1	2.98	0.50
3:U:3101[A]:PRO:HG2	3:U:3102[A]:TYR:CD1	2.46	0.50
3:U:3113[A]:ASP:O	3:U:3114[A]:PRO:C	2.53	0.50
3:U:3172[B]:SER:N	3:d:3152[B]:LYS:HZ1	2.10	0.50
3:U:3176[B]:LYS:N	3:U:3176[B]:LYS:CE	2.73	0.50
3:U:3217[A]:PHE:CB	3:U:3219[A]:LEU:HD21	2.42	0.50
3:U:3219[B]:LEU:O	3:d:2972[B]:GLY:C	2.55	0.50
3:U:3254[B]:MET:O	3:d:2975[B]:PHE:CZ	2.63	0.50
3:U:3288[A]:MET:CA	3:U:3295[A]:LEU:HG	2.42	0.50
3:U:3300[A]:LEU:CD2	3:U:3300[A]:LEU:H	2.24	0.50
1:V:622:HIS:HE1	1:V:767:LYS:H	1.60	0.50
1:V:963:ALA:HB3	1:V:1038:PHE:O	2.10	0.50
2:W:2742:MET:HE3	2:W:2769:PHE:HE2	1.76	0.50
3:X:3276[B]:ASP:O	3:X:3277[B]:ALA:HB3	2.12	0.50
1:Y:492:ARG:NH1	1:Y:638:ASP:OD1	2.45	0.50
1:Y:566:ARG:N	1:Y:567:LEU:HA	2.25	0.50
2:Z:2486:ILE:HB	1:b:1487:PRO:HD3	1.92	0.50
3:a:3023[B]:ILE:O	3:a:3025[B]:VAL:N	2.44	0.50
3:a:3151[B]:LEU:CB	3:a:3175[B]:TYR:CD2	2.93	0.50
3:a:3196[B]:THR:O	3:a:3199[B]:GLN:HB2	2.11	0.50
1:b:573:LYS:HB3	1:b:574:GLY:HA2	1.93	0.50
1:b:704:ASP:N	1:b:704:ASP:OD1	2.44	0.50
1:b:1421:VAL:HG23	1:b:1422:HIS:HD1	1.76	0.50
2:c:2107:LEU:HA	2:c:2110:MET:HG2	1.94	0.50
2:c:2571:ARG:NH1	2:c:2715:ASP:OD1	2.44	0.50
3:d:2966[B]:SER:C	3:d:2967[B]:CYS:SG	2.94	0.50
3:d:3176[A]:LYS:N	3:d:3176[A]:LYS:CE	2.73	0.50
3:d:3217[A]:PHE:CB	3:d:3219[A]:LEU:HD21	2.42	0.50
3:C:2966[A]:SER:C	3:C:2967[A]:CYS:SG	2.94	0.50
3:C:3285[A]:VAL:CG2	3:C:3286[A]:THR:N	2.73	0.50
3:F:2985[B]:PHE:CE2	3:a:2970[B]:PRO:HA	2.40	0.50
3:F:3028[B]:PRO:HG2	3:F:3029[B]:LYS:CG	2.40	0.50
3:F:3219[B]:LEU:N	3:F:3219[B]:LEU:CD2	2.73	0.50
3:F:3288[A]:MET:CA	3:F:3295[A]:LEU:HG	2.42	0.50
1:G:307:ARG:HH12	1:G:484:MET:HE1	1.77	0.50
1:G:474:LEU:HD22	1:G:475:ASN:H	1.77	0.50
1:G:594:ASP:OD1	1:G:775:ARG:NH1	2.45	0.50
1:G:896:HIS:HB2	1:G:905:TRP:CG	2.47	0.50
1:G:931:TRP:CZ3	1:G:995:ILE:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2568:HIS:NE2	2:H:2669:TYR:OH	2.44	0.50
2:H:2800:LYS:O	3:I:3023[A]:ILE:HD13	2.03	0.50
3:I:3147[A]:GLU:CG	3:I:3149[A]:ASN:ND2	2.73	0.50
3:I:3252[B]:TYR:CD1	3:R:3108[B]:HIS:CE1	2.99	0.50
3:I:3284[A]:LYS:HD3	3:I:3284[A]:LYS:C	2.32	0.50
1:J:1427:HIS:CE1	1:J:1457:HIS:CE1	2.99	0.50
3:L:2952[B]:ALA:CB	3:L:2956[B]:LYS:HB3	2.40	0.50
3:L:2969[A]:TYR:CD2	3:L:2970[A]:PRO:HD2	2.47	0.50
3:L:3217[B]:PHE:CB	3:L:3219[B]:LEU:HD21	2.42	0.50
3:L:3300[A]:LEU:CD2	3:L:3300[A]:LEU:H	2.24	0.50
3:L:3300[B]:LEU:CD2	3:L:3300[B]:LEU:H	2.24	0.50
1:M:157:GLU:OE2	1:M:296:ARG:NH2	2.41	0.50
1:M:1323:HIS:CD2	1:M:1458:HIS:CE1	3.00	0.50
1:M:1339:SER:CB	1:M:1340:GLY:HA2	2.42	0.50
2:N:2548:CYS:HB2	2:N:2558:CYS:HA	1.93	0.50
2:N:2647:LEU:HD12	2:N:2656:LEU:HB2	1.94	0.50
3:O:2965[B]:LEU:CG	3:O:2974[B]:ALA:CB	2.85	0.50
3:O:3141[B]:TYR:CD2	3:O:3141[B]:TYR:C	2.86	0.50
3:O:3276[A]:ASP:O	3:O:3277[A]:ALA:HB3	2.12	0.50
2:Q:2394:VAL:HG11	2:Q:2451:LEU:HD12	1.93	0.50
3:R:3217[A]:PHE:CB	3:R:3219[A]:LEU:HD21	2.42	0.50
3:R:3300[B]:LEU:CD2	3:R:3300[B]:LEU:H	2.24	0.50
2:T:2303:ARG:NH2	2:T:2372:GLU:O	2.44	0.50
3:U:3023[B]:ILE:O	3:U:3025[B]:VAL:N	2.44	0.50
3:U:3176[B]:LYS:NZ	3:U:3176[B]:LYS:CB	2.73	0.50
3:U:3196[B]:THR:O	3:U:3199[B]:GLN:HB2	2.11	0.50
3:U:3273[A]:LEU:O	3:U:3275[A]:LEU:HD12	2.11	0.50
3:U:3291[B]:ASP:OD2	3:U:3293[B]:LYS:NZ	2.43	0.50
1:V:904:HIS:O	1:V:907:ARG:HB3	2.12	0.50
2:W:2390:GLN:NE2	2:W:2494:GLN:O	2.44	0.50
3:X:3196[A]:THR:OG1	3:X:3199[A]:GLN:HB2	2.12	0.50
3:X:3196[B]:THR:OG1	3:X:3199[B]:GLN:HB2	2.11	0.50
3:X:3264[B]:TYR:C	3:X:3264[B]:TYR:CD1	2.86	0.50
3:X:3285[B]:VAL:CG2	3:X:3286[B]:THR:N	2.73	0.50
3:X:3300[B]:LEU:CD2	3:X:3300[B]:LEU:H	2.24	0.50
1:Y:1315:GLY:HA3	1:Y:1601:TRP:CB	2.42	0.50
2:Z:2244:PHE:HZ	2:Z:2376:MET:HE1	1.76	0.50
3:a:2935[B]:ILE:CD1	3:a:2936[B]:GLU:N	2.73	0.50
3:a:2969[A]:TYR:CD2	3:a:2970[A]:PRO:HD2	2.47	0.50
3:a:3101[B]:PRO:HG2	3:a:3102[B]:TYR:CD1	2.46	0.50
3:a:3217[A]:PHE:CB	3:a:3219[A]:LEU:HD21	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3023[A]:ILE:O	3:d:3025[A]:VAL:N	2.44	0.50
3:d:3135[B]:LYS:HB2	3:d:3141[B]:TYR:HD1	1.76	0.50
1:A:500:ASN:O	1:A:504:THR:OG1	2.23	0.50
2:B:2242:TRP:O	2:B:2246:ASN:ND2	2.36	0.50
3:C:3196[A]:THR:CA	3:C:3199[A]:GLN:OE1	2.58	0.50
3:C:3196[B]:THR:O	3:C:3199[B]:GLN:HB2	2.11	0.50
3:C:3249[B]:GLY:O	3:L:3252[B]:TYR:CD2	2.65	0.50
1:D:1279:LYS:O	1:D:1282:ALA:N	2.42	0.50
3:F:2966[A]:SER:C	3:F:2967[A]:CYS:SG	2.94	0.50
3:F:2969[A]:TYR:CD2	3:F:2970[A]:PRO:HD2	2.47	0.50
3:F:3160[B]:SER:OG	3:a:2982[B]:MET:C	2.54	0.50
3:F:3160[B]:SER:OG	3:a:2983[B]:VAL:HG23	2.12	0.50
2:H:2546:LEU:HA	2:H:2557:ALA:HA	1.93	0.50
3:I:3135[A]:LYS:HB2	3:I:3141[A]:TYR:HD1	1.76	0.50
3:I:3156[B]:MET:N	3:R:2979[B]:GLN:NE2	2.56	0.50
1:J:516:TRP:HZ3	1:J:633:HIS:HD1	1.60	0.50
1:J:718:ARG:HG3	1:J:832:LYS:HB2	1.92	0.50
3:L:3201[A]:GLU:O	3:L:3205[A]:LYS:HB2	2.11	0.50
3:L:3288[B]:MET:CA	3:L:3295[B]:LEU:HG	2.42	0.50
1:M:1141:ARG:HB2	1:M:1197:THR:OG1	2.12	0.50
3:O:2965[B]:LEU:C	3:X:3254[B]:MET:HE1	2.34	0.50
3:O:3147[A]:GLU:CG	3:O:3149[A]:ASN:ND2	2.73	0.50
3:O:3291[B]:ASP:OD2	3:O:3293[B]:LYS:NZ	2.43	0.50
1:P:898:GLY:HA2	1:P:1186:TRP:HB2	1.93	0.50
3:R:2949[B]:LYS:C	3:R:2949[B]:LYS:CD	2.85	0.50
3:R:3298[B]:ASN:HA	3:R:3299[B]:LEU:HB3	1.88	0.50
2:T:2261:VAL:HG21	2:T:2441:ARG:HG3	1.93	0.50
2:T:2415:PRO:HD3	2:T:2454:MET:HE1	1.93	0.50
2:T:2830:GLN:OE1	2:T:2863:ARG:NH1	2.44	0.50
1:V:166:GLU:OE2	1:V:297:ARG:NH1	2.45	0.50
1:V:718:ARG:HH11	1:V:830:ASN:ND2	2.10	0.50
3:X:2949[B]:LYS:C	3:X:2949[B]:LYS:CD	2.85	0.50
3:X:2949[B]:LYS:C	3:X:2949[B]:LYS:HZ3	2.12	0.50
3:X:3196[B]:THR:CA	3:X:3199[B]:GLN:OE1	2.58	0.50
3:a:2961[A]:HIS:CD2	3:a:2988[A]:TRP:CZ3	2.96	0.50
3:a:3110[B]:THR:C	3:a:3112[B]:TYR:N	2.68	0.50
3:a:3196[A]:THR:O	3:a:3199[A]:GLN:HB2	2.11	0.50
3:a:3217[B]:PHE:CB	3:a:3219[B]:LEU:HD21	2.42	0.50
3:a:3288[A]:MET:CA	3:a:3295[A]:LEU:HG	2.42	0.50
3:d:3147[A]:GLU:CG	3:d:3149[A]:ASN:ND2	2.73	0.50
3:d:3211[B]:ASP:OD1	3:d:3211[B]:ASP:N	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:HB3	1:A:120:LYS:HD2	1.93	0.50
1:A:637:VAL:HA	1:A:640:LEU:HD12	1.94	0.50
1:A:1078:ARG:NH2	2:E:2877:ILE:O	2.45	0.50
2:B:2749:PHE:O	2:B:2754:ASN:ND2	2.31	0.50
3:C:2935[A]:ILE:CD1	3:C:2935[A]:ILE:H	2.25	0.50
3:C:3110[B]:THR:O	3:C:3111[B]:SER:C	2.53	0.50
3:C:3135[B]:LYS:HB2	3:C:3141[B]:TYR:HD1	1.76	0.50
1:D:443:MET:HE3	1:D:447:MET:HE2	1.93	0.50
2:E:2157:LEU:O	2:E:2160:VAL:HG22	2.12	0.50
2:E:2248:ILE:HG13	2:E:2373:MET:HE2	1.94	0.50
3:F:2939[B]:ARG:NE	3:F:3031[B]:ASN:ND2	2.60	0.50
3:F:2962[B]:GLY:N	3:F:3111[B]:SER:OG	2.44	0.50
3:F:2986[A]:PRO:CB	3:F:3127[A]:TRP:CZ3	2.94	0.50
3:F:3255[B]:PRO:CA	3:a:2966[B]:SER:N	2.75	0.50
3:F:3273[A]:LEU:HB2	3:F:3275[A]:LEU:CD1	2.34	0.50
3:F:3300[B]:LEU:CD2	3:F:3300[B]:LEU:H	2.24	0.50
1:G:120:LYS:HB3	1:G:122:VAL:N	2.27	0.50
1:G:1087:ALA:HB3	1:G:1090:ILE:HG13	1.92	0.50
3:I:2949[B]:LYS:C	3:I:2949[B]:LYS:CD	2.85	0.50
3:I:2960[A]:PHE:CD1	3:I:2960[A]:PHE:N	2.72	0.50
3:I:3155[B]:MET:HE3	3:R:3156[B]:MET:H	1.77	0.50
1:J:1582:ASN:HB3	1:J:1583:CYS:HB3	1.94	0.50
3:L:3220[A]:ARG:HH11	3:L:3220[A]:ARG:CG	2.12	0.50
3:L:3293[B]:LYS:HB2	3:L:3294[B]:SER:CA	2.41	0.50
3:O:2969[A]:TYR:CD2	3:O:2970[A]:PRO:HD2	2.47	0.50
3:O:3159[B]:SER:C	3:X:3151[B]:LEU:HD12	2.37	0.50
3:O:3228[B]:VAL:O	3:O:3228[B]:VAL:HG23	2.10	0.50
1:P:450:LYS:HE3	1:P:451:SER:H	1.77	0.50
1:P:843:VAL:HG22	1:P:928:TYR:O	2.12	0.50
1:P:1132:GLU:OE2	1:P:1136:ARG:NE	2.31	0.50
3:R:2937[B]:ASN:ND2	3:R:3006[B]:LYS:CD	2.73	0.50
3:R:2962[A]:GLY:N	3:R:3111[A]:SER:OG	2.44	0.50
3:R:3042[B]:ASP:N	3:R:3042[B]:ASP:OD2	2.41	0.50
3:R:3113[A]:ASP:O	3:R:3114[A]:PRO:C	2.53	0.50
3:R:3151[B]:LEU:CB	3:R:3175[B]:TYR:CD2	2.93	0.50
1:S:855:ARG:HD2	1:S:947:TYR:CD2	2.46	0.50
1:S:930:ASP:OD1	1:S:1051:ARG:NH2	2.44	0.50
2:T:2097:LEU:HD12	2:W:2235:PRO:HG2	1.94	0.50
3:U:2948[A]:ASP:CB	3:U:2949[A]:LYS:CA	2.78	0.50
3:U:2949[A]:LYS:C	3:U:2949[A]:LYS:CD	2.85	0.50
3:U:2949[B]:LYS:C	3:U:2949[B]:LYS:CD	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2960[B]:PHE:CD1	3:U:2960[B]:PHE:N	2.72	0.50
3:U:3258[B]:PHE:N	3:d:2969[B]:TYR:O	2.45	0.50
3:U:3293[B]:LYS:HB2	3:U:3294[B]:SER:CA	2.41	0.50
1:V:1423:TYR:OH	1:V:1461:VAL:O	2.25	0.50
1:V:1427:HIS:HD2	1:V:1457:HIS:HE1	1.59	0.50
2:W:2128:LEU:HD23	2:W:2216:PHE:HZ	1.76	0.50
3:X:3004[B]:GLY:O	3:X:3006[B]:LYS:N	2.44	0.50
3:X:3110[A]:THR:C	3:X:3112[A]:TYR:H	2.20	0.50
3:X:3135[A]:LYS:HB2	3:X:3141[A]:TYR:HD1	1.76	0.50
3:X:3217[A]:PHE:CB	3:X:3219[A]:LEU:HD21	2.42	0.50
3:X:3288[A]:MET:CA	3:X:3295[A]:LEU:HG	2.42	0.50
1:Y:305:ASN:HB3	1:Y:400:ILE:HB	1.94	0.50
1:Y:1008:GLU:HA	1:Y:1011:TYR:HB3	1.93	0.50
3:a:3004[A]:GLY:O	3:a:3006[A]:LYS:N	2.44	0.50
3:a:3291[A]:ASP:OD2	3:a:3293[A]:LYS:NZ	2.43	0.50
1:b:1170:MET:HB3	1:b:1203:MET:HE2	1.94	0.50
2:c:2740:ASP:OD2	2:c:2741:GLN:HG2	2.12	0.50
3:d:2949[A]:LYS:C	3:d:2949[A]:LYS:CD	2.85	0.50
3:d:3110[A]:THR:O	3:d:3111[A]:SER:C	2.53	0.50
3:d:3288[B]:MET:CA	3:d:3295[B]:LEU:HG	2.42	0.50
1:A:1639:LYS:CB	1:b:472:ASP:HB3	2.40	0.50
2:B:2161:GLN:NE2	2:B:2348:THR:HG21	2.27	0.50
3:C:2928[B]:ASN:C	3:C:2930[B]:LEU:HD22	2.36	0.50
3:C:3151[B]:LEU:CA	3:L:3154[B]:PRO:HB2	2.40	0.50
3:C:3152[B]:LYS:HG3	3:L:3172[B]:SER:HG	1.75	0.50
3:C:3276[A]:ASP:O	3:C:3277[A]:ALA:HB3	2.12	0.50
1:D:1321:HIS:O	1:D:1324:ARG:HB3	2.11	0.50
2:E:2603:PRO:HG2	2:E:2606:LEU:HD12	1.93	0.50
3:F:3196[B]:THR:OG1	3:F:3199[B]:GLN:HG3	2.12	0.50
3:F:3262[A]:PHE:C	3:F:3263[A]:LEU:HD12	2.37	0.50
1:G:127:GLU:CG	1:G:135:THR:H	2.24	0.50
3:I:2952[B]:ALA:CA	3:I:2956[B]:LYS:HB3	2.38	0.50
3:I:2969[A]:TYR:CE2	3:I:2970[A]:PRO:CG	2.86	0.50
3:I:2971[B]:ASP:CG	3:I:2973[B]:THR:HG1	2.15	0.50
3:I:3276[A]:ASP:O	3:I:3277[A]:ALA:HB3	2.12	0.50
1:J:41:HIS:NE2	1:J:58:CYS:SG	2.85	0.50
1:J:69:HIS:CD2	9:J:5001:CUO:O1	2.64	0.50
1:J:931:TRP:CZ3	1:J:995:ILE:HD11	2.46	0.50
2:K:2282:LEU:HD21	2:K:2294:PHE:HA	1.94	0.50
3:L:2981[A]:GLY:N	3:L:3086[A]:GLU:OE1	2.45	0.50
3:L:3262[A]:PHE:C	3:L:3263[A]:LEU:HD12	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2960[B]:PHE:CD2	3:O:3157[B]:PRO:CG	2.74	0.50
3:O:3102[B]:TYR:HA	3:X:2971[B]:ASP:CA	2.42	0.50
3:O:3196[B]:THR:O	3:O:3199[B]:GLN:HB2	2.11	0.50
1:P:1604:ASP:OD1	1:P:1605:ARG:NH1	2.44	0.50
3:R:2966[A]:SER:C	3:R:2967[A]:CYS:SG	2.94	0.50
3:R:3110[B]:THR:C	3:R:3112[B]:TYR:N	2.68	0.50
1:S:514:TRP:CZ2	1:S:606:ILE:HD11	2.47	0.50
1:S:1231:VAL:O	1:S:1233:SER:N	2.44	0.50
1:S:1467:ILE:HD13	1:S:1532:PHE:HB2	1.93	0.50
2:T:2107:LEU:O	2:T:2111:GLN:HB2	2.12	0.50
3:U:2935[B]:ILE:CD1	3:U:2935[B]:ILE:H	2.25	0.50
3:U:2966[B]:SER:C	3:U:2967[B]:CYS:SG	2.94	0.50
3:U:2969[B]:TYR:CD2	3:U:2970[B]:PRO:HD2	2.47	0.50
3:U:3159[B]:SER:HB2	3:d:3150[B]:LYS:HE3	1.90	0.50
3:U:3283[A]:ILE:C	3:U:3283[A]:ILE:CD1	2.85	0.50
1:V:372:ALA:O	1:V:375:SER:OG	2.26	0.50
1:V:730:PHE:N	1:V:821:ILE:O	2.27	0.50
1:V:882:TRP:CD1	1:V:1086:LEU:HD11	2.47	0.50
1:V:1324:ARG:NH1	1:V:1519:TYR:HB3	2.26	0.50
3:X:2928[B]:ASN:C	3:X:2930[B]:LEU:HD22	2.36	0.50
3:X:3093[B]:HIS:HB2	3:X:3248[B]:LEU:HD13	1.94	0.50
3:X:3262[B]:PHE:C	3:X:3263[B]:LEU:HD12	2.37	0.50
2:Z:2736:TYR:HB3	1:b:1236:TYR:HB3	1.93	0.50
3:a:3004[B]:GLY:O	3:a:3006[B]:LYS:N	2.44	0.50
3:a:3300[A]:LEU:CD2	3:a:3300[A]:LEU:H	2.24	0.50
1:b:132:ASN:OD1	1:b:132:ASN:N	2.45	0.50
1:b:757:VAL:O	1:b:779:HIS:HE1	1.95	0.50
1:b:931:TRP:NE1	1:b:1048:ASN:HD22	2.10	0.50
2:c:2807:GLY:O	2:c:2899:PRO:HA	2.12	0.50
3:d:2954[A]:TYR:C	3:d:2957[A]:ILE:HG22	2.37	0.50
3:d:3288[A]:MET:CA	3:d:3295[A]:LEU:HG	2.42	0.50
3:d:3293[A]:LYS:HB2	3:d:3294[A]:SER:CA	2.41	0.50
1:A:874:ALA:HA	1:A:913:PHE:HZ	1.76	0.49
3:C:2952[A]:ALA:CA	3:C:2956[A]:LYS:HB3	2.38	0.49
3:C:2962[B]:GLY:N	3:C:3111[B]:SER:OG	2.44	0.49
3:C:3135[A]:LYS:HB2	3:C:3141[A]:TYR:HD1	1.76	0.49
3:C:3173[B]:THR:HA	3:L:3153[B]:LYS:C	2.37	0.49
3:C:3183[B]:LEU:N	3:C:3184[B]:ASN:HA	2.12	0.49
3:C:3201[B]:GLU:O	3:C:3205[B]:LYS:HB2	2.11	0.49
3:C:3262[A]:PHE:C	3:C:3263[A]:LEU:HD12	2.37	0.49
1:D:567:LEU:HD11	1:D:579:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:891:LYS:HB2	1:D:892:TYR:CD2	2.47	0.49
1:D:1361:GLU:HG3	1:D:1363:THR:H	1.77	0.49
3:F:3150[B]:LYS:C	3:a:3172[B]:SER:CB	2.85	0.49
3:F:3151[A]:LEU:CB	3:F:3175[A]:TYR:CD2	2.93	0.49
3:F:3151[B]:LEU:CB	3:F:3175[B]:TYR:CD2	2.93	0.49
3:F:3154[B]:PRO:CG	3:a:3174[B]:GLY:CA	2.86	0.49
3:F:3160[B]:SER:CB	3:a:2983[B]:VAL:HG23	2.37	0.49
3:F:3173[B]:THR:HG22	3:F:3174[B]:GLY:H	1.67	0.49
3:F:3252[B]:TYR:O	3:a:3253[B]:GLU:HA	2.12	0.49
3:F:3255[B]:PRO:HG3	3:a:2963[B]:MET:CA	2.41	0.49
1:G:1033:LEU:HD11	1:G:1183:GLU:HB2	1.93	0.49
3:I:2949[A]:LYS:C	3:I:2949[A]:LYS:CD	2.85	0.49
3:I:2952[A]:ALA:N	3:I:2953[A]:GLY:HA2	2.06	0.49
3:I:3110[B]:THR:C	3:I:3112[B]:TYR:H	2.20	0.49
3:I:3196[B]:THR:O	3:I:3199[B]:GLN:HB2	2.11	0.49
3:I:3288[B]:MET:CA	3:I:3295[B]:LEU:HG	2.42	0.49
1:J:329:ARG:HB3	1:M:1584:GLY:N	2.26	0.49
1:J:972:SER:HA	1:J:1028:VAL:HG22	1.94	0.49
1:J:1316:MET:HB3	1:J:1318:VAL:HG22	1.94	0.49
3:L:2954[A]:TYR:C	3:L:2957[A]:ILE:HG22	2.37	0.49
3:L:2986[A]:PRO:CB	3:L:3127[A]:TRP:CZ3	2.94	0.49
3:L:2986[B]:PRO:CB	3:L:3127[B]:TRP:CZ3	2.94	0.49
3:L:3176[B]:LYS:NZ	3:L:3176[B]:LYS:CB	2.73	0.49
3:O:2939[B]:ARG:NE	3:O:3031[B]:ASN:ND2	2.60	0.49
3:O:2969[B]:TYR:CG	3:O:2970[B]:PRO:HD2	2.42	0.49
3:O:3038[A]:ILE:HG23	3:O:3040[A]:VAL:HG22	1.90	0.49
3:O:3093[A]:HIS:HB2	3:O:3248[A]:LEU:HD13	1.94	0.49
1:P:1034:GLU:HB2	1:P:1180:SER:OG	2.12	0.49
1:P:1475:ARG:NE	1:P:1541:GLU:OE2	2.30	0.49
3:R:3066[A]:TYR:CE1	3:R:3193[A]:HIS:CE1	2.98	0.49
3:R:3176[A]:LYS:N	3:R:3176[A]:LYS:CE	2.73	0.49
3:R:3196[B]:THR:OG1	3:R:3199[B]:GLN:HG3	2.12	0.49
3:R:3262[B]:PHE:C	3:R:3263[B]:LEU:HD12	2.37	0.49
3:R:3293[A]:LYS:HB2	3:R:3294[A]:SER:CA	2.41	0.49
3:U:2939[A]:ARG:NE	3:U:3031[A]:ASN:ND2	2.60	0.49
3:U:2954[B]:TYR:C	3:U:2957[B]:ILE:HG22	2.37	0.49
3:U:3093[B]:HIS:HB2	3:U:3248[B]:LEU:HD13	1.94	0.49
3:U:3104[A]:MET:HA	3:U:3110[A]:THR:CG2	2.17	0.49
3:U:3135[A]:LYS:HB2	3:U:3141[A]:TYR:HD1	1.76	0.49
3:U:3196[A]:THR:OG1	3:U:3199[A]:GLN:HB2	2.12	0.49
3:U:3256[B]:TRP:CA	3:d:2969[B]:TYR:H	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:843:VAL:HG11	1:V:1044:LEU:HD13	1.93	0.49
1:V:1396:GLU:OE2	1:V:1569:ARG:NH2	2.45	0.49
2:W:2257:CYS:O	2:W:2261:VAL:HG23	2.12	0.49
3:X:2935[A]:ILE:CD1	3:X:2935[A]:ILE:H	2.25	0.49
3:X:2939[A]:ARG:NE	3:X:3031[A]:ASN:ND2	2.60	0.49
3:X:3113[B]:ASP:O	3:X:3114[B]:PRO:C	2.53	0.49
3:X:3135[B]:LYS:HB2	3:X:3141[B]:TYR:HD1	1.76	0.49
1:Y:126:GLY:HA3	1:Y:202:TYR:O	2.11	0.49
1:Y:238:ASN:OD1	1:Y:238:ASN:N	2.40	0.49
1:Y:1492:PRO:HA	1:Y:1512:ARG:HA	1.94	0.49
2:Z:2154:TRP:HD1	2:Z:2333:LEU:HD12	1.77	0.49
3:a:3151[A]:LEU:CB	3:a:3175[A]:TYR:CD2	2.93	0.49
3:a:3201[B]:GLU:O	3:a:3205[B]:LYS:HB2	2.11	0.49
3:a:3273[B]:LEU:O	3:a:3275[B]:LEU:HD12	2.11	0.49
2:c:2570:HIS:HD2	2:c:2711:HIS:HE1	1.58	0.49
2:c:2606:LEU:HD21	2:c:2709:VAL:HG21	1.92	0.49
3:d:2935[B]:ILE:CD1	3:d:2935[B]:ILE:H	2.25	0.49
3:d:3141[A]:TYR:CD2	3:d:3141[A]:TYR:C	2.86	0.49
3:C:2935[B]:ILE:CD1	3:C:2935[B]:ILE:H	2.25	0.49
3:C:3024[B]:LEU:CD1	3:C:3024[B]:LEU:C	2.85	0.49
3:C:3217[B]:PHE:CB	3:C:3219[B]:LEU:HD21	2.42	0.49
3:C:3262[B]:PHE:C	3:C:3263[B]:LEU:HD12	2.37	0.49
1:D:711:LEU:HD21	1:D:719:TYR:HD2	1.76	0.49
2:E:2647:LEU:HG	2:E:2656:LEU:HG	1.93	0.49
3:F:2935[B]:ILE:CD1	3:F:2935[B]:ILE:H	2.25	0.49
3:F:3196[B]:THR:OG1	3:F:3199[B]:GLN:HB2	2.11	0.49
1:G:37:ILE:HD13	1:G:75:GLN:HG3	1.94	0.49
3:I:2935[A]:ILE:CD1	3:I:2935[A]:ILE:H	2.25	0.49
3:I:2939[A]:ARG:NE	3:I:3031[A]:ASN:ND2	2.60	0.49
3:I:3066[A]:TYR:CE1	3:I:3193[A]:HIS:CE1	2.98	0.49
3:I:3113[B]:ASP:O	3:I:3114[B]:PRO:C	2.53	0.49
3:I:3155[B]:MET:HA	3:R:2979[B]:GLN:HE21	1.77	0.49
3:I:3196[A]:THR:O	3:I:3199[A]:GLN:HB2	2.11	0.49
3:I:3219[A]:LEU:N	3:I:3219[A]:LEU:CD2	2.73	0.49
1:J:1583:CYS:O	1:M:329:ARG:HA	2.12	0.49
2:K:2746:MET:HE2	2:K:2765:PRO:HG3	1.93	0.49
3:L:2935[A]:ILE:CD1	3:L:2936[A]:GLU:N	2.73	0.49
3:L:2935[B]:ILE:CD1	3:L:2936[B]:GLU:N	2.73	0.49
3:L:3066[B]:TYR:CE1	3:L:3193[B]:HIS:CE1	2.98	0.49
3:L:3096[A]:VAL:HG11	3:L:3115[A]:LEU:HD12	1.89	0.49
3:L:3110[A]:THR:C	3:L:3112[A]:TYR:N	2.68	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3284[B]:LYS:CE	3:L:3284[B]:LYS:CA	2.85	0.49
3:L:3298[A]:ASN:CA	3:L:3299[A]:LEU:C	2.85	0.49
1:M:81:VAL:HA	1:M:85:SER:HB3	1.94	0.49
1:M:137:ARG:NH2	1:M:203:ASP:OD1	2.37	0.49
1:M:329:ARG:HH11	1:M:329:ARG:HB3	1.76	0.49
1:M:804:ASP:H	1:M:810:LEU:HD13	1.77	0.49
1:M:861:PHE:CD2	1:M:870:TYR:HB2	2.47	0.49
1:M:1622:GLN:HG2	1:M:1652:PHE:CD1	2.47	0.49
3:O:2948[B]:ASP:CB	3:O:2949[B]:LYS:CA	2.78	0.49
3:O:3066[B]:TYR:CE1	3:O:3193[B]:HIS:CE1	2.98	0.49
3:O:3113[B]:ASP:O	3:O:3114[B]:PRO:C	2.53	0.49
3:O:3135[A]:LYS:HB2	3:O:3141[A]:TYR:HD1	1.76	0.49
3:O:3201[B]:GLU:O	3:O:3205[B]:LYS:HB2	2.11	0.49
3:O:3262[A]:PHE:C	3:O:3263[A]:LEU:HD12	2.37	0.49
3:O:3275[A]:LEU:N	3:O:3275[A]:LEU:CD1	2.73	0.49
3:O:3275[B]:LEU:N	3:O:3275[B]:LEU:CD1	2.73	0.49
3:R:3232[B]:VAL:HG23	3:R:3273[B]:LEU:HD11	1.94	0.49
3:R:3291[A]:ASP:OD2	3:R:3293[A]:LYS:NZ	2.43	0.49
1:S:1219:ASP:N	1:S:1223:ALA:O	2.36	0.49
1:S:1362:ALA:HA	1:S:1378:PHE:CG	2.47	0.49
2:T:2867:PRO:HG2	3:U:2932[A]:PRO:HG2	1.93	0.49
3:U:2939[B]:ARG:NE	3:U:3031[B]:ASN:ND2	2.60	0.49
3:U:3023[A]:ILE:O	3:U:3025[A]:VAL:N	2.44	0.49
3:U:3232[A]:VAL:HG23	3:U:3273[A]:LEU:HD11	1.94	0.49
3:U:3276[B]:ASP:O	3:U:3277[B]:ALA:HB3	2.12	0.49
1:V:559:THR:HG21	1:V:627:ASP:HA	1.94	0.49
1:V:1322:TRP:CD1	1:V:1493:MET:HB3	2.47	0.49
3:X:2954[A]:TYR:C	3:X:2957[A]:ILE:HG22	2.37	0.49
3:X:3176[B]:LYS:CE	3:X:3176[B]:LYS:N	2.73	0.49
1:Y:483:GLY:HA2	1:Y:773:PHE:CZ	2.46	0.49
1:Y:499:GLU:HG3	1:Y:511:VAL:HG12	1.95	0.49
3:a:2949[A]:LYS:C	3:a:2949[A]:LYS:CD	2.85	0.49
3:a:2962[B]:GLY:N	3:a:3111[B]:SER:OG	2.44	0.49
3:a:3093[A]:HIS:HB2	3:a:3248[A]:LEU:HD13	1.94	0.49
3:a:3135[A]:LYS:HB2	3:a:3141[A]:TYR:HD1	1.76	0.49
3:d:2935[A]:ILE:CD1	3:d:2935[A]:ILE:H	2.26	0.49
3:d:3151[A]:LEU:CB	3:d:3175[A]:TYR:CD2	2.93	0.49
3:d:3219[B]:LEU:N	3:d:3219[B]:LEU:CD2	2.73	0.49
1:A:449:ASP:HB3	1:A:1276:ASN:OD1	2.12	0.49
1:A:572:SER:O	1:A:578:PHE:HB2	2.12	0.49
3:C:3151[B]:LEU:CB	3:C:3175[B]:TYR:CD2	2.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:ILE:O	1:D:260:ASN:ND2	2.45	0.49
1:D:668:MET:HE2	1:D:668:MET:HA	1.95	0.49
2:E:2451:LEU:HD22	2:E:2456:LEU:HD11	1.94	0.49
3:F:2949[B]:LYS:C	3:F:2949[B]:LYS:CD	2.85	0.49
3:F:2985[B]:PHE:CD2	3:a:2968[B]:GLN:O	2.64	0.49
3:F:3114[B]:PRO:CD	3:F:3115[B]:LEU:N	2.72	0.49
3:F:3196[A]:THR:OG1	3:F:3199[A]:GLN:HB2	2.11	0.49
3:F:3276[B]:ASP:O	3:F:3277[B]:ALA:HB3	2.12	0.49
1:G:489:HIS:HB3	1:G:689:PRO:HB3	1.95	0.49
2:H:2542:TYR:HB2	2:H:2573:TYR:HE1	1.77	0.49
2:H:2650:GLY:N	2:H:2651:GLN:HA	2.27	0.49
3:I:2954[A]:TYR:C	3:I:2957[A]:ILE:HG22	2.37	0.49
3:I:2954[B]:TYR:C	3:I:2957[B]:ILE:HG22	2.37	0.49
3:I:3110[A]:THR:C	3:I:3112[A]:TYR:H	2.20	0.49
3:I:3160[B]:SER:CA	3:R:2983[B]:VAL:HB	2.42	0.49
3:I:3176[A]:LYS:H	3:I:3176[A]:LYS:CE	2.17	0.49
3:I:3196[A]:THR:OG1	3:I:3199[A]:GLN:HG3	2.12	0.49
3:I:3201[B]:GLU:O	3:I:3205[B]:LYS:HB2	2.11	0.49
2:K:2735:ALA:HB2	2:K:2769:PHE:CZ	2.47	0.49
3:L:3023[B]:ILE:O	3:L:3025[B]:VAL:N	2.44	0.49
3:L:3110[A]:THR:O	3:L:3111[A]:SER:C	2.53	0.49
3:L:3191[A]:ASN:C	3:L:3192[A]:PHE:O	2.52	0.49
3:L:3283[B]:ILE:C	3:L:3283[B]:ILE:CD1	2.85	0.49
1:M:639:ARG:HB2	1:M:703:TYR:CE2	2.47	0.49
2:N:2595:TRP:CE2	2:N:2683:ILE:HG13	2.47	0.49
3:O:3114[A]:PRO:CD	3:O:3115[A]:LEU:N	2.72	0.49
3:O:3217[A]:PHE:CB	3:O:3219[A]:LEU:HD21	2.42	0.49
1:P:324:PRO:HG2	1:P:376:ASN:OD1	2.12	0.49
1:P:744:VAL:HG12	1:P:802:ILE:HG23	1.94	0.49
3:R:2939[A]:ARG:NE	3:R:3031[A]:ASN:ND2	2.60	0.49
3:R:2969[A]:TYR:CD2	3:R:2970[A]:PRO:HD2	2.47	0.49
3:R:2981[B]:GLY:N	3:R:3086[B]:GLU:OE1	2.45	0.49
3:U:2935[A]:ILE:CD1	3:U:2935[A]:ILE:H	2.25	0.49
3:U:2952[A]:ALA:CA	3:U:2956[A]:LYS:HB3	2.38	0.49
3:U:3004[A]:GLY:O	3:U:3006[A]:LYS:N	2.44	0.49
1:V:567:LEU:HD13	1:V:609:TRP:CD1	2.46	0.49
3:X:2935[B]:ILE:CD1	3:X:2935[B]:ILE:H	2.25	0.49
3:X:3027[B]:GLU:CD	3:X:3028[B]:PRO:CD	2.86	0.49
3:X:3191[B]:ASN:C	3:X:3192[B]:PHE:O	2.52	0.49
3:X:3201[B]:GLU:O	3:X:3205[B]:LYS:HB2	2.11	0.49
3:X:3298[B]:ASN:CA	3:X:3299[B]:LEU:C	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1302:SER:HB3	1:Y:1303:GLU:CD	2.37	0.49
1:Y:1312:CYS:HA	1:Y:1322:TRP:CE2	2.47	0.49
1:Y:1492:PRO:HB2	1:Y:1497:SER:HB3	1.94	0.49
3:a:2939[B]:ARG:NE	3:a:3031[B]:ASN:ND2	2.60	0.49
3:a:3291[B]:ASP:OD2	3:a:3293[B]:LYS:NZ	2.43	0.49
1:b:552:PHE:HZ	1:b:623:TYR:HE1	1.58	0.49
3:d:2949[B]:LYS:C	3:d:2949[B]:LYS:CD	2.85	0.49
3:d:2961[A]:HIS:CD2	3:d:2988[A]:TRP:CZ3	2.96	0.49
3:d:3110[B]:THR:C	3:d:3112[B]:TYR:H	2.20	0.49
3:d:3293[A]:LYS:CB	3:d:3294[A]:SER:CB	2.54	0.49
3:d:3298[B]:ASN:CB	3:d:3299[B]:LEU:C	2.85	0.49
7:z:3:BMA:H2	7:z:4:MAN:C3	2.31	0.49
1:A:456:GLN:HG2	1:A:551:GLU:HB3	1.95	0.49
1:A:1441:SER:OG	1:A:1442:MET:N	2.43	0.49
2:B:2680:HIS:CD2	2:B:2684:HIS:HD2	2.31	0.49
3:C:2949[B]:LYS:C	3:C:2949[B]:LYS:CD	2.85	0.49
3:C:2960[A]:PHE:CD2	3:C:3157[A]:PRO:CG	2.74	0.49
3:C:3066[B]:TYR:CE1	3:C:3193[B]:HIS:CE1	2.98	0.49
1:D:730:PHE:CE1	1:D:780:GLU:HG2	2.47	0.49
1:D:1324:ARG:NH1	1:D:1516:VAL:O	2.46	0.49
3:F:2978[B]:CYS:O	3:a:2975[B]:PHE:HB3	2.11	0.49
3:F:2982[B]:MET:C	3:a:3160[B]:SER:OG	2.53	0.49
3:F:3135[B]:LYS:HB2	3:F:3141[B]:TYR:HD1	1.76	0.49
3:F:3283[B]:ILE:C	3:F:3283[B]:ILE:CD1	2.85	0.49
2:H:2361:LYS:HD2	2:H:2362:GLN:H	1.77	0.49
3:I:2935[B]:ILE:CD1	3:I:2935[B]:ILE:H	2.25	0.49
3:I:2965[B]:LEU:CD2	3:R:3250[B]:GLY:H	2.25	0.49
3:I:3066[B]:TYR:CE1	3:I:3193[B]:HIS:CE1	2.98	0.49
3:I:3268[A]:LYS:CG	1:J:1539:GLN:HE22	2.25	0.49
1:J:194:MET:HA	1:J:200:THR:HA	1.95	0.49
3:L:3014[B]:TRP:HH2	3:L:3123[B]:THR:HG23	1.78	0.49
3:L:3276[A]:ASP:O	3:L:3277[A]:ALA:HB3	2.12	0.49
3:L:3291[A]:ASP:OD2	3:L:3293[A]:LYS:NZ	2.43	0.49
1:M:127:GLU:OE2	1:M:135:THR:N	2.42	0.49
3:O:2963[B]:MET:SD	3:X:2975[B]:PHE:CZ	3.02	0.49
3:O:3110[A]:THR:C	3:O:3112[A]:TYR:H	2.20	0.49
3:O:3196[A]:THR:O	3:O:3200[A]:LEU:N	2.43	0.49
3:O:3201[A]:GLU:O	3:O:3205[A]:LYS:HB2	2.11	0.49
3:O:3252[B]:TYR:CB	3:X:3156[B]:MET:CB	2.66	0.49
3:O:3291[A]:ASP:OD2	3:O:3293[A]:LYS:NZ	2.43	0.49
1:P:432:THR:HG23	1:P:435:GLU:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1562:ILE:HD11	1:P:1645:PHE:CZ	2.48	0.49
2:Q:2568:HIS:ND1	2:Q:2765:PRO:HB3	2.28	0.49
3:R:3014[B]:TRP:HH2	3:R:3123[B]:THR:HG23	1.78	0.49
3:R:3298[B]:ASN:CB	3:R:3299[B]:LEU:C	2.85	0.49
1:S:598:GLN:O	1:S:602:THR:OG1	2.23	0.49
1:S:949:ASP:OD1	1:S:950:ALA:N	2.40	0.49
3:U:3110[A]:THR:C	3:U:3112[A]:TYR:H	2.20	0.49
3:U:3147[B]:GLU:CG	3:U:3149[B]:ASN:ND2	2.73	0.49
1:V:460:GLU:O	1:V:467:LYS:NZ	2.36	0.49
1:V:1019:HIS:CE1	1:V:1046:HIS:HE1	2.31	0.49
3:X:2939[B]:ARG:HG3	3:X:2939[B]:ARG:NH1	2.28	0.49
3:X:2939[B]:ARG:NE	3:X:3031[B]:ASN:ND2	2.60	0.49
3:X:2969[A]:TYR:CD2	3:X:2970[A]:PRO:HD2	2.47	0.49
3:X:3298[A]:ASN:CA	3:X:3299[A]:LEU:C	2.85	0.49
1:Y:1470:GLU:HB3	1:Y:1537:ILE:CD1	2.42	0.49
3:a:2954[B]:TYR:C	3:a:2957[B]:ILE:HG22	2.37	0.49
3:a:3262[A]:PHE:C	3:a:3263[A]:LEU:HD12	2.37	0.49
3:a:3284[B]:LYS:HE2	3:a:3284[B]:LYS:CA	2.30	0.49
1:b:567:LEU:HB3	1:b:570:GLN:O	2.12	0.49
2:c:2312:GLN:OE1	2:c:2315:ARG:NH1	2.46	0.49
2:c:2404:GLY:HA2	2:c:2405:SER:C	2.37	0.49
2:c:2722:GLN:NE2	2:c:2769:PHE:O	2.39	0.49
3:d:2988[B]:TRP:HE3	3:d:2989[B]:HIS:CE1	2.25	0.49
3:d:3027[A]:GLU:CD	3:d:3028[A]:PRO:CD	2.86	0.49
3:d:3201[B]:GLU:O	3:d:3205[B]:LYS:HB2	2.11	0.49
3:d:3217[B]:PHE:CB	3:d:3219[B]:LEU:HD21	2.42	0.49
3:d:3298[A]:ASN:CA	3:d:3299[A]:LEU:C	2.86	0.49
1:A:1301:PRO:HA	1:A:1308:VAL:HA	1.95	0.49
2:B:2680:HIS:HB2	2:B:2714:VAL:HG11	1.93	0.49
3:C:2969[A]:TYR:CD2	3:C:2970[A]:PRO:HD2	2.47	0.49
3:C:2986[B]:PRO:CB	3:C:3127[B]:TRP:CZ3	2.94	0.49
3:C:3014[A]:TRP:HH2	3:C:3123[A]:THR:HG23	1.78	0.49
3:C:3086[B]:GLU:CG	3:L:2968[B]:GLN:NE2	2.70	0.49
3:C:3217[A]:PHE:CB	3:C:3219[A]:LEU:HD21	2.42	0.49
3:C:3256[B]:TRP:CD1	3:L:2975[B]:PHE:O	2.65	0.49
3:C:3298[B]:ASN:CB	3:C:3299[B]:LEU:C	2.85	0.49
2:E:2533:ASP:OD1	2:E:2533:ASP:N	2.44	0.49
3:F:3027[B]:GLU:CD	3:F:3028[B]:PRO:CD	2.86	0.49
3:F:3155[B]:MET:O	3:a:3153[B]:LYS:HD2	2.07	0.49
3:F:3298[B]:ASN:CB	3:F:3299[B]:LEU:C	2.86	0.49
1:G:1339:SER:CB	1:G:1340:GLY:HA2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2553:ALA:N	2:H:2554:PRO:HD2	2.28	0.49
3:I:2933[B]:SER:CB	3:I:2936[B]:GLU:CB	2.85	0.49
3:I:2980[B]:HIS:HD2	3:R:2969[B]:TYR:O	1.94	0.49
3:I:3248[B]:LEU:C	3:R:2974[B]:ALA:H	2.20	0.49
3:I:3252[B]:TYR:CD2	3:R:3108[B]:HIS:CE1	3.00	0.49
3:I:3283[B]:ILE:C	3:I:3283[B]:ILE:CD1	2.85	0.49
3:I:3288[A]:MET:CA	3:I:3295[A]:LEU:HG	2.42	0.49
3:I:3298[A]:ASN:CA	3:I:3299[A]:LEU:C	2.86	0.49
1:J:428:ILE:HD12	1:J:514:TRP:HB3	1.94	0.49
1:J:1215:LEU:HD22	1:J:1229:LYS:NZ	2.27	0.49
3:L:3285[B]:VAL:CG2	3:L:3286[B]:THR:N	2.73	0.49
3:L:3298[B]:ASN:HA	3:L:3299[B]:LEU:HB3	1.88	0.49
2:N:2866:PRO:HB2	2:N:2868:GLU:OE1	2.11	0.49
3:O:3109[B]:TYR:CD2	3:X:2969[B]:TYR:C	2.81	0.49
3:O:3110[B]:THR:C	3:O:3112[B]:TYR:H	2.20	0.49
3:O:3183[B]:LEU:H	3:O:3184[B]:ASN:CA	2.22	0.49
3:O:3228[A]:VAL:HG23	3:O:3228[A]:VAL:O	2.10	0.49
1:P:483:GLY:HA2	1:P:773:PHE:CZ	2.48	0.49
1:P:1015:HIS:CD2	1:P:1045:HIS:HE1	2.31	0.49
2:Q:2525:LYS:NZ	2:Q:2526:ARG:HH12	2.11	0.49
2:Q:2553:ALA:N	2:Q:2554:PRO:HD2	2.28	0.49
2:Q:2805:PHE:CE1	2:Q:2855:ASP:HB3	2.47	0.49
3:R:2939[A]:ARG:HG3	3:R:2939[A]:ARG:NH1	2.28	0.49
3:R:3110[A]:THR:C	3:R:3112[A]:TYR:H	2.21	0.49
3:R:3262[A]:PHE:C	3:R:3263[A]:LEU:HD12	2.37	0.49
3:R:3283[B]:ILE:C	3:R:3283[B]:ILE:CD1	2.85	0.49
1:S:462:HIS:HA	1:S:490:TRP:CH2	2.47	0.49
2:T:2825:ILE:HG22	2:T:2863:ARG:HH21	1.76	0.49
1:V:898:GLY:N	1:V:899:MET:SD	2.73	0.49
1:V:1351:PRO:HA	1:V:1400:ASN:HB2	1.92	0.49
2:W:2180:TRP:CH2	2:W:2300:ASN:HB3	2.48	0.49
2:W:2571:ARG:NH1	2:W:2771:TYR:HB3	2.27	0.49
3:X:3110[B]:THR:C	3:X:3112[B]:TYR:H	2.20	0.49
3:X:3232[B]:VAL:HG23	3:X:3273[B]:LEU:HD11	1.95	0.49
3:X:3276[A]:ASP:O	3:X:3277[A]:ALA:HB3	2.12	0.49
1:Y:215:ARG:NE	1:Y:279:LEU:HA	2.28	0.49
2:Z:2090:LYS:NZ	2:Z:2099:GLU:OE2	2.45	0.49
2:Z:2121:THR:O	2:Z:2124:SER:HB3	2.13	0.49
3:a:2935[B]:ILE:CD1	3:a:2935[B]:ILE:H	2.25	0.49
3:a:3196[B]:THR:OG1	3:a:3199[B]:GLN:HG3	2.12	0.49
3:a:3201[A]:GLU:O	3:a:3205[A]:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3232[A]:VAL:HG23	3:a:3273[A]:LEU:HD11	1.94	0.49
1:b:1582:ASN:HB3	1:b:1583:CYS:CB	2.34	0.49
2:c:2603:PRO:HG2	2:c:2606:LEU:HD12	1.93	0.49
3:d:3014[A]:TRP:HH2	3:d:3123[A]:THR:HG23	1.78	0.49
3:d:3089[B]:HIS:CE1	3:d:3093[B]:HIS:CE1	3.01	0.49
3:d:3176[B]:LYS:N	3:d:3176[B]:LYS:CE	2.73	0.49
3:d:3196[B]:THR:OG1	3:d:3199[B]:GLN:HB2	2.12	0.49
1:A:105:VAL:HB	1:A:137:ARG:HH12	1.77	0.49
1:A:372:ALA:O	1:A:375:SER:OG	2.31	0.49
1:A:646:ALA:O	1:A:649:ILE:HG12	2.12	0.49
3:C:2954[B]:TYR:C	3:C:2957[B]:ILE:HG22	2.37	0.49
3:C:2971[B]:ASP:OD2	3:L:3248[B]:LEU:CD2	2.60	0.49
3:C:3113[A]:ASP:O	3:C:3114[A]:PRO:C	2.53	0.49
3:C:3228[B]:VAL:O	3:C:3228[B]:VAL:HG23	2.10	0.49
3:C:3232[A]:VAL:HG23	3:C:3273[A]:LEU:HD11	1.95	0.49
3:C:3275[A]:LEU:N	3:C:3275[A]:LEU:CD1	2.73	0.49
3:C:3300[A]:LEU:CD2	3:C:3300[A]:LEU:H	2.24	0.49
9:C:3401[A]:CUO:O1	3:L:3120[A]:HIS:CE1	2.66	0.49
1:D:467:LYS:HB2	1:D:471:PRO:HG3	1.94	0.49
2:E:2472:ASN:HB2	2:E:2474:THR:N	2.28	0.49
3:F:3120[A]:HIS:CE1	9:a:3401[A]:CUO:O1	2.66	0.49
3:F:3191[B]:ASN:C	3:F:3192[B]:PHE:O	2.52	0.49
3:F:3201[B]:GLU:O	3:F:3205[B]:LYS:HB2	2.11	0.49
3:F:3255[B]:PRO:CB	3:a:2964[B]:PRO:HD2	2.43	0.49
3:F:3262[B]:PHE:C	3:F:3263[B]:LEU:HD12	2.37	0.49
3:F:3283[A]:ILE:C	3:F:3283[A]:ILE:CD1	2.85	0.49
1:G:145:GLN:HG2	1:G:151:GLN:HB2	1.95	0.49
1:G:293:LEU:O	1:G:296:ARG:HG2	2.12	0.49
2:H:2866:PRO:CB	2:H:2868:GLU:HG3	2.43	0.49
3:I:3107[B]:LEU:HD12	3:R:2973[B]:THR:C	2.37	0.49
3:L:3151[A]:LEU:CB	3:L:3175[A]:TYR:CD2	2.93	0.49
1:M:899:MET:HB3	1:M:1012:GLU:OE1	2.13	0.49
1:M:901:THR:HG22	1:M:904:HIS:HB2	1.94	0.49
1:M:1166:THR:H	1:M:1167:ASP:HA	1.77	0.49
1:M:1290:ILE:HD13	1:M:1329:LEU:HG	1.93	0.49
1:M:1315:GLY:HA3	1:M:1601:TRP:CG	2.47	0.49
3:O:2939[B]:ARG:HG3	3:O:2939[B]:ARG:NH1	2.28	0.49
3:O:3014[A]:TRP:HH2	3:O:3123[A]:THR:HG23	1.78	0.49
3:O:3120[B]:HIS:CE1	9:O:3401[B]:CUO:O1	2.66	0.49
3:O:3196[B]:THR:OG1	3:O:3199[B]:GLN:HG3	2.12	0.49
3:O:3232[A]:VAL:HG23	3:O:3273[A]:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2935[B]:ILE:CD1	3:R:2936[B]:GLU:N	2.73	0.49
3:R:2939[B]:ARG:NE	3:R:3031[B]:ASN:ND2	2.60	0.49
3:R:3196[A]:THR:CA	3:R:3199[A]:GLN:OE1	2.58	0.49
3:R:3276[A]:ASP:O	3:R:3277[A]:ALA:HB3	2.12	0.49
3:R:3283[A]:ILE:C	3:R:3283[A]:ILE:CD1	2.85	0.49
1:S:49:ALA:H	1:S:55:ILE:HD12	1.78	0.49
1:S:462:HIS:HA	1:S:490:TRP:HH2	1.77	0.49
2:T:2808:PHE:HZ	2:T:2821:LEU:HD13	1.78	0.49
3:U:2975[B]:PHE:CZ	3:d:3256[B]:TRP:HD1	2.30	0.49
3:U:3089[B]:HIS:CE1	3:U:3093[B]:HIS:CE1	3.01	0.49
3:U:3191[A]:ASN:ND2	3:U:3191[A]:ASN:N	2.60	0.49
3:U:3211[B]:ASP:OD1	3:U:3211[B]:ASP:N	2.28	0.49
2:W:2762:VAL:O	2:W:2768:LEU:HD23	2.13	0.49
3:X:3089[B]:HIS:CE1	3:X:3093[B]:HIS:CE1	3.01	0.49
3:X:3293[A]:LYS:HB2	3:X:3294[A]:SER:CA	2.41	0.49
3:X:3300[A]:LEU:CD2	3:X:3300[A]:LEU:H	2.24	0.49
2:Z:2849:ASP:HB3	2:Z:2850:ARG:NE	2.27	0.49
3:a:3027[B]:GLU:CD	3:a:3028[B]:PRO:CD	2.86	0.49
3:a:3110[A]:THR:O	3:a:3111[A]:SER:C	2.53	0.49
3:a:3283[B]:ILE:C	3:a:3283[B]:ILE:CD1	2.85	0.49
3:a:3298[A]:ASN:CB	3:a:3299[A]:LEU:C	2.85	0.49
1:b:411:ASP:OD1	1:b:411:ASP:N	2.46	0.49
3:d:3027[B]:GLU:CD	3:d:3028[B]:PRO:CD	2.86	0.49
3:d:3196[B]:THR:OG1	3:d:3199[B]:GLN:HG3	2.12	0.49
1:A:480:CYS:HA	1:A:490:TRP:CE2	2.48	0.49
1:A:717:GLN:O	1:A:720:VAL:HG22	2.13	0.49
1:A:1074:ILE:HB	2:E:2901:LEU:HB2	1.94	0.49
2:B:2573:TYR:CE2	2:B:2707:PHE:HE2	2.28	0.49
3:C:2939[B]:ARG:NE	3:C:3031[B]:ASN:ND2	2.60	0.49
3:C:2949[A]:LYS:C	3:C:2949[A]:LYS:CD	2.85	0.49
3:C:2954[A]:TYR:C	3:C:2957[A]:ILE:HG22	2.37	0.49
3:C:3089[A]:HIS:CE1	3:C:3093[A]:HIS:CE1	3.01	0.49
3:C:3120[B]:HIS:NE2	9:L:3401[B]:CUO:O1	2.30	0.49
3:C:3196[B]:THR:O	3:C:3200[B]:LEU:N	2.43	0.49
1:D:644:TRP:O	1:D:647:LEU:HB2	2.12	0.49
1:D:830:ASN:HB3	1:D:832:LYS:HB2	1.95	0.49
3:F:2967[B]:CYS:HB3	3:a:2980[B]:HIS:N	2.16	0.49
3:F:3014[B]:TRP:HH2	3:F:3123[B]:THR:HG23	1.78	0.49
3:F:3093[A]:HIS:HB2	3:F:3248[A]:LEU:HD13	1.94	0.49
3:F:3110[A]:THR:C	3:F:3112[A]:TYR:H	2.20	0.49
3:F:3110[B]:THR:C	3:F:3112[B]:TYR:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:306:PHE:HB3	1:G:308:LEU:HD13	1.94	0.49
1:G:655:TYR:HE2	1:G:693:TYR:HB3	1.78	0.49
1:G:1284:GLU:OE1	1:G:1337:ARG:NH1	2.46	0.49
1:G:1636:ASN:OD1	6:r:1:NAG:C7	2.60	0.49
1:G:1636:ASN:OD1	6:r:1:NAG:N2	2.46	0.49
2:H:2457:LYS:HZ1	1:J:1206:HIS:HB3	1.78	0.49
2:H:2680:HIS:NE2	2:H:2684:HIS:CD2	2.81	0.49
3:I:3262[A]:PHE:C	3:I:3263[A]:LEU:HD12	2.38	0.49
1:J:63:PRO:HA	1:J:172:GLU:HG3	1.94	0.49
1:J:618:MET:HE2	1:J:629:MET:HE2	1.95	0.49
1:J:1361:GLU:HG3	1:J:1363:THR:H	1.77	0.49
2:K:2279:LEU:HD12	2:K:2284:HIS:HD2	1.78	0.49
3:L:2935[B]:ILE:CD1	3:L:2935[B]:ILE:H	2.25	0.49
3:L:2939[B]:ARG:NE	3:L:3031[B]:ASN:ND2	2.60	0.49
3:L:2949[A]:LYS:C	3:L:2949[A]:LYS:CD	2.85	0.49
3:L:3110[B]:THR:O	3:L:3111[B]:SER:C	2.53	0.49
3:L:3196[B]:THR:OG1	3:L:3199[B]:GLN:HG3	2.12	0.49
1:M:1103:PHE:HE2	2:Q:2871:PHE:HA	1.78	0.49
2:N:2536:PHE:HE1	2:N:2708:TYR:HE2	1.60	0.49
3:O:2949[B]:LYS:C	3:O:2949[B]:LYS:HZ3	2.11	0.49
3:O:2968[B]:GLN:CD	3:X:2984[B]:THR:HG1	2.11	0.49
3:O:2981[A]:GLY:N	3:O:3086[A]:GLU:OE1	2.45	0.49
3:O:3120[A]:HIS:CE1	9:O:3401[A]:CUO:O1	2.66	0.49
2:Q:2336:PHE:HB3	2:Q:2348:THR:HG22	1.94	0.49
3:R:2935[A]:ILE:CD1	3:R:2935[A]:ILE:H	2.25	0.49
3:R:2935[B]:ILE:CD1	3:R:2935[B]:ILE:H	2.25	0.49
3:R:2954[A]:TYR:C	3:R:2957[A]:ILE:HG22	2.37	0.49
3:R:3027[B]:GLU:CD	3:R:3028[B]:PRO:CD	2.86	0.49
3:R:3093[A]:HIS:HB2	3:R:3248[A]:LEU:HD13	1.94	0.49
3:R:3288[B]:MET:CA	3:R:3295[B]:LEU:HG	2.42	0.49
1:S:1063:ARG:HB3	1:S:1065:LYS:HE3	1.95	0.49
1:S:1558:LEU:HD13	2:W:2440:ASP:HA	1.94	0.49
2:T:2665:GLU:OE1	2:T:2798:GLN:NE2	2.46	0.49
3:U:2939[B]:ARG:HG3	3:U:2939[B]:ARG:NH1	2.28	0.49
3:U:3176[A]:LYS:NZ	3:U:3176[A]:LYS:CB	2.73	0.49
3:U:3176[B]:LYS:C	3:U:3177[B]:SER:HG	2.08	0.49
3:U:3196[A]:THR:CA	3:U:3199[A]:GLN:OE1	2.58	0.49
3:U:3262[A]:PHE:C	3:U:3263[A]:LEU:HD12	2.37	0.49
3:U:3298[A]:ASN:CA	3:U:3299[A]:LEU:C	2.85	0.49
3:X:2960[A]:PHE:CD2	3:X:3157[A]:PRO:CG	2.74	0.49
3:X:3014[B]:TRP:HH2	3:X:3123[B]:THR:HG23	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3201[A]:GLU:O	3:X:3205[A]:LYS:HB2	2.11	0.49
3:X:3217[B]:PHE:CB	3:X:3219[B]:LEU:HD21	2.42	0.49
3:a:2939[A]:ARG:NE	3:a:3031[A]:ASN:ND2	2.60	0.49
3:a:2960[A]:PHE:CD2	3:a:3157[A]:PRO:CG	2.74	0.49
3:a:3176[A]:LYS:C	3:a:3177[A]:SER:HG	2.10	0.49
3:a:3191[B]:ASN:C	3:a:3192[B]:PHE:O	2.52	0.49
3:a:3276[B]:ASP:O	3:a:3277[B]:ALA:HB3	2.12	0.49
1:b:389:THR:OG1	6:NA:1:NAG:H82	2.12	0.49
1:b:464:LEU:HD13	1:b:622:HIS:CE1	2.47	0.49
1:b:1148:LEU:HB2	1:b:1188:PHE:HD2	1.78	0.49
1:b:1316:MET:HB3	1:b:1318:VAL:HG22	1.95	0.49
3:d:3196[A]:THR:CA	3:d:3199[A]:GLN:OE1	2.58	0.49
3:d:3275[A]:LEU:N	3:d:3275[A]:LEU:CD1	2.73	0.49
1:A:611:GLY:HA2	1:A:617:SER:HB2	1.94	0.49
1:A:1018:ILE:HA	1:A:1021:LEU:HB2	1.95	0.49
2:B:2252:GLU:CD	2:B:2393:ARG:HH12	2.20	0.49
3:C:3027[A]:GLU:CD	3:C:3028[A]:PRO:CD	2.86	0.49
2:E:2099:GLU:HA	2:E:2172:ILE:HD11	1.95	0.49
3:F:2939[B]:ARG:HG3	3:F:2939[B]:ARG:NH1	2.28	0.49
3:F:3293[A]:LYS:CG	3:F:3294[A]:SER:HB2	2.36	0.49
3:F:3298[A]:ASN:CB	3:F:3299[A]:LEU:C	2.85	0.49
9:F:3401[A]:CUO:O1	3:a:3120[A]:HIS:CE1	2.66	0.49
3:I:2989[B]:HIS:HD2	3:R:2970[B]:PRO:HA	1.72	0.49
3:I:3014[A]:TRP:HH2	3:I:3123[A]:THR:HG23	1.78	0.49
3:I:3160[B]:SER:CB	3:R:3150[B]:LYS:NZ	2.62	0.49
1:J:135:THR:HG22	1:J:192:HIS:HB3	1.94	0.49
1:J:139:VAL:HG11	1:J:144:TYR:OH	2.13	0.49
1:J:1279:LYS:HE3	1:J:1376:PRO:HG3	1.93	0.49
3:L:3147[B]:GLU:CG	3:L:3149[B]:ASN:ND2	2.73	0.49
3:L:3219[A]:LEU:N	3:L:3219[A]:LEU:CD2	2.73	0.49
1:M:142:ARG:NH1	1:M:340:GLN:OE1	2.45	0.49
1:M:552:PHE:HZ	1:M:623:TYR:HE1	1.61	0.49
1:M:801:ASP:N	1:M:801:ASP:OD1	2.45	0.49
1:M:1081:MET:HG2	1:M:1100:SER:O	2.12	0.49
3:O:3027[A]:GLU:CD	3:O:3028[A]:PRO:CD	2.86	0.49
3:O:3157[B]:PRO:HB3	3:X:3150[B]:LYS:HA	1.93	0.49
3:O:3169[B]:LYS:HA	3:X:3148[B]:ILE:HG21	1.91	0.49
3:O:3255[B]:PRO:N	3:X:3169[B]:LYS:HG3	2.27	0.49
3:R:2954[B]:TYR:C	3:R:2957[B]:ILE:HG22	2.37	0.49
3:R:2961[B]:HIS:CD2	3:R:2988[B]:TRP:CZ3	2.96	0.49
3:R:3110[B]:THR:C	3:R:3112[B]:TYR:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1315:GLY:HA3	1:S:1601:TRP:HB2	1.94	0.49
1:S:1333:GLU:O	1:S:1337:ARG:HG3	2.12	0.49
2:T:2625:LEU:HA	2:T:2638:ARG:NH2	2.27	0.49
3:U:2954[B]:TYR:CA	3:U:2957[B]:ILE:HG22	2.43	0.49
3:U:2960[B]:PHE:CD2	3:U:3157[B]:PRO:CG	2.74	0.49
3:U:3014[B]:TRP:HH2	3:U:3123[B]:THR:HG23	1.78	0.49
3:U:3089[A]:HIS:CE1	3:U:3093[A]:HIS:CE1	3.01	0.49
3:U:3288[B]:MET:CA	3:U:3295[B]:LEU:HG	2.42	0.49
2:W:2903:TYR:OH	3:X:2932[A]:PRO:HD2	2.12	0.49
3:X:3014[A]:TRP:HH2	3:X:3123[A]:THR:HG23	1.77	0.49
3:a:2949[B]:LYS:C	3:a:2949[B]:LYS:CD	2.85	0.49
3:a:3014[B]:TRP:HH2	3:a:3123[B]:THR:HG23	1.78	0.49
3:a:3110[B]:THR:C	3:a:3112[B]:TYR:H	2.20	0.49
3:a:3298[B]:ASN:CA	3:a:3299[B]:LEU:C	2.85	0.49
1:b:318:ARG:HB2	1:b:382:GLU:HB2	1.94	0.49
1:b:1505:ARG:O	1:b:1509:THR:OG1	2.31	0.49
1:b:1636:ASN:ND2	4:QA:1:NAG:O7	2.46	0.49
2:c:2599:SER:O	2:c:2645:PHE:HB3	2.13	0.49
2:c:2687:ILE:HD11	2:c:2695:MET:HE3	1.95	0.49
3:d:2954[B]:TYR:C	3:d:2957[B]:ILE:HG22	2.37	0.49
3:d:3066[A]:TYR:CE1	3:d:3193[A]:HIS:CE1	2.98	0.49
3:d:3110[B]:THR:C	3:d:3112[B]:TYR:N	2.68	0.49
5:l:1:NAG:H61	5:l:2:NAG:C1	2.43	0.49
1:A:980:TYR:HE1	1:A:1021:LEU:HD13	1.77	0.49
1:A:1205:LEU:HD23	1:A:1211:TYR:HB2	1.94	0.49
1:A:1348:TRP:HD1	1:A:1403:LEU:HD13	1.76	0.49
3:C:2969[B]:TYR:CD2	3:L:3093[B]:HIS:NE2	2.79	0.49
3:C:3004[A]:GLY:O	3:C:3006[A]:LYS:N	2.44	0.49
3:C:3014[B]:TRP:HH2	3:C:3123[B]:THR:HG23	1.78	0.49
3:C:3156[B]:MET:CE	3:L:2979[B]:GLN:HB3	2.32	0.49
3:C:3196[A]:THR:O	3:C:3200[A]:LEU:N	2.44	0.49
3:C:3232[B]:VAL:HG23	3:C:3273[B]:LEU:HD11	1.94	0.49
3:C:3255[B]:PRO:CD	3:L:2959[B]:SER:O	2.61	0.49
3:C:3276[B]:ASP:O	3:C:3277[B]:ALA:HB3	2.12	0.49
3:C:3293[B]:LYS:HB2	3:C:3294[B]:SER:CA	2.41	0.49
3:C:3298[A]:ASN:CB	3:C:3299[A]:LEU:C	2.86	0.49
1:D:398:ARG:NH2	1:D:484:MET:HE2	2.28	0.49
3:F:2949[A]:LYS:C	3:F:2949[A]:LYS:CD	2.85	0.49
3:F:2954[B]:TYR:C	3:F:2957[B]:ILE:HG22	2.37	0.49
3:F:2968[B]:GLN:HG2	3:a:2980[B]:HIS:CA	2.34	0.49
3:F:3172[B]:SER:HB2	3:a:3150[B]:LYS:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3196[B]:THR:CA	3:F:3199[B]:GLN:OE1	2.58	0.49
2:H:2411:PHE:HE2	2:H:2445:MET:HE3	1.77	0.49
2:H:2615:TRP:NE1	2:K:2121:THR:HG23	2.28	0.49
2:H:2813:ILE:CG2	2:H:2896:LEU:HD21	2.42	0.49
3:I:2935[B]:ILE:CD1	3:I:2936[B]:GLU:N	2.73	0.49
3:I:2969[A]:TYR:CD2	3:I:2970[A]:PRO:HD2	2.47	0.49
3:I:2970[B]:PRO:HD3	3:R:2989[B]:HIS:ND1	2.21	0.49
3:I:3183[B]:LEU:N	3:I:3184[B]:ASN:HA	2.11	0.49
3:I:3262[B]:PHE:C	3:I:3263[B]:LEU:HD12	2.37	0.49
3:I:3283[A]:ILE:C	3:I:3283[A]:ILE:CD1	2.85	0.49
1:J:195:SER:CB	1:J:386:ILE:HD11	2.43	0.49
1:J:570:GLN:HA	1:J:571:PRO:C	2.38	0.49
2:K:2679:ILE:O	2:K:2682:SER:HB3	2.13	0.49
3:L:2933[B]:SER:CB	3:L:2936[B]:GLU:CB	2.85	0.49
3:L:2949[B]:LYS:C	3:L:2949[B]:LYS:CD	2.85	0.49
3:L:3027[A]:GLU:CD	3:L:3028[A]:PRO:CD	2.86	0.49
3:L:3066[A]:TYR:CE1	3:L:3193[A]:HIS:CE1	2.98	0.49
3:L:3196[B]:THR:CA	3:L:3199[B]:GLN:HB2	2.43	0.49
3:L:3275[B]:LEU:N	3:L:3275[B]:LEU:CD1	2.73	0.49
1:M:289:LEU:HD22	1:M:293:LEU:HD13	1.93	0.49
1:M:425:ARG:NE	1:M:499:GLU:OE2	2.38	0.49
1:M:898:GLY:HA2	1:M:1186:TRP:HB2	1.95	0.49
2:N:2329:MET:HA	2:N:2354:PRO:HG2	1.95	0.49
2:N:2866:PRO:HB2	2:N:2868:GLU:CD	2.37	0.49
3:O:2954[A]:TYR:C	3:O:2957[A]:ILE:HG22	2.37	0.49
3:O:3089[A]:HIS:CE1	3:O:3093[A]:HIS:CE1	3.01	0.49
3:O:3196[A]:THR:CG2	1:P:416:ASN:ND2	2.59	0.49
3:O:3196[B]:THR:CA	3:O:3199[B]:GLN:OE1	2.58	0.49
1:P:449:ASP:HB3	1:P:1280:GLN:NE2	2.28	0.49
1:P:1086:LEU:CD1	1:P:1090:ILE:HD11	2.43	0.49
2:Q:2340:ALA:HB1	2:Q:2341:PRO:CD	2.42	0.49
3:R:3089[A]:HIS:CE1	3:R:3093[A]:HIS:CE1	3.01	0.49
3:R:3211[B]:ASP:OD1	3:R:3211[B]:ASP:N	2.28	0.49
1:S:557:VAL:HB	1:S:558:HIS:HA	1.95	0.49
3:U:2965[B]:LEU:HG	3:d:3220[B]:ARG:C	2.37	0.49
3:U:3120[A]:HIS:CE1	9:U:3401[A]:CUO:O1	2.66	0.49
3:U:3196[B]:THR:OG1	3:U:3199[B]:GLN:HG3	2.12	0.49
3:U:3217[B]:PHE:CB	3:U:3219[B]:LEU:HD21	2.42	0.49
2:W:2240:GLN:HE21	2:W:2241:THR:HG22	1.78	0.49
2:W:2451:LEU:HD22	2:W:2456:LEU:HD11	1.95	0.49
3:X:2954[B]:TYR:C	3:X:2957[B]:ILE:HG22	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2961[B]:HIS:CD2	3:X:2988[B]:TRP:CZ3	2.96	0.49
3:X:3151[A]:LEU:CB	3:X:3175[A]:TYR:CD2	2.93	0.49
3:X:3200[A]:LEU:HD22	3:X:3204[A]:LEU:HD11	1.95	0.49
3:X:3262[A]:PHE:C	3:X:3263[A]:LEU:HD12	2.37	0.49
1:Y:1422:HIS:NE2	1:Y:1608:ARG:HB2	2.28	0.49
2:Z:2240:GLN:HG2	2:Z:2244:PHE:CD1	2.48	0.49
3:a:3014[A]:TRP:HH2	3:a:3123[A]:THR:HG23	1.78	0.49
3:a:3110[A]:THR:C	3:a:3112[A]:TYR:H	2.21	0.49
3:a:3284[B]:LYS:CD	3:a:3284[B]:LYS:C	2.86	0.49
1:b:1494:ARG:HG3	1:b:1494:ARG:HH11	1.77	0.49
2:c:2110:MET:HE1	2:c:2122:ILE:HD12	1.94	0.49
3:d:2939[A]:ARG:HG3	3:d:2939[A]:ARG:NH1	2.28	0.49
3:d:2939[B]:ARG:NE	3:d:3031[B]:ASN:ND2	2.60	0.49
3:d:3014[B]:TRP:HH2	3:d:3123[B]:THR:HG23	1.78	0.49
3:d:3141[B]:TYR:CD2	3:d:3141[B]:TYR:C	2.86	0.49
3:d:3196[A]:THR:OG1	3:d:3199[A]:GLN:HG3	2.12	0.49
3:d:3262[A]:PHE:C	3:d:3263[A]:LEU:HD12	2.38	0.49
3:d:3276[B]:ASP:O	3:d:3277[B]:ALA:HB3	2.12	0.49
2:B:2887:ASP:OD1	2:B:2887:ASP:N	2.34	0.49
3:C:3086[B]:GLU:HG2	3:L:2968[B]:GLN:HE21	1.78	0.49
3:C:3151[A]:LEU:CB	3:C:3175[A]:TYR:CD2	2.93	0.49
3:C:3253[B]:GLU:HB3	3:L:3252[B]:TYR:CB	2.42	0.49
1:D:215:ARG:NE	1:D:279:LEU:HA	2.27	0.49
1:D:947:TYR:HE1	1:D:956:PRO:HG2	1.78	0.49
2:E:2819:VAL:HG22	2:E:2883:ILE:HG13	1.94	0.49
3:F:2971[B]:ASP:N	3:a:3093[B]:HIS:NE2	2.13	0.49
3:F:3089[A]:HIS:CE1	3:F:3093[A]:HIS:CE1	3.01	0.49
3:F:3143[B]:SER:OG	3:F:3144[B]:ALA:N	2.46	0.49
3:F:3232[A]:VAL:HG23	3:F:3273[A]:LEU:HD11	1.94	0.49
1:G:277:ASP:OD1	1:G:278:ASP:N	2.46	0.49
1:G:1245:GLU:CD	1:G:1245:GLU:H	2.17	0.49
1:G:1260:ARG:HD3	1:G:1331:GLU:OE1	2.13	0.49
2:H:2572:VAL:HG22	2:H:2768:LEU:HD22	1.95	0.49
2:H:2744:PHE:HZ	1:J:1212:HIS:HB3	1.78	0.49
3:I:2939[A]:ARG:HG3	3:I:2939[A]:ARG:NH1	2.28	0.49
3:I:2965[B]:LEU:CG	3:I:2974[B]:ALA:CB	2.85	0.49
3:I:3096[A]:VAL:HG11	3:I:3115[A]:LEU:HD12	1.89	0.49
3:I:3151[B]:LEU:HB2	3:I:3175[B]:TYR:HE2	1.68	0.49
3:I:3155[B]:MET:SD	3:R:3154[B]:PRO:HD2	2.53	0.49
3:I:3183[A]:LEU:H	3:I:3184[A]:ASN:CA	2.22	0.49
3:I:3217[A]:PHE:CB	3:I:3219[A]:LEU:HD21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:120:LYS:N	1:J:121:ASN:HA	2.27	0.49
1:J:1335:LEU:HA	1:J:1339:SER:HB3	1.93	0.49
3:L:2954[B]:TYR:C	3:L:2957[B]:ILE:HG22	2.37	0.49
3:L:3176[B]:LYS:N	3:L:3176[B]:LYS:CE	2.73	0.49
1:M:1400:ASN:ND2	1:M:1433:TRP:HZ3	2.11	0.49
2:N:2374:ASN:ND2	2:Q:2098:GLN:HE22	2.11	0.49
2:N:2805:PHE:CE1	2:N:2855:ASP:HB3	2.48	0.49
3:O:2949[A]:LYS:C	3:O:2949[A]:LYS:CD	2.85	0.49
3:O:3196[A]:THR:OG1	3:O:3199[A]:GLN:HG3	2.12	0.49
3:O:3196[A]:THR:CA	3:O:3199[A]:GLN:HB2	2.43	0.49
3:O:3217[B]:PHE:HD2	3:O:3300[B]:LEU:HD12	1.78	0.49
3:R:3113[B]:ASP:O	3:R:3114[B]:PRO:C	2.53	0.49
3:R:3191[B]:ASN:C	3:R:3192[B]:PHE:O	2.52	0.49
3:R:3196[A]:THR:O	3:R:3200[A]:LEU:N	2.43	0.49
3:R:3219[A]:LEU:N	3:R:3219[A]:LEU:CD2	2.73	0.49
1:S:834:ASP:OD1	1:S:834:ASP:N	2.38	0.49
3:U:2952[A]:ALA:CB	3:U:2953[A]:GLY:CA	2.82	0.49
3:U:2969[B]:TYR:C	3:d:2981[B]:GLY:N	2.70	0.49
3:U:2975[B]:PHE:HB2	3:d:3256[B]:TRP:CB	1.78	0.49
3:U:3154[B]:PRO:HG3	3:d:2984[B]:THR:HG22	1.77	0.49
3:U:3191[B]:ASN:ND2	3:U:3191[B]:ASN:N	2.60	0.49
3:U:3196[A]:THR:OG1	3:U:3199[A]:GLN:HG3	2.12	0.49
3:U:3196[A]:THR:O	3:U:3200[A]:LEU:N	2.43	0.49
3:U:3262[B]:PHE:C	3:U:3263[B]:LEU:HD12	2.37	0.49
1:V:49:ALA:HB3	1:V:55:ILE:HD12	1.94	0.49
1:V:137:ARG:NH1	1:V:203:ASP:OD1	2.46	0.49
1:V:745:ASP:HB2	1:V:801:ASP:OD1	2.12	0.49
1:V:949:ASP:C	1:V:952:GLY:H	2.21	0.49
3:X:2933[B]:SER:HA	3:X:2935[B]:ILE:HD11	1.95	0.49
1:Y:22:LEU:HG	1:Y:122:VAL:HG11	1.94	0.49
1:Y:392:PRO:HB2	1:Y:394:GLN:HG2	1.95	0.49
1:Y:1299:GLN:HB2	1:Y:1311:CYS:SG	2.53	0.49
1:Y:1365:TYR:CD1	1:Y:1372:ILE:HG22	2.35	0.49
1:Y:1622:GLN:O	2:c:2326:ILE:HD11	2.13	0.49
1:Y:1639:LYS:NZ	1:Y:1642:GLN:HG3	2.28	0.49
3:a:3196[A]:THR:CA	3:a:3199[A]:GLN:HB2	2.43	0.49
3:a:3196[B]:THR:OG1	3:a:3199[B]:GLN:HB2	2.12	0.49
3:a:3217[A]:PHE:HD2	3:a:3300[A]:LEU:HD12	1.78	0.49
3:a:3232[B]:VAL:HG23	3:a:3273[B]:LEU:HD11	1.94	0.49
1:b:1390:ASP:HB2	1:b:1438:ASP:OD2	2.12	0.49
3:d:2954[B]:TYR:CA	3:d:2957[B]:ILE:HG22	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3196[A]:THR:O	3:d:3200[A]:LEU:N	2.44	0.49
3:d:3232[B]:VAL:HG23	3:d:3273[B]:LEU:HD11	1.95	0.49
1:A:187:GLY:HA3	1:A:195:SER:N	2.27	0.48
1:A:1627:ARG:NH2	1:A:1629:GLU:OE1	2.43	0.48
2:B:2597:MET:HE2	2:B:2598:PRO:HD2	1.93	0.48
2:B:2670:CYS:N	2:B:2737:CYS:SG	2.86	0.48
2:B:2740:ASP:OD2	1:D:1232:THR:OG1	2.23	0.48
3:C:2939[B]:ARG:HG3	3:C:2939[B]:ARG:NH1	2.28	0.48
3:C:2961[B]:HIS:CD2	3:C:2988[B]:TRP:CZ3	2.96	0.48
3:C:3089[B]:HIS:CE1	3:L:2971[B]:ASP:HB3	2.47	0.48
3:C:3283[A]:ILE:C	3:C:3283[A]:ILE:CD1	2.85	0.48
3:C:3288[A]:MET:CA	3:C:3295[A]:LEU:HG	2.42	0.48
1:D:104:LEU:HB3	1:D:123:PHE:HD2	1.77	0.48
1:D:514:TRP:CZ2	1:D:606:ILE:HD11	2.48	0.48
1:D:664:VAL:O	1:D:689:PRO:HD2	2.13	0.48
1:D:902:PHE:HB3	1:D:903:PRO:HD3	1.93	0.48
1:D:1296:VAL:HG13	1:D:1384:PHE:HZ	1.78	0.48
3:F:2969[B]:TYR:HE2	3:a:3120[B]:HIS:NE2	2.09	0.48
3:F:3089[B]:HIS:CE1	3:F:3093[B]:HIS:CE1	3.01	0.48
3:F:3147[B]:GLU:CG	3:F:3149[B]:ASN:ND2	2.73	0.48
3:F:3149[B]:ASN:HB3	3:a:3165[B]:ASN:O	2.12	0.48
3:F:3217[A]:PHE:CB	3:F:3219[A]:LEU:HD21	2.42	0.48
1:G:954:ALA:O	1:G:956:PRO:HD3	2.13	0.48
2:H:2402:GLY:HA3	2:H:2403:PHE:HD1	1.78	0.48
3:I:2971[B]:ASP:O	3:R:3093[B]:HIS:HB2	2.13	0.48
3:I:2981[A]:GLY:N	3:I:3086[A]:GLU:OE1	2.45	0.48
3:I:2991[A]:LEU:HD23	3:I:3158[A]:PHE:CE1	2.48	0.48
3:I:3089[A]:HIS:CE1	3:I:3093[A]:HIS:CE1	3.01	0.48
3:I:3256[B]:TRP:NE1	3:R:2965[B]:LEU:HD12	2.26	0.48
1:J:1302:SER:HB3	1:J:1494:ARG:NH2	2.28	0.48
3:L:2939[B]:ARG:HG3	3:L:2939[B]:ARG:NH1	2.28	0.48
3:L:2948[A]:ASP:CB	3:L:2949[A]:LYS:CA	2.78	0.48
3:L:3110[A]:THR:C	3:L:3112[A]:TYR:H	2.20	0.48
3:L:3135[B]:LYS:HB2	3:L:3141[B]:TYR:HD1	1.76	0.48
3:L:3284[A]:LYS:CE	3:L:3284[A]:LYS:CA	2.85	0.48
1:M:622:HIS:HE1	1:M:767:LYS:H	1.59	0.48
1:M:1324:ARG:NH1	1:M:1519:TYR:HB3	2.28	0.48
1:M:1427:HIS:CE1	1:M:1458:HIS:CE1	3.00	0.48
3:O:2935[B]:ILE:CD1	3:O:2935[B]:ILE:H	2.25	0.48
3:O:2949[B]:LYS:C	3:O:2949[B]:LYS:CD	2.85	0.48
3:O:2954[B]:TYR:C	3:O:2957[B]:ILE:HG22	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2954[B]:TYR:CA	3:O:2957[B]:ILE:HG22	2.43	0.48
3:O:3157[B]:PRO:CA	3:X:3153[B]:LYS:N	2.60	0.48
3:O:3252[B]:TYR:CD2	3:X:2966[B]:SER:O	2.53	0.48
1:P:563:ILE:O	1:P:612:GLY:HA3	2.13	0.48
3:R:2937[B]:ASN:CB	3:R:3006[B]:LYS:CE	2.86	0.48
3:R:2952[A]:ALA:CB	3:R:2953[A]:GLY:CA	2.82	0.48
3:R:3135[A]:LYS:HB2	3:R:3141[A]:TYR:HD1	1.76	0.48
3:R:3147[B]:GLU:CG	3:R:3149[B]:ASN:ND2	2.73	0.48
3:R:3191[A]:ASN:ND2	3:R:3191[A]:ASN:N	2.60	0.48
3:R:3196[A]:THR:OG1	3:R:3199[A]:GLN:HG3	2.12	0.48
3:R:3298[B]:ASN:CA	3:R:3299[B]:LEU:C	2.85	0.48
1:S:14:GLU:O	1:S:17:ASN:ND2	2.46	0.48
2:T:2341:PRO:HG2	2:T:2342:TYR:CD1	2.47	0.48
3:U:2954[A]:TYR:C	3:U:2957[A]:ILE:HG22	2.37	0.48
3:U:3183[B]:LEU:H	3:U:3184[B]:ASN:CA	2.22	0.48
3:U:3217[A]:PHE:HD2	3:U:3300[A]:LEU:HD12	1.79	0.48
1:V:140:ASP:OD1	1:V:142:ARG:NE	2.38	0.48
1:V:1156:LEU:HD13	1:V:1176:TYR:CE1	2.48	0.48
1:V:1583:CYS:C	1:Y:329:ARG:HB3	2.38	0.48
2:W:2370:MET:HE3	2:W:2370:MET:HB2	1.75	0.48
2:W:2612:TYR:OH	2:W:2617:ASP:OD1	2.28	0.48
2:W:2786:MET:HE1	2:W:2794:LEU:HD13	1.94	0.48
3:X:3120[B]:HIS:CE1	9:X:3401[B]:CUO:O1	2.66	0.48
3:X:3232[A]:VAL:HG23	3:X:3273[A]:LEU:HD11	1.94	0.48
1:Y:826:ILE:HG12	1:Y:827:ALA:N	2.28	0.48
1:Y:975:PRO:HG3	1:Y:1026:GLU:HG3	1.95	0.48
3:a:3114[A]:PRO:CD	3:a:3115[A]:LEU:N	2.72	0.48
3:d:2954[A]:TYR:CA	3:d:2957[A]:ILE:HG22	2.43	0.48
3:d:3191[A]:ASN:ND2	3:d:3191[A]:ASN:N	2.60	0.48
3:d:3276[A]:ASP:O	3:d:3277[A]:ALA:HB3	2.12	0.48
6:GA:1:NAG:O3	6:GA:2:NAG:C1	2.60	0.48
3:C:2933[B]:SER:HA	3:C:2935[B]:ILE:HD11	1.95	0.48
3:C:2971[A]:ASP:CG	3:C:2973[A]:THR:HG1	2.17	0.48
3:C:3027[B]:GLU:CD	3:C:3028[B]:PRO:CD	2.86	0.48
3:C:3110[A]:THR:C	3:C:3112[A]:TYR:H	2.20	0.48
3:C:3149[B]:ASN:O	3:L:3172[B]:SER:CA	2.60	0.48
3:C:3191[B]:ASN:ND2	3:C:3191[B]:ASN:N	2.60	0.48
1:D:462:HIS:HA	1:D:490:TRP:CH2	2.47	0.48
3:F:2939[A]:ARG:NE	3:F:3031[A]:ASN:ND2	2.60	0.48
3:F:2954[B]:TYR:CA	3:F:2957[B]:ILE:HG22	2.43	0.48
3:F:3027[A]:GLU:CD	3:F:3028[A]:PRO:CD	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3298[B]:ASN:CA	3:F:3299[B]:LEU:C	2.86	0.48
1:G:902:PHE:HB3	1:G:903:PRO:HD3	1.93	0.48
3:I:2939[B]:ARG:NE	3:I:3031[B]:ASN:ND2	2.60	0.48
3:I:2985[B]:PHE:CD2	3:R:2968[B]:GLN:O	2.67	0.48
3:I:3027[A]:GLU:CD	3:I:3028[A]:PRO:CD	2.86	0.48
3:I:3150[B]:LYS:CD	3:R:3160[B]:SER:CB	2.91	0.48
3:I:3155[B]:MET:H	3:R:3153[B]:LYS:C	2.10	0.48
3:I:3157[B]:PRO:HD3	3:R:2982[B]:MET:CE	2.43	0.48
3:I:3171[B]:HIS:HA	3:R:3152[B]:LYS:HB3	1.95	0.48
3:I:3176[B]:LYS:N	3:I:3176[B]:LYS:CE	2.73	0.48
3:I:3217[B]:PHE:CB	3:I:3219[B]:LEU:HD21	2.42	0.48
3:I:3298[B]:ASN:CB	3:I:3299[B]:LEU:C	2.85	0.48
2:K:2179:ASP:HB3	2:K:2303:ARG:HH12	1.78	0.48
3:L:3014[A]:TRP:HH2	3:L:3123[A]:THR:HG23	1.78	0.48
3:L:3191[A]:ASN:ND2	3:L:3191[A]:ASN:N	2.60	0.48
3:L:3196[A]:THR:O	3:L:3199[A]:GLN:HB2	2.11	0.48
1:M:294:LYS:HA	1:M:297:ARG:HD2	1.95	0.48
2:N:2373:MET:HB3	2:N:2381:LEU:HD11	1.96	0.48
3:O:2939[A]:ARG:NE	3:O:3031[A]:ASN:ND2	2.60	0.48
3:O:2949[A]:LYS:C	3:O:2949[A]:LYS:HZ3	2.15	0.48
3:O:3110[B]:THR:C	3:O:3112[B]:TYR:N	2.68	0.48
3:O:3143[A]:SER:OG	3:O:3144[A]:ALA:N	2.46	0.48
3:O:3217[A]:PHE:HD2	3:O:3300[A]:LEU:HD12	1.79	0.48
1:P:1145:THR:OG1	1:P:1233:SER:HB3	2.13	0.48
3:R:2933[A]:SER:HA	3:R:2935[A]:ILE:HD11	1.95	0.48
3:R:2939[B]:ARG:HG3	3:R:2939[B]:ARG:NH1	2.28	0.48
3:R:3183[B]:LEU:H	3:R:3184[B]:ASN:CA	2.22	0.48
1:S:597:VAL:O	1:S:601:VAL:HG12	2.13	0.48
2:T:2172:ILE:HG13	2:T:2173:VAL:HG13	1.95	0.48
2:T:2265:ILE:HD12	2:T:2443:TYR:CD1	2.47	0.48
2:T:2279:LEU:HD12	2:T:2284:HIS:HD2	1.78	0.48
2:T:2504:ARG:HD3	2:T:2775:GLY:O	2.13	0.48
3:U:3004[B]:GLY:O	3:U:3006[B]:LYS:N	2.44	0.48
3:U:3298[B]:ASN:CA	3:U:3299[B]:LEU:C	2.85	0.48
1:V:904:HIS:HB3	1:V:1105:VAL:HG21	1.95	0.48
3:X:3024[A]:LEU:CD1	3:X:3024[A]:LEU:C	2.85	0.48
2:Z:2562:GLY:H	2:Z:2846:TRP:HB2	1.78	0.48
3:a:2935[A]:ILE:CD1	3:a:2935[A]:ILE:H	2.25	0.48
3:a:3027[A]:GLU:CD	3:a:3028[A]:PRO:CD	2.86	0.48
3:a:3262[B]:PHE:C	3:a:3263[B]:LEU:HD12	2.37	0.48
1:b:22:LEU:HD23	1:b:122:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3298[A]:ASN:CB	3:d:3299[A]:LEU:C	2.86	0.48
3:d:3298[B]:ASN:CB	3:d:3300[B]:LEU:CD2	2.61	0.48
1:A:213:VAL:HA	1:A:216:HIS:ND1	2.29	0.48
1:A:494:VAL:HG23	1:A:671:PHE:CZ	2.48	0.48
1:A:1148:LEU:HB2	1:A:1188:PHE:CD2	2.48	0.48
2:B:2268:ASN:HD22	2:B:2428:VAL:HA	1.78	0.48
3:C:2939[A]:ARG:NE	3:C:3031[A]:ASN:ND2	2.60	0.48
3:C:2961[A]:HIS:CD2	3:C:2988[A]:TRP:CZ3	2.97	0.48
3:C:3093[B]:HIS:HB2	3:C:3248[B]:LEU:HD13	1.94	0.48
3:C:3196[B]:THR:OG1	3:C:3199[B]:GLN:HG3	2.12	0.48
3:C:3219[A]:LEU:N	3:C:3219[A]:LEU:CD2	2.73	0.48
1:D:145:GLN:HB3	1:D:146:ALA:H	1.48	0.48
1:D:449:ASP:OD1	1:D:449:ASP:N	2.46	0.48
3:F:2933[B]:SER:HA	3:F:2935[B]:ILE:HD11	1.95	0.48
3:F:3155[B]:MET:CB	3:a:3153[B]:LYS:HB3	2.43	0.48
3:F:3228[B]:VAL:CG2	3:F:3245[B]:PHE:CE1	2.97	0.48
1:G:398:ARG:HH21	1:G:663:GLU:CD	2.21	0.48
2:H:2300:ASN:OD1	2:H:2303:ARG:NH1	2.47	0.48
2:H:2887:ASP:HB2	2:H:2890:VAL:HG23	1.95	0.48
3:I:2933[A]:SER:CB	3:I:2936[A]:GLU:CB	2.85	0.48
3:I:2975[B]:PHE:CB	3:R:3107[B]:LEU:HD11	2.19	0.48
3:I:3014[B]:TRP:HH2	3:I:3123[B]:THR:HG23	1.78	0.48
3:I:3090[B]:ASN:CB	3:R:2971[B]:ASP:O	2.61	0.48
3:I:3153[B]:LYS:HB3	3:R:3155[B]:MET:CA	2.42	0.48
3:I:3196[B]:THR:O	3:I:3200[B]:LEU:N	2.44	0.48
3:I:3276[B]:ASP:O	3:I:3277[B]:ALA:HB3	2.12	0.48
3:I:3291[A]:ASP:OD2	3:I:3293[A]:LYS:NZ	2.43	0.48
1:J:308:LEU:O	1:J:772:ARG:NH2	2.46	0.48
1:J:555:ALA:HB3	1:J:558:HIS:HE1	1.77	0.48
1:J:1157:VAL:HG21	1:J:1229:LYS:HE2	1.93	0.48
1:J:1403:LEU:HD21	1:J:1429:THR:HG21	1.96	0.48
1:J:1563:LYS:H	1:J:1563:LYS:HG2	1.38	0.48
2:K:2336:PHE:HB3	2:K:2348:THR:HG22	1.95	0.48
2:K:2903:TYR:OH	3:L:2932[A]:PRO:HD2	2.13	0.48
3:L:3093[B]:HIS:HB2	3:L:3248[B]:LEU:HD13	1.94	0.48
3:L:3191[B]:ASN:C	3:L:3192[B]:PHE:O	2.52	0.48
3:L:3196[A]:THR:CA	3:L:3199[A]:GLN:HB2	2.43	0.48
3:L:3220[B]:ARG:HH11	3:L:3220[B]:ARG:CG	2.12	0.48
3:L:3262[B]:PHE:C	3:L:3263[B]:LEU:HD12	2.37	0.48
3:L:3283[A]:ILE:C	3:L:3283[A]:ILE:CD1	2.85	0.48
1:M:1028:VAL:HA	1:M:1035:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1078:ARG:NH1	2:Q:2870:LEU:O	2.45	0.48
2:N:2240:GLN:HG2	2:N:2244:PHE:CD1	2.48	0.48
3:O:2933[A]:SER:CB	3:O:2936[A]:GLU:CB	2.85	0.48
3:O:2935[A]:ILE:CD1	3:O:2935[A]:ILE:H	2.25	0.48
3:O:2991[B]:LEU:HD23	3:O:3158[B]:PHE:CE1	2.47	0.48
3:O:3262[B]:PHE:C	3:O:3263[B]:LEU:HD12	2.37	0.48
1:P:4:ARG:HD3	1:P:77:GLU:OE2	2.13	0.48
1:P:879:SER:O	1:P:879:SER:OG	2.31	0.48
1:P:999:LEU:HB3	1:P:1133:ILE:HD11	1.95	0.48
1:P:1348:TRP:CG	1:P:1430:ILE:HD11	2.48	0.48
2:Q:2627:GLY:HA3	2:Q:2703:PHE:O	2.13	0.48
3:R:2952[A]:ALA:HB3	3:R:2954[A]:TYR:N	2.17	0.48
3:R:3027[A]:GLU:CD	3:R:3028[A]:PRO:CD	2.86	0.48
3:R:3114[A]:PRO:CD	3:R:3115[A]:LEU:N	2.72	0.48
3:R:3196[B]:THR:HG23	3:R:3199[B]:GLN:OE1	2.14	0.48
3:R:3228[A]:VAL:CG2	3:R:3245[A]:PHE:CE1	2.97	0.48
3:R:3291[B]:ASP:OD2	3:R:3293[B]:LYS:NZ	2.43	0.48
3:R:3298[A]:ASN:CA	3:R:3299[A]:LEU:C	2.86	0.48
1:S:1465:TRP:O	1:S:1469:GLN:HG3	2.12	0.48
2:T:2730:LEU:HA	1:V:1245:GLU:HB3	1.95	0.48
3:U:3027[B]:GLU:CD	3:U:3028[B]:PRO:CD	2.86	0.48
3:U:3110[B]:THR:C	3:U:3112[B]:TYR:H	2.21	0.48
3:U:3120[B]:HIS:CE1	9:U:3401[B]:CUO:O1	2.66	0.48
3:U:3170[B]:ALA:HA	3:d:3148[B]:ILE:CB	2.38	0.48
3:U:3196[A]:THR:CA	3:U:3199[A]:GLN:HB2	2.43	0.48
3:U:3298[A]:ASN:CB	3:U:3299[A]:LEU:C	2.85	0.48
1:V:307:ARG:HH21	1:V:397:PRO:HB3	1.78	0.48
1:V:914:GLU:OE1	1:V:926:LEU:N	2.35	0.48
1:V:1013:ILE:HD11	1:V:1148:LEU:CD1	2.43	0.48
1:V:1037:ALA:C	1:V:1039:ASP:H	2.21	0.48
1:V:1150:GLY:N	1:V:1186:TRP:O	2.41	0.48
1:V:1427:HIS:CD2	1:V:1457:HIS:HE1	2.31	0.48
3:X:3143[A]:SER:OG	3:X:3144[A]:ALA:N	2.46	0.48
3:X:3217[A]:PHE:HD2	3:X:3300[A]:LEU:HD12	1.78	0.48
1:Y:1613:ASP:OD1	3:d:3185[B]:TYR:CA	2.61	0.48
1:Y:1656:ASP:C	3:d:2937[B]:ASN:HD21	2.03	0.48
3:a:2933[B]:SER:HA	3:a:2935[B]:ILE:HD11	1.95	0.48
3:a:2954[A]:TYR:C	3:a:2957[A]:ILE:HG22	2.37	0.48
3:a:3096[A]:VAL:HG11	3:a:3115[A]:LEU:HD12	1.89	0.48
3:a:3141[B]:TYR:CD2	3:a:3141[B]:TYR:C	2.86	0.48
3:a:3196[A]:THR:O	3:a:3200[A]:LEU:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3217[B]:PHE:HD2	3:a:3300[B]:LEU:HD12	1.79	0.48
1:b:914:GLU:OE1	1:b:926:LEU:N	2.34	0.48
2:c:2569:TRP:HZ2	2:c:2748:PRO:HG3	1.78	0.48
2:c:2627:GLY:HA3	2:c:2703:PHE:O	2.13	0.48
2:c:2830:GLN:HB2	2:c:2863:ARG:NH2	2.28	0.48
3:d:2931[A]:THR:HG1	3:d:2934[A]:GLU:CD	2.04	0.48
3:d:3004[A]:GLY:O	3:d:3006[A]:LYS:N	2.44	0.48
3:d:3232[A]:VAL:HG23	3:d:3273[A]:LEU:HD11	1.95	0.48
3:d:3262[B]:PHE:C	3:d:3263[B]:LEU:HD12	2.37	0.48
1:A:989:THR:OG1	1:A:990:HIS:N	2.44	0.48
3:C:3089[B]:HIS:CE1	3:C:3093[B]:HIS:CE1	3.01	0.48
3:C:3153[B]:LYS:NZ	3:L:3158[B]:PHE:HE2	2.03	0.48
3:C:3196[B]:THR:CA	3:C:3199[B]:GLN:HB2	2.43	0.48
1:D:897:HIS:HB3	1:D:899:MET:HE1	1.94	0.48
3:F:2935[A]:ILE:CD1	3:F:2935[A]:ILE:H	2.25	0.48
3:F:2969[B]:TYR:C	3:a:2985[B]:PHE:HE2	2.21	0.48
3:F:2969[B]:TYR:HE1	3:a:2992[B]:TYR:HE2	1.61	0.48
3:F:3143[A]:SER:OG	3:F:3144[A]:ALA:N	2.46	0.48
3:F:3200[B]:LEU:HD22	3:F:3204[B]:LEU:HD11	1.95	0.48
3:F:3219[A]:LEU:N	3:F:3219[A]:LEU:CD2	2.73	0.48
1:G:572:SER:O	1:G:578:PHE:HB2	2.13	0.48
1:G:931:TRP:CD1	1:G:1048:ASN:HD22	2.32	0.48
1:G:1494:ARG:HG3	1:G:1494:ARG:NH1	2.28	0.48
2:H:2180:TRP:HB3	2:H:2184:MET:HE2	1.95	0.48
2:H:2797:LYS:HZ3	3:I:3028[A]:PRO:CD	2.13	0.48
3:I:2951[A]:ASP:C	3:I:2956[A]:LYS:HZ1	2.15	0.48
3:I:2961[A]:HIS:CD2	3:I:2988[A]:TRP:CZ3	2.96	0.48
3:I:2973[B]:THR:C	3:R:3107[B]:LEU:HD12	2.38	0.48
3:I:2982[B]:MET:CG	3:R:3156[B]:MET:CB	2.84	0.48
3:I:3027[B]:GLU:CD	3:I:3028[B]:PRO:CD	2.86	0.48
3:I:3113[A]:ASP:O	3:I:3114[A]:PRO:C	2.53	0.48
3:I:3120[A]:HIS:CE1	9:R:3401[A]:CUO:O1	2.66	0.48
3:I:3147[B]:GLU:N	3:R:3161[B]:GLU:HA	2.27	0.48
3:I:3149[B]:ASN:ND2	3:R:3163[B]:ASN:CA	2.76	0.48
3:I:3196[B]:THR:HG23	3:I:3199[B]:GLN:OE1	2.14	0.48
1:J:1414:THR:HG23	1:J:1477:LEU:HD13	1.95	0.48
1:J:1427:HIS:HE1	1:J:1458:HIS:CD2	2.32	0.48
3:L:3089[A]:HIS:CE1	3:L:3093[A]:HIS:CE1	3.01	0.48
3:L:3196[A]:THR:OG1	3:L:3199[A]:GLN:HG3	2.12	0.48
3:L:3228[B]:VAL:CG2	3:L:3245[B]:PHE:CE1	2.97	0.48
3:L:3232[B]:VAL:HG23	3:L:3273[B]:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3298[B]:ASN:CA	3:L:3299[B]:LEU:C	2.85	0.48
1:M:841:LYS:HA	1:M:1117:ASP:HB2	1.95	0.48
3:O:2939[A]:ARG:HG3	3:O:2939[A]:ARG:NH1	2.28	0.48
3:O:2969[B]:TYR:HD1	3:X:3158[B]:PHE:HD1	1.44	0.48
3:O:3101[B]:PRO:O	3:X:2971[B]:ASP:CA	2.59	0.48
3:O:3163[B]:ASN:HB2	3:X:3149[B]:ASN:HB3	1.91	0.48
3:O:3298[B]:ASN:CB	3:O:3299[B]:LEU:C	2.86	0.48
1:P:61:GLY:HA3	1:P:352:TRP:CG	2.47	0.48
1:P:112:ASP:N	1:P:112:ASP:OD1	2.42	0.48
1:P:945:ALA:C	1:P:957:ASN:HD22	2.21	0.48
2:Q:2509:ILE:HD11	2:Q:2605:LEU:HD23	1.94	0.48
3:R:2949[A]:LYS:C	3:R:2949[A]:LYS:CD	2.85	0.48
3:R:3143[B]:SER:OG	3:R:3144[B]:ALA:N	2.47	0.48
3:R:3196[B]:THR:CA	3:R:3199[B]:GLN:HB2	2.43	0.48
1:S:633:HIS:C	1:S:633:HIS:HD1	2.20	0.48
1:S:717:GLN:O	1:S:721:GLU:HG2	2.14	0.48
2:T:2502:LEU:HD12	2:T:2505:ILE:HD11	1.96	0.48
2:T:2825:ILE:HG13	2:T:2877:ILE:HG12	1.94	0.48
3:U:2954[A]:TYR:CA	3:U:2957[A]:ILE:HG22	2.43	0.48
3:U:3014[A]:TRP:HH2	3:U:3123[A]:THR:HG23	1.78	0.48
3:U:3027[A]:GLU:CD	3:U:3028[A]:PRO:CD	2.86	0.48
3:U:3169[B]:LYS:C	3:d:3148[B]:ILE:CG2	2.78	0.48
3:U:3183[A]:LEU:H	3:U:3184[A]:ASN:CA	2.22	0.48
3:U:3196[B]:THR:HG23	3:U:3199[B]:GLN:OE1	2.14	0.48
3:U:3254[B]:MET:CE	3:d:3254[B]:MET:HE2	2.26	0.48
1:V:468:CYS:SG	1:V:669:LYS:HB3	2.53	0.48
1:V:597:VAL:HG11	1:V:775:ARG:HB2	1.95	0.48
1:V:1143:ALA:HA	1:V:1195:ASP:HA	1.96	0.48
2:W:2671:ASP:O	2:W:2675:GLN:HG2	2.14	0.48
3:X:3004[A]:GLY:O	3:X:3006[A]:LYS:N	2.44	0.48
3:X:3066[A]:TYR:CE1	3:X:3193[A]:HIS:CE1	2.98	0.48
3:X:3275[A]:LEU:N	3:X:3275[A]:LEU:CD1	2.73	0.48
1:Y:566:ARG:HH12	1:Y:745:ASP:CG	2.21	0.48
1:Y:668:MET:N	1:Y:687:SER:O	2.27	0.48
1:Y:1074:ILE:HA	1:Y:1077:LEU:HB2	1.96	0.48
3:a:2933[A]:SER:HA	3:a:2935[A]:ILE:HD11	1.95	0.48
3:a:3104[A]:MET:HA	3:a:3110[A]:THR:CG2	2.17	0.48
1:b:1053:TRP:O	1:b:1057:GLN:HG3	2.13	0.48
1:b:1494:ARG:HG3	1:b:1494:ARG:NH1	2.28	0.48
2:c:2212:GLY:HA3	2:c:2290:TYR:O	2.13	0.48
3:d:2960[A]:PHE:CD1	3:d:2960[A]:PHE:N	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3200[B]:LEU:HD22	3:d:3204[B]:LEU:HD11	1.95	0.48
3:C:2939[A]:ARG:HG3	3:C:2939[A]:ARG:NH1	2.28	0.48
3:C:2952[B]:ALA:CA	3:C:2956[B]:LYS:HB3	2.38	0.48
3:C:2965[B]:LEU:HB3	3:L:3256[B]:TRP:CH2	2.39	0.48
3:C:2982[B]:MET:HG3	3:L:3156[B]:MET:HG3	1.84	0.48
3:C:3149[B]:ASN:CB	3:L:3169[B]:LYS:H	2.22	0.48
3:C:3155[B]:MET:H	3:L:3153[B]:LYS:CA	2.25	0.48
3:C:3170[B]:ALA:CA	3:L:3148[B]:ILE:HG22	2.44	0.48
3:C:3180[B]:TYR:CB	3:C:3183[B]:LEU:CD2	2.90	0.48
3:C:3298[A]:ASN:CB	3:C:3300[A]:LEU:CD2	2.61	0.48
1:D:447:MET:HA	1:D:455:TYR:HB3	1.96	0.48
1:D:806:ASN:OD1	1:D:808:THR:OG1	2.28	0.48
3:F:2954[A]:TYR:C	3:F:2957[A]:ILE:HG22	2.37	0.48
3:F:2969[B]:TYR:HA	3:a:2989[B]:HIS:NE2	2.29	0.48
3:F:2982[B]:MET:HG3	3:a:3156[B]:MET:CB	2.41	0.48
3:F:3293[B]:LYS:CD	3:F:3294[B]:SER:N	2.64	0.48
3:I:2939[B]:ARG:HG3	3:I:2939[B]:ARG:NH1	2.28	0.48
3:I:3093[B]:HIS:HB2	3:I:3248[B]:LEU:HD13	1.94	0.48
3:I:3155[B]:MET:HA	3:R:3155[B]:MET:HE3	1.94	0.48
3:I:3173[A]:THR:HG22	3:I:3174[A]:GLY:H	1.67	0.48
3:I:3196[A]:THR:CA	3:I:3199[A]:GLN:HB2	2.43	0.48
1:J:92:TRP:CE3	1:J:102:PRO:HD3	2.49	0.48
1:J:497:GLN:NE2	1:J:683:THR:OG1	2.46	0.48
1:J:885:SER:HB2	1:J:886:PRO:HA	1.96	0.48
3:L:3024[A]:LEU:CD1	3:L:3024[A]:LEU:C	2.85	0.48
3:L:3196[A]:THR:HG23	3:L:3199[A]:GLN:OE1	2.14	0.48
1:M:473:ALA:O	1:M:476:ARG:NH1	2.45	0.48
1:M:904:HIS:HB3	1:M:1105:VAL:HG21	1.96	0.48
1:M:1520:GLN:HE21	1:M:1526:LYS:HG3	1.78	0.48
3:O:3089[B]:HIS:CE1	3:O:3093[B]:HIS:CE1	3.01	0.48
3:O:3217[B]:PHE:CB	3:O:3219[B]:LEU:HD21	2.42	0.48
1:P:120:LYS:H	1:P:121:ASN:HA	1.78	0.48
2:Q:2310:GLU:HG3	2:Q:2371:LEU:HD13	1.94	0.48
2:Q:2628:HIS:HB2	2:Q:2635:TYR:CE2	2.49	0.48
3:R:2933[B]:SER:HA	3:R:2935[B]:ILE:HD11	1.95	0.48
3:R:2991[A]:LEU:HD23	3:R:3158[A]:PHE:CE1	2.48	0.48
3:R:3004[A]:GLY:O	3:R:3006[A]:LYS:N	2.44	0.48
3:R:3093[B]:HIS:HB2	3:R:3248[B]:LEU:HD13	1.94	0.48
3:R:3232[A]:VAL:HG23	3:R:3273[A]:LEU:HD11	1.95	0.48
3:R:3298[A]:ASN:CB	3:R:3299[A]:LEU:C	2.86	0.48
1:S:691:ASP:O	1:S:698:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1002:GLU:HG3	1:S:1065:LYS:HD2	1.93	0.48
1:S:1163:ALA:O	1:S:1167:ASP:HB3	2.13	0.48
2:T:2156:ARG:HD2	2:T:2357:VAL:HG12	1.95	0.48
3:U:2965[B]:LEU:HD23	3:d:3220[B]:ARG:NH1	2.29	0.48
3:U:3171[B]:HIS:CA	3:d:3152[B]:LYS:HZ1	2.27	0.48
3:U:3191[A]:ASN:C	3:U:3192[A]:PHE:O	2.52	0.48
3:U:3232[B]:VAL:HG23	3:U:3273[B]:LEU:HD11	1.94	0.48
1:V:1356:PRO:HD2	1:V:1359:ILE:HD11	1.94	0.48
3:X:2949[A]:LYS:C	3:X:2949[A]:LYS:CD	2.85	0.48
3:X:3120[A]:HIS:CE1	9:X:3401[A]:CUO:O1	2.66	0.48
3:X:3196[A]:THR:OG1	3:X:3199[A]:GLN:CD	2.57	0.48
3:X:3283[B]:ILE:C	3:X:3283[B]:ILE:CD1	2.85	0.48
1:Y:306:PHE:HB3	1:Y:308:LEU:HD13	1.96	0.48
2:Z:2116:SER:HA	2:Z:2121:THR:HG21	1.94	0.48
3:a:3191[A]:ASN:ND2	3:a:3191[A]:ASN:N	2.60	0.48
2:c:2471:HIS:ND1	2:c:2471:HIS:O	2.46	0.48
3:d:2933[B]:SER:HA	3:d:2935[B]:ILE:HD11	1.96	0.48
3:d:2952[B]:ALA:HB3	3:d:2954[B]:TYR:N	2.17	0.48
3:d:3196[A]:THR:OG1	3:d:3199[A]:GLN:CD	2.57	0.48
3:d:3196[A]:THR:CA	3:d:3199[A]:GLN:HB2	2.43	0.48
3:d:3283[B]:ILE:C	3:d:3283[B]:ILE:CD1	2.85	0.48
3:d:3291[B]:ASP:OD2	3:d:3293[B]:LYS:NZ	2.43	0.48
1:A:201:SER:HA	1:A:206:PHE:CD2	2.49	0.48
1:A:240:PHE:HA	1:A:263:ALA:HB3	1.94	0.48
2:B:2263:PHE:HE1	2:B:2304:LEU:HB3	1.79	0.48
2:B:2412:GLN:HG2	2:B:2422:GLU:HA	1.94	0.48
3:C:2968[B]:GLN:HA	3:C:2973[B]:THR:O	2.14	0.48
3:C:3217[A]:PHE:HD2	3:C:3300[A]:LEU:HD12	1.79	0.48
3:C:3220[A]:ARG:HH11	3:C:3220[A]:ARG:CG	2.12	0.48
1:D:1149:GLU:HG3	1:D:1187:LYS:HB3	1.95	0.48
2:E:2868:GLU:CG	3:F:2932[A]:PRO:C	2.71	0.48
3:F:2939[A]:ARG:HG3	3:F:2939[A]:ARG:NH1	2.28	0.48
3:F:2982[B]:MET:HA	3:a:3160[B]:SER:OG	2.12	0.48
3:F:2994[B]:LYS:HE2	3:F:3183[B]:LEU:O	2.14	0.48
3:F:3196[A]:THR:OG1	3:F:3199[A]:GLN:HG3	2.12	0.48
3:F:3284[B]:LYS:CD	3:F:3284[B]:LYS:C	2.86	0.48
1:G:430:SER:O	1:G:933:ARG:NH2	2.46	0.48
3:I:2954[B]:TYR:CA	3:I:2957[B]:ILE:HG22	2.43	0.48
3:I:2982[B]:MET:HB2	3:R:3156[B]:MET:HB3	1.94	0.48
3:I:3153[B]:LYS:HE3	3:R:3158[B]:PHE:N	1.92	0.48
3:I:3160[B]:SER:OG	3:R:2983[B]:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3251[B]:ASP:HB2	3:R:3251[B]:ASP:CG	2.38	0.48
9:I:3401[A]:CUO:O1	3:R:3120[A]:HIS:CE1	2.66	0.48
1:J:903:PRO:HG2	1:J:904:HIS:CD2	2.49	0.48
1:J:991:LEU:O	1:J:995:ILE:HG13	2.14	0.48
2:K:2457:LYS:O	2:K:2460:SER:OG	2.30	0.48
3:L:2939[A]:ARG:NE	3:L:3031[A]:ASN:ND2	2.60	0.48
3:L:2952[B]:ALA:HB3	3:L:2954[B]:TYR:N	2.17	0.48
3:L:2994[B]:LYS:HE2	3:L:3183[B]:LEU:O	2.14	0.48
3:L:3217[A]:PHE:HD2	3:L:3300[A]:LEU:HD12	1.78	0.48
1:M:897:HIS:HB3	1:M:899:MET:HE1	1.95	0.48
1:M:1361:GLU:HG3	1:M:1363:THR:H	1.78	0.48
2:N:2128:LEU:HD13	2:N:2286:HIS:HB3	1.96	0.48
3:O:3004[A]:GLY:O	3:O:3006[A]:LYS:N	2.44	0.48
3:O:3038[B]:ILE:HG23	3:X:2969[B]:TYR:HE1	1.71	0.48
3:O:3093[B]:HIS:HB2	3:O:3248[B]:LEU:HD13	1.94	0.48
3:O:3196[A]:THR:OG1	3:O:3199[A]:GLN:CD	2.57	0.48
3:O:3298[B]:ASN:CA	3:O:3299[B]:LEU:C	2.86	0.48
1:P:164:GLU:OE1	1:P:296:ARG:NH1	2.46	0.48
1:P:361:GLU:HG2	1:P:363:THR:HG22	1.94	0.48
1:P:954:ALA:O	1:P:956:PRO:HD3	2.13	0.48
3:R:3200[A]:LEU:HD22	3:R:3204[A]:LEU:HD11	1.95	0.48
3:R:3217[A]:PHE:HD2	3:R:3300[A]:LEU:HD12	1.79	0.48
3:U:3143[B]:SER:OG	3:U:3144[B]:ALA:N	2.47	0.48
1:V:450:LYS:HD2	1:V:450:LYS:HA	1.40	0.48
1:V:757:VAL:HG21	1:V:781:ILE:HG22	1.94	0.48
1:V:858:MET:HG3	1:V:959:PHE:CZ	2.48	0.48
3:X:3110[A]:THR:C	3:X:3112[A]:TYR:N	2.68	0.48
1:Y:133:LYS:HE3	1:Y:134:VAL:HG23	1.95	0.48
1:Y:547:LYS:HD2	1:Y:558:HIS:HD2	1.78	0.48
1:Y:854:LEU:HD23	1:Y:941:LEU:HD21	1.96	0.48
1:Y:862:ALA:HA	1:Y:870:TYR:HB3	1.95	0.48
2:Z:2189:GLY:HA2	2:Z:2192:THR:HG22	1.94	0.48
3:a:3093[B]:HIS:HB2	3:a:3248[B]:LEU:HD13	1.94	0.48
3:a:3151[B]:LEU:HB2	3:a:3175[B]:TYR:HE2	1.67	0.48
1:b:483:GLY:HA2	1:b:773:PHE:CE1	2.48	0.48
2:c:2265:ILE:HD12	2:c:2443:TYR:CD1	2.49	0.48
3:d:3093[B]:HIS:HB2	3:d:3248[B]:LEU:HD13	1.94	0.48
3:d:3183[A]:LEU:H	3:d:3184[A]:ASN:CA	2.22	0.48
3:d:3191[A]:ASN:C	3:d:3192[A]:PHE:O	2.52	0.48
4:7:1:NAG:H61	4:7:2:NAG:C1	2.43	0.48
4:OA:1:NAG:O4	4:OA:2:NAG:O7	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:LYS:HD3	1:A:554:LYS:HA	1.72	0.48
2:B:2500:ILE:HD11	2:B:2775:GLY:O	2.13	0.48
3:C:3110[B]:THR:C	3:C:3112[B]:TYR:H	2.20	0.48
3:C:3120[A]:HIS:CE1	9:L:3401[A]:CUO:O1	2.66	0.48
3:C:3176[A]:LYS:N	3:C:3176[A]:LYS:CE	2.73	0.48
3:C:3191[B]:ASN:C	3:C:3192[B]:PHE:O	2.52	0.48
3:C:3200[A]:LEU:HD22	3:C:3204[A]:LEU:HD11	1.95	0.48
3:C:3298[A]:ASN:CA	3:C:3299[A]:LEU:C	2.85	0.48
1:D:69:HIS:NE2	9:D:5001:CUO:O1	2.47	0.48
2:E:2086:ASN:OD1	2:E:2086:ASN:N	2.44	0.48
3:F:2975[B]:PHE:CA	3:a:3107[B]:LEU:CD1	2.92	0.48
3:F:3013[B]:ASP:CG	3:F:3015[B]:THR:HG1	2.21	0.48
3:F:3148[B]:ILE:HG22	3:F:3152[B]:LYS:CE	2.44	0.48
3:F:3183[B]:LEU:H	3:F:3184[B]:ASN:CA	2.21	0.48
3:F:3229[A]:ASN:OD1	3:F:3244[A]:THR:HB	2.14	0.48
1:G:1392:ASP:OD2	1:G:1437:ARG:NE	2.46	0.48
2:H:2097:LEU:HD12	2:K:2235:PRO:HG2	1.96	0.48
2:H:2130:PRO:HG2	2:H:2140:ARG:HB2	1.94	0.48
2:H:2515:ARG:HD2	2:K:2168:ARG:NH2	2.29	0.48
3:I:3093[A]:HIS:HB2	3:I:3248[A]:LEU:HD13	1.94	0.48
3:I:3153[B]:LYS:NZ	3:R:3157[B]:PRO:N	2.62	0.48
3:I:3159[B]:SER:O	3:R:3150[B]:LYS:CB	2.55	0.48
3:I:3196[B]:THR:OG1	3:I:3199[B]:GLN:CD	2.57	0.48
3:I:3217[A]:PHE:HD2	3:I:3300[A]:LEU:HD12	1.78	0.48
3:I:3221[B]:ALA:HB3	3:R:2964[B]:PRO:HB2	1.81	0.48
3:I:3285[B]:VAL:CG2	3:I:3286[B]:THR:H	2.27	0.48
1:J:447:MET:HA	1:J:455:TYR:CB	2.43	0.48
3:L:2933[A]:SER:HA	3:L:2935[A]:ILE:HD11	1.95	0.48
3:L:3027[B]:GLU:CD	3:L:3028[B]:PRO:CD	2.86	0.48
3:L:3093[A]:HIS:HB2	3:L:3248[A]:LEU:HD13	1.94	0.48
3:L:3217[B]:PHE:HD2	3:L:3300[B]:LEU:HD12	1.79	0.48
1:M:494:VAL:HG13	1:M:631:TRP:HZ3	1.79	0.48
2:N:2440:ASP:OD2	2:N:2441:ARG:NH1	2.47	0.48
2:N:2819:VAL:HB	2:N:2835:ILE:HB	1.96	0.48
3:O:2937[A]:ASN:CB	3:O:3006[A]:LYS:CE	2.86	0.48
3:O:2981[B]:GLY:N	3:O:3086[B]:GLU:OE1	2.45	0.48
3:O:2994[A]:LYS:HE2	3:O:3183[A]:LEU:O	2.14	0.48
3:O:3027[B]:GLU:CD	3:O:3028[B]:PRO:CD	2.86	0.48
3:O:3161[B]:GLU:HG2	3:X:3146[B]:CYS:SG	2.54	0.48
3:O:3196[A]:THR:HG23	3:O:3199[A]:GLN:OE1	2.14	0.48
3:O:3196[B]:THR:CA	3:O:3199[B]:GLN:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:43:GLU:HG3	1:P:44:PRO:HA	1.94	0.48
3:R:3066[B]:TYR:CE1	3:R:3193[B]:HIS:CE1	2.98	0.48
3:R:3228[B]:VAL:CG2	3:R:3245[B]:PHE:CE1	2.97	0.48
3:R:3229[A]:ASN:OD1	3:R:3244[A]:THR:HB	2.14	0.48
1:S:236:GLY:HA2	1:S:819:ILE:HB	1.96	0.48
1:S:980:TYR:OH	1:S:1021:LEU:HD22	2.14	0.48
1:S:1346:TRP:O	1:S:1460:ASN:ND2	2.47	0.48
3:U:2937[A]:ASN:CB	3:U:3006[A]:LYS:CE	2.86	0.48
3:U:2971[B]:ASP:HA	3:d:3090[B]:ASN:CG	2.31	0.48
3:U:2994[B]:LYS:HE2	3:U:3183[B]:LEU:O	2.14	0.48
1:V:597:VAL:HG12	1:V:773:PHE:CD1	2.49	0.48
1:V:1005:CYS:O	1:V:1009:VAL:HG23	2.14	0.48
3:X:2933[A]:SER:HA	3:X:2935[A]:ILE:HD11	1.95	0.48
1:Y:527:LEU:HD22	1:Y:629:MET:HG3	1.96	0.48
2:Z:2546:LEU:H	2:Z:2557:ALA:HA	1.79	0.48
3:a:3089[A]:HIS:CE1	3:a:3093[A]:HIS:CE1	3.01	0.48
3:a:3183[B]:LEU:H	3:a:3184[B]:ASN:CA	2.22	0.48
3:a:3196[A]:THR:OG1	3:a:3199[A]:GLN:CD	2.57	0.48
3:a:3276[A]:ASP:O	3:a:3277[A]:ALA:HB3	2.12	0.48
1:b:137:ARG:NH1	1:b:203:ASP:OD1	2.47	0.48
1:b:957:ASN:HB3	1:b:960:PHE:H	1.77	0.48
2:c:2107:LEU:O	2:c:2111:GLN:HB2	2.13	0.48
3:d:2939[A]:ARG:NE	3:d:3031[A]:ASN:ND2	2.60	0.48
3:d:3120[A]:HIS:CE1	9:d:3401[A]:CUO:O1	2.66	0.48
1:A:572:SER:HA	1:A:573:LYS:HA	1.47	0.48
1:A:835:GLU:C	1:A:836:GLN:HE21	2.21	0.48
2:B:2157:LEU:O	2:B:2160:VAL:HG22	2.14	0.48
3:C:3196[A]:THR:CA	3:C:3199[A]:GLN:HB2	2.43	0.48
3:C:3196[B]:THR:HG23	3:C:3199[B]:GLN:OE1	2.14	0.48
1:D:47:CYS:N	1:D:57:CYS:SG	2.87	0.48
1:D:203:ASP:O	1:D:206:PHE:HB3	2.14	0.48
1:D:480:CYS:HA	1:D:490:TRP:CE2	2.49	0.48
1:D:1013:ILE:HG21	1:D:1192:TYR:CD1	2.48	0.48
1:D:1584:GLY:HA3	1:G:329:ARG:HB2	1.96	0.48
3:F:2952[B]:ALA:HB1	3:F:2957[B]:ILE:H	1.79	0.48
3:F:3196[A]:THR:OG1	3:F:3199[A]:GLN:CD	2.57	0.48
3:F:3220[B]:ARG:HH11	3:F:3220[B]:ARG:CG	2.12	0.48
1:G:387:ASN:ND2	4:o:1:NAG:C6	2.77	0.48
2:H:2807:GLY:O	2:H:2899:PRO:HA	2.14	0.48
3:I:2988[B]:TRP:CZ2	3:R:2975[B]:PHE:HE2	2.31	0.48
3:I:3148[A]:ILE:HG22	3:I:3152[A]:LYS:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3183[B]:LEU:H	3:I:3184[B]:ASN:CA	2.22	0.48
3:I:3196[A]:THR:OG1	3:I:3199[A]:GLN:CD	2.57	0.48
3:I:3196[B]:THR:OG1	3:I:3199[B]:GLN:HG3	2.12	0.48
3:I:3217[B]:PHE:HD2	3:I:3300[B]:LEU:HD12	1.78	0.48
2:K:2265:ILE:HD12	2:K:2443:TYR:CD1	2.49	0.48
3:L:2935[A]:ILE:CD1	3:L:2935[A]:ILE:H	2.25	0.48
3:L:3089[B]:HIS:CE1	3:L:3093[B]:HIS:CE1	3.01	0.48
3:L:3228[A]:VAL:CG2	3:L:3245[A]:PHE:CE1	2.97	0.48
3:O:2954[A]:TYR:CA	3:O:2957[A]:ILE:HG22	2.43	0.48
3:O:2976[B]:ALA:CB	3:X:3156[B]:MET:CG	2.91	0.48
3:O:3200[A]:LEU:HD22	3:O:3204[A]:LEU:HD11	1.95	0.48
3:O:3228[A]:VAL:CG2	3:O:3245[A]:PHE:CE1	2.97	0.48
1:P:695:TYR:OH	1:P:703:TYR:HD2	1.97	0.48
1:P:855:ARG:HH21	1:P:941:LEU:HA	1.79	0.48
2:Q:2184:MET:HE3	2:Q:2231:LEU:HD11	1.96	0.48
2:Q:2668:ASP:OD1	2:Q:2669:TYR:N	2.47	0.48
2:Q:2825:ILE:HG23	2:Q:2826:GLU:N	2.28	0.48
2:Q:2856:ILE:HG22	2:Q:2859:VAL:HB	1.95	0.48
1:S:873:VAL:HA	1:S:876:PHE:CE2	2.48	0.48
1:S:1239:GLY:O	1:S:1242:ASN:ND2	2.46	0.48
1:S:1491:GLN:OE1	1:S:1491:GLN:N	2.46	0.48
2:T:2682:SER:HA	2:T:2836:PHE:CD1	2.48	0.48
2:T:2824:CYS:O	2:T:2877:ILE:HA	2.13	0.48
3:U:2952[B]:ALA:HB1	3:U:2957[B]:ILE:H	1.79	0.48
3:U:2961[A]:HIS:CD2	3:U:2988[A]:TRP:CZ3	2.97	0.48
3:U:2973[B]:THR:HG21	3:d:3222[B]:ILE:O	2.14	0.48
3:U:3143[A]:SER:OG	3:U:3144[A]:ALA:N	2.47	0.48
3:U:3151[B]:LEU:CB	3:U:3175[B]:TYR:CD2	2.93	0.48
3:U:3229[A]:ASN:OD1	3:U:3244[A]:THR:HB	2.14	0.48
1:V:951:ASN:N	1:V:951:ASN:OD1	2.46	0.48
3:X:2952[B]:ALA:N	3:X:2953[B]:GLY:CA	2.71	0.48
3:X:2994[A]:LYS:HE2	3:X:3183[A]:LEU:O	2.14	0.48
3:X:3027[A]:GLU:CD	3:X:3028[A]:PRO:CD	2.86	0.48
3:X:3089[A]:HIS:CE1	3:X:3093[A]:HIS:CE1	3.01	0.48
3:X:3114[B]:PRO:CD	3:X:3115[B]:LEU:N	2.72	0.48
3:X:3196[A]:THR:OG1	3:X:3199[A]:GLN:HG3	2.12	0.48
1:Y:972:SER:HA	1:Y:1028:VAL:HG22	1.96	0.48
2:Z:2134:ASN:HD22	2:Z:2134:ASN:C	2.22	0.48
3:a:2939[A]:ARG:HG3	3:a:2939[A]:ARG:NH1	2.28	0.48
3:a:3196[B]:THR:OG1	3:a:3199[B]:GLN:CD	2.57	0.48
1:b:843:VAL:HG13	1:b:927:PRO:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:1636:ASN:HB3	1:b:1638:SER:H	1.79	0.48
2:c:2658:LYS:NZ	2:c:2858:ASP:OD2	2.30	0.48
3:d:3093[A]:HIS:HB2	3:d:3248[A]:LEU:HD13	1.94	0.48
3:d:3110[A]:THR:C	3:d:3112[A]:TYR:H	2.20	0.48
3:d:3120[B]:HIS:CE1	9:d:3401[B]:CUO:O1	2.66	0.48
3:d:3143[A]:SER:OG	3:d:3144[A]:ALA:N	2.47	0.48
1:A:646:ALA:HB1	1:A:713:ILE:HD12	1.95	0.48
1:A:893:ALA:HB2	1:A:1182:ASN:HB2	1.96	0.48
1:A:899:MET:HE2	1:A:1186:TRP:CD2	2.49	0.48
1:A:1145:THR:HB	1:A:1191:PRO:HB2	1.96	0.48
2:B:2826:GLU:OE1	2:B:2876:LYS:NZ	2.44	0.48
3:C:2976[B]:ALA:HB2	3:L:3253[B]:GLU:HG3	1.96	0.48
3:C:2985[B]:PHE:CZ	3:L:2969[B]:TYR:O	2.66	0.48
1:D:258:LYS:O	1:D:261:SER:OG	2.32	0.48
1:D:630:PHE:O	1:D:633:HIS:HB3	2.14	0.48
1:D:1058:ALA:HB1	1:D:1126:ILE:HD12	1.95	0.48
1:D:1171:LYS:HG2	1:D:1173:GLY:H	1.79	0.48
1:D:1630:MET:HE2	1:D:1648:PRO:HD3	1.96	0.48
2:E:2225:ARG:NH1	2:E:2291:ASP:OD1	2.47	0.48
2:E:2575:LEU:HD23	2:E:2575:LEU:HA	1.73	0.48
3:F:2952[A]:ALA:N	3:F:2953[A]:GLY:HA2	2.06	0.48
3:F:3217[A]:PHE:HD2	3:F:3300[A]:LEU:HD12	1.78	0.48
3:F:3252[B]:TYR:O	3:a:3253[B]:GLU:N	2.46	0.48
3:F:3298[A]:ASN:CA	3:F:3299[A]:LEU:C	2.85	0.48
1:G:278:ASP:O	1:G:279:LEU:HG	2.13	0.48
1:G:1574:VAL:HG22	1:G:1620:LEU:HD21	1.95	0.48
3:I:2954[A]:TYR:CA	3:I:2957[A]:ILE:HG22	2.43	0.48
3:I:3004[A]:GLY:O	3:I:3006[A]:LYS:N	2.44	0.48
3:I:3108[B]:HIS:CE1	3:R:3251[B]:ASP:CB	2.97	0.48
3:I:3151[A]:LEU:CB	3:I:3175[A]:TYR:CD2	2.93	0.48
3:I:3196[A]:THR:HG23	3:I:3199[A]:GLN:OE1	2.14	0.48
3:I:3211[B]:ASP:OD1	3:I:3211[B]:ASP:N	2.27	0.48
1:J:331:SER:HA	1:M:1581:GLU:HG3	1.94	0.48
1:J:753:ASN:OD1	1:J:753:ASN:N	2.46	0.48
1:J:1400:ASN:HD22	1:J:1403:LEU:HG	1.79	0.48
3:L:2937[A]:ASN:CB	3:L:3006[A]:LYS:CE	2.85	0.48
3:L:2952[B]:ALA:HB1	3:L:2957[B]:ILE:H	1.79	0.48
3:L:3104[A]:MET:HA	3:L:3110[A]:THR:CG2	2.17	0.48
3:L:3141[B]:TYR:CD2	3:L:3141[B]:TYR:C	2.86	0.48
3:L:3148[A]:ILE:HG22	3:L:3152[A]:LYS:CE	2.44	0.48
3:L:3196[A]:THR:OG1	3:L:3199[A]:GLN:CD	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3225[A]:SER:C	3:L:3290[A]:ILE:HG23	2.39	0.48
1:M:151:GLN:N	1:M:151:GLN:OE1	2.47	0.48
1:M:588:GLU:OE2	1:M:728:ARG:NH2	2.36	0.48
1:M:1348:TRP:CH2	1:M:1461:VAL:HG23	2.49	0.48
3:O:2968[B]:GLN:C	3:X:2988[B]:TRP:CB	2.87	0.48
3:O:3014[B]:TRP:HH2	3:O:3123[B]:THR:HG23	1.78	0.48
3:O:3196[B]:THR:OG1	3:O:3199[B]:GLN:CD	2.57	0.48
3:O:3225[B]:SER:C	3:O:3290[B]:ILE:HG23	2.39	0.48
3:R:2970[A]:PRO:C	3:R:2972[A]:GLY:N	2.72	0.48
3:R:3196[A]:THR:OG1	3:R:3199[A]:GLN:CD	2.57	0.48
3:R:3284[A]:LYS:CE	3:R:3284[A]:LYS:CA	2.85	0.48
1:S:906:HIS:CD2	9:S:2104:CUO:O1	2.67	0.48
1:S:1421:VAL:HG23	1:S:1422:HIS:HD1	1.78	0.48
1:S:1596:GLU:O	1:S:1597:THR:HG22	2.14	0.48
1:S:1604:ASP:OD1	1:S:1605:ARG:NH1	2.47	0.48
2:T:2168:ARG:NH2	2:W:2515:ARG:HD2	2.28	0.48
3:U:2933[A]:SER:HA	3:U:2935[A]:ILE:HD11	1.96	0.48
3:U:2968[A]:GLN:HA	3:U:2973[A]:THR:O	2.14	0.48
3:U:2994[A]:LYS:HE2	3:U:3183[A]:LEU:O	2.14	0.48
3:U:3151[A]:LEU:CB	3:U:3175[A]:TYR:CD2	2.93	0.48
3:U:3196[A]:THR:HG23	3:U:3199[A]:GLN:OE1	2.14	0.48
2:W:2336:PHE:HB3	2:W:2348:THR:HG22	1.95	0.48
2:W:2343:ASN:HD22	2:W:2349:THR:HG23	1.77	0.48
2:W:2802:ASP:OD2	3:X:2932[A]:PRO:CD	2.62	0.48
3:X:3217[B]:PHE:HD2	3:X:3300[B]:LEU:HD12	1.78	0.48
1:Y:1471:LEU:HD12	1:Y:1537:ILE:HD13	1.95	0.48
1:Y:1565:SER:HB3	1:Y:1594:GLY:H	1.79	0.48
2:Z:2746:MET:O	2:Z:2750:ILE:HG13	2.14	0.48
3:a:2968[A]:GLN:HA	3:a:2973[A]:THR:O	2.14	0.48
3:a:3143[B]:SER:OG	3:a:3144[B]:ALA:N	2.46	0.48
3:a:3147[A]:GLU:CG	3:a:3149[A]:ASN:ND2	2.73	0.48
3:a:3298[A]:ASN:CA	3:a:3299[A]:LEU:C	2.86	0.48
2:c:2547:MET:O	2:c:2751:TRP:HH2	1.96	0.48
3:d:3089[A]:HIS:CE1	3:d:3093[A]:HIS:CE1	3.01	0.48
4:q:2:NAG:H83	4:q:2:NAG:O3	2.14	0.48
1:A:177:VAL:HA	1:A:180:ASN:OD1	2.14	0.48
1:A:641:TRP:C	1:A:641:TRP:CD1	2.91	0.48
1:A:944:GLU:O	1:A:957:ASN:ND2	2.47	0.48
1:A:954:ALA:O	1:A:956:PRO:HD3	2.13	0.48
2:B:2370:MET:HE3	2:B:2370:MET:HB2	1.73	0.48
2:B:2650:GLY:N	2:B:2651:GLN:HA	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2952[B]:ALA:N	3:C:2953[B]:GLY:HA2	2.06	0.48
3:C:2970[B]:PRO:C	3:C:2972[B]:GLY:N	2.72	0.48
3:C:3093[A]:HIS:HB2	3:C:3248[A]:LEU:HD13	1.94	0.48
3:C:3104[B]:MET:HA	3:C:3110[B]:THR:CG2	2.17	0.48
3:C:3172[B]:SER:CB	3:L:3152[B]:LYS:HB2	2.42	0.48
3:C:3196[A]:THR:HG23	3:C:3199[A]:GLN:OE1	2.14	0.48
3:C:3285[B]:VAL:CG2	3:C:3286[B]:THR:H	2.27	0.48
1:D:456:GLN:HG2	1:D:551:GLU:HB3	1.96	0.48
1:D:928:TYR:HB2	1:D:1048:ASN:HB2	1.95	0.48
1:D:1257:SER:O	1:D:1525:TYR:HA	2.13	0.48
1:D:1396:GLU:O	1:D:1400:ASN:ND2	2.47	0.48
2:E:2158:TYR:O	2:E:2161:GLN:HB3	2.14	0.48
2:E:2652:LYS:HE2	2:E:2657:PHE:CZ	2.49	0.48
2:E:2800:LYS:HB3	3:F:3023[A]:ILE:HD13	1.95	0.48
3:F:2983[B]:VAL:CG2	3:a:3162[B]:ASP:OD1	2.62	0.48
3:F:3125[B]:ARG:O	3:F:3129[B]:ILE:HG13	2.14	0.48
3:F:3196[A]:THR:HG23	3:F:3199[A]:GLN:OE1	2.14	0.48
3:F:3196[B]:THR:CA	3:F:3199[B]:GLN:HB2	2.43	0.48
3:F:3217[B]:PHE:HD2	3:F:3300[B]:LEU:HD12	1.78	0.48
3:F:3275[B]:LEU:N	3:F:3275[B]:LEU:CD1	2.73	0.48
1:G:346:GLY:O	1:G:349:GLU:HB3	2.14	0.48
2:H:2414:CYS:SG	2:H:2465:LYS:HD2	2.54	0.48
2:H:2622:ASN:O	2:H:2625:LEU:HD12	2.14	0.48
2:H:2695:MET:CE	2:H:2707:PHE:HB2	2.43	0.48
2:H:2866:PRO:HB2	2:H:2868:GLU:HG3	1.96	0.48
1:J:415:VAL:HG21	1:J:697:ALA:HB2	1.94	0.48
2:K:2322:SER:HB3	2:K:2329:MET:HE2	1.96	0.48
2:K:2653:GLU:H	2:K:2653:GLU:HG3	1.53	0.48
3:L:2933[B]:SER:HA	3:L:2935[B]:ILE:HD11	1.96	0.48
3:L:2952[A]:ALA:HB1	3:L:2957[A]:ILE:H	1.79	0.48
3:L:2970[A]:PRO:C	3:L:2972[A]:GLY:N	2.72	0.48
3:L:2994[A]:LYS:HE2	3:L:3183[A]:LEU:O	2.14	0.48
3:L:3135[A]:LYS:HB2	3:L:3141[A]:TYR:HD1	1.76	0.48
1:M:127:GLU:CD	1:M:134:VAL:HB	2.39	0.48
1:M:494:VAL:HG23	1:M:671:PHE:CZ	2.49	0.48
2:N:2153:GLN:HG3	2:N:2305:TRP:HH2	1.79	0.48
3:O:3066[A]:TYR:CE1	3:O:3193[A]:HIS:CE1	2.98	0.48
3:O:3232[B]:VAL:HG23	3:O:3273[B]:LEU:HD11	1.94	0.48
1:P:447:MET:HA	1:P:455:TYR:CB	2.42	0.48
1:P:904:HIS:O	1:P:907:ARG:HB3	2.14	0.48
2:Q:2504:ARG:HG2	2:Q:2582:ARG:HH21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2968[A]:GLN:HA	3:R:2973[A]:THR:O	2.14	0.48
3:R:2968[B]:GLN:HA	3:R:2973[B]:THR:O	2.14	0.48
3:R:3014[A]:TRP:HH2	3:R:3123[A]:THR:HG23	1.78	0.48
3:R:3151[A]:LEU:CB	3:R:3175[A]:TYR:CD2	2.93	0.48
3:R:3196[B]:THR:O	3:R:3200[B]:LEU:N	2.44	0.48
1:S:904:HIS:O	1:S:907:ARG:HB3	2.13	0.48
1:V:560:SER:O	1:V:617:SER:HB3	2.14	0.48
1:V:597:VAL:O	1:V:601:VAL:HG12	2.14	0.48
3:X:2994[B]:LYS:HE2	3:X:3183[B]:LEU:O	2.14	0.48
3:X:3161[A]:GLU:H	3:X:3161[A]:GLU:CD	2.18	0.48
3:X:3196[B]:THR:OG1	3:X:3199[B]:GLN:CD	2.57	0.48
3:X:3196[B]:THR:OG1	3:X:3199[B]:GLN:HG3	2.12	0.48
3:X:3288[B]:MET:CA	3:X:3295[B]:LEU:HG	2.42	0.48
1:Y:593:CYS:HB3	1:Y:775:ARG:NE	2.29	0.48
1:Y:896:HIS:HB2	1:Y:905:TRP:CG	2.48	0.48
1:Y:1055:THR:HA	1:Y:1119:LEU:HD13	1.95	0.48
1:Y:1315:GLY:HA3	1:Y:1601:TRP:HB2	1.95	0.48
2:Z:2131:LEU:HD12	2:Z:2335:PRO:HB3	1.95	0.48
2:Z:2805:PHE:CE1	2:Z:2855:ASP:HB3	2.49	0.48
3:a:2994[B]:LYS:HE2	3:a:3183[B]:LEU:O	2.14	0.48
3:a:3089[B]:HIS:CE1	3:a:3093[B]:HIS:CE1	3.01	0.48
3:a:3125[B]:ARG:O	3:a:3129[B]:ILE:HG13	2.14	0.48
1:b:126:GLY:HA2	1:b:127:GLU:HA	1.35	0.48
1:b:240:PHE:HA	1:b:263:ALA:HB3	1.96	0.48
2:c:2142:ALA:HB1	2:c:2143:CYS:HB2	1.95	0.48
2:c:2225:ARG:HD2	2:c:2274:LEU:HD22	1.95	0.48
2:c:2552:GLU:HB3	2:c:2553:ALA:HB2	1.95	0.48
2:c:2573:TYR:HE2	2:c:2707:PHE:HE2	1.61	0.48
3:d:2937[B]:ASN:CB	3:d:3006[B]:LYS:CE	2.85	0.48
3:d:2969[A]:TYR:CD2	3:d:2970[A]:PRO:HD2	2.47	0.48
3:d:2994[B]:LYS:HE2	3:d:3183[B]:LEU:O	2.14	0.48
3:d:3196[B]:THR:CA	3:d:3199[B]:GLN:HB2	2.43	0.48
3:d:3228[A]:VAL:CG2	3:d:3245[A]:PHE:CE1	2.97	0.48
1:A:611:GLY:HA3	1:A:619:SER:HB3	1.96	0.47
1:A:905:TRP:HE1	1:A:1083:PRO:HD2	1.79	0.47
1:A:1571:TYR:HE1	1:A:1631:GLU:HB3	1.78	0.47
3:C:2949[B]:LYS:C	3:C:2953[B]:GLY:N	2.72	0.47
3:C:2981[A]:GLY:N	3:C:3086[A]:GLU:OE1	2.45	0.47
3:C:3125[A]:ARG:O	3:C:3129[A]:ILE:HG13	2.14	0.47
3:C:3125[B]:ARG:O	3:C:3129[B]:ILE:HG13	2.14	0.47
3:C:3191[A]:ASN:ND2	3:C:3191[A]:ASN:N	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3217[B]:PHE:HD2	3:C:3300[B]:LEU:HD12	1.78	0.47
1:D:464:LEU:HD11	1:D:767:LYS:HD3	1.96	0.47
2:E:2783:PHE:HB3	2:E:2791:LEU:HD21	1.95	0.47
3:F:2965[B]:LEU:HB3	3:a:3256[B]:TRP:CZ2	2.48	0.47
3:F:3196[A]:THR:CA	3:F:3199[A]:GLN:HB2	2.43	0.47
3:F:3284[A]:LYS:CE	3:F:3284[A]:LYS:CA	2.85	0.47
1:G:148:GLN:HA	1:G:149:GLU:C	2.38	0.47
1:G:301:ARG:HD2	1:G:361:GLU:OE2	2.14	0.47
3:I:2968[B]:GLN:HG2	3:R:2981[B]:GLY:N	2.28	0.47
3:I:3298[B]:ASN:CA	3:I:3299[B]:LEU:C	2.86	0.47
1:J:1085:SER:HB2	1:J:1100:SER:HB2	1.96	0.47
3:L:3200[A]:LEU:HD22	3:L:3204[A]:LEU:HD11	1.95	0.47
1:M:1018:ILE:HD12	1:M:1045:HIS:CD2	2.49	0.47
1:M:1348:TRP:CZ3	1:M:1460:ASN:HB3	2.49	0.47
2:N:2603:PRO:HG2	2:N:2606:LEU:HD12	1.96	0.47
2:N:2665:GLU:HB2	2:N:2798:GLN:NE2	2.29	0.47
3:O:2975[B]:PHE:CA	3:X:3156[B]:MET:CG	2.90	0.47
3:O:2991[A]:LEU:HD23	3:O:3158[A]:PHE:CE1	2.48	0.47
3:O:3104[B]:MET:HA	3:O:3110[B]:THR:CG2	2.17	0.47
3:O:3160[B]:SER:HB3	3:X:3149[B]:ASN:N	2.28	0.47
3:O:3196[A]:THR:CA	3:O:3199[A]:GLN:OE1	2.58	0.47
3:O:3283[A]:ILE:C	3:O:3283[A]:ILE:CD1	2.85	0.47
1:P:979:LEU:HB2	1:P:980:TYR:CA	2.38	0.47
1:P:1033:LEU:HG	1:P:1180:SER:HB3	1.96	0.47
3:R:3125[B]:ARG:O	3:R:3129[B]:ILE:HG13	2.14	0.47
1:S:194:MET:HA	1:S:200:THR:HA	1.96	0.47
1:S:906:HIS:NE2	9:S:2104:CUO:O1	2.47	0.47
1:S:1228:LEU:H	1:S:1228:LEU:HD13	1.78	0.47
2:T:2361:LYS:HD2	2:T:2362:GLN:N	2.29	0.47
3:U:3093[A]:HIS:HB2	3:U:3248[A]:LEU:HD13	1.95	0.47
3:U:3191[B]:ASN:C	3:U:3192[B]:PHE:O	2.52	0.47
3:U:3196[B]:THR:OG1	3:U:3199[B]:GLN:CD	2.57	0.47
3:U:3229[B]:ASN:OD1	3:U:3244[B]:THR:HB	2.14	0.47
3:U:3230[A]:PHE:H	3:U:3243[A]:GLY:HA3	1.79	0.47
1:V:668:MET:HE2	1:V:668:MET:HA	1.95	0.47
3:X:2968[A]:GLN:HA	3:X:2973[A]:THR:O	2.14	0.47
3:X:3093[A]:HIS:HB2	3:X:3248[A]:LEU:HD13	1.95	0.47
3:X:3125[A]:ARG:O	3:X:3129[A]:ILE:HG13	2.14	0.47
3:X:3228[B]:VAL:CG2	3:X:3245[B]:PHE:CE1	2.97	0.47
3:X:3291[A]:ASP:OD2	3:X:3293[A]:LYS:NZ	2.43	0.47
3:X:3298[A]:ASN:CB	3:X:3299[A]:LEU:C	2.85	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:321:LEU:HD11	1:Y:377:TYR:CD1	2.49	0.47
1:Y:664:VAL:O	1:Y:689:PRO:HD2	2.14	0.47
1:Y:684:ARG:HH11	1:Y:684:ARG:HB3	1.78	0.47
1:Y:906:HIS:CD2	9:Y:2104:CUO:O1	2.66	0.47
1:Y:1013:ILE:HG21	1:Y:1192:TYR:CD1	2.49	0.47
1:Y:1563:LYS:HE3	6:LA:2:NAG:H3	1.96	0.47
1:Y:1617:LYS:HE2	3:d:3180[B]:TYR:CD2	2.48	0.47
2:Z:2168:ARG:NH2	2:c:2515:ARG:HD2	2.29	0.47
2:Z:2823:ILE:HG13	2:Z:2832:ALA:HB2	1.96	0.47
3:a:2952[B]:ALA:HB1	3:a:2957[B]:ILE:H	1.79	0.47
3:a:2968[B]:GLN:HA	3:a:2973[B]:THR:O	2.14	0.47
3:a:3066[B]:TYR:CE1	3:a:3193[B]:HIS:CE1	2.98	0.47
3:a:3196[A]:THR:OG1	3:a:3199[A]:GLN:HG3	2.12	0.47
3:a:3196[A]:THR:HG23	3:a:3199[A]:GLN:OE1	2.14	0.47
3:a:3196[B]:THR:HG23	3:a:3199[B]:GLN:OE1	2.14	0.47
3:a:3230[B]:PHE:H	3:a:3243[B]:GLY:HA3	1.79	0.47
1:b:1162:ALA:HB3	1:b:1212:HIS:CE1	2.49	0.47
1:b:1315:GLY:HA3	1:b:1601:TRP:CB	2.43	0.47
2:c:2411:PHE:HE1	2:c:2445:MET:HE3	1.79	0.47
3:d:3089[A]:HIS:CE1	3:d:3119[A]:HIS:CE1	2.81	0.47
3:d:3125[A]:ARG:O	3:d:3129[A]:ILE:HG13	2.14	0.47
3:d:3285[B]:VAL:CG2	3:d:3286[B]:THR:H	2.27	0.47
1:A:72:TYR:HE2	1:A:206:PHE:HE2	1.61	0.47
2:B:2472:ASN:ND2	4:i:1:NAG:C7	2.75	0.47
2:B:2551:PRO:HA	2:B:2552:GLU:HA	1.49	0.47
2:B:2887:ASP:C	2:B:2889:ALA:HA	2.40	0.47
3:C:2937[A]:ASN:CB	3:C:3006[A]:LYS:CE	2.86	0.47
3:C:2954[A]:TYR:CA	3:C:2957[A]:ILE:HG22	2.43	0.47
3:C:2971[B]:ASP:HA	3:L:3089[B]:HIS:C	2.38	0.47
3:C:2972[B]:GLY:CA	3:L:3086[B]:GLU:HG2	2.42	0.47
3:C:2985[B]:PHE:CZ	3:L:2970[B]:PRO:CB	2.84	0.47
3:C:3120[B]:HIS:HD2	3:L:2969[B]:TYR:OH	1.91	0.47
3:C:3149[B]:ASN:CG	3:L:3169[B]:LYS:HE3	2.17	0.47
3:C:3153[B]:LYS:HZ2	3:L:3156[B]:MET:C	2.17	0.47
1:D:670:PRO:HD2	1:D:671:PHE:HD1	1.79	0.47
1:D:1002:GLU:HB3	1:D:1065:LYS:NZ	2.29	0.47
2:E:2651:GLN:HE21	2:E:2652:LYS:HG3	1.78	0.47
2:E:2672:PHE:HZ	2:E:2718:TRP:HA	1.79	0.47
3:F:2968[B]:GLN:HA	3:F:2973[B]:THR:O	2.14	0.47
3:F:3150[B]:LYS:HZ1	3:a:3162[B]:ASP:C	2.20	0.47
3:F:3165[B]:ASN:O	3:a:3149[B]:ASN:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3169[B]:LYS:CE	3:a:3147[B]:GLU:N	2.58	0.47
3:F:3225[A]:SER:C	3:F:3290[A]:ILE:HG23	2.39	0.47
3:F:3229[B]:ASN:OD1	3:F:3244[B]:THR:HB	2.14	0.47
3:F:3230[A]:PHE:H	3:F:3243[A]:GLY:HA3	1.79	0.47
3:F:3255[B]:PRO:O	3:a:2966[B]:SER:HA	2.13	0.47
1:G:177:VAL:HG11	1:G:358:TYR:CE1	2.50	0.47
1:G:1034:GLU:HB2	1:G:1182:ASN:ND2	2.29	0.47
2:H:2122:ILE:O	2:H:2125:PHE:HB2	2.13	0.47
2:H:2644:LEU:HB2	2:H:2686:LEU:HB3	1.96	0.47
3:I:2952[B]:ALA:HB1	3:I:2957[B]:ILE:H	1.79	0.47
3:I:3004[B]:GLY:O	3:I:3006[B]:LYS:N	2.44	0.47
3:I:3196[A]:THR:O	3:I:3200[A]:LEU:N	2.43	0.47
3:I:3200[B]:LEU:HD22	3:I:3204[B]:LEU:HD11	1.95	0.47
3:I:3228[B]:VAL:CG2	3:I:3245[B]:PHE:CE1	2.97	0.47
3:I:3232[A]:VAL:HG23	3:I:3273[A]:LEU:HD11	1.95	0.47
1:J:1438:ASP:HB2	1:M:1372:ILE:HD12	1.96	0.47
2:K:2496:LEU:HB3	2:K:2498:VAL:HG22	1.95	0.47
3:L:2968[B]:GLN:HA	3:L:2973[B]:THR:O	2.14	0.47
3:L:3110[B]:THR:C	3:L:3112[B]:TYR:H	2.21	0.47
3:L:3196[B]:THR:HG23	3:L:3199[B]:GLN:OE1	2.14	0.47
1:M:1442:MET:HE1	1:M:1454:PHE:HA	1.95	0.47
1:M:1575:PRO:HA	1:M:1581:GLU:O	2.14	0.47
2:N:2129:PRO:O	2:N:2131:LEU:HD23	2.14	0.47
3:O:2933[B]:SER:HA	3:O:2935[B]:ILE:HD11	1.95	0.47
3:O:2976[B]:ALA:H	3:X:3156[B]:MET:CG	1.99	0.47
3:O:3125[A]:ARG:O	3:O:3129[A]:ILE:HG13	2.14	0.47
3:O:3143[B]:SER:OG	3:O:3144[B]:ALA:N	2.46	0.47
3:O:3151[B]:LEU:CB	3:O:3175[B]:TYR:CD2	2.93	0.47
3:O:3191[A]:ASN:C	3:O:3192[A]:PHE:O	2.52	0.47
3:O:3293[A]:LYS:HB2	3:O:3294[A]:SER:CA	2.41	0.47
1:P:829:ALA:HA	1:P:830:ASN:CG	2.39	0.47
1:P:961:SER:HB2	1:P:973:ARG:HA	1.95	0.47
1:P:981:GLU:HG2	1:P:983:PRO:HD2	1.96	0.47
1:P:1551:ASP:OD1	1:P:1551:ASP:N	2.47	0.47
2:Q:2240:GLN:HG2	2:Q:2244:PHE:CD1	2.49	0.47
2:Q:2840:GLY:O	2:Q:2843:GLU:HB2	2.15	0.47
3:R:2994[A]:LYS:HE2	3:R:3183[A]:LEU:O	2.14	0.47
3:R:3110[A]:THR:C	3:R:3112[A]:TYR:N	2.68	0.47
3:R:3125[A]:ARG:O	3:R:3129[A]:ILE:HG13	2.14	0.47
3:R:3298[A]:ASN:CA	3:R:3299[A]:LEU:CB	2.85	0.47
1:S:411:ASP:HB2	1:S:654:PRO:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:750:ALA:HA	1:S:796:TYR:HB3	1.96	0.47
1:S:929:TRP:O	1:S:1048:ASN:ND2	2.47	0.47
2:T:2327:GLU:H	2:T:2327:GLU:HG3	1.44	0.47
2:T:2597:MET:SD	2:T:2651:GLN:NE2	2.76	0.47
3:U:2933[B]:SER:HA	3:U:2935[B]:ILE:HD11	1.95	0.47
3:U:3200[A]:LEU:HD22	3:U:3204[A]:LEU:HD11	1.95	0.47
1:V:215:ARG:HE	1:V:279:LEU:HA	1.78	0.47
1:V:564:ASP:OD1	1:V:564:ASP:N	2.38	0.47
1:V:1642:GLN:CD	1:V:1642:GLN:H	2.21	0.47
3:X:2991[A]:LEU:HD23	3:X:3158[A]:PHE:CE1	2.47	0.47
3:X:3143[B]:SER:OG	3:X:3144[B]:ALA:N	2.47	0.47
3:X:3147[A]:GLU:CG	3:X:3149[A]:ASN:ND2	2.73	0.47
3:X:3196[A]:THR:HG23	3:X:3199[A]:GLN:OE1	2.14	0.47
3:X:3196[B]:THR:HG23	3:X:3199[B]:GLN:OE1	2.14	0.47
1:Y:127:GLU:HA	1:Y:134:VAL:HG13	1.95	0.47
1:Y:760:ILE:HG21	1:Y:777:TYR:HE2	1.79	0.47
1:Y:871:GLN:NE2	1:Y:964:ILE:O	2.47	0.47
1:Y:1161:ILE:O	1:Y:1203:MET:HE1	2.14	0.47
2:Z:2730:LEU:HA	1:b:1245:GLU:HB3	1.95	0.47
2:Z:2879:LEU:HD12	2:Z:2899:PRO:HB2	1.96	0.47
2:Z:2901:LEU:HB2	1:b:1074:ILE:HB	1.96	0.47
3:a:2949[A]:LYS:C	3:a:2953[A]:GLY:N	2.72	0.47
3:a:3298[B]:ASN:CB	3:a:3299[B]:LEU:C	2.85	0.47
1:b:1018:ILE:HD12	1:b:1045:HIS:CD2	2.49	0.47
3:d:2968[A]:GLN:HA	3:d:2973[A]:THR:O	2.14	0.47
3:d:3196[B]:THR:OG1	3:d:3199[B]:GLN:CD	2.57	0.47
3:d:3196[B]:THR:HG23	3:d:3199[B]:GLN:OE1	2.14	0.47
3:d:3230[A]:PHE:H	3:d:3243[A]:GLY:HA3	1.80	0.47
3:d:3230[B]:PHE:H	3:d:3243[B]:GLY:HA3	1.80	0.47
4:7:1:NAG:H61	4:7:2:NAG:N2	2.30	0.47
1:A:466:ALA:HB1	1:A:476:ARG:HG3	1.95	0.47
1:A:1145:THR:OG1	1:A:1233:SER:HB3	2.14	0.47
1:A:1154:SER:HB2	1:A:1220:MET:HE2	1.95	0.47
1:A:1578:ILE:HA	1:A:1579:GLY:HA2	1.58	0.47
2:B:2568:HIS:HD2	2:B:2765:PRO:HB3	1.79	0.47
3:C:2952[B]:ALA:HB1	3:C:2957[B]:ILE:H	1.79	0.47
3:C:3143[B]:SER:OG	3:C:3144[B]:ALA:N	2.47	0.47
3:C:3169[B]:LYS:O	3:L:3152[B]:LYS:CD	2.62	0.47
3:C:3172[B]:SER:CB	3:L:3150[B]:LYS:HA	2.27	0.47
3:C:3228[B]:VAL:CG2	3:C:3245[B]:PHE:CE1	2.97	0.47
3:F:2991[B]:LEU:HD23	3:F:3158[B]:PHE:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3157[B]:PRO:O	3:a:3150[B]:LYS:CG	2.54	0.47
3:F:3163[B]:ASN:HD22	3:a:3150[B]:LYS:CG	2.07	0.47
3:F:3228[A]:VAL:CG2	3:F:3245[A]:PHE:CE1	2.97	0.47
3:F:3257[B]:ALA:HB3	3:a:2956[B]:LYS:HD2	1.97	0.47
3:F:3285[A]:VAL:CG2	3:F:3286[A]:THR:H	2.27	0.47
1:G:872:GLN:O	1:G:875:ALA:N	2.45	0.47
1:G:1358:LEU:O	1:G:1375:ASN:ND2	2.42	0.47
1:G:1559:LEU:HD21	1:G:1590:PHE:CE1	2.49	0.47
2:H:2166:LEU:HA	2:H:2169:HIS:HB2	1.95	0.47
2:H:2728:ARG:HB3	2:H:2730:LEU:HD12	1.96	0.47
3:I:2933[A]:SER:HA	3:I:2935[A]:ILE:HD11	1.95	0.47
3:I:2949[B]:LYS:C	3:I:2953[B]:GLY:N	2.72	0.47
3:I:2959[B]:SER:HA	3:R:3255[B]:PRO:HG2	1.50	0.47
3:I:3148[B]:ILE:HG22	3:I:3152[B]:LYS:CE	2.44	0.47
3:I:3221[B]:ALA:HB2	3:R:2964[B]:PRO:C	2.23	0.47
3:I:3225[B]:SER:C	3:I:3290[B]:ILE:HG23	2.39	0.47
3:I:3293[A]:LYS:HB2	3:I:3294[A]:SER:CA	2.41	0.47
3:I:3298[A]:ASN:CB	3:I:3299[A]:LEU:C	2.86	0.47
1:J:40:TYR:HE2	1:J:75:GLN:HE21	1.61	0.47
1:J:324:PRO:HA	1:J:332:ASP:OD1	2.14	0.47
1:J:855:ARG:HH21	1:J:941:LEU:HA	1.79	0.47
1:J:946:GLU:HA	1:J:955:LYS:HB3	1.96	0.47
2:K:2240:GLN:HE21	2:K:2241:THR:HG22	1.79	0.47
3:L:2954[A]:TYR:CA	3:L:2957[A]:ILE:HG22	2.43	0.47
3:L:3125[A]:ARG:O	3:L:3129[A]:ILE:HG13	2.14	0.47
3:L:3143[B]:SER:OG	3:L:3144[B]:ALA:N	2.46	0.47
3:L:3196[B]:THR:OG1	3:L:3199[B]:GLN:CD	2.57	0.47
3:L:3200[B]:LEU:HD22	3:L:3204[B]:LEU:HD11	1.95	0.47
3:L:3229[B]:ASN:OD1	3:L:3244[B]:THR:HB	2.14	0.47
3:L:3230[A]:PHE:H	3:L:3243[A]:GLY:HA3	1.80	0.47
3:O:2968[A]:GLN:HA	3:O:2973[A]:THR:O	2.14	0.47
3:O:3191[B]:ASN:C	3:O:3192[B]:PHE:O	2.52	0.47
3:O:3196[B]:THR:HG23	3:O:3199[B]:GLN:OE1	2.14	0.47
3:O:3298[A]:ASN:CB	3:O:3299[A]:LEU:C	2.85	0.47
1:P:837:HIS:HA	1:P:1113:HIS:O	2.13	0.47
1:P:1279:LYS:HB2	1:P:1376:PRO:HG3	1.96	0.47
1:P:1324:ARG:NE	1:P:1462:ASP:OD1	2.44	0.47
3:R:2994[B]:LYS:HE2	3:R:3183[B]:LEU:O	2.14	0.47
3:R:3141[A]:TYR:CD2	3:R:3141[A]:TYR:C	2.86	0.47
3:R:3148[A]:ILE:HG22	3:R:3152[A]:LYS:CE	2.44	0.47
3:R:3217[B]:PHE:HD2	3:R:3300[B]:LEU:HD12	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:898:GLY:N	1:S:899:MET:SD	2.74	0.47
1:S:1179:GLY:HA2	1:S:1183:GLU:OE1	2.14	0.47
1:S:1286:ARG:HG3	1:S:1337:ARG:NH2	2.29	0.47
2:T:2435:MET:SD	2:T:2436:PRO:HD2	2.54	0.47
1:V:1578:ILE:HA	1:V:1579:GLY:HA2	1.55	0.47
2:W:2728:ARG:HB3	2:W:2730:LEU:HD12	1.96	0.47
3:X:2968[B]:GLN:HA	3:X:2973[B]:THR:O	2.14	0.47
3:X:2981[B]:GLY:N	3:X:3086[B]:GLU:OE1	2.45	0.47
3:X:3200[B]:LEU:HD22	3:X:3204[B]:LEU:HD11	1.95	0.47
3:X:3225[A]:SER:C	3:X:3290[A]:ILE:HG23	2.39	0.47
3:X:3230[A]:PHE:H	3:X:3243[A]:GLY:HA3	1.79	0.47
3:X:3230[B]:PHE:H	3:X:3243[B]:GLY:HA3	1.79	0.47
1:Y:325:THR:N	1:Y:332:ASP:OD1	2.47	0.47
1:Y:1475:ARG:NE	1:Y:1541:GLU:OE2	2.32	0.47
2:Z:2286:HIS:NE2	2:Z:2433:THR:HG22	2.29	0.47
2:Z:2625:LEU:O	2:Z:2638:ARG:NH2	2.47	0.47
3:a:2994[A]:LYS:HE2	3:a:3183[A]:LEU:O	2.14	0.47
3:a:3229[A]:ASN:OD1	3:a:3244[A]:THR:HB	2.14	0.47
1:b:1077:LEU:HD23	1:b:1103:PHE:HE1	1.79	0.47
1:b:1161:ILE:O	1:b:1203:MET:HE1	2.14	0.47
3:d:3143[B]:SER:OG	3:d:3144[B]:ALA:N	2.46	0.47
3:d:3146[A]:CYS:HA	3:d:3147[A]:GLU:HA	1.70	0.47
3:d:3217[A]:PHE:HD2	3:d:3300[A]:LEU:HD12	1.79	0.47
3:d:3229[B]:ASN:OD1	3:d:3244[B]:THR:HB	2.14	0.47
1:A:398:ARG:NH2	1:A:484:MET:HE2	2.29	0.47
3:C:3074[A]:GLU:CD	3:C:3212[A]:ARG:NH2	2.73	0.47
3:C:3154[B]:PRO:CA	3:L:3174[B]:GLY:N	2.77	0.47
1:D:841:LYS:HA	1:D:1117:ASP:HB2	1.95	0.47
2:E:2823:ILE:HD11	2:E:2859:VAL:HG12	1.96	0.47
3:F:2949[B]:LYS:NZ	3:F:2949[B]:LYS:C	2.73	0.47
3:F:2994[A]:LYS:HE2	3:F:3183[A]:LEU:O	2.14	0.47
3:F:3150[B]:LYS:HD2	3:a:3160[B]:SER:O	2.06	0.47
1:G:293:LEU:O	1:G:297:ARG:HG3	2.14	0.47
1:G:1348:TRP:HD1	1:G:1403:LEU:HD13	1.78	0.47
1:G:1578:ILE:HA	1:G:1579:GLY:HA2	1.55	0.47
2:H:2340:ALA:HB1	2:H:2341:PRO:CD	2.41	0.47
3:I:2933[B]:SER:HA	3:I:2935[B]:ILE:HD11	1.96	0.47
3:I:2994[A]:LYS:HE2	3:I:3183[A]:LEU:O	2.14	0.47
3:I:2994[B]:LYS:HE2	3:I:3183[B]:LEU:O	2.14	0.47
3:I:3146[A]:CYS:HA	3:I:3147[A]:GLU:HA	1.70	0.47
3:I:3169[B]:LYS:HE2	3:R:3147[B]:GLU:H	1.07	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3196[B]:THR:CA	3:I:3199[B]:GLN:HB2	2.43	0.47
1:J:73:LEU:HD21	1:J:210:HIS:HB2	1.96	0.47
2:K:2400:LEU:HB2	2:K:2439:PHE:HD2	1.80	0.47
3:L:2932[B]:PRO:CA	3:L:2935[B]:ILE:CD1	2.85	0.47
3:L:2949[A]:LYS:C	3:L:2953[A]:GLY:N	2.72	0.47
1:M:394:GLN:H	1:M:394:GLN:HG3	1.36	0.47
1:M:516:TRP:CD1	1:M:579:LEU:HD22	2.50	0.47
1:M:979:LEU:HB3	1:M:980:TYR:HA	1.96	0.47
1:M:1470:GLU:OE2	1:M:1473:ARG:NH1	2.47	0.47
3:O:2952[A]:ALA:HB1	3:O:2957[A]:ILE:H	1.79	0.47
3:O:3183[A]:LEU:H	3:O:3184[A]:ASN:CA	2.22	0.47
3:O:3229[A]:ASN:OD1	3:O:3244[A]:THR:HB	2.14	0.47
3:O:3288[B]:MET:CA	3:O:3295[B]:LEU:HG	2.42	0.47
1:P:1258:ARG:HD2	1:P:1524:HIS:O	2.14	0.47
3:R:2981[A]:GLY:N	3:R:3086[A]:GLU:OE1	2.45	0.47
3:R:3196[A]:THR:HG23	3:R:3199[A]:GLN:OE1	2.14	0.47
3:R:3229[B]:ASN:OD1	3:R:3244[B]:THR:HB	2.14	0.47
1:S:151:GLN:OE1	1:S:151:GLN:N	2.42	0.47
1:V:618:MET:HE3	1:V:618:MET:HB3	1.77	0.47
1:V:838:ARG:NH2	1:V:915:ASN:OD1	2.47	0.47
3:X:3229[B]:ASN:OD1	3:X:3244[B]:THR:HB	2.14	0.47
1:Y:25:MET:HE2	1:Y:34:TYR:HA	1.95	0.47
1:Y:387:ASN:OD1	1:Y:387:ASN:N	2.39	0.47
1:Y:836:GLN:HB2	1:Y:1113:HIS:CG	2.49	0.47
1:Y:1619:GLY:N	3:d:3190[B]:LEU:HG	2.30	0.47
2:Z:2565:THR:OG1	2:Z:2741:GLN:NE2	2.47	0.47
3:a:2939[B]:ARG:HG3	3:a:2939[B]:ARG:NH1	2.28	0.47
3:a:2952[A]:ALA:HB1	3:a:2957[A]:ILE:H	1.79	0.47
3:a:2954[B]:TYR:CA	3:a:2957[B]:ILE:HG22	2.43	0.47
3:a:3066[A]:TYR:CE1	3:a:3193[A]:HIS:CE1	2.98	0.47
3:a:3143[A]:SER:OG	3:a:3144[A]:ALA:N	2.46	0.47
3:a:3229[B]:ASN:OD1	3:a:3244[B]:THR:HB	2.14	0.47
3:a:3288[B]:MET:CA	3:a:3295[B]:LEU:HG	2.42	0.47
1:b:806:ASN:ND2	4:OA:1:NAG:O7	2.47	0.47
1:b:1280:GLN:HG2	1:b:1337:ARG:HD2	1.96	0.47
1:b:1578:ILE:HA	1:b:1579:GLY:HA2	1.71	0.47
3:d:2939[B]:ARG:HG3	3:d:2939[B]:ARG:NH1	2.28	0.47
3:d:2985[A]:PHE:CE2	3:d:2989[A]:HIS:NE2	2.83	0.47
3:d:2994[A]:LYS:HE2	3:d:3183[A]:LEU:O	2.14	0.47
4:MA:1:NAG:C6	4:MA:2:NAG:HN2	2.27	0.47
1:A:907:ARG:HG3	1:A:1112:PHE:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2940[A]:ASN:O	3:C:2944[A]:ALA:N	2.48	0.47
3:C:2991[B]:LEU:HD23	3:C:3158[B]:PHE:CE1	2.48	0.47
3:C:2994[B]:LYS:HE2	3:C:3183[B]:LEU:O	2.14	0.47
3:C:3089[B]:HIS:CE1	3:C:3119[B]:HIS:CE1	2.81	0.47
3:C:3096[B]:VAL:HG11	3:C:3115[B]:LEU:HD12	1.89	0.47
3:C:3196[B]:THR:OG1	3:C:3199[B]:GLN:CD	2.57	0.47
3:C:3223[B]:GLY:C	3:L:3252[B]:TYR:CD1	2.88	0.47
3:C:3228[A]:VAL:CG2	3:C:3245[A]:PHE:CE1	2.97	0.47
1:D:1156:LEU:HB2	1:D:1176:TYR:CE1	2.50	0.47
2:E:2090:LYS:NZ	2:E:2099:GLU:OE2	2.46	0.47
2:E:2570:HIS:CD2	2:E:2711:HIS:CE1	2.98	0.47
3:F:2965[B]:LEU:C	3:a:3255[B]:PRO:CA	2.83	0.47
3:F:2968[A]:GLN:HA	3:F:2973[A]:THR:O	2.14	0.47
3:F:3096[A]:VAL:HG11	3:F:3115[A]:LEU:HD12	1.89	0.47
3:F:3141[A]:TYR:CD2	3:F:3141[A]:TYR:C	2.86	0.47
3:F:3148[A]:ILE:HG22	3:F:3152[A]:LYS:CE	2.44	0.47
3:F:3169[B]:LYS:HA	3:a:3150[B]:LYS:CA	2.16	0.47
3:F:3200[A]:LEU:HD22	3:F:3204[A]:LEU:HD11	1.95	0.47
3:F:3293[B]:LYS:HB2	3:F:3294[B]:SER:CA	2.41	0.47
1:G:497:GLN:HG2	1:G:683:THR:HG21	1.96	0.47
2:H:2704:ASP:O	2:H:2707:PHE:HB3	2.15	0.47
3:I:3150[B]:LYS:HG3	3:R:3163[B]:ASN:CG	2.34	0.47
3:I:3285[A]:VAL:CG2	3:I:3286[A]:THR:H	2.27	0.47
1:J:1019:HIS:HD1	1:J:1030:MET:HE2	1.80	0.47
1:J:1280:GLN:NE2	1:J:1337:ARG:HD3	2.30	0.47
2:K:2128:LEU:O	2:K:2130:PRO:HD3	2.13	0.47
2:K:2158:TYR:O	2:K:2161:GLN:HB3	2.14	0.47
2:K:2309:GLN:NE2	2:K:2319:ALA:O	2.40	0.47
2:K:2572:VAL:HG22	2:K:2768:LEU:HD13	1.96	0.47
3:L:2961[A]:HIS:CD2	3:L:2988[A]:TRP:CZ3	2.96	0.47
3:L:3180[B]:TYR:CB	3:L:3183[B]:LEU:CD2	2.90	0.47
3:L:3191[B]:ASN:ND2	3:L:3191[B]:ASN:N	2.60	0.47
3:O:2949[B]:LYS:C	3:O:2953[B]:GLY:N	2.72	0.47
3:O:2960[A]:PHE:CD1	3:O:2960[A]:PHE:N	2.72	0.47
3:O:3229[B]:ASN:OD1	3:O:3244[B]:THR:HB	2.14	0.47
3:O:3283[A]:ILE:HB	3:O:3305[A]:ILE:HD11	1.97	0.47
3:O:3298[A]:ASN:CA	3:O:3299[A]:LEU:C	2.85	0.47
1:P:1638:SER:OG	1:S:472:ASP:OD2	2.29	0.47
3:R:2949[A]:LYS:NZ	3:R:2949[A]:LYS:C	2.73	0.47
3:R:3225[B]:SER:C	3:R:3290[B]:ILE:HG23	2.39	0.47
3:R:3230[A]:PHE:H	3:R:3243[A]:GLY:HA3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:43:GLU:HG3	1:S:44:PRO:HA	1.97	0.47
1:S:187:GLY:HA2	1:S:193:SER:HB2	1.97	0.47
1:S:277:ASP:OD1	1:S:278:ASP:N	2.46	0.47
1:S:876:PHE:CD1	1:S:1083:PRO:HB2	2.48	0.47
2:T:2844:MET:O	2:T:2846:TRP:HD1	1.98	0.47
3:U:2940[B]:ASN:O	3:U:2944[B]:ALA:N	2.48	0.47
1:V:92:TRP:CE3	1:V:102:PRO:HD3	2.49	0.47
1:V:547:LYS:HE2	1:V:558:HIS:CD2	2.50	0.47
1:V:843:VAL:HG13	1:V:927:PRO:HB2	1.97	0.47
1:V:1407:THR:HG22	1:V:1426:LEU:HD21	1.96	0.47
1:V:1574:VAL:HG22	1:V:1620:LEU:HD21	1.96	0.47
3:X:2935[A]:ILE:CG1	3:X:2936[A]:GLU:N	2.78	0.47
1:Y:1487:PRO:HD3	2:c:2486:ILE:HB	1.95	0.47
1:Y:1546:LYS:HG3	3:d:3001[B]:LYS:CD	2.44	0.47
1:Y:1550:ARG:NE	3:d:3008[B]:GLY:C	2.72	0.47
2:Z:2279:LEU:HD12	2:Z:2284:HIS:HD2	1.77	0.47
3:a:2940[A]:ASN:O	3:a:2944[A]:ALA:N	2.48	0.47
3:a:2940[B]:ASN:O	3:a:2944[B]:ALA:N	2.48	0.47
3:a:2970[B]:PRO:C	3:a:2972[B]:GLY:N	2.72	0.47
3:a:2971[B]:ASP:OD1	9:a:3401[B]:CUO:O2	2.33	0.47
1:b:479:CYS:HB3	1:b:670:PRO:HD3	1.96	0.47
1:b:572:SER:HA	1:b:573:LYS:HA	1.39	0.47
2:c:2370:MET:HE3	2:c:2370:MET:HB2	1.71	0.47
2:c:2462:PHE:CE1	2:c:2486:ILE:HD13	2.49	0.47
2:c:2699:MET:HG3	2:c:2840:GLY:HA3	1.96	0.47
3:d:2935[B]:ILE:CG1	3:d:2936[B]:GLU:N	2.78	0.47
3:d:3196[A]:THR:HG23	3:d:3199[A]:GLN:OE1	2.14	0.47
3:d:3285[B]:VAL:CG2	3:d:3286[B]:THR:N	2.73	0.47
1:A:490:TRP:HE1	1:A:670:PRO:HD3	1.79	0.47
2:B:2294:PHE:O	2:B:2297:HIS:HB3	2.14	0.47
3:C:2933[A]:SER:HA	3:C:2935[A]:ILE:HD11	1.95	0.47
3:C:2937[B]:ASN:CB	3:C:3006[B]:LYS:CE	2.86	0.47
3:C:2952[A]:ALA:HB1	3:C:2957[A]:ILE:H	1.79	0.47
3:C:2968[A]:GLN:HA	3:C:2973[A]:THR:O	2.14	0.47
3:C:3151[B]:LEU:C	3:L:3154[B]:PRO:HB3	2.36	0.47
3:C:3255[B]:PRO:HA	3:L:2964[B]:PRO:O	2.12	0.47
1:D:745:ASP:HB2	1:D:801:ASP:OD1	2.14	0.47
1:D:855:ARG:HD3	1:D:959:PHE:CD2	2.49	0.47
1:D:1018:ILE:HA	1:D:1021:LEU:HB2	1.96	0.47
1:D:1258:ARG:HB3	1:D:1342:ALA:HB2	1.97	0.47
1:D:1283:ASP:OD1	1:D:1283:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3014[A]:TRP:HH2	3:F:3123[A]:THR:HG23	1.78	0.47
3:F:3151[A]:LEU:HB2	3:F:3175[A]:TYR:HE2	1.68	0.47
1:G:321:LEU:HD11	1:G:377:TYR:CD2	2.50	0.47
1:G:597:VAL:O	1:G:601:VAL:HG12	2.14	0.47
2:H:2800:LYS:HB3	3:I:3023[A]:ILE:CD1	2.45	0.47
3:I:2959[B]:SER:HB3	3:R:3255[B]:PRO:CB	2.36	0.47
3:I:2985[B]:PHE:CE2	3:I:2989[B]:HIS:NE2	2.83	0.47
3:I:3078[B]:PHE:HE2	3:R:3161[B]:GLU:OE1	1.98	0.47
3:I:3155[B]:MET:HA	3:R:2979[B]:GLN:NE2	2.29	0.47
3:I:3173[B]:THR:HA	3:R:3154[B]:PRO:HA	1.96	0.47
3:I:3255[B]:PRO:N	3:R:2966[B]:SER:OG	2.47	0.47
1:J:177:VAL:O	1:J:181:PRO:HD3	2.14	0.47
1:J:980:TYR:CE1	1:J:1021:LEU:HD13	2.49	0.47
2:K:2521:MET:HE3	2:K:2605:LEU:HD12	1.97	0.47
2:K:2616:THR:HB	2:K:2618:SER:H	1.78	0.47
3:L:2935[B]:ILE:CG1	3:L:2936[B]:GLU:N	2.78	0.47
3:L:3183[B]:LEU:H	3:L:3184[B]:ASN:CA	2.22	0.47
3:L:3229[A]:ASN:OD1	3:L:3244[A]:THR:HB	2.14	0.47
3:L:3230[B]:PHE:H	3:L:3243[B]:GLY:HA3	1.79	0.47
1:M:127:GLU:CD	1:M:135:THR:H	2.22	0.47
1:M:909:ILE:HG12	1:M:1084:PHE:HZ	1.79	0.47
3:O:2949[A]:LYS:NZ	3:O:2949[A]:LYS:C	2.73	0.47
1:P:1462:ASP:OD2	1:P:1525:TYR:OH	2.23	0.47
3:R:2949[B]:LYS:C	3:R:2953[B]:GLY:N	2.72	0.47
3:R:2952[A]:ALA:N	3:R:2953[A]:GLY:HA2	2.06	0.47
1:S:500:ASN:O	1:S:504:THR:OG1	2.32	0.47
3:U:2935[A]:ILE:CG1	3:U:2936[A]:GLU:N	2.78	0.47
3:U:2939[A]:ARG:HG3	3:U:2939[A]:ARG:NH1	2.28	0.47
3:U:2965[B]:LEU:CG	3:d:3221[B]:ALA:H	2.18	0.47
3:U:3257[B]:ALA:C	3:d:2969[B]:TYR:O	2.58	0.47
3:U:3284[B]:LYS:CD	3:U:3284[B]:LYS:C	2.86	0.47
1:V:840:ARG:HD2	1:V:1116:TYR:CZ	2.50	0.47
2:W:2225:ARG:HD2	2:W:2274:LEU:HD22	1.96	0.47
2:W:2560:LEU:HD13	2:W:2569:TRP:CD1	2.50	0.47
2:W:2867:PRO:HG2	3:X:2932[A]:PRO:CG	2.45	0.47
3:X:3148[A]:ILE:HG22	3:X:3152[A]:LYS:CE	2.44	0.47
3:X:3228[A]:VAL:CG2	3:X:3245[A]:PHE:CE1	2.97	0.47
3:X:3298[B]:ASN:CB	3:X:3299[B]:LEU:C	2.86	0.47
1:Y:4:ARG:NH1	1:Y:77:GLU:OE1	2.48	0.47
1:Y:81:VAL:HA	1:Y:85:SER:H	1.79	0.47
1:Y:1075:GLU:HG2	2:c:2901:LEU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:2985[A]:PHE:CE2	3:a:2989[A]:HIS:NE2	2.83	0.47
3:a:3074[B]:GLU:CD	3:a:3212[B]:ARG:NH2	2.73	0.47
3:a:3141[A]:TYR:CD2	3:a:3141[A]:TYR:C	2.86	0.47
3:a:3151[A]:LEU:HB2	3:a:3175[A]:TYR:HE2	1.68	0.47
3:a:3283[B]:ILE:HB	3:a:3305[B]:ILE:HD11	1.97	0.47
1:b:858:MET:HE1	1:b:870:TYR:CE2	2.50	0.47
3:d:3148[B]:ILE:HG22	3:d:3152[B]:LYS:CE	2.44	0.47
3:d:3219[A]:LEU:N	3:d:3219[A]:LEU:CD2	2.73	0.47
1:A:81:VAL:HA	1:A:85:SER:HB3	1.96	0.47
1:A:482:HIS:CE1	1:A:621:LEU:HD11	2.50	0.47
1:A:760:ILE:HG21	1:A:777:TYR:HE2	1.80	0.47
1:A:965:ASP:HB3	1:A:1038:PHE:CE2	2.50	0.47
1:A:1156:LEU:HB2	1:A:1176:TYR:CE2	2.50	0.47
1:A:1403:LEU:HD21	1:A:1429:THR:HG21	1.96	0.47
2:B:2554:PRO:HA	2:B:2555:GLU:CB	2.45	0.47
2:B:2903:TYR:OH	3:C:2932[A]:PRO:HD2	2.14	0.47
3:C:2951[A]:ASP:C	3:C:2956[A]:LYS:HZ1	2.09	0.47
3:C:2968[B]:GLN:CG	3:L:2981[B]:GLY:N	2.75	0.47
3:C:2994[A]:LYS:HE2	3:C:3183[A]:LEU:O	2.14	0.47
3:C:3148[A]:ILE:HG22	3:C:3152[A]:LYS:CE	2.44	0.47
3:C:3196[A]:THR:OG1	3:C:3199[A]:GLN:CD	2.57	0.47
3:C:3200[B]:LEU:CD2	3:C:3204[B]:LEU:CD1	2.93	0.47
3:C:3229[A]:ASN:OD1	3:C:3244[A]:THR:HB	2.14	0.47
3:C:3283[B]:ILE:C	3:C:3283[B]:ILE:CD1	2.85	0.47
1:D:118:ALA:HB1	1:D:119:LYS:HA	1.96	0.47
1:D:353:ASN:HD22	1:D:772:ARG:NH2	2.13	0.47
1:D:961:SER:HB3	1:D:972:SER:O	2.14	0.47
1:D:964:ILE:HG22	1:D:970:SER:C	2.40	0.47
3:F:2935[B]:ILE:CG1	3:F:2936[B]:GLU:N	2.78	0.47
3:F:2952[A]:ALA:CB	3:F:2953[A]:GLY:CA	2.82	0.47
3:F:2969[B]:TYR:CE2	3:F:2970[B]:PRO:CG	2.86	0.47
3:F:2983[B]:VAL:H	3:a:3160[B]:SER:CA	2.27	0.47
3:F:2985[B]:PHE:CE2	3:F:2989[B]:HIS:NE2	2.83	0.47
3:F:3152[B]:LYS:CB	3:a:3170[B]:ALA:C	2.86	0.47
3:F:3183[A]:LEU:H	3:F:3184[A]:ASN:CA	2.22	0.47
3:F:3196[B]:THR:HG23	3:F:3199[B]:GLN:OE1	2.14	0.47
3:F:3232[B]:VAL:HG23	3:F:3273[B]:LEU:HD11	1.95	0.47
3:F:3253[B]:GLU:HB3	3:a:3252[B]:TYR:HB3	1.97	0.47
3:F:3255[B]:PRO:CD	3:a:2962[B]:GLY:C	2.69	0.47
1:G:440:ARG:O	1:G:444:GLU:HB2	2.14	0.47
1:G:460:GLU:CD	1:G:1368:ARG:HH21	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:664:VAL:O	1:G:689:PRO:HD2	2.15	0.47
1:G:1636:ASN:HB3	1:G:1639:LYS:HD3	1.95	0.47
2:H:2564:PRO:HA	2:H:2673:GLU:HG3	1.97	0.47
2:H:2900:SER:HA	1:J:1075:GLU:HG2	1.97	0.47
3:I:2935[A]:ILE:CG1	3:I:2936[A]:GLU:N	2.78	0.47
3:I:2935[B]:ILE:CG1	3:I:2936[B]:GLU:N	2.78	0.47
3:I:2952[A]:ALA:HB1	3:I:2957[A]:ILE:H	1.79	0.47
3:I:2964[B]:PRO:N	3:R:3255[B]:PRO:HG3	2.30	0.47
3:I:2968[B]:GLN:HA	3:I:2973[B]:THR:O	2.14	0.47
3:I:2969[A]:TYR:CD2	3:I:2970[A]:PRO:N	2.83	0.47
3:I:2985[A]:PHE:CE2	3:I:2989[A]:HIS:NE2	2.83	0.47
3:I:2992[B]:TYR:CE2	3:R:2969[B]:TYR:HE1	2.31	0.47
3:I:3107[B]:LEU:HD22	3:R:3252[B]:TYR:HB3	1.97	0.47
3:I:3125[A]:ARG:O	3:I:3129[A]:ILE:HG13	2.14	0.47
3:I:3125[B]:ARG:O	3:I:3129[B]:ILE:HG13	2.14	0.47
3:I:3143[B]:SER:OG	3:I:3144[B]:ALA:N	2.46	0.47
3:I:3155[B]:MET:HB2	3:R:3153[B]:LYS:HG2	1.83	0.47
3:I:3191[A]:ASN:ND2	3:I:3191[A]:ASN:N	2.60	0.47
3:I:3229[B]:ASN:OD1	3:I:3244[B]:THR:HB	2.14	0.47
3:I:3232[B]:VAL:HG23	3:I:3273[B]:LEU:HD11	1.94	0.47
1:J:163:LEU:HB3	1:J:293:LEU:HD21	1.96	0.47
1:J:882:TRP:HB3	1:J:1086:LEU:HD11	1.97	0.47
1:J:1596:GLU:O	1:J:1597:THR:HG22	2.14	0.47
2:K:2149:ALA:HA	2:K:2260:GLU:HG2	1.97	0.47
2:K:2235:PRO:HG3	2:K:2240:GLN:NE2	2.27	0.47
2:K:2568:HIS:HD2	2:K:2718:TRP:CH2	2.33	0.47
3:L:2954[B]:TYR:CA	3:L:2957[B]:ILE:HG22	2.43	0.47
3:L:2985[B]:PHE:CE2	3:L:2989[B]:HIS:NE2	2.83	0.47
3:L:3125[B]:ARG:O	3:L:3129[B]:ILE:HG13	2.14	0.47
3:L:3141[A]:TYR:CD2	3:L:3141[A]:TYR:C	2.86	0.47
3:L:3182[B]:GLN:H	3:L:3182[B]:GLN:HG2	1.56	0.47
3:L:3200[B]:LEU:CD2	3:L:3204[B]:LEU:CD1	2.93	0.47
3:L:3225[B]:SER:C	3:L:3290[B]:ILE:HG23	2.39	0.47
3:L:3285[A]:VAL:CG2	3:L:3286[A]:THR:H	2.27	0.47
1:M:1019:HIS:NE2	1:M:1046:HIS:CE1	2.83	0.47
1:M:1274:LEU:HD21	1:M:1344:PRO:HD3	1.96	0.47
2:N:2509:ILE:HD11	2:N:2605:LEU:HD23	1.97	0.47
2:N:2567:MET:HE3	2:N:2718:TRP:HB2	1.97	0.47
3:O:2933[A]:SER:HA	3:O:2935[A]:ILE:HD11	1.95	0.47
3:O:3148[B]:ILE:HG22	3:O:3152[B]:LYS:CE	2.44	0.47
3:O:3154[B]:PRO:CG	3:X:3175[B]:TYR:CG	2.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3162[B]:ASP:OD2	3:X:3150[B]:LYS:CE	2.62	0.47
1:P:419:THR:HA	1:P:420:SER:HA	1.68	0.47
1:P:480:CYS:SG	1:P:621:LEU:HD11	2.54	0.47
1:P:832:LYS:HA	1:P:832:LYS:NZ	2.29	0.47
1:P:879:SER:HA	1:P:893:ALA:HA	1.96	0.47
1:P:979:LEU:HD23	1:P:980:TYR:HD1	1.80	0.47
1:P:1199:VAL:O	1:P:1203:MET:HG3	2.15	0.47
2:Q:2149:ALA:HA	2:Q:2260:GLU:HG2	1.97	0.47
2:Q:2551:PRO:HA	2:Q:2552:GLU:HA	1.56	0.47
2:Q:2726:LYS:HB2	2:Q:2726:LYS:HE3	1.77	0.47
2:Q:2833:GLY:HA3	2:Q:2854:MET:HE1	1.95	0.47
3:R:2935[A]:ILE:CG1	3:R:2936[A]:GLU:N	2.78	0.47
3:R:2937[A]:ASN:CB	3:R:3006[A]:LYS:CE	2.85	0.47
3:R:2940[A]:ASN:O	3:R:2944[A]:ALA:N	2.48	0.47
3:R:2952[A]:ALA:HB1	3:R:2957[A]:ILE:H	1.79	0.47
3:R:2952[B]:ALA:HB1	3:R:2957[B]:ILE:H	1.79	0.47
3:R:3143[A]:SER:OG	3:R:3144[A]:ALA:N	2.46	0.47
3:R:3196[B]:THR:OG1	3:R:3199[B]:GLN:CD	2.57	0.47
3:R:3200[B]:LEU:HD22	3:R:3204[B]:LEU:HD11	1.95	0.47
3:R:3225[A]:SER:C	3:R:3290[A]:ILE:HG23	2.39	0.47
3:R:3285[B]:VAL:CG2	3:R:3286[B]:THR:H	2.27	0.47
1:S:931:TRP:CZ3	1:S:995:ILE:HD11	2.50	0.47
1:S:962:GLY:HA2	1:S:971:THR:HB	1.97	0.47
2:T:2240:GLN:HG2	2:T:2244:PHE:CD1	2.50	0.47
2:T:2749:PHE:HA	2:T:2754:ASN:HD22	1.79	0.47
3:U:2970[B]:PRO:C	3:U:2972[B]:GLY:H	2.23	0.47
3:U:2970[B]:PRO:C	3:d:3086[B]:GLU:HG2	2.40	0.47
3:U:2985[A]:PHE:CE2	3:U:2989[A]:HIS:NE2	2.83	0.47
3:U:3125[A]:ARG:O	3:U:3129[A]:ILE:HG13	2.14	0.47
3:U:3228[A]:VAL:CG2	3:U:3245[A]:PHE:CE1	2.97	0.47
3:U:3255[B]:PRO:HB3	3:d:2974[B]:ALA:O	2.12	0.47
1:V:547:LYS:HG3	1:V:559:THR:O	2.15	0.47
1:V:583:LEU:HG	1:V:602:THR:HG21	1.97	0.47
1:V:843:VAL:HG22	1:V:928:TYR:O	2.14	0.47
1:V:1302:SER:HA	1:V:1303:GLU:HA	1.66	0.47
1:V:1493:MET:HG2	1:V:1511:SER:O	2.14	0.47
2:W:2177:TYR:HB2	2:W:2300:ASN:HB2	1.97	0.47
3:X:2935[B]:ILE:CG1	3:X:2936[B]:GLU:N	2.78	0.47
3:X:2949[A]:LYS:NZ	3:X:2949[A]:LYS:C	2.73	0.47
3:X:2949[B]:LYS:NZ	3:X:2949[B]:LYS:C	2.73	0.47
3:X:2954[B]:TYR:CA	3:X:2957[B]:ILE:HG22	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2988[B]:TRP:HE3	3:X:2989[B]:HIS:CE1	2.25	0.47
3:X:3014[B]:TRP:CD2	3:X:3092[B]:ILE:CD1	2.98	0.47
3:X:3074[A]:GLU:CD	3:X:3212[A]:ARG:NH2	2.73	0.47
3:X:3125[B]:ARG:O	3:X:3129[B]:ILE:HG13	2.14	0.47
3:X:3137[A]:ARG:HB3	3:X:3139[A]:LEU:HD21	1.97	0.47
3:X:3182[A]:GLN:H	3:X:3182[A]:GLN:HG2	1.56	0.47
3:X:3196[A]:THR:CA	3:X:3199[A]:GLN:HB2	2.43	0.47
3:X:3283[A]:ILE:C	3:X:3283[A]:ILE:CD1	2.85	0.47
1:Y:327:ASP:HB3	1:Y:329:ARG:HG3	1.97	0.47
1:Y:860:ALA:HB3	1:Y:920:ASN:ND2	2.29	0.47
1:Y:867:VAL:HG12	1:Y:872:GLN:NE2	2.30	0.47
1:Y:977:GLU:HG2	1:Y:1021:LEU:HD22	1.97	0.47
1:Y:1536:SER:O	1:Y:1539:GLN:HG2	2.15	0.47
2:Z:2556:TYR:HE1	2:Z:2845:PRO:HD2	1.78	0.47
3:a:2969[A]:TYR:CD2	3:a:2970[A]:PRO:N	2.83	0.47
3:a:3148[A]:ILE:HG22	3:a:3152[A]:LYS:CE	2.44	0.47
3:a:3228[B]:VAL:CG2	3:a:3245[B]:PHE:CE1	2.97	0.47
3:a:3284[A]:LYS:CE	3:a:3284[A]:LYS:CA	2.85	0.47
1:b:490:TRP:HE1	1:b:670:PRO:CD	2.28	0.47
1:b:566:ARG:H	1:b:567:LEU:HD12	1.80	0.47
1:b:618:MET:HE3	1:b:618:MET:HB3	1.72	0.47
1:b:741:SER:O	1:b:805:VAL:HG23	2.14	0.47
1:b:879:SER:HA	1:b:893:ALA:HA	1.95	0.47
1:b:1160:PHE:HD1	1:b:1171:LYS:HA	1.80	0.47
2:c:2190:LEU:HD23	2:c:2296:LEU:HD21	1.96	0.47
3:d:2933[A]:SER:HA	3:d:2935[A]:ILE:HD11	1.95	0.47
3:d:3066[B]:TYR:CE1	3:d:3193[B]:HIS:CE1	2.98	0.47
3:d:3125[B]:ARG:O	3:d:3129[B]:ILE:HG13	2.14	0.47
3:d:3148[A]:ILE:HG22	3:d:3152[A]:LYS:CE	2.44	0.47
3:d:3200[A]:LEU:HD22	3:d:3204[A]:LEU:HD11	1.95	0.47
3:d:3217[B]:PHE:HD2	3:d:3300[B]:LEU:HD12	1.79	0.47
3:d:3218[A]:LEU:HD12	3:d:3218[A]:LEU:HA	1.78	0.47
3:d:3228[B]:VAL:CG2	3:d:3245[B]:PHE:CE1	2.97	0.47
3:d:3298[B]:ASN:CA	3:d:3299[B]:LEU:C	2.85	0.47
4:q:2:NAG:C3	4:q:2:NAG:C8	2.85	0.47
4:BA:1:NAG:O7	4:BA:1:NAG:H3	2.15	0.47
5:PA:1:NAG:H62	5:PA:2:NAG:C7	2.45	0.47
1:A:1211:TYR:O	1:A:1211:TYR:CG	2.67	0.47
1:A:1316:MET:SD	1:A:1316:MET:N	2.88	0.47
3:C:2940[B]:ASN:O	3:C:2944[B]:ALA:N	2.48	0.47
3:C:2984[B]:THR:OG1	3:L:3156[B]:MET:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2985[A]:PHE:CE2	3:C:2989[A]:HIS:NE2	2.83	0.47
3:C:3169[B]:LYS:HG3	3:L:3150[B]:LYS:N	2.30	0.47
3:C:3230[A]:PHE:H	3:C:3243[A]:GLY:HA3	1.79	0.47
3:C:3230[B]:PHE:H	3:C:3243[B]:GLY:HA3	1.80	0.47
3:C:3252[B]:TYR:CZ	3:L:3224[B]:GLN:HA	2.49	0.47
3:C:3285[A]:VAL:CG2	3:C:3286[A]:THR:H	2.27	0.47
3:C:3288[B]:MET:CA	3:C:3295[B]:LEU:HG	2.42	0.47
1:D:188:GLY:O	1:D:386:ILE:HD11	2.15	0.47
1:D:589:GLN:HG2	1:D:594:ASP:HB3	1.97	0.47
2:E:2272:SER:HA	2:E:2283:ASN:ND2	2.29	0.47
2:E:2844:MET:O	2:E:2846:TRP:HD1	1.97	0.47
3:F:2952[A]:ALA:HB1	3:F:2957[A]:ILE:H	1.79	0.47
3:F:2975[B]:PHE:CE1	3:a:3107[B]:LEU:CD1	2.86	0.47
3:F:2985[A]:PHE:CE2	3:F:2989[A]:HIS:NE2	2.83	0.47
3:F:3004[B]:GLY:O	3:F:3006[B]:LYS:N	2.44	0.47
3:F:3152[B]:LYS:HG3	3:a:3172[B]:SER:OG	2.06	0.47
3:F:3196[A]:THR:O	3:F:3200[A]:LEU:N	2.44	0.47
1:G:1321:HIS:ND1	1:G:1513:PRO:HB3	2.29	0.47
1:G:1348:TRP:CD1	1:G:1403:LEU:HD13	2.50	0.47
2:H:2270:ILE:HB	2:H:2297:HIS:CD2	2.50	0.47
3:I:2981[B]:GLY:N	3:I:3086[B]:GLU:OE1	2.45	0.47
3:I:3089[B]:HIS:CD2	3:R:2972[B]:GLY:H	2.32	0.47
3:I:3147[B]:GLU:OE2	3:R:3163[B]:ASN:O	2.33	0.47
3:I:3171[B]:HIS:C	3:R:3152[B]:LYS:O	2.53	0.47
3:I:3176[A]:LYS:C	3:I:3177[A]:SER:HG	2.09	0.47
1:J:634:HIS:HA	1:J:637:VAL:HG23	1.95	0.47
1:J:745:ASP:HB2	1:J:801:ASP:OD1	2.15	0.47
1:J:1242:ASN:HB3	1:J:1479:TYR:OH	2.15	0.47
2:K:2302:ASP:HB3	2:K:2368:TYR:OH	2.15	0.47
2:K:2506:ARG:HG3	2:K:2589:ALA:HB1	1.97	0.47
2:K:2879:LEU:HD22	2:K:2901:LEU:HD11	1.96	0.47
3:L:2968[A]:GLN:HA	3:L:2973[A]:THR:O	2.14	0.47
3:L:3074[B]:GLU:OE2	3:L:3208[B]:GLN:HG2	2.15	0.47
3:L:3298[B]:ASN:CB	3:L:3299[B]:LEU:C	2.86	0.47
1:M:995:ILE:HG22	1:M:999:LEU:HD22	1.97	0.47
3:O:2968[B]:GLN:C	3:X:2988[B]:TRP:CA	2.70	0.47
3:O:3109[B]:TYR:OH	3:X:2973[B]:THR:OG1	2.14	0.47
3:O:3137[A]:ARG:HB3	3:O:3139[A]:LEU:HD21	1.97	0.47
1:P:4:ARG:HD2	1:P:89:ILE:O	2.14	0.47
1:P:329:ARG:NH2	1:S:1574:VAL:H	2.13	0.47
1:P:411:ASP:HB3	1:P:658:TYR:OH	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:473:ALA:HB3	1:P:476:ARG:HG2	1.96	0.47
2:Q:2685:TYR:OH	2:Q:2886:VAL:HA	2.15	0.47
3:R:2935[B]:ILE:CG1	3:R:2936[B]:GLU:N	2.78	0.47
3:R:2970[B]:PRO:C	3:R:2972[B]:GLY:H	2.23	0.47
3:R:3230[B]:PHE:H	3:R:3243[B]:GLY:HA3	1.80	0.47
1:S:210:HIS:HA	1:S:213:VAL:HG22	1.97	0.47
1:S:245:GLU:OE1	1:S:249:ARG:NH1	2.48	0.47
1:S:428:ILE:HD12	1:S:514:TRP:HB3	1.96	0.47
1:S:904:HIS:HB3	1:S:1105:VAL:HG21	1.96	0.47
1:S:920:ASN:OD1	1:S:920:ASN:N	2.47	0.47
3:U:2935[B]:ILE:CG1	3:U:2936[B]:GLU:N	2.78	0.47
3:U:2960[A]:PHE:CD2	3:U:3157[A]:PRO:CG	2.74	0.47
3:U:3180[A]:TYR:CB	3:U:3183[A]:LEU:CD2	2.90	0.47
3:U:3196[B]:THR:CA	3:U:3199[B]:GLN:HB2	2.43	0.47
3:U:3200[B]:LEU:CD2	3:U:3204[B]:LEU:CD1	2.93	0.47
3:U:3217[B]:PHE:HD2	3:U:3300[B]:LEU:HD12	1.78	0.47
3:U:3228[B]:VAL:CG2	3:U:3245[B]:PHE:CE1	2.97	0.47
3:U:3256[B]:TRP:CE3	3:d:2973[B]:THR:N	2.77	0.47
3:U:3298[B]:ASN:CB	3:U:3299[B]:LEU:C	2.86	0.47
1:V:103:GLU:OE2	1:V:106:GLN:NE2	2.48	0.47
1:V:847:THR:O	1:V:851:MET:HG3	2.14	0.47
2:W:2286:HIS:CD2	2:W:2433:THR:HG22	2.50	0.47
3:X:2952[B]:ALA:N	3:X:2953[B]:GLY:HA2	2.06	0.47
3:X:3173[A]:THR:HG22	3:X:3174[A]:GLY:H	1.67	0.47
3:X:3196[B]:THR:O	3:X:3200[B]:LEU:N	2.44	0.47
3:X:3229[A]:ASN:OD1	3:X:3244[A]:THR:HB	2.14	0.47
3:X:3298[A]:ASN:CA	3:X:3299[A]:LEU:HB2	2.44	0.47
1:Y:59:LEU:HD13	1:Y:68:TRP:CD1	2.49	0.47
2:Z:2426:PHE:HB3	2:Z:2445:MET:HE1	1.97	0.47
2:Z:2661:MET:HE2	2:Z:2794:LEU:HD23	1.97	0.47
3:a:2937[A]:ASN:CB	3:a:3006[A]:LYS:CE	2.86	0.47
3:a:2960[B]:PHE:CD2	3:a:3157[B]:PRO:CG	2.74	0.47
3:a:2970[A]:PRO:C	3:a:2972[A]:GLY:H	2.23	0.47
3:a:2985[B]:PHE:CE2	3:a:2989[B]:HIS:NE2	2.83	0.47
3:a:3038[A]:ILE:HG23	3:a:3040[A]:VAL:HG22	1.90	0.47
2:c:2544:GLY:HA3	2:c:2699:MET:O	2.14	0.47
2:c:2571:ARG:HG3	2:c:2715:ASP:OD1	2.15	0.47
3:d:2952[A]:ALA:HB1	3:d:2957[A]:ILE:H	1.79	0.47
3:d:2952[B]:ALA:HB1	3:d:2957[B]:ILE:H	1.79	0.47
3:d:3161[A]:GLU:H	3:d:3161[A]:GLU:CD	2.19	0.47
3:d:3229[A]:ASN:OD1	3:d:3244[A]:THR:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ARG:HH12	1:A:743:ASN:CB	2.25	0.47
1:A:854:LEU:HG	1:A:959:PHE:HE2	1.80	0.47
1:A:1493:MET:O	1:A:1497:SER:HB3	2.15	0.47
1:A:1500:THR:HA	1:A:1501:ALA:HA	1.67	0.47
2:B:2189:GLY:HA2	2:B:2192:THR:HG22	1.96	0.47
3:C:2985[B]:PHE:CE2	3:C:2989[B]:HIS:NE2	2.83	0.47
3:C:3196[A]:THR:OG1	3:C:3199[A]:GLN:HG3	2.12	0.47
3:C:3225[A]:SER:C	3:C:3290[A]:ILE:HG23	2.39	0.47
1:D:830:ASN:HA	1:D:831:VAL:C	2.39	0.47
2:E:2504:ARG:HD3	2:E:2775:GLY:O	2.15	0.47
3:F:2970[A]:PRO:C	3:F:2972[A]:GLY:N	2.72	0.47
3:F:3074[B]:GLU:OE2	3:F:3208[B]:GLN:HG2	2.15	0.47
3:F:3074[B]:GLU:CD	3:F:3212[B]:ARG:NH2	2.73	0.47
3:F:3093[B]:HIS:HB2	3:F:3248[B]:LEU:HD13	1.94	0.47
3:F:3096[B]:VAL:HG11	3:F:3115[B]:LEU:HD12	1.89	0.47
3:F:3125[A]:ARG:O	3:F:3129[A]:ILE:HG13	2.14	0.47
3:F:3160[B]:SER:CB	3:a:2982[B]:MET:HB3	2.45	0.47
3:F:3196[B]:THR:OG1	3:F:3199[B]:GLN:CD	2.57	0.47
3:F:3255[B]:PRO:HG3	3:a:2963[B]:MET:N	2.30	0.47
3:F:3283[B]:ILE:HB	3:F:3305[B]:ILE:HD11	1.97	0.47
3:F:3284[A]:LYS:CE	3:F:3285[A]:VAL:H	2.28	0.47
1:G:180:ASN:OD1	1:G:344:LEU:HB2	2.15	0.47
1:G:223:LEU:HG	1:G:290:GLU:OE2	2.14	0.47
1:G:391:MET:HE3	1:G:391:MET:HB3	1.79	0.47
1:G:533:VAL:HG12	1:G:540:THR:HG22	1.96	0.47
1:G:852:ASN:O	1:G:856:THR:OG1	2.33	0.47
1:G:1302:SER:OG	1:G:1494:ARG:NH2	2.48	0.47
2:H:2151:PHE:HB3	2:H:2152:PRO:HD3	1.96	0.47
2:H:2161:GLN:OE1	2:H:2348:THR:HG21	2.14	0.47
2:H:2603:PRO:HG2	2:H:2606:LEU:HD12	1.96	0.47
3:I:3143[A]:SER:OG	3:I:3144[A]:ALA:N	2.46	0.47
3:I:3176[A]:LYS:N	3:I:3176[A]:LYS:CE	2.73	0.47
3:I:3196[A]:THR:CA	3:I:3199[A]:GLN:OE1	2.58	0.47
1:J:458:LEU:O	1:J:461:PHE:HB2	2.15	0.47
2:K:2571:ARG:HG3	2:K:2715:ASP:OD1	2.15	0.47
3:L:3004[B]:GLY:O	3:L:3006[B]:LYS:N	2.44	0.47
3:L:3014[B]:TRP:CD2	3:L:3092[B]:ILE:CD1	2.98	0.47
3:L:3196[A]:THR:CA	3:L:3199[A]:GLN:OE1	2.58	0.47
1:M:51:ASP:HA	1:M:52:GLY:HA2	1.58	0.47
1:M:931:TRP:HE3	1:M:991:LEU:HD13	1.80	0.47
1:M:958:PRO:O	1:M:959:PHE:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1596:GLU:O	1:M:1597:THR:HG22	2.14	0.47
3:O:2952[B]:ALA:HB1	3:O:2957[B]:ILE:H	1.79	0.47
3:O:3014[B]:TRP:CG	3:O:3092[B]:ILE:CD1	2.98	0.47
1:P:1018:ILE:HD12	1:P:1045:HIS:HD2	1.80	0.47
3:R:2985[A]:PHE:CE2	3:R:2989[A]:HIS:NE2	2.83	0.47
1:S:372:ALA:HB3	1:S:375:SER:HB3	1.96	0.47
1:S:855:ARG:HH21	1:S:941:LEU:HA	1.79	0.47
1:S:931:TRP:CD1	1:S:1048:ASN:HD22	2.33	0.47
1:S:1639:LYS:HZ1	4:BA:2:NAG:C8	2.28	0.47
2:T:2556:TYR:CE1	2:T:2844:MET:HG3	2.50	0.47
2:T:2745:PRO:HB2	2:T:2750:ILE:HD12	1.97	0.47
3:U:3125[B]:ARG:O	3:U:3129[B]:ILE:HG13	2.14	0.47
3:U:3148[A]:ILE:HG22	3:U:3152[A]:LYS:CE	2.44	0.47
3:U:3196[A]:THR:OG1	3:U:3199[A]:GLN:CD	2.57	0.47
1:V:1147:MET:HE1	1:V:1191:PRO:HG3	1.96	0.47
3:X:2933[B]:SER:CB	3:X:2936[B]:GLU:CB	2.85	0.47
3:X:2939[A]:ARG:HG3	3:X:2939[A]:ARG:NH1	2.28	0.47
3:X:2952[A]:ALA:HB1	3:X:2957[A]:ILE:H	1.79	0.47
3:X:3137[B]:ARG:HB3	3:X:3139[B]:LEU:HD21	1.97	0.47
3:X:3183[B]:LEU:N	3:X:3184[B]:ASN:HA	2.12	0.47
1:Y:531:THR:HG22	1:Y:542:PRO:HA	1.95	0.47
1:Y:602:THR:O	1:Y:605:SER:OG	2.29	0.47
1:Y:1620:LEU:CD1	3:d:3189[B]:ASN:CB	2.93	0.47
3:a:2954[A]:TYR:CA	3:a:2957[A]:ILE:HG22	2.43	0.47
3:a:3180[B]:TYR:CB	3:a:3183[B]:LEU:CD2	2.90	0.47
3:a:3196[B]:THR:O	3:a:3200[B]:LEU:N	2.44	0.47
1:b:48:LYS:HA	1:b:55:ILE:HG13	1.97	0.47
1:b:119:LYS:HB2	1:b:120:LYS:C	2.40	0.47
2:c:2180:TRP:HB2	2:c:2243:LEU:HD13	1.97	0.47
3:d:3014[A]:TRP:CD2	3:d:3092[A]:ILE:CD1	2.98	0.47
3:d:3284[B]:LYS:CE	3:d:3284[B]:LYS:CA	2.85	0.47
3:d:3284[B]:LYS:CE	3:d:3285[B]:VAL:H	2.28	0.47
1:A:467:LYS:HB2	1:A:479:CYS:SG	2.54	0.47
1:A:874:ALA:HA	1:A:913:PHE:CZ	2.50	0.47
1:A:949:ASP:OD1	1:A:950:ALA:N	2.47	0.47
3:C:3298[B]:ASN:CA	3:C:3299[B]:LEU:HB2	2.44	0.47
1:D:17:ASN:OD1	1:D:85:SER:N	2.47	0.47
1:D:456:GLN:O	1:D:460:GLU:HG3	2.15	0.47
3:F:2933[A]:SER:HA	3:F:2935[A]:ILE:HD11	1.95	0.47
3:F:2949[A]:LYS:C	3:F:2953[A]:GLY:N	2.73	0.47
3:F:2949[B]:LYS:C	3:F:2953[B]:GLY:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2965[A]:LEU:HD22	3:F:2975[A]:PHE:O	2.15	0.47
3:F:2967[B]:CYS:HB2	3:a:2980[B]:HIS:N	2.30	0.47
3:F:2970[B]:PRO:C	3:F:2972[B]:GLY:N	2.72	0.47
3:F:3150[B]:LYS:CA	3:a:3172[B]:SER:HB3	2.45	0.47
3:F:3191[A]:ASN:C	3:F:3192[A]:PHE:O	2.52	0.47
3:F:3200[B]:LEU:CD2	3:F:3204[B]:LEU:CD1	2.93	0.47
1:G:1319:PHE:CE2	1:G:1424:GLU:HG3	2.50	0.47
3:I:3283[A]:ILE:HB	3:I:3305[A]:ILE:HD11	1.97	0.47
1:J:1209:ASP:O	1:J:1211:TYR:HD2	1.98	0.47
2:K:2132:CYS:HB2	2:K:2142:ALA:CB	2.45	0.47
3:L:2935[A]:ILE:CG1	3:L:2936[A]:GLU:N	2.78	0.47
3:L:2940[B]:ASN:O	3:L:2944[B]:ALA:N	2.48	0.47
3:L:3148[B]:ILE:HG22	3:L:3152[B]:LYS:CE	2.44	0.47
1:M:67:MET:HE1	1:M:233:PRO:CG	2.45	0.47
2:N:2115:SER:OG	2:N:2116:SER:N	2.47	0.47
2:N:2382:GLU:O	2:N:2386:ARG:HG3	2.14	0.47
3:O:2940[A]:ASN:O	3:O:2944[A]:ALA:N	2.48	0.47
3:O:2985[A]:PHE:CE2	3:O:2989[A]:HIS:NE2	2.83	0.47
3:O:3200[B]:LEU:CD2	3:O:3204[B]:LEU:CD1	2.93	0.47
3:O:3220[B]:ARG:HH11	3:O:3220[B]:ARG:CG	2.12	0.47
3:O:3293[B]:LYS:HB2	3:O:3294[B]:SER:CA	2.41	0.47
1:P:103:GLU:OE2	1:P:106:GLN:NE2	2.48	0.47
1:P:739:GLN:N	1:P:739:GLN:OE1	2.48	0.47
1:P:797:THR:HG22	1:P:798:LEU:H	1.80	0.47
2:Q:2190:LEU:O	2:Q:2209:PHE:HB2	2.15	0.47
3:R:2954[A]:TYR:CA	3:R:2957[A]:ILE:HG22	2.43	0.47
3:R:2965[B]:LEU:HD22	3:R:2975[B]:PHE:O	2.15	0.47
3:R:2980[A]:HIS:ND1	3:R:2980[A]:HIS:N	2.60	0.47
3:R:3074[A]:GLU:OE2	3:R:3208[A]:GLN:HG2	2.15	0.47
1:S:712:SER:O	1:S:716:LEU:N	2.48	0.47
1:S:1019:HIS:CE1	1:S:1046:HIS:HE1	2.31	0.47
1:S:1462:ASP:O	1:S:1465:TRP:HB3	2.15	0.47
1:S:1578:ILE:HA	1:S:1579:GLY:HA2	1.64	0.47
2:T:2569:TRP:O	2:T:2572:VAL:HG23	2.14	0.47
3:U:2985[B]:PHE:CE2	3:U:2989[B]:HIS:NE2	2.83	0.47
3:U:3014[B]:TRP:CD2	3:U:3092[B]:ILE:CD1	2.98	0.47
3:U:3148[B]:ILE:HG22	3:U:3152[B]:LYS:CE	2.44	0.47
3:U:3196[B]:THR:O	3:U:3200[B]:LEU:N	2.43	0.47
3:U:3298[A]:ASN:CB	3:U:3300[A]:LEU:CD2	2.61	0.47
1:V:430:SER:O	1:V:933:ARG:NH2	2.41	0.47
1:V:554:LYS:HA	1:V:554:LYS:HD3	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:871:GLN:O	1:V:875:ALA:N	2.48	0.47
1:V:1019:HIS:NE2	1:V:1046:HIS:HE1	2.13	0.47
2:W:2089:ARG:HB2	2:W:2368:TYR:CD1	2.50	0.47
2:W:2344:LEU:HD23	2:W:2349:THR:OG1	2.15	0.47
2:W:2562:GLY:H	2:W:2846:TRP:HB2	1.79	0.47
3:X:2940[B]:ASN:O	3:X:2944[B]:ALA:N	2.48	0.47
3:X:2952[A]:ALA:N	3:X:2953[A]:GLY:HA2	2.06	0.47
3:X:2952[B]:ALA:HB1	3:X:2957[B]:ILE:H	1.79	0.47
3:X:3203[B]:HIS:O	3:X:3206[B]:LYS:HB3	2.15	0.47
3:X:3218[B]:LEU:HD12	3:X:3218[B]:LEU:HA	1.78	0.47
1:Y:830:ASN:OD1	1:Y:832:LYS:HB2	2.15	0.47
1:Y:1427:HIS:HD2	1:Y:1457:HIS:CE1	2.33	0.47
1:Y:1617:LYS:CE	3:d:3180[B]:TYR:CZ	2.97	0.47
3:a:2949[B]:LYS:C	3:a:2953[B]:GLY:N	2.73	0.47
3:a:3014[B]:TRP:CG	3:a:3092[B]:ILE:CD1	2.98	0.47
3:a:3148[B]:ILE:HG22	3:a:3152[B]:LYS:CE	2.44	0.47
3:a:3228[A]:VAL:CG2	3:a:3245[A]:PHE:CE1	2.97	0.47
1:b:1013:ILE:HG21	1:b:1192:TYR:CD1	2.49	0.47
1:b:1142:VAL:HG22	1:b:1236:TYR:HD1	1.80	0.47
2:c:2669:TYR:HA	2:c:2721:TRP:CH2	2.50	0.47
3:d:2935[A]:ILE:CG1	3:d:2936[A]:GLU:N	2.78	0.47
3:d:3191[B]:ASN:C	3:d:3192[B]:PHE:O	2.52	0.47
3:d:3225[A]:SER:C	3:d:3290[A]:ILE:HG23	2.39	0.47
5:FA:1:NAG:H61	5:FA:2:NAG:C1	2.45	0.47
1:A:104:LEU:HD23	1:A:123:PHE:CE2	2.50	0.46
1:A:1160:PHE:HB3	1:A:1171:LYS:HA	1.97	0.46
1:A:1324:ARG:NH1	1:A:1516:VAL:O	2.48	0.46
3:C:2965[B]:LEU:HD22	3:C:2975[B]:PHE:O	2.16	0.46
3:C:3293[A]:LYS:HB2	3:C:3294[A]:SER:CA	2.41	0.46
1:D:637:VAL:HA	1:D:640:LEU:HD12	1.96	0.46
2:E:2128:LEU:HD13	2:E:2286:HIS:CG	2.50	0.46
2:E:2867:PRO:O	2:E:2870:LEU:HB3	2.14	0.46
3:F:3014[B]:TRP:CG	3:F:3092[B]:ILE:CD1	2.98	0.46
3:F:3079[A]:CYS:SG	3:F:3146[A]:CYS:O	2.73	0.46
3:F:3160[B]:SER:CB	3:a:2983[B]:VAL:H	2.28	0.46
1:G:695:TYR:N	1:G:695:TYR:CD1	2.81	0.46
1:G:883:CYS:O	1:G:885:SER:N	2.48	0.46
3:I:2940[A]:ASN:O	3:I:2944[A]:ALA:N	2.48	0.46
3:I:2940[B]:ASN:O	3:I:2944[B]:ALA:N	2.48	0.46
3:I:2968[B]:GLN:HE21	3:R:3086[B]:GLU:HG2	0.41	0.46
3:I:2970[A]:PRO:C	3:I:2972[A]:GLY:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2982[B]:MET:SD	3:R:2967[B]:CYS:SG	3.13	0.46
3:I:3074[B]:GLU:OE2	3:I:3208[B]:GLN:HG2	2.15	0.46
3:I:3119[B]:HIS:NE2	3:R:2971[B]:ASP:HA	2.24	0.46
3:I:3160[B]:SER:CA	3:R:2983[B]:VAL:N	2.35	0.46
3:I:3229[A]:ASN:OD1	3:I:3244[A]:THR:HB	2.14	0.46
3:I:3283[B]:ILE:HB	3:I:3305[B]:ILE:HD11	1.97	0.46
1:J:232:ARG:HA	1:J:233:PRO:HD3	1.79	0.46
1:J:1299:GLN:O	1:J:1301:PRO:HD3	2.14	0.46
1:J:1404:TYR:O	1:J:1407:THR:OG1	2.29	0.46
2:K:2822:LYS:HG2	2:K:2831:GLU:HA	1.96	0.46
3:L:3014[A]:TRP:CD2	3:L:3092[A]:ILE:CD1	2.98	0.46
3:L:3014[B]:TRP:CG	3:L:3092[B]:ILE:CD1	2.98	0.46
3:L:3183[A]:LEU:H	3:L:3184[A]:ASN:CA	2.22	0.46
3:L:3284[A]:LYS:CE	3:L:3285[A]:VAL:H	2.28	0.46
3:L:3284[B]:LYS:HD3	3:L:3285[B]:VAL:O	2.16	0.46
1:M:306:PHE:HB3	1:M:308:LEU:HD13	1.96	0.46
1:M:330:GLN:H	1:M:330:GLN:HG3	1.49	0.46
1:M:1505:ARG:O	1:M:1509:THR:OG1	2.33	0.46
2:N:2377:SER:HB3	2:N:2380:GLN:HG3	1.96	0.46
2:N:2622:ASN:O	2:N:2625:LEU:HD12	2.15	0.46
3:O:2994[B]:LYS:HE2	3:O:3183[B]:LEU:O	2.14	0.46
3:O:3200[A]:LEU:CD2	3:O:3204[A]:LEU:CD1	2.93	0.46
3:O:3230[A]:PHE:H	3:O:3243[A]:GLY:HA3	1.79	0.46
3:O:3255[B]:PRO:HG2	3:X:3163[B]:ASN:ND2	2.29	0.46
1:P:643:ILE:HD13	1:P:708:PHE:HB2	1.97	0.46
1:P:656:LYS:HB2	1:P:658:TYR:CE1	2.50	0.46
1:P:867:VAL:O	1:P:868:THR:OG1	2.22	0.46
1:P:949:ASP:CG	1:P:950:ALA:H	2.22	0.46
1:P:1046:HIS:HA	1:P:1049:VAL:HB	1.97	0.46
1:P:1143:ALA:HA	1:P:1195:ASP:O	2.15	0.46
1:P:1180:SER:OG	1:P:1181:GLU:N	2.47	0.46
1:P:1313:LEU:HD23	1:P:1318:VAL:HG23	1.96	0.46
2:Q:2572:VAL:HG13	2:Q:2768:LEU:HD21	1.95	0.46
2:Q:2599:SER:O	2:Q:2645:PHE:HB3	2.15	0.46
3:R:2965[B]:LEU:CD1	3:R:2974[B]:ALA:CA	2.89	0.46
3:R:2987[A]:HIS:O	3:R:2991[A]:LEU:HB2	2.15	0.46
3:R:3014[A]:TRP:CD2	3:R:3092[A]:ILE:CD1	2.98	0.46
3:R:3079[B]:CYS:SG	3:R:3146[B]:CYS:O	2.74	0.46
3:R:3148[B]:ILE:HG22	3:R:3152[B]:LYS:CE	2.44	0.46
1:S:353:ASN:HD22	1:S:772:ARG:NH2	2.12	0.46
1:S:588:GLU:HG3	1:S:724:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:2871:PHE:HZ	1:V:1071:ASN:HD22	1.61	0.46
3:U:2961[B]:HIS:CD2	3:U:2988[B]:TRP:CZ3	2.96	0.46
3:U:3014[A]:TRP:CG	3:U:3092[A]:ILE:CD1	2.98	0.46
3:U:3074[B]:GLU:CD	3:U:3212[B]:ARG:NH2	2.73	0.46
1:V:324:PRO:HG2	1:V:376:ASN:ND2	2.30	0.46
1:V:331:SER:HB2	1:Y:1581:GLU:OE2	2.14	0.46
2:W:2218:SER:OG	2:W:2221:THR:OG1	2.24	0.46
3:X:2932[B]:PRO:CA	3:X:2935[B]:ILE:CD1	2.85	0.46
3:X:3074[A]:GLU:OE2	3:X:3208[A]:GLN:HG2	2.15	0.46
3:X:3074[B]:GLU:OE2	3:X:3208[B]:GLN:HG2	2.15	0.46
3:X:3225[B]:SER:C	3:X:3290[B]:ILE:HG23	2.39	0.46
1:Y:630:PHE:O	1:Y:633:HIS:HB3	2.15	0.46
1:Y:859:ALA:N	1:Y:957:ASN:HD21	2.13	0.46
2:Z:2866:PRO:CG	3:a:2933[A]:SER:CB	2.93	0.46
3:a:3114[B]:PRO:CD	3:a:3115[B]:LEU:N	2.72	0.46
3:a:3180[A]:TYR:CB	3:a:3183[A]:LEU:CD2	2.89	0.46
1:b:385:ALA:HB2	1:b:391:MET:HG3	1.97	0.46
2:c:2638:ARG:NH1	2:c:2706:ILE:HG13	2.30	0.46
3:d:3273[B]:LEU:HB2	3:d:3275[B]:LEU:CD1	2.34	0.46
3:d:3284[B]:LYS:HD3	3:d:3285[B]:VAL:O	2.16	0.46
1:A:121:ASN:HD21	1:A:123:PHE:HB2	1.80	0.46
1:A:1163:ALA:HA	1:A:1211:TYR:H	1.80	0.46
2:B:2539:ILE:O	2:B:2573:TYR:OH	2.14	0.46
2:B:2830:GLN:HB2	2:B:2863:ARG:NH1	2.31	0.46
3:C:2969[B]:TYR:CD2	3:C:2970[B]:PRO:N	2.83	0.46
3:C:2975[B]:PHE:O	3:L:3256[B]:TRP:NE1	2.49	0.46
3:C:3229[B]:ASN:OD1	3:C:3244[B]:THR:HB	2.14	0.46
1:D:452:ILE:HD11	1:D:676:PRO:O	2.16	0.46
1:D:729:VAL:HG11	1:D:785:LEU:HD12	1.97	0.46
1:D:1551:ASP:HB3	1:D:1652:PHE:HE1	1.79	0.46
2:E:2131:LEU:HD12	2:E:2335:PRO:HG3	1.97	0.46
3:F:2940[B]:ASN:O	3:F:2944[B]:ALA:N	2.48	0.46
3:F:2949[A]:LYS:NZ	3:F:2949[A]:LYS:C	2.73	0.46
3:F:2954[A]:TYR:CA	3:F:2957[A]:ILE:HG22	2.43	0.46
3:F:2987[B]:HIS:O	3:F:2991[B]:LEU:HB2	2.16	0.46
3:F:3004[B]:GLY:C	3:F:3006[B]:LYS:N	2.74	0.46
3:F:3014[A]:TRP:CG	3:F:3092[A]:ILE:CD1	2.98	0.46
3:F:3151[B]:LEU:HB2	3:F:3175[B]:TYR:HE2	1.68	0.46
3:F:3153[B]:LYS:HB3	3:a:3155[B]:MET:N	2.30	0.46
3:F:3258[B]:PHE:HA	3:a:3162[B]:ASP:OD2	2.15	0.46
3:F:3284[B]:LYS:HD3	3:F:3285[B]:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:801:ASP:OD1	1:G:801:ASP:N	2.46	0.46
1:G:1013:ILE:HG21	1:G:1192:TYR:CD1	2.50	0.46
1:G:1482:ALA:HB2	1:G:1517:PHE:HZ	1.80	0.46
3:I:3014[B]:TRP:CD2	3:I:3092[B]:ILE:CD1	2.98	0.46
3:I:3079[A]:CYS:SG	3:I:3146[A]:CYS:O	2.74	0.46
3:I:3223[B]:GLY:N	3:R:2963[B]:MET:HE1	2.30	0.46
1:J:136:ALA:HB3	2:N:2619:VAL:HB	1.97	0.46
3:L:2949[B]:LYS:C	3:L:2953[B]:GLY:N	2.73	0.46
3:L:3146[A]:CYS:HA	3:L:3147[A]:GLU:HA	1.70	0.46
3:L:3146[B]:CYS:HA	3:L:3147[B]:GLU:HA	1.70	0.46
3:L:3288[A]:MET:CA	3:L:3295[A]:LEU:HG	2.42	0.46
1:M:302:ALA:H	1:M:363:THR:HB	1.81	0.46
1:M:464:LEU:HD22	1:M:622:HIS:HB3	1.97	0.46
1:M:996:ILE:HG23	1:M:1133:ILE:HG22	1.97	0.46
1:M:1045:HIS:HB3	1:M:1046:HIS:HD1	1.81	0.46
1:M:1303:GLU:N	1:M:1303:GLU:OE1	2.48	0.46
1:M:1331:GLU:HB2	1:M:1343:VAL:CG2	2.45	0.46
2:N:2590:VAL:HA	2:N:2591:PRO:HD3	1.81	0.46
3:O:2949[A]:LYS:C	3:O:2953[A]:GLY:N	2.72	0.46
3:O:2970[A]:PRO:C	3:O:2972[A]:GLY:H	2.23	0.46
3:O:2971[B]:ASP:C	3:X:2988[B]:TRP:HE3	2.23	0.46
3:O:3014[B]:TRP:CD2	3:O:3092[B]:ILE:CD1	2.98	0.46
3:O:3147[B]:GLU:CG	3:O:3149[B]:ASN:ND2	2.73	0.46
3:O:3151[A]:LEU:CB	3:O:3175[A]:TYR:CD2	2.93	0.46
3:O:3203[B]:HIS:O	3:O:3206[B]:LYS:HB3	2.16	0.46
3:O:3298[B]:ASN:CA	3:O:3299[B]:LEU:HB2	2.44	0.46
1:P:416:ASN:HD22	1:P:416:ASN:H	1.62	0.46
2:Q:2903:TYR:O	2:Q:2905:PRO:HD3	2.16	0.46
3:R:2965[A]:LEU:HD13	3:R:2975[A]:PHE:O	2.16	0.46
3:R:3151[A]:LEU:HB2	3:R:3175[A]:TYR:HE2	1.68	0.46
3:R:3284[A]:LYS:HD3	3:R:3285[A]:VAL:O	2.16	0.46
3:R:3298[B]:ASN:CA	3:R:3299[B]:LEU:CB	2.85	0.46
1:S:4:ARG:HD2	1:S:89:ILE:O	2.15	0.46
1:S:1438:ASP:OD1	1:S:1439:VAL:N	2.48	0.46
2:T:2131:LEU:CD1	2:T:2335:PRO:HB3	2.46	0.46
3:U:2949[A]:LYS:NZ	3:U:2949[A]:LYS:C	2.73	0.46
3:U:2949[B]:LYS:NZ	3:U:2949[B]:LYS:C	2.73	0.46
3:U:2970[A]:PRO:C	3:U:2972[A]:GLY:H	2.23	0.46
3:U:3074[B]:GLU:OE2	3:U:3208[B]:GLN:HG2	2.15	0.46
3:U:3137[A]:ARG:HB3	3:U:3139[A]:LEU:HD21	1.97	0.46
3:X:3219[A]:LEU:N	3:X:3219[A]:LEU:CD2	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3284[A]:LYS:HD3	3:X:3285[A]:VAL:O	2.16	0.46
1:Y:220:TRP:CZ3	1:Y:223:LEU:HD22	2.50	0.46
3:a:2935[B]:ILE:CG1	3:a:2936[B]:GLU:N	2.78	0.46
3:a:3014[B]:TRP:CD2	3:a:3092[B]:ILE:CD1	2.98	0.46
3:a:3104[B]:MET:HA	3:a:3110[B]:THR:CG2	2.17	0.46
3:a:3125[A]:ARG:O	3:a:3129[A]:ILE:HG13	2.14	0.46
3:a:3230[A]:PHE:H	3:a:3243[A]:GLY:HA3	1.79	0.46
3:d:2938[B]:LEU:O	3:d:2939[B]:ARG:C	2.58	0.46
3:d:2940[B]:ASN:O	3:d:2944[B]:ALA:N	2.48	0.46
3:d:2965[A]:LEU:HD22	3:d:2975[A]:PHE:O	2.15	0.46
3:d:2969[B]:TYR:CD2	3:d:2970[B]:PRO:N	2.83	0.46
3:d:3146[B]:CYS:HA	3:d:3147[B]:GLU:HA	1.70	0.46
1:A:733:PHE:CE2	1:A:818:PRO:HG3	2.51	0.46
2:B:2743:ALA:HB1	1:D:1210:LYS:HG3	1.97	0.46
3:C:2965[A]:LEU:HD13	3:C:2975[A]:PHE:O	2.16	0.46
3:C:2969[A]:TYR:CD2	3:C:2970[A]:PRO:N	2.83	0.46
3:C:3014[A]:TRP:CD2	3:C:3092[A]:ILE:CD1	2.98	0.46
3:C:3137[A]:ARG:HD3	3:C:3137[A]:ARG:HA	1.71	0.46
3:C:3284[B]:LYS:CE	3:C:3285[B]:VAL:H	2.29	0.46
1:D:493:LEU:HD12	1:D:668:MET:HG3	1.97	0.46
1:D:1271:MET:HG2	1:D:1358:LEU:HD13	1.97	0.46
1:D:1323:HIS:CD2	9:D:5004:CUO:O1	2.68	0.46
1:D:1622:GLN:HG2	1:D:1652:PHE:CD1	2.50	0.46
2:E:2582:ARG:HA	2:E:2586:ALA:HB3	1.97	0.46
2:E:2720:ILE:HG12	2:E:2781:LEU:HG	1.97	0.46
3:F:3074[A]:GLU:OE2	3:F:3208[A]:GLN:HG2	2.16	0.46
3:F:3230[B]:PHE:H	3:F:3243[B]:GLY:HA3	1.80	0.46
1:G:252:ASN:HD22	1:G:258:LYS:HB2	1.81	0.46
1:G:357:PRO:HB3	1:G:774:ASP:HB2	1.97	0.46
1:G:403:TYR:O	1:G:658:TYR:HB3	2.15	0.46
1:G:928:TYR:HB2	1:G:1048:ASN:HB2	1.98	0.46
1:G:1146:PHE:HZ	1:G:1159:TYR:CG	2.33	0.46
1:G:1250:ILE:O	1:G:1473:ARG:NH2	2.47	0.46
3:I:2965[A]:LEU:HD22	3:I:2975[A]:PHE:O	2.15	0.46
3:I:2968[A]:GLN:HA	3:I:2973[A]:THR:O	2.14	0.46
3:I:2968[B]:GLN:OE1	3:R:2981[B]:GLY:HA2	2.15	0.46
3:I:2970[B]:PRO:C	3:I:2972[B]:GLY:H	2.23	0.46
3:I:2988[B]:TRP:CD1	3:R:3153[B]:LYS:HD3	2.51	0.46
3:I:2992[B]:TYR:HE2	3:R:2969[B]:TYR:CE1	2.33	0.46
3:I:3004[B]:GLY:C	3:I:3006[B]:LYS:N	2.74	0.46
3:I:3074[A]:GLU:OE2	3:I:3208[A]:GLN:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3106[B]:THR:C	3:R:2973[B]:THR:HG21	2.40	0.46
1:J:55:ILE:HG21	1:J:350:MET:HA	1.97	0.46
1:J:640:LEU:HD23	1:J:643:ILE:HD12	1.98	0.46
2:K:2533:ASP:OD1	2:K:2533:ASP:N	2.49	0.46
3:L:2965[A]:LEU:HD22	3:L:2975[A]:PHE:O	2.15	0.46
3:L:3074[A]:GLU:OE2	3:L:3208[A]:GLN:HG2	2.15	0.46
3:L:3200[A]:LEU:CD2	3:L:3204[A]:LEU:CD1	2.93	0.46
3:L:3298[A]:ASN:CB	3:L:3299[A]:LEU:C	2.86	0.46
1:M:4:ARG:NH1	1:M:77:GLU:OE1	2.48	0.46
1:M:148:GLN:O	1:M:150:GLY:N	2.49	0.46
1:M:450:LYS:HE3	1:M:451:SER:H	1.80	0.46
3:O:2935[A]:ILE:CG1	3:O:2936[A]:GLU:N	2.78	0.46
3:O:2935[B]:ILE:CG1	3:O:2936[B]:GLU:N	2.78	0.46
3:O:2970[A]:PRO:C	3:O:2972[A]:GLY:N	2.72	0.46
3:O:2970[B]:PRO:O	3:X:2989[B]:HIS:CB	2.63	0.46
3:O:3074[A]:GLU:CD	3:O:3212[A]:ARG:NH2	2.73	0.46
3:O:3074[B]:GLU:CD	3:O:3212[B]:ARG:NH2	2.73	0.46
3:O:3079[B]:CYS:SG	3:O:3146[B]:CYS:O	2.73	0.46
3:O:3156[B]:MET:CE	3:X:3173[B]:THR:HG23	2.45	0.46
3:O:3159[B]:SER:N	3:X:3148[B]:ILE:O	2.47	0.46
3:O:3203[A]:HIS:O	3:O:3206[A]:LYS:HB3	2.16	0.46
3:O:3284[A]:LYS:HD3	3:O:3285[A]:VAL:O	2.16	0.46
1:P:53:SER:O	1:P:55:ILE:HG13	2.15	0.46
3:R:2985[B]:PHE:CE2	3:R:2989[B]:HIS:NE2	2.83	0.46
3:R:3014[A]:TRP:CG	3:R:3092[A]:ILE:CD1	2.98	0.46
1:S:227:ARG:HE	1:S:227:ARG:HB2	1.34	0.46
1:S:355:ALA:HA	1:S:734:LEU:HD12	1.97	0.46
1:S:881:GLN:OE1	1:S:891:LYS:HE2	2.15	0.46
1:S:1403:LEU:HD21	1:S:1429:THR:HG21	1.95	0.46
2:T:2168:ARG:O	2:W:2503:ASN:HB3	2.15	0.46
2:T:2235:PRO:HG3	2:T:2240:GLN:NE2	2.30	0.46
2:T:2528:LYS:HA	2:T:2536:PHE:HB3	1.97	0.46
2:T:2651:GLN:H	2:T:2652:LYS:HE2	1.79	0.46
3:U:2987[B]:HIS:O	3:U:2991[B]:LEU:HB2	2.16	0.46
3:U:3014[A]:TRP:CD2	3:U:3092[A]:ILE:CD1	2.98	0.46
3:U:3220[B]:ARG:HG2	3:U:3221[B]:ALA:N	2.09	0.46
3:U:3220[B]:ARG:HH11	3:U:3220[B]:ARG:CG	2.12	0.46
3:U:3293[A]:LYS:HB2	3:U:3294[A]:SER:CA	2.41	0.46
1:V:133:LYS:HA	1:V:134:VAL:HA	1.82	0.46
1:V:1016:ASN:HD22	1:V:1177:VAL:HA	1.81	0.46
3:X:2985[B]:PHE:CE2	3:X:2989[B]:HIS:NE2	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3014[B]:TRP:CG	3:X:3092[B]:ILE:CD1	2.98	0.46
3:X:3079[A]:CYS:SG	3:X:3146[A]:CYS:O	2.74	0.46
3:X:3151[B]:LEU:CB	3:X:3175[B]:TYR:CD2	2.93	0.46
3:X:3203[A]:HIS:O	3:X:3206[A]:LYS:HB3	2.16	0.46
1:Y:250:ASP:HA	1:Y:258:LYS:NZ	2.30	0.46
1:Y:1149:GLU:HG3	1:Y:1187:LYS:HB3	1.97	0.46
1:Y:1166:THR:N	1:Y:1167:ASP:HA	2.30	0.46
2:Z:2094:ARG:CZ	2:c:2370:MET:HE1	2.45	0.46
2:Z:2156:ARG:HD2	2:Z:2357:VAL:HG12	1.97	0.46
2:Z:2572:VAL:HG22	2:Z:2768:LEU:CD2	2.44	0.46
2:Z:2800:LYS:C	3:a:3023[A]:ILE:HD13	2.40	0.46
2:Z:2816:SER:HB2	2:Z:2886:VAL:HB	1.97	0.46
3:a:3024[B]:LEU:CD1	3:a:3024[B]:LEU:C	2.85	0.46
3:a:3185[B]:TYR:CE2	3:a:3187[B]:TYR:HE2	2.31	0.46
1:b:306:PHE:HB3	1:b:308:LEU:HD13	1.98	0.46
2:c:2495:ASN:HD22	2:c:2495:ASN:HA	1.57	0.46
2:c:2885:SER:OG	2:c:2886:VAL:N	2.49	0.46
3:d:2940[A]:ASN:O	3:d:2944[A]:ALA:N	2.48	0.46
3:d:2965[A]:LEU:HD13	3:d:2975[A]:PHE:O	2.16	0.46
3:d:2965[B]:LEU:HD22	3:d:2975[B]:PHE:O	2.15	0.46
3:d:2985[B]:PHE:CE2	3:d:2989[B]:HIS:NE2	2.83	0.46
3:d:3014[A]:TRP:CG	3:d:3092[A]:ILE:CD1	2.98	0.46
3:d:3074[B]:GLU:OE2	3:d:3208[B]:GLN:HG2	2.15	0.46
3:d:3180[B]:TYR:CB	3:d:3183[B]:LEU:CD2	2.89	0.46
3:d:3225[B]:SER:C	3:d:3290[B]:ILE:HG23	2.39	0.46
4:7:1:NAG:H62	4:7:2:NAG:N2	2.31	0.46
1:A:150:GLY:HA2	1:A:152:LYS:N	2.30	0.46
1:A:361:GLU:HG2	1:A:363:THR:HG22	1.97	0.46
1:A:885:SER:HB3	1:A:891:LYS:NZ	2.29	0.46
1:A:1059:LEU:HD11	1:A:1129:LEU:HD23	1.97	0.46
1:A:1485:ALA:O	1:A:1489:MET:HG2	2.15	0.46
2:B:2394:VAL:HG11	2:B:2451:LEU:HD12	1.98	0.46
3:C:2970[B]:PRO:C	3:C:2972[B]:GLY:H	2.23	0.46
3:C:2987[B]:HIS:O	3:C:2991[B]:LEU:HB2	2.16	0.46
3:C:3004[B]:GLY:C	3:C:3006[B]:LYS:N	2.73	0.46
3:C:3079[A]:CYS:SG	3:C:3146[A]:CYS:O	2.74	0.46
3:C:3159[B]:SER:OG	3:L:3151[B]:LEU:HA	2.15	0.46
3:C:3169[B]:LYS:CG	3:L:3149[B]:ASN:CG	2.49	0.46
3:C:3173[B]:THR:HG23	3:L:3173[B]:THR:OG1	2.16	0.46
3:C:3283[B]:ILE:HB	3:C:3305[B]:ILE:HD11	1.97	0.46
3:C:3284[B]:LYS:HD3	3:C:3285[B]:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:987:LYS:HD2	1:D:988:TYR:CE1	2.51	0.46
2:E:2472:ASN:HB2	2:E:2474:THR:H	1.80	0.46
3:F:2940[A]:ASN:O	3:F:2944[A]:ALA:N	2.48	0.46
3:F:3155[B]:MET:HG3	3:a:3154[B]:PRO:HD2	1.97	0.46
3:F:3161[A]:GLU:H	3:F:3161[A]:GLU:CD	2.19	0.46
3:F:3174[B]:GLY:CA	3:a:3154[B]:PRO:CD	2.85	0.46
3:F:3209[B]:GLU:O	3:F:3310[B]:GLY:C	2.59	0.46
3:F:3288[B]:MET:CA	3:F:3295[B]:LEU:HG	2.42	0.46
1:G:1617:LYS:O	3:L:3197[B]:ILE:HD12	2.14	0.46
3:I:2937[A]:ASN:CB	3:I:3006[A]:LYS:CE	2.86	0.46
3:I:3161[B]:GLU:C	3:R:3147[B]:GLU:HG3	2.40	0.46
3:I:3161[B]:GLU:CA	3:R:3147[B]:GLU:HG2	2.46	0.46
3:I:3255[B]:PRO:CB	3:R:2959[B]:SER:HB3	2.40	0.46
3:I:3264[A]:TYR:HD1	3:I:3265[A]:ASP:N	2.14	0.46
3:I:3284[B]:LYS:HD3	3:I:3285[B]:VAL:O	2.15	0.46
1:J:164:GLU:CG	1:J:297:ARG:HE	2.28	0.46
1:J:518:LYS:HD2	1:J:519:PRO:HD2	1.96	0.46
1:J:912:ASN:ND2	1:J:1093:ASP:OD2	2.48	0.46
1:J:1163:ALA:O	1:J:1167:ASP:HB3	2.16	0.46
2:K:2682:SER:HA	2:K:2836:PHE:CD2	2.51	0.46
2:K:2792:GLU:OE2	2:K:2796:GLN:NE2	2.41	0.46
3:L:2965[B]:LEU:HD13	3:L:2975[B]:PHE:O	2.16	0.46
3:L:2969[A]:TYR:CD2	3:L:2970[A]:PRO:N	2.83	0.46
3:L:2985[A]:PHE:CE2	3:L:2989[A]:HIS:NE2	2.83	0.46
3:L:3196[B]:THR:CA	3:L:3199[B]:GLN:OE1	2.58	0.46
3:L:3203[B]:HIS:O	3:L:3206[B]:LYS:HB3	2.16	0.46
3:L:3232[A]:VAL:HG23	3:L:3273[A]:LEU:HD11	1.95	0.46
3:L:3298[B]:ASN:CA	3:L:3299[B]:LEU:CB	2.86	0.46
1:M:729:VAL:HG11	1:M:785:LEU:HD12	1.98	0.46
2:N:2631:TYR:H	2:N:2631:TYR:HD1	1.63	0.46
3:O:2965[A]:LEU:HD22	3:O:2975[A]:PHE:O	2.15	0.46
3:O:2969[A]:TYR:CD2	3:O:2970[A]:PRO:N	2.83	0.46
3:O:2985[B]:PHE:CE2	3:O:2989[B]:HIS:NE2	2.83	0.46
3:O:3014[A]:TRP:CD2	3:O:3092[A]:ILE:CD1	2.98	0.46
3:O:3038[B]:ILE:HG23	3:O:3040[B]:VAL:HG22	1.90	0.46
3:O:3074[A]:GLU:OE2	3:O:3208[A]:GLN:HG2	2.15	0.46
3:O:3209[A]:GLU:O	3:O:3310[A]:GLY:C	2.59	0.46
3:O:3283[B]:ILE:C	3:O:3283[B]:ILE:CD1	2.85	0.46
3:O:3284[B]:LYS:HD3	3:O:3285[B]:VAL:O	2.16	0.46
1:P:187:GLY:HA3	1:P:195:SER:HB3	1.97	0.46
1:P:575:ASP:OD1	1:P:575:ASP:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:792:MET:HB2	1:P:793:PHE:HD1	1.80	0.46
3:R:2970[A]:PRO:C	3:R:2972[A]:GLY:H	2.23	0.46
3:R:3014[B]:TRP:CD2	3:R:3092[B]:ILE:CD1	2.98	0.46
3:R:3203[B]:HIS:O	3:R:3206[B]:LYS:HB3	2.16	0.46
3:R:3288[A]:MET:CA	3:R:3295[A]:LEU:HG	2.42	0.46
3:R:3298[A]:ASN:CA	3:R:3299[A]:LEU:HB2	2.44	0.46
1:S:120:LYS:HB3	1:S:121:ASN:HA	1.98	0.46
1:S:226:HIS:HA	1:S:227:ARG:HB2	1.97	0.46
2:T:2370:MET:HE2	2:T:2370:MET:HB2	1.66	0.46
3:U:2949[B]:LYS:C	3:U:2953[B]:GLY:N	2.73	0.46
3:U:3079[A]:CYS:SG	3:U:3146[A]:CYS:O	2.74	0.46
3:U:3079[B]:CYS:SG	3:U:3146[B]:CYS:O	2.74	0.46
3:U:3284[B]:LYS:CE	3:U:3285[B]:VAL:H	2.28	0.46
1:V:949:ASP:CB	1:V:953:GLU:HB2	2.41	0.46
1:V:1250:ILE:O	1:V:1473:ARG:NH2	2.49	0.46
2:W:2398:PHE:HE1	2:W:2466:THR:HG21	1.79	0.46
3:X:2965[B]:LEU:HD22	3:X:2975[B]:PHE:O	2.15	0.46
3:X:2987[A]:HIS:O	3:X:2991[A]:LEU:HB2	2.16	0.46
3:X:3196[B]:THR:CA	3:X:3199[B]:GLN:HB2	2.43	0.46
3:X:3298[B]:ASN:CA	3:X:3299[B]:LEU:HB2	2.44	0.46
1:Y:212:ASN:OD1	1:Y:215:ARG:NH1	2.48	0.46
1:Y:1166:THR:HB	1:Y:1167:ASP:C	2.40	0.46
1:Y:1423:TYR:OH	1:Y:1461:VAL:O	2.31	0.46
2:Z:2168:ARG:HA	2:c:2502:LEU:HB3	1.96	0.46
2:Z:2225:ARG:NH1	2:Z:2291:ASP:OD1	2.48	0.46
3:a:2970[A]:PRO:C	3:a:2972[A]:GLY:N	2.72	0.46
3:a:3079[A]:CYS:SG	3:a:3146[A]:CYS:O	2.74	0.46
3:a:3203[B]:HIS:O	3:a:3206[B]:LYS:HB3	2.16	0.46
1:b:462:HIS:CE1	1:b:621:LEU:HD12	2.51	0.46
1:b:1392:ASP:H	1:b:1435:GLY:HA2	1.80	0.46
2:c:2702:SER:HA	2:c:2707:PHE:CD2	2.49	0.46
3:d:2949[B]:LYS:C	3:d:2953[B]:GLY:N	2.72	0.46
3:d:3014[B]:TRP:CD2	3:d:3092[B]:ILE:CD1	2.98	0.46
3:d:3079[B]:CYS:SG	3:d:3146[B]:CYS:O	2.74	0.46
3:d:3182[A]:GLN:H	3:d:3182[A]:GLN:HG2	1.56	0.46
3:d:3200[B]:LEU:CD2	3:d:3204[B]:LEU:CD1	2.93	0.46
3:d:3284[A]:LYS:HD3	3:d:3285[A]:VAL:O	2.16	0.46
1:A:184:TYR:CE2	1:A:386:ILE:HG12	2.50	0.46
1:A:877:HIS:CE1	1:A:905:TRP:HZ3	2.33	0.46
1:A:979:LEU:HB2	1:A:980:TYR:CD1	2.50	0.46
2:B:2472:ASN:N	2:B:2473:GLY:HA2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2935[B]:ILE:CG1	3:C:2936[B]:GLU:N	2.78	0.46
3:C:2938[A]:LEU:O	3:C:2939[A]:ARG:C	2.58	0.46
3:C:2961[B]:HIS:C	3:L:3255[B]:PRO:CD	2.88	0.46
3:C:3141[A]:TYR:CD2	3:C:3141[A]:TYR:C	2.86	0.46
3:C:3203[A]:HIS:O	3:C:3206[A]:LYS:HB3	2.16	0.46
1:D:432:THR:HG23	1:D:435:GLU:H	1.81	0.46
1:D:440:ARG:O	1:D:444:GLU:HB2	2.15	0.46
3:F:2935[A]:ILE:CG1	3:F:2936[A]:GLU:N	2.78	0.46
3:F:2970[B]:PRO:C	3:F:2972[B]:GLY:H	2.23	0.46
3:F:2984[B]:THR:CB	3:a:3159[B]:SER:CB	2.80	0.46
3:F:2985[A]:PHE:CE2	3:F:2989[A]:HIS:CD2	3.04	0.46
3:F:3004[A]:GLY:C	3:F:3006[A]:LYS:N	2.73	0.46
3:F:3180[B]:TYR:CB	3:F:3183[B]:LEU:CD2	2.90	0.46
3:F:3264[B]:TYR:HD1	3:F:3265[B]:ASP:N	2.14	0.46
1:G:163:LEU:HB3	1:G:293:LEU:HD21	1.96	0.46
1:G:630:PHE:O	1:G:633:HIS:HB3	2.16	0.46
1:G:956:PRO:HB2	1:G:957:ASN:C	2.40	0.46
2:H:2344:LEU:HA	2:H:2345:ASN:C	2.40	0.46
2:H:2779:ASP:HA	2:H:2780:HIS:HA	1.45	0.46
3:I:2949[A]:LYS:NZ	3:I:2949[A]:LYS:C	2.73	0.46
3:I:2949[B]:LYS:NZ	3:I:2949[B]:LYS:C	2.73	0.46
3:I:3150[B]:LYS:HE2	3:R:3157[B]:PRO:HB2	1.96	0.46
3:I:3200[A]:LEU:HD22	3:I:3204[A]:LEU:HD11	1.95	0.46
3:I:3200[B]:LEU:CD2	3:I:3204[B]:LEU:CD1	2.93	0.46
3:I:3203[B]:HIS:O	3:I:3206[B]:LYS:HB3	2.16	0.46
3:I:3228[A]:VAL:CG2	3:I:3245[A]:PHE:CE1	2.96	0.46
3:I:3230[B]:PHE:H	3:I:3243[B]:GLY:HA3	1.79	0.46
3:I:3284[B]:LYS:CE	3:I:3284[B]:LYS:CA	2.85	0.46
3:I:3293[B]:LYS:HB2	3:I:3294[B]:SER:CA	2.41	0.46
3:I:3298[A]:ASN:CA	3:I:3299[A]:LEU:HB2	2.44	0.46
3:L:3284[B]:LYS:CE	3:L:3285[B]:VAL:H	2.28	0.46
3:L:3298[B]:ASN:CA	3:L:3299[B]:LEU:HB2	2.45	0.46
1:M:1059:LEU:HD13	1:M:1063:ARG:NH2	2.31	0.46
2:N:2234:GLN:HG3	2:N:2235:PRO:HD2	1.98	0.46
2:N:2235:PRO:HG3	2:N:2240:GLN:NE2	2.31	0.46
2:N:2426:PHE:HB3	2:N:2445:MET:HE1	1.96	0.46
3:O:2968[B]:GLN:HA	3:X:2979[B]:GLN:HG2	1.96	0.46
3:O:2976[A]:ALA:O	3:O:2978[A]:CYS:N	2.46	0.46
3:O:2987[A]:HIS:O	3:O:2991[A]:LEU:HB2	2.15	0.46
3:O:3176[A]:LYS:C	3:O:3177[A]:SER:HG	2.10	0.46
3:O:3284[A]:LYS:CE	3:O:3285[A]:VAL:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3284[B]:LYS:CE	3:O:3285[B]:VAL:H	2.28	0.46
1:P:1339:SER:HB2	1:P:1340:GLY:CA	2.46	0.46
2:Q:2885:SER:HB3	2:Q:2890:VAL:HG12	1.96	0.46
3:R:2949[A]:LYS:C	3:R:2953[A]:GLY:N	2.73	0.46
3:R:3146[B]:CYS:HA	3:R:3147[B]:GLU:HA	1.70	0.46
3:R:3196[B]:THR:CA	3:R:3199[B]:GLN:OE1	2.58	0.46
3:R:3281[A]:PHE:HE1	3:R:3305[A]:ILE:HG21	1.81	0.46
3:R:3293[B]:LYS:HB2	3:R:3294[B]:SER:CA	2.41	0.46
1:S:191:THR:HG1	1:S:192:HIS:HD1	1.62	0.46
1:S:618:MET:HA	1:S:624:THR:HB	1.97	0.46
1:S:673:PHE:HB3	1:S:677:LEU:HB2	1.97	0.46
1:S:748:VAL:HG22	1:S:781:ILE:HD11	1.97	0.46
1:S:760:ILE:HG21	1:S:777:TYR:HE2	1.80	0.46
1:S:1487:PRO:HD3	2:W:2486:ILE:HB	1.97	0.46
2:T:2786:MET:HE1	2:T:2794:LEU:HD22	1.97	0.46
3:U:2969[B]:TYR:C	3:d:2981[B]:GLY:CA	2.88	0.46
3:U:3264[A]:TYR:HD1	3:U:3265[A]:ASP:N	2.14	0.46
3:U:3284[A]:LYS:HD3	3:U:3285[A]:VAL:O	2.16	0.46
3:U:3284[B]:LYS:HD3	3:U:3285[B]:VAL:O	2.16	0.46
1:V:883:CYS:N	1:V:894:CYS:SG	2.88	0.46
1:V:1002:GLU:HB3	1:V:1065:LYS:HD3	1.97	0.46
1:V:1082:SER:OG	1:V:1083:PRO:HD3	2.16	0.46
3:X:2965[A]:LEU:HD22	3:X:2975[A]:PHE:O	2.15	0.46
3:X:3209[A]:GLU:O	3:X:3310[A]:GLY:C	2.59	0.46
3:X:3209[B]:GLU:O	3:X:3310[B]:GLY:C	2.59	0.46
3:X:3284[A]:LYS:CE	3:X:3285[A]:VAL:H	2.29	0.46
3:X:3284[B]:LYS:HD3	3:X:3285[B]:VAL:O	2.16	0.46
1:Y:958:PRO:CA	1:Y:959:PHE:HB2	2.44	0.46
2:Z:2155:HIS:O	2:Z:2159:VAL:HG23	2.15	0.46
2:Z:2244:PHE:CZ	2:Z:2376:MET:HE1	2.51	0.46
2:Z:2795:ILE:O	2:Z:2799:LYS:HG3	2.16	0.46
3:a:2935[A]:ILE:CG1	3:a:2936[A]:GLU:N	2.78	0.46
3:a:3203[A]:HIS:O	3:a:3206[A]:LYS:HB3	2.16	0.46
3:a:3209[A]:GLU:O	3:a:3310[A]:GLY:C	2.59	0.46
3:a:3284[A]:LYS:HD3	3:a:3285[A]:VAL:O	2.15	0.46
3:a:3284[A]:LYS:CE	3:a:3285[A]:VAL:H	2.28	0.46
1:b:1302:SER:CB	1:b:1303:GLU:HA	2.45	0.46
3:d:2949[A]:LYS:C	3:d:2953[A]:GLY:N	2.72	0.46
3:d:2969[A]:TYR:CD2	3:d:2970[A]:PRO:N	2.83	0.46
3:d:3079[A]:CYS:SG	3:d:3146[A]:CYS:O	2.74	0.46
6:r:1:NAG:O4	6:r:1:NAG:O6	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:THR:HB	1:A:193:SER:HB3	1.96	0.46
1:A:904:HIS:HE2	1:A:1004:PHE:HE2	1.62	0.46
1:A:1210:LYS:HG3	2:E:2743:ALA:CB	2.46	0.46
2:B:2086:ASN:ND2	2:B:2086:ASN:H	2.14	0.46
2:B:2344:LEU:O	2:E:2515:ARG:HB3	2.15	0.46
3:C:2935[A]:ILE:CG1	3:C:2936[A]:GLU:N	2.78	0.46
3:C:2949[A]:LYS:C	3:C:2953[A]:GLY:N	2.72	0.46
3:C:2956[B]:LYS:O	3:C:2959[B]:SER:OG	2.33	0.46
3:C:2985[B]:PHE:CE2	3:C:2989[B]:HIS:CD2	3.04	0.46
3:C:2987[A]:HIS:O	3:C:2991[A]:LEU:HB2	2.15	0.46
3:C:2991[A]:LEU:HD23	3:C:3158[A]:PHE:CE1	2.48	0.46
3:C:3090[B]:ASN:HB3	3:L:2973[B]:THR:N	2.29	0.46
3:C:3104[A]:MET:HA	3:C:3110[A]:THR:CG2	2.17	0.46
3:C:3151[A]:LEU:HB2	3:C:3175[A]:TYR:HE2	1.68	0.46
3:C:3151[B]:LEU:C	3:L:3154[B]:PRO:CB	2.88	0.46
3:C:3153[B]:LYS:C	3:L:3173[B]:THR:C	2.84	0.46
3:C:3283[A]:ILE:HB	3:C:3305[A]:ILE:HD11	1.97	0.46
3:C:3284[A]:LYS:HD3	3:C:3284[A]:LYS:C	2.32	0.46
3:C:3284[A]:LYS:CE	3:C:3285[A]:VAL:H	2.28	0.46
1:D:673:PHE:HB3	1:D:677:LEU:HD13	1.98	0.46
3:F:2961[A]:HIS:CD2	3:F:2988[A]:TRP:CZ3	2.96	0.46
3:F:2987[A]:HIS:O	3:F:2991[A]:LEU:HB2	2.16	0.46
3:F:3014[A]:TRP:CD2	3:F:3092[A]:ILE:CD1	2.98	0.46
3:F:3251[B]:ASP:CB	3:a:3251[B]:ASP:HB2	2.08	0.46
1:G:177:VAL:O	1:G:181:PRO:HD3	2.15	0.46
1:G:1576:THR:H	1:G:1581:GLU:CB	2.28	0.46
2:H:2094:ARG:HE	2:K:2094:ARG:HH21	1.63	0.46
3:I:2965[A]:LEU:HD13	3:I:2975[A]:PHE:O	2.16	0.46
3:I:3153[B]:LYS:O	3:R:3154[B]:PRO:HA	2.15	0.46
3:I:3203[A]:HIS:O	3:I:3206[A]:LYS:HB3	2.16	0.46
3:I:3264[B]:TYR:HD1	3:I:3265[B]:ASP:N	2.14	0.46
1:J:1077:LEU:HB3	1:J:1103:PHE:CE1	2.51	0.46
1:J:1494:ARG:NH1	1:J:1494:ARG:HG3	2.30	0.46
3:L:2976[A]:ALA:O	3:L:2978[A]:CYS:N	2.46	0.46
3:L:2987[A]:HIS:O	3:L:2991[A]:LEU:HB2	2.15	0.46
1:M:1315:GLY:HA3	1:M:1601:TRP:HB2	1.96	0.46
2:N:2550:THR:O	2:N:2554:PRO:HD3	2.16	0.46
3:O:2965[B]:LEU:CD1	3:O:2974[B]:ALA:CA	2.89	0.46
3:O:2969[B]:TYR:HB3	3:X:3158[B]:PHE:CE2	2.45	0.46
3:O:3004[A]:GLY:C	3:O:3006[A]:LYS:N	2.74	0.46
3:O:3116[A]:PHE:CD1	3:O:3116[A]:PHE:C	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3209[B]:GLU:O	3:O:3310[B]:GLY:C	2.59	0.46
3:O:3254[B]:MET:C	3:X:3160[B]:SER:C	2.84	0.46
3:O:3264[B]:TYR:HD1	3:O:3265[B]:ASP:N	2.14	0.46
1:P:64:THR:HG21	1:P:239:LEU:HB2	1.97	0.46
1:P:625:SER:HA	1:P:630:PHE:CG	2.51	0.46
2:Q:2180:TRP:HH2	2:Q:2297:HIS:O	1.99	0.46
3:R:2952[A]:ALA:N	3:R:2953[A]:GLY:CA	2.71	0.46
3:R:2954[B]:TYR:CA	3:R:2957[B]:ILE:HG22	2.43	0.46
3:R:3074[B]:GLU:OE2	3:R:3208[B]:GLN:HG2	2.15	0.46
3:R:3104[A]:MET:HA	3:R:3110[A]:THR:CG2	2.17	0.46
3:R:3209[B]:GLU:O	3:R:3310[B]:GLY:C	2.59	0.46
3:R:3264[B]:TYR:HD1	3:R:3265[B]:ASP:N	2.14	0.46
2:T:2644:LEU:HD11	2:T:2683:ILE:HD13	1.96	0.46
3:U:2949[B]:LYS:C	3:U:2949[B]:LYS:HZ3	2.18	0.46
3:U:2968[B]:GLN:HG2	3:d:3258[B]:PHE:CE1	2.42	0.46
3:U:2970[A]:PRO:C	3:U:2972[A]:GLY:N	2.72	0.46
3:U:2981[A]:GLY:N	3:U:3086[A]:GLU:OE1	2.45	0.46
3:U:3169[B]:LYS:O	3:d:3149[B]:ASN:N	2.42	0.46
3:U:3203[A]:HIS:O	3:U:3206[A]:LYS:HB3	2.16	0.46
3:U:3283[B]:ILE:HB	3:U:3305[B]:ILE:HD11	1.97	0.46
1:V:149:GLU:HG3	1:V:150:GLY:N	2.29	0.46
1:V:514:TRP:CZ2	1:V:606:ILE:HD11	2.50	0.46
1:V:717:GLN:O	1:V:720:VAL:HG22	2.15	0.46
2:W:2401:GLU:HG2	2:W:2402:GLY:H	1.80	0.46
3:X:2949[B]:LYS:C	3:X:2953[B]:GLY:N	2.72	0.46
3:X:3004[A]:GLY:C	3:X:3006[A]:LYS:N	2.74	0.46
3:X:3079[B]:CYS:SG	3:X:3146[B]:CYS:O	2.74	0.46
3:X:3191[A]:ASN:ND2	3:X:3191[A]:ASN:N	2.60	0.46
3:X:3263[B]:LEU:N	3:X:3263[B]:LEU:CD1	2.79	0.46
3:X:3283[B]:ILE:HB	3:X:3305[B]:ILE:HD11	1.97	0.46
1:Y:578:PHE:H	1:Y:578:PHE:HD1	1.63	0.46
1:Y:1546:LYS:HB3	3:d:3001[B]:LYS:HZ2	1.76	0.46
2:Z:2109:ARG:NH1	2:Z:2169:HIS:O	2.48	0.46
2:Z:2572:VAL:HG22	2:Z:2768:LEU:HD22	1.97	0.46
3:a:2976[A]:ALA:O	3:a:2978[A]:CYS:N	2.46	0.46
3:a:3171[B]:HIS:C	3:a:3173[B]:THR:N	2.73	0.46
3:a:3200[A]:LEU:CD2	3:a:3204[A]:LEU:CD1	2.93	0.46
3:a:3263[B]:LEU:N	3:a:3263[B]:LEU:CD1	2.79	0.46
3:a:3265[A]:ASP:CG	3:a:3267[A]:SER:HG	2.13	0.46
3:a:3284[B]:LYS:CE	3:a:3285[B]:VAL:H	2.28	0.46
1:b:1195:ASP:O	1:b:1196:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2987[B]:HIS:O	3:d:2991[B]:LEU:HB2	2.16	0.46
3:d:2991[A]:LEU:HD23	3:d:3158[A]:PHE:CE1	2.48	0.46
3:d:3264[A]:TYR:HD1	3:d:3265[A]:ASP:N	2.14	0.46
1:A:120:LYS:HB3	1:A:121:ASN:HA	1.97	0.46
1:A:462:HIS:HA	1:A:490:TRP:HH2	1.80	0.46
1:A:949:ASP:HB2	1:A:953:GLU:HB2	1.98	0.46
2:B:2158:TYR:O	2:B:2161:GLN:HB3	2.15	0.46
2:B:2802:ASP:OD1	2:B:2906:ALA:N	2.44	0.46
3:C:3148[B]:ILE:HG22	3:C:3152[B]:LYS:CE	2.44	0.46
3:C:3200[B]:LEU:HD22	3:C:3204[B]:LEU:HD11	1.95	0.46
3:C:3298[B]:ASN:CA	3:C:3299[B]:LEU:C	2.85	0.46
1:D:447:MET:HA	1:D:455:TYR:CB	2.46	0.46
1:D:905:TRP:HE1	1:D:1083:PRO:HD2	1.81	0.46
2:E:2525:LYS:NZ	2:E:2526:ARG:HH12	2.14	0.46
2:E:2715:ASP:HB3	2:E:2778:TYR:OH	2.16	0.46
3:F:3284[B]:LYS:CE	3:F:3285[B]:VAL:H	2.29	0.46
1:G:548:ALA:O	1:G:559:THR:HG22	2.15	0.46
1:G:999:LEU:HD12	1:G:1059:LEU:HD12	1.98	0.46
1:G:1166:THR:OG1	1:G:1168:GLN:OE1	2.30	0.46
1:G:1315:GLY:HA3	1:G:1601:TRP:HB2	1.98	0.46
2:H:2121:THR:O	2:H:2124:SER:HB3	2.16	0.46
2:H:2286:HIS:NE2	2:H:2433:THR:HG22	2.31	0.46
1:J:22:LEU:HG	1:J:122:VAL:HB	1.97	0.46
3:L:2940[A]:ASN:O	3:L:2944[A]:ALA:N	2.48	0.46
3:L:2970[A]:PRO:C	3:L:2972[A]:GLY:H	2.23	0.46
3:L:3264[A]:TYR:HD1	3:L:3265[A]:ASP:N	2.14	0.46
3:L:3281[A]:PHE:HE1	3:L:3305[A]:ILE:HG21	1.81	0.46
3:L:3284[A]:LYS:HD3	3:L:3285[A]:VAL:O	2.16	0.46
1:M:1129:LEU:O	1:M:1133:ILE:HG23	2.16	0.46
1:M:1189:ASP:HA	2:Q:2809:LEU:HD12	1.96	0.46
1:M:1394:GLN:HG3	1:M:1433:TRP:HA	1.98	0.46
1:M:1438:ASP:OD1	1:M:1439:VAL:N	2.49	0.46
2:N:2116:SER:HA	2:N:2121:THR:HG21	1.97	0.46
3:O:2940[B]:ASN:O	3:O:2944[B]:ALA:N	2.48	0.46
3:O:2965[A]:LEU:HD13	3:O:2975[A]:PHE:O	2.16	0.46
3:O:2965[B]:LEU:HD13	3:O:2975[B]:PHE:O	2.16	0.46
3:O:2987[B]:HIS:O	3:O:2991[B]:LEU:HB2	2.16	0.46
3:O:3074[B]:GLU:OE2	3:O:3208[B]:GLN:HG2	2.15	0.46
3:O:3116[B]:PHE:C	3:O:3116[B]:PHE:CD1	2.94	0.46
3:O:3125[B]:ARG:O	3:O:3129[B]:ILE:HG13	2.14	0.46
3:O:3148[A]:ILE:HG22	3:O:3152[A]:LYS:CE	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3200[B]:LEU:HD22	3:O:3204[B]:LEU:HD11	1.95	0.46
2:Q:2568:HIS:HE1	2:Q:2742:MET:SD	2.38	0.46
3:R:2938[B]:LEU:O	3:R:2939[B]:ARG:C	2.58	0.46
3:R:3283[A]:ILE:HB	3:R:3305[A]:ILE:HD11	1.97	0.46
1:S:250:ASP:HA	1:S:258:LYS:NZ	2.31	0.46
1:S:780:GLU:C	1:S:782:THR:H	2.24	0.46
1:S:807:GLY:HA2	1:S:808:THR:HB	1.97	0.46
1:S:931:TRP:CE3	1:S:991:LEU:HD13	2.51	0.46
3:U:2961[A]:HIS:HB2	3:U:2992[A]:TYR:HE2	1.81	0.46
3:U:2965[B]:LEU:HD22	3:U:2975[B]:PHE:O	2.16	0.46
3:U:3074[A]:GLU:CD	3:U:3212[A]:ARG:NH2	2.73	0.46
3:U:3116[B]:PHE:C	3:U:3116[B]:PHE:CD1	2.94	0.46
3:U:3162[B]:ASP:OD1	3:d:3260[B]:ARG:HD2	2.16	0.46
3:U:3203[B]:HIS:O	3:U:3206[B]:LYS:HB3	2.16	0.46
3:U:3225[B]:SER:C	3:U:3290[B]:ILE:HG23	2.39	0.46
3:U:3298[A]:ASN:CA	3:U:3299[A]:LEU:HB2	2.44	0.46
1:V:1260:ARG:HD2	1:V:1343:VAL:O	2.16	0.46
1:V:1309:HIS:N	1:V:1309:HIS:CD2	2.83	0.46
1:V:1390:ASP:HB2	1:V:1438:ASP:OD2	2.15	0.46
2:W:2327:GLU:H	2:W:2327:GLU:HG3	1.57	0.46
3:X:2940[A]:ASN:O	3:X:2944[A]:ALA:N	2.48	0.46
3:X:2954[A]:TYR:CA	3:X:2957[A]:ILE:HG22	2.43	0.46
3:X:3200[A]:LEU:CD2	3:X:3204[A]:LEU:CD1	2.93	0.46
3:X:3285[A]:VAL:CG2	3:X:3286[A]:THR:H	2.27	0.46
3:X:3298[B]:ASN:CB	3:X:3300[B]:LEU:CD2	2.61	0.46
1:Y:472:ASP:HA	1:Y:473:ALA:HA	1.67	0.46
1:Y:1546:LYS:HA	3:d:3002[B]:ALA:HA	1.60	0.46
1:Y:1656:ASP:N	3:d:3006[B]:LYS:HD2	2.30	0.46
2:Z:2128:LEU:HD22	2:Z:2286:HIS:HB3	1.98	0.46
2:Z:2680:HIS:NE2	2:Z:2684:HIS:CD2	2.83	0.46
3:a:2949[A]:LYS:NZ	3:a:2949[A]:LYS:C	2.73	0.46
3:a:2965[B]:LEU:HD13	3:a:2975[B]:PHE:O	2.16	0.46
3:a:3004[A]:GLY:C	3:a:3006[A]:LYS:N	2.74	0.46
3:a:3298[A]:ASN:CA	3:a:3299[A]:LEU:HB2	2.45	0.46
2:c:2142:ALA:HA	2:c:2143:CYS:HA	1.76	0.46
2:c:2185:THR:HG23	2:c:2186:GLU:HG2	1.98	0.46
2:c:2726:LYS:HB2	2:c:2726:LYS:HE3	1.75	0.46
2:c:2863:ARG:HB2	2:c:2865:ILE:HG12	1.97	0.46
3:d:3299[B]:LEU:HB3	3:d:3300[B]:LEU:H	1.53	0.46
4:9:1:NAG:O6	4:9:2:NAG:C1	2.63	0.46
1:A:183:HIS:CG	1:A:344:LEU:HD21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASN:O	1:A:821:ILE:HA	2.16	0.46
1:A:376:ASN:HB2	1:A:665:TYR:CG	2.51	0.46
1:A:483:GLY:HA2	1:A:773:PHE:CZ	2.51	0.46
1:A:980:TYR:CE1	1:A:1021:LEU:HD13	2.50	0.46
3:C:2965[A]:LEU:HD22	3:C:2975[A]:PHE:O	2.15	0.46
3:C:2971[B]:ASP:OD2	3:L:3248[B]:LEU:HD21	2.16	0.46
3:C:3079[B]:CYS:SG	3:C:3146[B]:CYS:O	2.74	0.46
3:C:3143[A]:SER:OG	3:C:3144[A]:ALA:N	2.46	0.46
3:C:3209[A]:GLU:O	3:C:3310[A]:GLY:C	2.59	0.46
1:D:22:LEU:HD12	1:D:25:MET:HG2	1.97	0.46
1:D:398:ARG:HH21	1:D:663:GLU:CD	2.23	0.46
2:E:2657:PHE:O	2:E:2661:MET:HG2	2.15	0.46
2:E:2890:VAL:HG13	2:E:2891:LEU:C	2.40	0.46
3:F:3137[B]:ARG:O	3:F:3139[B]:LEU:HD22	2.16	0.46
1:G:23:ARG:HD3	1:G:120:LYS:HD3	1.97	0.46
1:G:444:GLU:O	1:G:448:SER:OG	2.13	0.46
1:G:597:VAL:HG23	1:G:598:GLN:H	1.81	0.46
1:G:1166:THR:H	1:G:1166:THR:HG1	1.34	0.46
1:G:1287:TYR:HA	1:G:1290:ILE:HB	1.98	0.46
2:H:2803:ARG:HH21	2:H:2805:PHE:HZ	1.64	0.46
3:I:2961[B]:HIS:CD2	3:I:2988[B]:TRP:CZ3	2.96	0.46
3:I:2966[B]:SER:CA	3:R:3255[B]:PRO:C	2.89	0.46
3:I:2985[B]:PHE:CE2	3:I:2989[B]:HIS:CD2	3.04	0.46
3:I:2987[A]:HIS:O	3:I:2991[A]:LEU:HB2	2.16	0.46
3:I:3079[B]:CYS:SG	3:I:3146[B]:CYS:O	2.74	0.46
3:I:3154[B]:PRO:N	3:R:3173[B]:THR:C	2.74	0.46
3:I:3191[A]:ASN:C	3:I:3192[A]:PHE:O	2.52	0.46
3:I:3209[A]:GLU:O	3:I:3310[A]:GLY:C	2.59	0.46
3:I:3225[A]:SER:C	3:I:3290[A]:ILE:HG23	2.39	0.46
3:I:3284[B]:LYS:CE	3:I:3285[B]:VAL:H	2.29	0.46
3:I:3301[B]:PRO:HB2	3:I:3302[B]:SER:H	1.33	0.46
1:J:1324:ARG:NH1	1:J:1519:TYR:HB3	2.31	0.46
3:L:3283[A]:ILE:HB	3:L:3305[A]:ILE:HD11	1.97	0.46
1:M:525:SER:HA	1:M:528:ALA:HB3	1.98	0.46
1:M:1206:HIS:CD2	1:M:1207:TYR:H	2.34	0.46
1:M:1578:ILE:HA	1:M:1579:GLY:HA2	1.64	0.46
2:N:2177:TYR:HB2	2:N:2300:ASN:HB2	1.98	0.46
2:N:2325:ALA:HA	1:P:1649:THR:HG23	1.97	0.46
2:N:2638:ARG:HG2	2:N:2687:ILE:O	2.15	0.46
2:N:2762:VAL:O	2:N:2768:LEU:HD23	2.16	0.46
3:O:2961[A]:HIS:CD2	3:O:2988[A]:TRP:CZ3	2.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2961[B]:HIS:CD2	3:O:2988[B]:TRP:CZ3	2.96	0.46
3:O:2971[B]:ASP:CG	3:X:3158[B]:PHE:CZ	2.92	0.46
3:O:2976[B]:ALA:HB2	3:X:3156[B]:MET:HE2	1.98	0.46
3:O:3196[B]:THR:CB	3:O:3199[B]:GLN:OE1	2.64	0.46
1:P:109:LEU:HD21	2:T:2635:TYR:HB2	1.98	0.46
3:R:2991[B]:LEU:HD23	3:R:3158[B]:PHE:CE1	2.48	0.46
3:R:3079[A]:CYS:SG	3:R:3146[A]:CYS:O	2.74	0.46
3:R:3284[B]:LYS:HD3	3:R:3285[B]:VAL:O	2.16	0.46
1:S:1156:LEU:HB2	1:S:1176:TYR:CE1	2.51	0.46
3:U:2940[A]:ASN:O	3:U:2944[A]:ALA:N	2.48	0.46
3:U:2969[A]:TYR:CD2	3:U:2970[A]:PRO:N	2.83	0.46
3:U:2975[B]:PHE:CZ	3:d:3253[B]:GLU:HB2	2.51	0.46
3:U:2994[A]:LYS:O	3:U:2997[A]:GLU:N	2.49	0.46
3:U:3161[B]:GLU:H	3:U:3161[B]:GLU:CD	2.19	0.46
3:U:3196[A]:THR:CB	3:U:3199[A]:GLN:OE1	2.64	0.46
3:U:3263[B]:LEU:N	3:U:3263[B]:LEU:CD1	2.79	0.46
3:U:3285[B]:VAL:CG2	3:U:3286[B]:THR:H	2.27	0.46
1:V:854:LEU:HG	1:V:959:PHE:CE2	2.51	0.46
2:W:2089:ARG:HD3	2:W:2163:GLU:OE2	2.16	0.46
2:W:2885:SER:OG	2:W:2886:VAL:N	2.47	0.46
3:X:2949[A]:LYS:C	3:X:2953[A]:GLY:N	2.72	0.46
3:X:2969[A]:TYR:CD2	3:X:2970[A]:PRO:N	2.83	0.46
3:X:2981[A]:GLY:N	3:X:3086[A]:GLU:OE1	2.45	0.46
3:X:3137[B]:ARG:O	3:X:3139[B]:LEU:HD22	2.16	0.46
3:X:3196[A]:THR:CB	3:X:3199[A]:GLN:OE1	2.64	0.46
3:X:3263[A]:LEU:CD1	3:X:3263[A]:LEU:N	2.79	0.46
3:X:3284[B]:LYS:CE	3:X:3285[B]:VAL:H	2.28	0.46
1:Y:669:LYS:HB2	1:Y:670:PRO:HD3	1.98	0.46
3:a:2970[B]:PRO:C	3:a:2972[B]:GLY:H	2.23	0.46
3:a:2985[B]:PHE:CE2	3:a:2989[B]:HIS:CD2	3.04	0.46
3:a:2987[A]:HIS:O	3:a:2991[A]:LEU:HB2	2.15	0.46
3:a:3079[B]:CYS:SG	3:a:3146[B]:CYS:O	2.74	0.46
3:a:3283[A]:ILE:HB	3:a:3305[A]:ILE:HD11	1.97	0.46
1:b:1636:ASN:ND2	4:QA:1:NAG:C7	2.79	0.46
2:c:2115:SER:OG	2:c:2116:SER:N	2.48	0.46
2:c:2302:ASP:O	2:c:2306:VAL:HG23	2.16	0.46
3:d:2994[A]:LYS:O	3:d:2997[A]:GLU:N	2.49	0.46
3:d:3074[A]:GLU:CD	3:d:3212[A]:ARG:NH2	2.73	0.46
3:d:3263[B]:LEU:N	3:d:3263[B]:LEU:CD1	2.79	0.46
2:B:2126:HIS:O	2:B:2143:CYS:HB3	2.16	0.46
2:B:2218:SER:HB2	2:B:2221:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2888:GLY:N	2:B:2889:ALA:HA	2.31	0.46
3:C:2994[B]:LYS:O	3:C:2997[B]:GLU:N	2.49	0.46
3:C:3196[A]:THR:CB	3:C:3199[A]:GLN:OE1	2.64	0.46
1:D:956:PRO:HD2	1:D:957:ASN:HA	1.97	0.46
1:D:1433:TRP:HE3	1:D:1433:TRP:N	2.14	0.46
2:E:2639:GLU:OE1	2:E:2690:HIS:HB2	2.16	0.46
2:E:2805:PHE:CE1	2:E:2855:ASP:HB3	2.51	0.46
2:E:2822:LYS:HG3	2:E:2830:GLN:C	2.41	0.46
3:F:2965[B]:LEU:HD13	3:F:2975[B]:PHE:O	2.16	0.46
3:F:2968[B]:GLN:O	3:a:2980[B]:HIS:N	2.40	0.46
3:F:2970[A]:PRO:C	3:F:2972[A]:GLY:H	2.23	0.46
3:F:2973[B]:THR:HG21	3:a:3107[B]:LEU:N	2.31	0.46
3:F:2985[B]:PHE:CE2	3:F:2989[B]:HIS:CD2	3.04	0.46
3:F:2994[B]:LYS:O	3:F:2997[B]:GLU:N	2.49	0.46
3:F:3203[B]:HIS:O	3:F:3206[B]:LYS:HB3	2.16	0.46
3:F:3293[B]:LYS:CD	3:F:3293[B]:LYS:C	2.86	0.46
1:G:53:SER:O	1:G:55:ILE:HG13	2.16	0.46
1:G:792:MET:HB2	1:G:793:PHE:CD1	2.51	0.46
1:G:877:HIS:CE1	1:G:905:TRP:HZ3	2.34	0.46
2:H:2800:LYS:C	3:I:3023[A]:ILE:HD13	2.41	0.46
2:H:2870:LEU:HD11	2:H:2901:LEU:HD23	1.97	0.46
3:I:3014[A]:TRP:CD2	3:I:3092[A]:ILE:CD1	2.98	0.46
3:I:3135[A]:LYS:HB2	3:I:3141[A]:TYR:CD1	2.51	0.46
3:I:3157[B]:PRO:CD	3:R:2982[B]:MET:CE	2.93	0.46
1:J:730:PHE:CE2	1:J:780:GLU:HB3	2.51	0.46
1:J:913:PHE:HE2	1:J:1042:PHE:CD1	2.33	0.46
1:J:1494:ARG:HG3	1:J:1494:ARG:HH11	1.80	0.46
2:K:2115:SER:OG	2:K:2116:SER:N	2.49	0.46
3:L:2970[B]:PRO:C	3:L:2972[B]:GLY:N	2.72	0.46
3:L:2985[A]:PHE:CE2	3:L:2989[A]:HIS:CD2	3.04	0.46
1:M:854:LEU:HD23	1:M:941:LEU:HD21	1.98	0.46
2:N:2625:LEU:HD13	2:N:2626:ARG:HB2	1.98	0.46
2:N:2743:ALA:HB1	1:P:1210:LYS:HG3	1.98	0.46
2:N:2866:PRO:HA	2:N:2867:PRO:HD3	1.78	0.46
3:O:3014[A]:TRP:CG	3:O:3092[A]:ILE:CD1	2.98	0.46
3:O:3025[A]:VAL:CG2	3:O:3047[A]:ARG:NH1	2.73	0.46
3:O:3137[B]:ARG:O	3:O:3139[B]:LEU:HD22	2.16	0.46
3:O:3230[B]:PHE:H	3:O:3243[B]:GLY:HA3	1.79	0.46
3:O:3255[B]:PRO:HB3	3:X:3161[B]:GLU:CA	2.46	0.46
3:O:3283[B]:ILE:HB	3:O:3305[B]:ILE:HD11	1.97	0.46
1:P:239:LEU:H	1:P:239:LEU:HD12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:636:GLN:OE1	1:P:639:ARG:NH1	2.48	0.46
2:Q:2545:SER:CA	2:Q:2546:LEU:HB3	2.44	0.46
3:R:2940[B]:ASN:O	3:R:2944[B]:ALA:N	2.48	0.46
3:R:2965[A]:LEU:HD22	3:R:2975[A]:PHE:O	2.15	0.46
3:R:3023[B]:ILE:O	3:R:3026[B]:THR:OG1	2.34	0.46
3:R:3185[B]:TYR:CE2	3:R:3187[B]:TYR:HE2	2.31	0.46
3:R:3196[A]:THR:CB	3:R:3199[A]:GLN:OE1	2.64	0.46
3:R:3283[B]:ILE:HB	3:R:3305[B]:ILE:HD11	1.97	0.46
3:U:2952[A]:ALA:HB1	3:U:2957[A]:ILE:H	1.79	0.46
3:U:2991[B]:LEU:HD23	3:U:3158[B]:PHE:CE1	2.48	0.46
3:U:3074[A]:GLU:OE2	3:U:3208[A]:GLN:HG2	2.15	0.46
3:U:3106[B]:THR:O	3:U:3106[B]:THR:HG23	2.16	0.46
3:U:3116[A]:PHE:CD1	3:U:3116[A]:PHE:C	2.94	0.46
3:U:3200[B]:LEU:HD22	3:U:3204[B]:LEU:HD11	1.95	0.46
3:U:3220[B]:ARG:CG	3:d:2973[B]:THR:HA	2.43	0.46
1:V:780:GLU:O	1:V:781:ILE:HG12	2.14	0.46
1:V:902:PHE:CD2	1:V:1012:GLU:HB2	2.50	0.46
1:V:1321:HIS:ND1	1:V:1513:PRO:HB3	2.31	0.46
3:X:2970[A]:PRO:C	3:X:2972[A]:GLY:N	2.72	0.46
3:X:2985[A]:PHE:CE2	3:X:2989[A]:HIS:NE2	2.83	0.46
3:X:3137[A]:ARG:O	3:X:3139[A]:LEU:HD22	2.16	0.46
3:X:3191[A]:ASN:C	3:X:3192[A]:PHE:O	2.52	0.46
3:X:3281[B]:PHE:HE1	3:X:3305[B]:ILE:HG21	1.81	0.46
3:a:2994[A]:LYS:O	3:a:2997[A]:GLU:N	2.49	0.46
3:a:2994[B]:LYS:O	3:a:2997[B]:GLU:N	2.49	0.46
3:a:3023[B]:ILE:O	3:a:3026[B]:THR:OG1	2.34	0.46
1:b:22:LEU:O	1:b:26:GLN:HB2	2.16	0.46
1:b:434:GLU:O	1:b:438:GLU:HG3	2.16	0.46
1:b:930:ASP:OD1	1:b:1051:ARG:NH2	2.48	0.46
1:b:947:TYR:CE1	1:b:956:PRO:HD2	2.51	0.46
1:b:1300:CYS:HB3	1:b:1494:ARG:NH1	2.30	0.46
2:c:2549:PRO:CD	2:c:2554:PRO:HB3	2.37	0.46
2:c:2631:TYR:H	2:c:2631:TYR:HD1	1.64	0.46
3:d:2970[A]:PRO:C	3:d:2972[A]:GLY:H	2.23	0.46
3:d:2991[B]:LEU:HD23	3:d:3158[B]:PHE:CE1	2.48	0.46
3:d:3171[B]:HIS:C	3:d:3173[B]:THR:N	2.73	0.46
3:d:3203[B]:HIS:O	3:d:3206[B]:LYS:HB3	2.16	0.46
3:d:3263[A]:LEU:CD1	3:d:3263[A]:LEU:N	2.79	0.46
3:d:3283[B]:ILE:HB	3:d:3305[B]:ILE:HD11	1.97	0.46
5:l:3:BMA:H3	5:l:4:MAN:H2	1.54	0.46
1:A:321:LEU:HB2	1:A:338:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:PHE:HE1	1:A:756:PHE:HD2	1.64	0.46
1:A:832:LYS:O	1:A:832:LYS:HG3	2.15	0.46
1:A:912:ASN:HD21	1:A:1091:ASN:ND2	2.12	0.46
1:A:956:PRO:HB2	1:A:957:ASN:C	2.40	0.46
1:A:1225:VAL:HG12	1:A:1226:THR:H	1.80	0.46
1:A:1423:TYR:OH	1:A:1461:VAL:HG13	2.16	0.46
2:B:2394:VAL:H	2:B:2448:THR:CG2	2.20	0.46
2:B:2609:ALA:HA	2:B:2625:LEU:HD23	1.97	0.46
3:C:2970[A]:PRO:C	3:C:2972[A]:GLY:H	2.23	0.46
3:C:2994[A]:LYS:O	3:C:2997[A]:GLU:N	2.49	0.46
3:C:3014[A]:TRP:CG	3:C:3092[A]:ILE:CD1	2.98	0.46
3:C:3284[A]:LYS:HD3	3:C:3285[A]:VAL:O	2.16	0.46
1:D:904:HIS:HB3	1:D:1105:VAL:HG21	1.96	0.46
2:E:2627:GLY:HA3	2:E:2703:PHE:O	2.16	0.46
3:F:3116[B]:PHE:C	3:F:3116[B]:PHE:CD1	2.94	0.46
3:F:3150[B]:LYS:HZ3	3:a:3160[B]:SER:HB2	1.69	0.46
3:F:3169[B]:LYS:HA	3:a:3150[B]:LYS:HA	1.92	0.46
3:F:3209[A]:GLU:O	3:F:3310[A]:GLY:C	2.59	0.46
3:F:3263[B]:LEU:N	3:F:3263[B]:LEU:CD1	2.79	0.46
1:G:742:ALA:HA	1:G:805:VAL:HG23	1.97	0.46
1:G:1026:GLU:OE1	1:G:1028:VAL:N	2.49	0.46
1:G:1325:LEU:O	1:G:1328:SER:HB3	2.16	0.46
1:G:1636:ASN:HB2	1:G:1639:LYS:HD3	1.98	0.46
2:H:2128:LEU:HB2	2:H:2286:HIS:HB3	1.98	0.46
2:H:2695:MET:HE2	2:H:2695:MET:HA	1.98	0.46
3:I:2987[B]:HIS:O	3:I:2991[B]:LEU:HB2	2.15	0.46
3:I:2994[B]:LYS:O	3:I:2997[B]:GLU:N	2.49	0.46
3:I:3024[A]:LEU:CD1	3:I:3024[A]:LEU:C	2.85	0.46
3:I:3024[B]:LEU:CD1	3:I:3024[B]:LEU:C	2.85	0.46
3:I:3116[A]:PHE:CD1	3:I:3116[A]:PHE:C	2.94	0.46
3:I:3191[B]:ASN:ND2	3:I:3191[B]:ASN:N	2.60	0.46
3:I:3251[B]:ASP:HB3	3:I:3252[B]:TYR:CD1	2.40	0.46
3:I:3263[B]:LEU:N	3:I:3263[B]:LEU:CD1	2.79	0.46
1:J:480:CYS:HA	1:J:490:TRP:CE2	2.51	0.46
1:J:880:THR:HB	1:J:882:TRP:CZ2	2.50	0.46
3:L:2948[A]:ASP:CB	3:L:2949[A]:LYS:HA	2.16	0.46
3:L:3004[B]:GLY:C	3:L:3006[B]:LYS:N	2.74	0.46
3:L:3023[A]:ILE:O	3:L:3026[A]:THR:OG1	2.34	0.46
3:L:3116[A]:PHE:C	3:L:3116[A]:PHE:CD1	2.94	0.46
3:L:3137[A]:ARG:HB3	3:L:3139[A]:LEU:HD21	1.97	0.46
1:M:589:GLN:HG2	1:M:594:ASP:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:618:MET:HE3	1:M:618:MET:HB3	1.67	0.46
1:M:935:ILE:HD11	1:M:980:TYR:HD2	1.80	0.46
1:P:329:ARG:HH22	1:S:1574:VAL:H	1.63	0.46
1:P:376:ASN:HB2	1:P:665:TYR:CE1	2.51	0.46
2:Q:2115:SER:OG	2:Q:2116:SER:N	2.49	0.46
3:R:2985[A]:PHE:CE2	3:R:2989[A]:HIS:CD2	3.04	0.46
3:R:3074[A]:GLU:CD	3:R:3212[A]:ARG:NH2	2.73	0.46
3:R:3106[B]:THR:O	3:R:3106[B]:THR:HG23	2.16	0.46
3:R:3182[A]:GLN:H	3:R:3182[A]:GLN:HG2	1.56	0.46
3:R:3196[A]:THR:CA	3:R:3199[A]:GLN:HB2	2.43	0.46
3:R:3196[B]:THR:CB	3:R:3199[B]:GLN:OE1	2.64	0.46
3:R:3285[B]:VAL:CG2	3:R:3286[B]:THR:N	2.73	0.46
1:S:61:GLY:N	1:S:176:GLU:OE2	2.43	0.46
1:S:664:VAL:O	1:S:689:PRO:HD2	2.16	0.46
1:S:801:ASP:OD1	1:S:801:ASP:N	2.48	0.46
3:U:2970[B]:PRO:C	3:U:2972[B]:GLY:N	2.72	0.46
3:U:3004[B]:GLY:C	3:U:3006[B]:LYS:N	2.74	0.46
3:U:3014[B]:TRP:CG	3:U:3092[B]:ILE:CD1	2.98	0.46
3:U:3209[B]:GLU:O	3:U:3310[B]:GLY:C	2.59	0.46
3:U:3263[A]:LEU:N	3:U:3263[A]:LEU:CD1	2.79	0.46
3:U:3283[B]:ILE:C	3:U:3283[B]:ILE:CD1	2.85	0.46
3:U:3284[A]:LYS:CE	3:U:3285[A]:VAL:H	2.28	0.46
1:V:48:LYS:HE3	1:V:54:THR:HG22	1.97	0.46
1:V:1316:MET:HB3	1:V:1318:VAL:HG22	1.97	0.46
1:V:1498:ASN:ND2	1:V:1500:THR:O	2.49	0.46
2:W:2568:HIS:HD2	2:W:2718:TRP:CH2	2.34	0.46
2:W:2740:ASP:OD1	2:W:2740:ASP:N	2.49	0.46
3:X:2965[B]:LEU:HD13	3:X:2975[B]:PHE:O	2.16	0.46
3:X:2994[A]:LYS:O	3:X:2997[A]:GLU:N	2.49	0.46
3:X:3134[A]:GLN:O	3:X:3136[A]:TYR:N	2.49	0.46
3:X:3283[A]:ILE:HB	3:X:3305[A]:ILE:HD11	1.97	0.46
1:Y:92:TRP:O	1:Y:212:ASN:ND2	2.49	0.46
2:Z:2128:LEU:O	2:Z:2130:PRO:HD3	2.16	0.46
2:Z:2783:PHE:HB3	2:Z:2791:LEU:HD21	1.97	0.46
3:a:2938[A]:LEU:O	3:a:2939[A]:ARG:C	2.58	0.46
3:a:2965[A]:LEU:HD22	3:a:2975[A]:PHE:O	2.15	0.46
3:a:2965[B]:LEU:HD22	3:a:2975[B]:PHE:O	2.15	0.46
3:a:2987[B]:HIS:O	3:a:2991[B]:LEU:HB2	2.16	0.46
3:a:3014[A]:TRP:CD2	3:a:3092[A]:ILE:CD1	2.98	0.46
3:a:3074[B]:GLU:OE2	3:a:3208[B]:GLN:HG2	2.15	0.46
3:a:3191[A]:ASN:C	3:a:3192[A]:PHE:O	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3196[B]:THR:CA	3:a:3199[B]:GLN:HB2	2.43	0.46
3:a:3196[B]:THR:CB	3:a:3199[B]:GLN:OE1	2.64	0.46
3:a:3301[A]:PRO:HB2	3:a:3302[A]:SER:H	1.33	0.46
2:c:2802:ASP:OD2	2:c:2903:TYR:OH	2.28	0.46
2:c:2890:VAL:HG23	2:c:2891:LEU:C	2.40	0.46
3:d:2969[B]:TYR:CD2	3:d:2971[B]:ASP:N	2.73	0.46
3:d:2994[B]:LYS:O	3:d:2997[B]:GLU:N	2.49	0.46
3:d:3135[B]:LYS:HB2	3:d:3141[B]:TYR:CD1	2.51	0.46
3:d:3137[B]:ARG:HB3	3:d:3139[B]:LEU:HD21	1.97	0.46
3:d:3285[A]:VAL:CG2	3:d:3286[A]:THR:H	2.27	0.46
3:d:3298[B]:ASN:CA	3:d:3299[B]:LEU:HB2	2.44	0.46
8:0:1:NAG:H62	8:0:2:NAG:HN2	1.75	0.46
1:A:1145:THR:HG22	1:A:1193:LYS:HG2	1.97	0.45
2:B:2145:LEU:HG	2:B:2148:MET:SD	2.55	0.45
3:C:2932[A]:PRO:CA	3:C:2935[A]:ILE:CD1	2.85	0.45
3:C:2954[B]:TYR:CA	3:C:2957[B]:ILE:HG22	2.43	0.45
3:C:3004[A]:GLY:C	3:C:3006[A]:LYS:N	2.74	0.45
3:C:3116[A]:PHE:CD1	3:C:3116[A]:PHE:C	2.94	0.45
3:C:3116[B]:PHE:CD1	3:C:3116[B]:PHE:C	2.94	0.45
3:C:3119[B]:HIS:O	3:C:3122[B]:ASN:HB3	2.17	0.45
3:C:3204[B]:LEU:CD1	3:C:3204[B]:LEU:N	2.80	0.45
3:C:3263[B]:LEU:CD1	3:C:3263[B]:LEU:N	2.79	0.45
1:D:465:PRO:HD2	1:D:467:LYS:HZ1	1.79	0.45
1:D:522:ALA:HA	1:D:568:PHE:CZ	2.51	0.45
1:D:784:ALA:O	1:D:788:LEU:HG	2.16	0.45
1:D:1391:ARG:NH1	1:D:1451:ASP:OD1	2.49	0.45
2:E:2403:PHE:CZ	2:E:2428:VAL:HG21	2.51	0.45
3:F:2937[A]:ASN:CB	3:F:3006[A]:LYS:CE	2.85	0.45
3:F:3135[A]:LYS:HG3	3:F:3141[A]:TYR:HE1	1.29	0.45
3:F:3137[A]:ARG:HB3	3:F:3139[A]:LEU:HD21	1.97	0.45
3:F:3162[B]:ASP:C	3:a:3147[B]:GLU:OE1	2.59	0.45
3:F:3264[A]:TYR:HD1	3:F:3265[A]:ASP:N	2.14	0.45
1:G:22:LEU:HD23	1:G:123:PHE:CE1	2.51	0.45
1:G:1026:GLU:OE2	1:G:1028:VAL:HG12	2.15	0.45
1:G:1301:PRO:HA	1:G:1308:VAL:HA	1.99	0.45
2:H:2217:ILE:HD11	2:H:2287:TYR:HE1	1.81	0.45
2:H:2625:LEU:O	2:H:2638:ARG:NH2	2.49	0.45
2:H:2663:MET:HG3	2:H:2675:GLN:HB2	1.98	0.45
2:H:2822:LYS:HD2	2:H:2831:GLU:HA	1.97	0.45
3:I:3196[B]:THR:CB	3:I:3199[B]:GLN:OE1	2.64	0.45
3:I:3256[B]:TRP:NE1	3:R:2965[B]:LEU:HD13	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:494:VAL:HG23	1:J:671:PHE:HZ	1.81	0.45
1:J:901:THR:HG23	1:J:1077:LEU:HD12	1.97	0.45
1:J:949:ASP:CB	1:J:953:GLU:HB2	2.44	0.45
1:J:1578:ILE:HA	1:J:1579:GLY:HA2	1.59	0.45
3:L:2961[B]:HIS:CD2	3:L:2988[B]:TRP:CZ3	2.97	0.45
3:L:2987[B]:HIS:O	3:L:2991[B]:LEU:HB2	2.15	0.45
3:L:3137[B]:ARG:HB3	3:L:3139[B]:LEU:HD21	1.97	0.45
3:L:3242[A]:GLY:C	3:L:3243[A]:GLY:O	2.58	0.45
3:L:3264[B]:TYR:HD1	3:L:3265[B]:ASP:N	2.14	0.45
1:M:1145:THR:OG1	1:M:1233:SER:HB3	2.16	0.45
2:N:2110:MET:HE1	2:N:2122:ILE:HD12	1.98	0.45
2:N:2778:TYR:HB2	2:N:2781:LEU:HD12	1.97	0.45
3:O:3004[B]:GLY:C	3:O:3006[B]:LYS:N	2.74	0.45
3:O:3004[B]:GLY:O	3:O:3006[B]:LYS:N	2.44	0.45
3:O:3079[A]:CYS:SG	3:O:3146[A]:CYS:O	2.74	0.45
3:O:3191[B]:ASN:ND2	3:O:3191[B]:ASN:N	2.60	0.45
3:O:3196[A]:THR:CB	3:O:3199[A]:GLN:OE1	2.64	0.45
3:O:3263[B]:LEU:CD1	3:O:3263[B]:LEU:N	2.79	0.45
1:P:40:TYR:CE2	1:P:75:GLN:HG2	2.50	0.45
1:P:76:PHE:CD2	1:P:89:ILE:HG21	2.51	0.45
1:P:262:LYS:NZ	1:P:795:GLU:OE1	2.49	0.45
1:P:897:HIS:CD2	1:P:899:MET:HE1	2.51	0.45
1:P:1241:GLY:HA2	1:P:1252:PRO:HB3	1.97	0.45
3:R:2951[B]:ASP:CG	3:R:2952[B]:ALA:N	2.74	0.45
3:R:2994[A]:LYS:O	3:R:2997[A]:GLU:N	2.49	0.45
3:R:3074[B]:GLU:CD	3:R:3212[B]:ARG:NH2	2.73	0.45
3:R:3119[A]:HIS:O	3:R:3122[A]:ASN:HB3	2.17	0.45
3:R:3134[A]:GLN:O	3:R:3136[A]:TYR:N	2.49	0.45
3:R:3263[A]:LEU:N	3:R:3263[A]:LEU:CD1	2.79	0.45
1:S:308:LEU:O	1:S:772:ARG:NH2	2.50	0.45
1:S:961:SER:HB3	1:S:972:SER:O	2.16	0.45
1:S:1171:LYS:HG2	1:S:1173:GLY:H	1.81	0.45
2:T:2867:PRO:HG2	3:U:2932[A]:PRO:CG	2.45	0.45
2:T:2887:ASP:OD1	2:T:2887:ASP:N	2.48	0.45
3:U:2969[B]:TYR:CD2	3:U:2970[B]:PRO:N	2.83	0.45
3:U:2969[B]:TYR:CA	3:d:2981[B]:GLY:HA3	2.39	0.45
3:U:2985[B]:PHE:CE2	3:U:2989[B]:HIS:CD2	3.04	0.45
3:U:2987[A]:HIS:O	3:U:2991[A]:LEU:HB2	2.16	0.45
3:U:3087[B]:MET:HA	3:U:3090[B]:ASN:OD1	2.17	0.45
3:U:3134[A]:GLN:O	3:U:3136[A]:TYR:N	2.49	0.45
3:U:3134[B]:GLN:O	3:U:3136[B]:TYR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3264[B]:TYR:HD1	3:U:3265[B]:ASP:N	2.14	0.45
2:W:2723:GLU:HG2	2:W:2788:ILE:CD1	2.46	0.45
3:X:2937[A]:ASN:CB	3:X:3006[A]:LYS:CE	2.86	0.45
3:X:2951[A]:ASP:C	3:X:2956[A]:LYS:HZ1	2.13	0.45
3:X:3014[A]:TRP:CG	3:X:3092[A]:ILE:CD1	2.98	0.45
3:X:3014[A]:TRP:CD2	3:X:3092[A]:ILE:CD1	2.98	0.45
3:X:3116[B]:PHE:CD1	3:X:3116[B]:PHE:C	2.94	0.45
3:X:3119[A]:HIS:O	3:X:3122[A]:ASN:HB3	2.16	0.45
3:X:3134[B]:GLN:O	3:X:3136[B]:TYR:N	2.49	0.45
3:X:3137[A]:ARG:HD3	3:X:3137[A]:ARG:HA	1.71	0.45
3:X:3196[A]:THR:N	3:X:3199[A]:GLN:CB	2.65	0.45
3:X:3281[A]:PHE:HE1	3:X:3305[A]:ILE:HG21	1.81	0.45
3:a:3116[A]:PHE:CD1	3:a:3116[A]:PHE:C	2.94	0.45
3:a:3209[B]:GLU:O	3:a:3310[B]:GLY:C	2.59	0.45
3:a:3293[A]:LYS:HB2	3:a:3294[A]:SER:CA	2.41	0.45
1:b:418:ASP:C	1:b:420:SER:HA	2.41	0.45
1:b:468:CYS:SG	1:b:669:LYS:HB3	2.56	0.45
2:c:2867:PRO:HG2	3:d:2932[A]:PRO:O	2.16	0.45
3:d:2961[B]:HIS:HB2	3:d:2992[B]:TYR:HE2	1.81	0.45
3:d:2987[A]:HIS:O	3:d:2991[A]:LEU:HB2	2.16	0.45
3:d:3196[A]:THR:CB	3:d:3199[A]:GLN:OE1	2.64	0.45
1:A:428:ILE:HD12	1:A:514:TRP:HB3	1.99	0.45
1:A:1211:TYR:OH	2:E:2739:LEU:HD12	2.16	0.45
2:B:2462:PHE:CE1	2:B:2486:ILE:HD13	2.51	0.45
3:C:2965[B]:LEU:HD13	3:C:2975[B]:PHE:O	2.16	0.45
3:C:2973[B]:THR:HG22	3:L:3249[B]:GLY:N	2.31	0.45
3:C:3256[B]:TRP:NE1	3:L:2975[B]:PHE:O	2.49	0.45
1:D:28:ASP:HB3	1:D:33:GLY:HA2	1.98	0.45
1:D:613:SER:HA	1:D:805:VAL:HG12	1.97	0.45
1:D:962:GLY:HA2	1:D:971:THR:HB	1.97	0.45
1:D:1313:LEU:HD13	1:D:1322:TRP:CD1	2.51	0.45
2:E:2737:CYS:O	2:E:2739:LEU:HD23	2.15	0.45
3:F:2971[B]:ASP:CG	3:a:3248[B]:LEU:HD21	2.40	0.45
3:F:3148[A]:ILE:O	3:F:3148[A]:ILE:HG22	2.17	0.45
3:F:3252[B]:TYR:C	3:a:2976[B]:ALA:CB	2.88	0.45
1:G:1302:SER:HA	1:G:1303:GLU:HA	1.68	0.45
1:G:1331:GLU:OE1	1:G:1342:ALA:HB1	2.16	0.45
2:H:2114:ARG:HG3	2:K:2526:ARG:HE	1.81	0.45
2:H:2500:ILE:HD11	2:H:2775:GLY:O	2.16	0.45
3:I:2965[B]:LEU:HD22	3:I:2975[B]:PHE:O	2.15	0.45
3:I:2985[A]:PHE:CE2	3:I:2989[A]:HIS:CD2	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2992[B]:TYR:HE2	3:R:2969[B]:TYR:HE1	1.62	0.45
3:I:3134[B]:GLN:O	3:I:3136[B]:TYR:N	2.49	0.45
3:I:3137[B]:ARG:O	3:I:3139[B]:LEU:HD22	2.16	0.45
3:I:3151[B]:LEU:CB	3:I:3175[B]:TYR:CD2	2.93	0.45
3:I:3209[B]:GLU:O	3:I:3310[B]:GLY:C	2.59	0.45
1:J:1424:GLU:O	1:J:1427:HIS:HB3	2.16	0.45
2:K:2329:MET:HA	2:K:2354:PRO:HG2	1.96	0.45
3:L:2961[B]:HIS:HB2	3:L:2992[B]:TYR:HE2	1.81	0.45
3:L:2965[B]:LEU:HD22	3:L:2975[B]:PHE:O	2.15	0.45
3:L:3137[B]:ARG:O	3:L:3139[B]:LEU:HD22	2.16	0.45
3:L:3196[B]:THR:CB	3:L:3199[B]:GLN:OE1	2.64	0.45
3:L:3209[A]:GLU:O	3:L:3310[A]:GLY:C	2.59	0.45
2:N:2244:PHE:HE2	2:N:2374:ASN:HD22	1.64	0.45
3:O:2956[A]:LYS:O	3:O:2959[A]:SER:OG	2.33	0.45
3:O:2965[B]:LEU:HD22	3:O:2975[B]:PHE:O	2.15	0.45
3:O:2985[B]:PHE:CE2	3:O:2989[B]:HIS:CD2	3.04	0.45
3:O:3137[B]:ARG:HB3	3:O:3139[B]:LEU:HD21	1.97	0.45
3:O:3242[B]:GLY:C	3:O:3243[B]:GLY:O	2.58	0.45
3:O:3244[A]:THR:H	3:O:3264[A]:TYR:HE2	1.65	0.45
3:O:3301[B]:PRO:HB2	3:O:3302[B]:SER:H	1.33	0.45
1:P:899:MET:HE2	1:P:1012:GLU:OE2	2.16	0.45
1:P:931:TRP:CZ3	1:P:995:ILE:HD11	2.51	0.45
2:Q:2888:GLY:HA2	2:Q:2889:ALA:HA	1.70	0.45
3:R:2994[B]:LYS:O	3:R:2997[B]:GLU:N	2.49	0.45
3:R:3171[A]:HIS:C	3:R:3173[A]:THR:N	2.73	0.45
3:R:3176[B]:LYS:C	3:R:3177[B]:SER:HG	2.09	0.45
3:R:3191[B]:ASN:ND2	3:R:3191[B]:ASN:N	2.60	0.45
1:S:731:ALA:HB2	1:S:781:ILE:HD12	1.99	0.45
3:U:3135[A]:LYS:HB2	3:U:3141[A]:TYR:CD1	2.51	0.45
3:U:3158[B]:PHE:HB2	3:d:3149[B]:ASN:HB2	1.97	0.45
3:U:3255[B]:PRO:CD	3:d:3253[B]:GLU:N	2.78	0.45
1:V:133:LYS:HD2	1:V:134:VAL:HG22	1.98	0.45
1:V:428:ILE:HD12	1:V:514:TRP:HB3	1.97	0.45
1:V:688:VAL:HA	1:V:689:PRO:HD3	1.74	0.45
1:V:896:HIS:HB2	1:V:905:TRP:CD1	2.52	0.45
2:W:2340:ALA:HB1	2:W:2341:PRO:CD	2.42	0.45
3:X:3047[B]:ARG:NH2	3:X:3113[B]:ASP:OD1	2.43	0.45
3:X:3135[B]:LYS:HB2	3:X:3141[B]:TYR:CD1	2.51	0.45
3:X:3171[A]:HIS:C	3:X:3173[A]:THR:N	2.73	0.45
1:Y:25:MET:HA	1:Y:83:HIS:CD2	2.51	0.45
1:Y:950:ALA:HA	1:Y:951:ASN:HA	1.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:2606:LEU:HD13	2:Z:2706:ILE:HG13	1.96	0.45
3:a:3148[A]:ILE:O	3:a:3148[A]:ILE:HG22	2.17	0.45
3:a:3264[A]:TYR:HD1	3:a:3265[A]:ASP:N	2.14	0.45
1:b:490:TRP:HE1	1:b:670:PRO:HD2	1.80	0.45
3:d:3074[A]:GLU:OE2	3:d:3208[A]:GLN:HG2	2.15	0.45
3:d:3196[B]:THR:CB	3:d:3199[B]:GLN:OE1	2.64	0.45
2:B:2610:ASP:OD1	2:B:2610:ASP:N	2.49	0.45
3:C:2970[A]:PRO:C	3:C:2972[A]:GLY:N	2.72	0.45
3:C:2973[B]:THR:HG22	3:L:3248[B]:LEU:C	2.39	0.45
3:C:3134[B]:GLN:O	3:C:3136[B]:TYR:N	2.49	0.45
3:C:3155[B]:MET:C	3:L:3153[B]:LYS:HE3	2.40	0.45
3:C:3196[B]:THR:CB	3:C:3199[B]:GLN:OE1	2.64	0.45
3:C:3264[A]:TYR:HD1	3:C:3265[A]:ASP:N	2.14	0.45
1:D:17:ASN:HD21	1:D:86:THR:N	2.11	0.45
1:D:176:GLU:O	1:D:180:ASN:ND2	2.49	0.45
1:D:304:ALA:HB1	1:D:306:PHE:HE1	1.82	0.45
1:D:732:GLY:HA2	1:D:777:TYR:O	2.16	0.45
1:D:1167:ASP:OD1	1:D:1167:ASP:N	2.45	0.45
1:D:1562:ILE:C	1:D:1564:ALA:H	2.23	0.45
2:E:2274:LEU:HD23	2:E:2274:LEU:HA	1.77	0.45
2:E:2344:LEU:HA	2:E:2345:ASN:O	2.17	0.45
2:E:2672:PHE:CZ	2:E:2718:TRP:HA	2.52	0.45
3:F:2969[A]:TYR:CD2	3:F:2970[A]:PRO:N	2.83	0.45
3:F:3079[B]:CYS:SG	3:F:3146[B]:CYS:O	2.73	0.45
3:F:3106[A]:THR:O	3:F:3106[A]:THR:HG23	2.16	0.45
3:F:3116[A]:PHE:CD1	3:F:3116[A]:PHE:C	2.94	0.45
3:F:3120[B]:HIS:NE2	3:a:2969[B]:TYR:CD2	2.65	0.45
3:F:3150[B]:LYS:HZ2	3:a:3160[B]:SER:CB	1.99	0.45
3:F:3196[A]:THR:CB	3:F:3199[A]:GLN:OE1	2.64	0.45
3:F:3242[B]:GLY:C	3:F:3243[B]:GLY:O	2.58	0.45
3:F:3263[A]:LEU:N	3:F:3263[A]:LEU:CD1	2.79	0.45
3:F:3284[A]:LYS:HD3	3:F:3285[A]:VAL:O	2.16	0.45
1:G:883:CYS:HB3	1:G:884:PRO:CD	2.47	0.45
1:G:1169:LYS:HE3	1:G:1169:LYS:HB2	1.70	0.45
1:G:1189:ASP:HB2	2:K:2851:ASN:OD1	2.16	0.45
2:H:2625:LEU:HD13	2:H:2626:ARG:N	2.30	0.45
3:I:2931[A]:THR:HG1	3:I:2934[A]:GLU:CD	2.04	0.45
3:I:2949[A]:LYS:C	3:I:2953[A]:GLY:N	2.73	0.45
3:I:2974[B]:ALA:CA	3:R:3248[B]:LEU:C	2.87	0.45
3:I:2991[B]:LEU:HD23	3:I:3158[B]:PHE:CE1	2.48	0.45
3:I:3025[B]:VAL:CG2	3:I:3047[B]:ARG:NH1	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3087[A]:MET:HA	3:I:3090[A]:ASN:OD1	2.17	0.45
3:I:3153[B]:LYS:CD	3:R:3155[B]:MET:HB3	2.33	0.45
3:I:3204[A]:LEU:CD1	3:I:3204[A]:LEU:N	2.80	0.45
3:I:3253[B]:GLU:HB2	3:R:2965[B]:LEU:HD22	1.42	0.45
3:I:3284[A]:LYS:CE	3:I:3285[A]:VAL:H	2.28	0.45
1:J:961:SER:HB2	1:J:972:SER:O	2.16	0.45
1:J:1445:LEU:HD13	1:J:1594:GLY:HA2	1.99	0.45
2:K:2180:TRP:HB2	2:K:2243:LEU:HD13	1.98	0.45
2:K:2561:HIS:HA	2:K:2562:GLY:HA2	1.71	0.45
2:K:2783:PHE:HB3	2:K:2791:LEU:HD21	1.98	0.45
3:L:2994[B]:LYS:O	3:L:2997[B]:GLU:N	2.49	0.45
3:L:3074[B]:GLU:CD	3:L:3212[B]:ARG:NH2	2.73	0.45
3:L:3116[B]:PHE:CD1	3:L:3116[B]:PHE:C	2.94	0.45
3:L:3134[A]:GLN:O	3:L:3136[A]:TYR:N	2.50	0.45
3:L:3135[B]:LYS:HB2	3:L:3141[B]:TYR:CD1	2.52	0.45
3:L:3143[A]:SER:OG	3:L:3144[A]:ALA:N	2.47	0.45
3:L:3204[A]:LEU:CD1	3:L:3204[A]:LEU:N	2.80	0.45
3:L:3209[B]:GLU:O	3:L:3310[B]:GLY:C	2.59	0.45
1:M:573:LYS:NZ	1:M:780:GLU:O	2.49	0.45
1:M:931:TRP:CZ3	1:M:995:ILE:HD11	2.52	0.45
1:M:1279:LYS:O	1:M:1283:ASP:N	2.45	0.45
1:M:1280:GLN:HG2	1:M:1337:ARG:HH11	1.80	0.45
3:O:2994[B]:LYS:O	3:O:2997[B]:GLU:N	2.49	0.45
3:O:3087[A]:MET:HA	3:O:3090[A]:ASN:OD1	2.17	0.45
3:O:3146[B]:CYS:HA	3:O:3147[B]:GLU:HA	1.70	0.45
3:O:3156[B]:MET:SD	3:X:3173[B]:THR:CG2	3.05	0.45
3:O:3228[B]:VAL:CG2	3:O:3245[B]:PHE:CE1	2.97	0.45
1:P:944:GLU:O	1:P:957:ASN:ND2	2.48	0.45
1:P:1575:PRO:HA	1:P:1581:GLU:O	2.17	0.45
2:Q:2142:ALA:HA	2:Q:2143:CYS:HA	1.71	0.45
3:R:2965[B]:LEU:HD13	3:R:2975[B]:PHE:O	2.16	0.45
3:R:2985[B]:PHE:CE2	3:R:2989[B]:HIS:CD2	3.04	0.45
3:R:3148[B]:ILE:O	3:R:3148[B]:ILE:HG22	2.17	0.45
1:S:353:ASN:HD22	1:S:772:ARG:HH22	1.64	0.45
1:S:1017:HIS:C	1:S:1021:LEU:HG	2.41	0.45
2:T:2225:ARG:HB2	2:T:2274:LEU:O	2.17	0.45
2:T:2822:LYS:HE2	2:T:2882:GLU:OE1	2.16	0.45
3:U:3086[B]:GLU:OE1	3:d:2970[B]:PRO:HG2	2.17	0.45
1:V:452:ILE:HD11	1:V:676:PRO:O	2.15	0.45
1:V:938:LEU:HD23	1:V:1041:ILE:HD12	1.97	0.45
2:W:2181:THR:HB	2:W:2374:ASN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:2800:LYS:HB3	3:X:3023[A]:ILE:CD1	2.46	0.45
3:X:2937[B]:ASN:CB	3:X:3006[B]:LYS:CE	2.86	0.45
3:X:2965[A]:LEU:HD13	3:X:2975[A]:PHE:O	2.16	0.45
3:X:3013[B]:ASP:CG	3:X:3015[B]:THR:HG1	2.23	0.45
3:X:3106[B]:THR:O	3:X:3106[B]:THR:HG23	2.17	0.45
3:X:3285[B]:VAL:CG2	3:X:3286[B]:THR:H	2.27	0.45
1:Y:236:GLY:HA2	1:Y:819:ILE:HG13	1.98	0.45
1:Y:516:TRP:HD1	1:Y:579:LEU:HB3	1.82	0.45
1:Y:885:SER:HA	1:Y:888:ALA:H	1.80	0.45
1:Y:1427:HIS:CD2	1:Y:1457:HIS:HE1	2.33	0.45
1:Y:1596:GLU:O	1:Y:1597:THR:HG22	2.16	0.45
2:Z:2819:VAL:HG22	2:Z:2883:ILE:HG22	1.99	0.45
3:a:3134[A]:GLN:O	3:a:3136[A]:TYR:N	2.49	0.45
3:a:3196[A]:THR:CB	3:a:3199[A]:GLN:OE1	2.64	0.45
3:a:3200[A]:LEU:HD22	3:a:3204[A]:LEU:HD11	1.95	0.45
3:a:3200[B]:LEU:CD2	3:a:3204[B]:LEU:CD1	2.93	0.45
1:b:227:ARG:HA	1:b:227:ARG:NH1	2.30	0.45
1:b:402:THR:HG23	1:b:659:CYS:HA	1.98	0.45
3:d:2949[A]:LYS:NZ	3:d:2949[A]:LYS:C	2.73	0.45
3:d:2976[B]:ALA:O	3:d:2978[B]:CYS:N	2.46	0.45
3:d:3004[B]:GLY:C	3:d:3006[B]:LYS:N	2.74	0.45
3:d:3087[B]:MET:HA	3:d:3090[B]:ASN:OD1	2.17	0.45
3:d:3106[B]:THR:O	3:d:3106[B]:THR:HG23	2.16	0.45
3:d:3148[A]:ILE:O	3:d:3148[A]:ILE:HG22	2.17	0.45
3:d:3209[A]:GLU:O	3:d:3310[A]:GLY:C	2.59	0.45
1:A:277:ASP:OD1	1:A:277:ASP:N	2.24	0.45
1:A:364:ASP:O	1:A:368:SER:OG	2.31	0.45
1:A:601:VAL:HG11	1:A:777:TYR:CG	2.51	0.45
1:A:943:LEU:HD13	1:A:944:GLU:H	1.82	0.45
1:A:1000:GLU:HG2	1:A:1133:ILE:HB	1.99	0.45
1:A:1403:LEU:O	1:A:1407:THR:OG1	2.35	0.45
1:A:1422:HIS:NE2	1:A:1608:ARG:HB2	2.32	0.45
2:B:2738:ALA:HB1	2:B:2740:ASP:OD1	2.17	0.45
3:C:2966[B]:SER:CB	3:L:2982[B]:MET:CE	2.93	0.45
3:C:2976[B]:ALA:H	3:L:3253[B]:GLU:CA	2.30	0.45
3:C:3014[B]:TRP:CD2	3:C:3092[B]:ILE:CD1	2.98	0.45
3:C:3074[A]:GLU:OE2	3:C:3208[A]:GLN:HG2	2.15	0.45
3:C:3074[B]:GLU:OE2	3:C:3208[B]:GLN:HG2	2.15	0.45
3:C:3147[B]:GLU:CG	3:L:3161[B]:GLU:N	2.79	0.45
3:C:3250[B]:GLY:H	3:L:3252[B]:TYR:HB3	1.49	0.45
3:C:3263[A]:LEU:N	3:C:3263[A]:LEU:CD1	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1412:GLU:OE2	1:D:1552:ARG:NH1	2.40	0.45
2:E:2121:THR:O	2:E:2124:SER:OG	2.31	0.45
3:F:2965[B]:LEU:HD22	3:F:2975[B]:PHE:O	2.15	0.45
3:F:2994[A]:LYS:O	3:F:2997[A]:GLU:N	2.49	0.45
3:F:3013[A]:ASP:CG	3:F:3015[A]:THR:HG1	2.21	0.45
3:F:3134[A]:GLN:O	3:F:3136[A]:TYR:N	2.50	0.45
3:F:3137[A]:ARG:O	3:F:3139[A]:LEU:HD22	2.16	0.45
3:F:3146[A]:CYS:HA	3:F:3147[A]:GLU:HA	1.70	0.45
3:F:3169[B]:LYS:HG2	3:a:3151[B]:LEU:H	1.80	0.45
3:F:3196[B]:THR:CB	3:F:3199[B]:GLN:OE1	2.64	0.45
3:F:3244[B]:THR:H	3:F:3264[B]:TYR:HE2	1.65	0.45
3:F:3283[A]:ILE:HB	3:F:3305[A]:ILE:HD11	1.97	0.45
1:G:95:THR:O	1:G:153:ASN:ND2	2.50	0.45
1:G:304:ALA:HB3	1:G:360:HIS:HB3	1.99	0.45
1:G:415:VAL:HG11	1:G:697:ALA:N	2.32	0.45
1:G:902:PHE:CD1	1:G:1012:GLU:HB2	2.52	0.45
2:H:2572:VAL:HG22	2:H:2768:LEU:CD2	2.46	0.45
3:I:2951[B]:ASP:CG	3:I:2952[B]:ALA:N	2.74	0.45
3:I:2971[B]:ASP:C	3:R:3090[B]:ASN:HA	2.36	0.45
3:I:3023[B]:ILE:O	3:I:3026[B]:THR:OG1	2.34	0.45
3:I:3119[B]:HIS:O	3:I:3122[B]:ASN:HB3	2.17	0.45
3:I:3156[B]:MET:H	3:R:2979[B]:GLN:HE21	1.63	0.45
3:I:3284[A]:LYS:HD3	3:I:3285[A]:VAL:O	2.16	0.45
3:L:3047[B]:ARG:NH2	3:L:3113[B]:ASP:OD1	2.43	0.45
3:L:3079[A]:CYS:SG	3:L:3146[A]:CYS:O	2.74	0.45
3:L:3203[A]:HIS:O	3:L:3206[A]:LYS:HB3	2.15	0.45
3:L:3242[B]:GLY:C	3:L:3243[B]:GLY:O	2.58	0.45
3:L:3244[B]:THR:H	3:L:3264[B]:TYR:HE2	1.65	0.45
1:M:306:PHE:CE2	1:M:399:PRO:HG3	2.52	0.45
1:M:443:MET:HE1	1:M:455:TYR:CE1	2.51	0.45
1:M:695:TYR:HB3	1:M:696:GLN:HG3	1.99	0.45
2:N:2579:GLU:CD	2:N:2582:ARG:HH12	2.24	0.45
2:N:2872:GLU:O	1:P:1078:ARG:NH1	2.43	0.45
3:O:3134[B]:GLN:O	3:O:3136[B]:TYR:N	2.49	0.45
3:O:3204[A]:LEU:CD1	3:O:3204[A]:LEU:N	2.80	0.45
3:O:3264[A]:TYR:HD1	3:O:3265[A]:ASP:N	2.14	0.45
3:O:3281[B]:PHE:HE1	3:O:3305[B]:ILE:HG21	1.81	0.45
1:P:398:ARG:HH21	1:P:663:GLU:CD	2.23	0.45
1:P:730:PHE:CD1	1:P:780:GLU:HA	2.52	0.45
1:P:1427:HIS:HD2	1:P:1457:HIS:HE1	1.63	0.45
2:Q:2402:GLY:HA3	2:Q:2403:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:2732:HIS:CD2	2:Q:2732:HIS:H	2.35	0.45
3:R:2970[B]:PRO:C	3:R:2972[B]:GLY:N	2.72	0.45
3:R:3004[A]:GLY:C	3:R:3006[A]:LYS:N	2.74	0.45
3:R:3116[A]:PHE:C	3:R:3116[A]:PHE:CD1	2.94	0.45
3:R:3134[B]:GLN:O	3:R:3136[B]:TYR:N	2.49	0.45
3:R:3137[B]:ARG:O	3:R:3139[B]:LEU:HD22	2.16	0.45
3:R:3204[B]:LEU:CD1	3:R:3204[B]:LEU:N	2.80	0.45
3:R:3264[A]:TYR:HD1	3:R:3265[A]:ASP:N	2.14	0.45
1:S:622:HIS:HE1	1:S:767:LYS:H	1.64	0.45
1:S:1012:GLU:O	1:S:1015:HIS:N	2.50	0.45
2:T:2236:ALA:HB3	2:T:2239:LYS:HB3	1.98	0.45
2:T:2706:ILE:O	2:T:2710:HIS:N	2.44	0.45
3:U:2949[A]:LYS:C	3:U:2953[A]:GLY:N	2.73	0.45
3:U:2965[A]:LEU:HD13	3:U:2975[A]:PHE:O	2.16	0.45
3:U:2994[B]:LYS:O	3:U:2997[B]:GLU:N	2.49	0.45
3:U:3132[B]:ALA:HB3	3:U:3197[B]:ILE:HD13	1.98	0.45
3:U:3244[A]:THR:H	3:U:3264[A]:TYR:HE2	1.65	0.45
1:V:424:PHE:CZ	1:V:1125:SER:HB2	2.52	0.45
1:V:830:ASN:HB3	1:V:831:VAL:HA	1.98	0.45
1:V:1372:ILE:HD12	1:Y:1438:ASP:HB2	1.99	0.45
3:X:3087[B]:MET:HA	3:X:3090[B]:ASN:OD1	2.17	0.45
3:X:3204[A]:LEU:CD1	3:X:3204[A]:LEU:N	2.80	0.45
3:X:3264[A]:TYR:HD1	3:X:3265[A]:ASP:N	2.14	0.45
1:Y:86:THR:HB	1:Y:87:LEU:HD12	1.98	0.45
1:Y:483:GLY:HA3	1:Y:771:TRP:CE3	2.52	0.45
1:Y:515:ASP:OD1	1:Y:517:THR:OG1	2.25	0.45
1:Y:931:TRP:CG	1:Y:1018:ILE:HD11	2.51	0.45
1:Y:1019:HIS:NE2	1:Y:1046:HIS:HE1	2.12	0.45
1:Y:1612:THR:C	3:d:3186[B]:GLU:HB2	2.40	0.45
3:a:2937[B]:ASN:CB	3:a:3006[B]:LYS:CE	2.86	0.45
3:a:2961[B]:HIS:CD2	3:a:2988[B]:TRP:CZ3	2.96	0.45
3:a:3116[B]:PHE:CD1	3:a:3116[B]:PHE:C	2.94	0.45
3:a:3137[B]:ARG:O	3:a:3139[B]:LEU:HD22	2.16	0.45
3:a:3285[B]:VAL:CG2	3:a:3286[B]:THR:H	2.27	0.45
3:a:3293[B]:LYS:HB2	3:a:3294[B]:SER:CA	2.41	0.45
1:b:520:PHE:CD1	1:b:520:PHE:N	2.84	0.45
2:c:2477:PRO:O	2:c:2480:LEU:HD22	2.16	0.45
3:d:3196[B]:THR:O	3:d:3200[B]:LEU:N	2.43	0.45
3:d:3200[A]:LEU:CD2	3:d:3204[A]:LEU:CD1	2.93	0.45
3:d:3283[A]:ILE:HB	3:d:3305[A]:ILE:HD11	1.97	0.45
3:d:3298[A]:ASN:CA	3:d:3299[A]:LEU:HB2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2572:VAL:HG22	2:B:2768:LEU:CD2	2.46	0.45
2:B:2702:SER:HA	2:B:2707:PHE:CD2	2.52	0.45
3:C:2949[B]:LYS:NZ	3:C:2949[B]:LYS:C	2.73	0.45
3:C:2952[B]:ALA:N	3:C:2953[B]:GLY:CA	2.71	0.45
3:C:2964[B]:PRO:CA	3:L:3255[B]:PRO:HB3	2.47	0.45
3:C:2985[A]:PHE:CE2	3:C:2989[A]:HIS:CD2	3.04	0.45
3:C:3037[A]:TYR:C	3:C:3038[A]:ILE:HG13	2.42	0.45
3:C:3137[A]:ARG:HB3	3:C:3139[A]:LEU:HD21	1.97	0.45
3:C:3173[A]:THR:HG22	3:C:3174[A]:GLY:H	1.67	0.45
1:D:465:PRO:HD2	1:D:467:LYS:HZ3	1.81	0.45
1:D:587:PHE:HE2	1:D:643:ILE:HB	1.81	0.45
1:D:760:ILE:HG21	1:D:777:TYR:HE2	1.82	0.45
1:D:834:ASP:OD1	1:D:834:ASP:N	2.48	0.45
1:D:1470:GLU:OE2	1:D:1473:ARG:NH1	2.50	0.45
1:D:1562:ILE:HG13	1:D:1564:ALA:O	2.15	0.45
3:F:2938[A]:LEU:O	3:F:2939[A]:ARG:C	2.58	0.45
3:F:2956[B]:LYS:O	3:F:2959[B]:SER:OG	2.33	0.45
3:F:2957[B]:ILE:HA	3:F:2960[B]:PHE:HE1	1.64	0.45
3:F:2961[B]:HIS:HB2	3:F:2992[B]:TYR:HE2	1.81	0.45
3:F:2983[B]:VAL:HG23	3:a:3160[B]:SER:HG	1.76	0.45
3:F:3134[B]:GLN:O	3:F:3136[B]:TYR:N	2.49	0.45
3:F:3148[B]:ILE:O	3:F:3148[B]:ILE:HG22	2.17	0.45
3:F:3173[B]:THR:HA	3:a:3154[B]:PRO:CA	2.46	0.45
3:F:3281[B]:PHE:HE1	3:F:3305[B]:ILE:HG21	1.81	0.45
1:G:728:ARG:HE	1:G:730:PHE:HZ	1.65	0.45
1:G:1142:VAL:HG12	1:G:1143:ALA:N	2.32	0.45
2:H:2657:PHE:CD1	2:H:2783:PHE:HE2	2.35	0.45
3:I:3135[B]:LYS:HB2	3:I:3141[B]:TYR:CD1	2.51	0.45
2:K:2286:HIS:CD2	2:K:2433:THR:HG22	2.52	0.45
3:L:2939[A]:ARG:HG3	3:L:2939[A]:ARG:NH1	2.28	0.45
3:L:3037[A]:TYR:C	3:L:3038[A]:ILE:HG13	2.42	0.45
3:L:3119[A]:HIS:O	3:L:3122[A]:ASN:HB3	2.17	0.45
3:L:3263[A]:LEU:N	3:L:3263[A]:LEU:CD1	2.79	0.45
3:L:3281[B]:PHE:HE1	3:L:3305[B]:ILE:HG21	1.81	0.45
1:M:140:ASP:OD1	1:M:141:ALA:N	2.50	0.45
1:M:516:TRP:HH2	1:M:637:VAL:HG23	1.80	0.45
2:N:2132:CYS:H	2:N:2142:ALA:HB2	1.80	0.45
3:O:2937[B]:ASN:CB	3:O:3006[B]:LYS:CE	2.86	0.45
3:O:3037[A]:TYR:C	3:O:3038[A]:ILE:HG13	2.42	0.45
3:R:2969[A]:TYR:CD2	3:R:2970[A]:PRO:N	2.83	0.45
3:R:3004[B]:GLY:C	3:R:3006[B]:LYS:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3087[B]:MET:HA	3:R:3090[B]:ASN:OD1	2.17	0.45
3:R:3096[A]:VAL:HG11	3:R:3115[A]:LEU:HD12	1.89	0.45
3:R:3284[B]:LYS:CE	3:R:3285[B]:VAL:H	2.29	0.45
1:S:398:ARG:NH2	1:S:663:GLU:OE1	2.49	0.45
1:S:614:GLU:HA	1:S:615:PRO:HD3	1.87	0.45
1:S:903:PRO:HG2	1:S:904:HIS:CD2	2.52	0.45
1:S:1415:ASP:OD1	1:S:1416:PHE:N	2.48	0.45
2:T:2628:HIS:HB2	2:T:2635:TYR:CE2	2.52	0.45
3:U:2965[B]:LEU:HD13	3:U:2975[B]:PHE:O	2.16	0.45
3:U:3119[B]:HIS:O	3:U:3122[B]:ASN:HB3	2.16	0.45
3:U:3137[A]:ARG:O	3:U:3139[A]:LEU:HD22	2.16	0.45
3:U:3283[A]:ILE:HB	3:U:3305[A]:ILE:HD11	1.97	0.45
1:V:59:LEU:HD13	1:V:68:TRP:CD1	2.51	0.45
1:V:1243:PHE:CD2	1:V:1249:TRP:HD1	2.34	0.45
1:V:1599:MET:HG3	1:V:1600:PRO:HD2	1.97	0.45
2:W:2866:PRO:HB2	2:W:2868:GLU:HG3	1.98	0.45
1:Y:949:ASP:OD1	1:Y:950:ALA:N	2.49	0.45
1:Y:1077:LEU:HD23	1:Y:1103:PHE:HE1	1.82	0.45
2:Z:2568:HIS:CD2	2:Z:2718:TRP:CH2	3.05	0.45
2:Z:2568:HIS:HD2	2:Z:2718:TRP:CH2	2.35	0.45
2:Z:2568:HIS:HE1	2:Z:2742:MET:SD	2.40	0.45
3:a:2965[A]:LEU:HD13	3:a:2975[A]:PHE:O	2.16	0.45
3:a:3004[B]:GLY:C	3:a:3006[B]:LYS:N	2.74	0.45
1:b:664:VAL:HG12	1:b:690:THR:HG22	1.97	0.45
1:b:1642:GLN:N	1:b:1642:GLN:OE1	2.50	0.45
3:d:3087[A]:MET:HA	3:d:3090[A]:ASN:OD1	2.17	0.45
3:d:3264[B]:TYR:HD1	3:d:3265[B]:ASP:N	2.14	0.45
3:d:3281[B]:PHE:HE1	3:d:3305[B]:ILE:HG21	1.81	0.45
3:d:3284[A]:LYS:CE	3:d:3285[A]:VAL:H	2.29	0.45
1:A:567:LEU:CB	1:A:571:PRO:HG2	2.43	0.45
2:B:2114:ARG:HG3	2:E:2526:ARG:HH21	1.81	0.45
2:B:2382:GLU:O	2:B:2386:ARG:HG3	2.17	0.45
2:B:2805:PHE:CE1	2:B:2855:ASP:HB3	2.51	0.45
3:C:3004[B]:GLY:O	3:C:3006[B]:LYS:N	2.44	0.45
3:C:3014[B]:TRP:CG	3:C:3092[B]:ILE:CD1	2.98	0.45
3:C:3148[A]:ILE:O	3:C:3148[A]:ILE:HG22	2.17	0.45
3:C:3155[B]:MET:SD	3:L:3154[B]:PRO:N	2.88	0.45
3:C:3156[B]:MET:CB	3:L:2982[B]:MET:HB2	2.22	0.45
3:C:3163[B]:ASN:HD21	3:L:3149[B]:ASN:HB2	1.45	0.45
3:C:3191[A]:ASN:C	3:C:3192[A]:PHE:O	2.52	0.45
3:C:3222[B]:ILE:CD1	3:C:3223[B]:GLY:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3223[B]:GLY:N	3:L:2963[B]:MET:HE1	2.10	0.45
3:C:3253[B]:GLU:CB	3:L:2976[B]:ALA:H	1.90	0.45
3:C:3306[A]:LEU:C	3:C:3306[A]:LEU:CD1	2.86	0.45
3:F:3119[A]:HIS:O	3:F:3122[A]:ASN:HB3	2.17	0.45
3:F:3150[B]:LYS:CE	3:a:3163[B]:ASN:HB3	2.42	0.45
3:F:3203[A]:HIS:O	3:F:3206[A]:LYS:HB3	2.16	0.45
3:F:3244[A]:THR:H	3:F:3264[A]:TYR:HE2	1.65	0.45
3:F:3255[B]:PRO:CB	3:a:2964[B]:PRO:CD	2.94	0.45
3:I:2952[B]:ALA:N	3:I:2953[B]:GLY:HA2	2.06	0.45
3:I:2962[B]:GLY:N	3:R:3255[B]:PRO:HD3	2.32	0.45
3:I:2971[B]:ASP:C	3:R:3248[B]:LEU:HD22	2.42	0.45
3:I:2979[A]:GLN:HB2	3:I:2988[A]:TRP:CD1	2.52	0.45
3:I:3087[B]:MET:HA	3:I:3090[B]:ASN:OD1	2.17	0.45
3:I:3119[A]:HIS:O	3:I:3122[A]:ASN:HB3	2.17	0.45
3:I:3134[A]:GLN:O	3:I:3136[A]:TYR:N	2.49	0.45
1:J:92:TRP:CZ3	1:J:102:PRO:HD3	2.51	0.45
3:L:2949[B]:LYS:NZ	3:L:2949[B]:LYS:C	2.73	0.45
3:L:2971[A]:ASP:CG	3:L:2973[A]:THR:HG1	2.13	0.45
3:L:3134[B]:GLN:O	3:L:3136[B]:TYR:N	2.49	0.45
3:L:3137[A]:ARG:O	3:L:3139[A]:LEU:HD22	2.16	0.45
3:L:3283[B]:ILE:HB	3:L:3305[B]:ILE:HD11	1.97	0.45
1:M:991:LEU:O	1:M:995:ILE:HG13	2.17	0.45
1:M:1166:THR:N	1:M:1167:ASP:HA	2.32	0.45
1:M:1321:HIS:HE1	1:M:1489:MET:HE1	1.82	0.45
2:N:2128:LEU:HD22	2:N:2287:TYR:CE1	2.51	0.45
3:O:2951[A]:ASP:C	3:O:2956[A]:LYS:HZ1	2.12	0.45
3:O:2969[B]:TYR:CD2	3:O:2970[B]:PRO:N	2.83	0.45
3:O:3119[B]:HIS:O	3:O:3122[B]:ASN:HB3	2.17	0.45
1:P:398:ARG:NH2	1:P:663:GLU:OE1	2.42	0.45
1:P:1075:GLU:H	1:P:1075:GLU:HG3	1.35	0.45
1:P:1082:SER:HB3	1:P:1083:PRO:HD3	1.98	0.45
1:P:1400:ASN:HD22	1:P:1433:TRP:HZ3	1.64	0.45
1:P:1423:TYR:OH	1:P:1461:VAL:O	2.28	0.45
3:R:2948[B]:ASP:CB	3:R:2949[B]:LYS:HA	2.16	0.45
3:R:3209[A]:GLU:O	3:R:3310[A]:GLY:C	2.59	0.45
1:S:284:MET:HE1	1:S:292:LEU:HD22	1.99	0.45
1:S:730:PHE:O	1:S:820:VAL:HA	2.17	0.45
1:S:877:HIS:ND1	1:S:1036:SER:OG	2.49	0.45
1:S:1029:SER:OG	1:S:1030:MET:N	2.49	0.45
1:S:1153:LYS:H	1:S:1153:LYS:HG2	1.50	0.45
2:T:2217:ILE:HG22	2:T:2218:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:2823:ILE:O	2:T:2823:ILE:HG13	2.16	0.45
3:U:2965[A]:LEU:HD22	3:U:2975[A]:PHE:O	2.15	0.45
3:U:2969[B]:TYR:CB	3:d:3256[B]:TRP:NE1	2.80	0.45
3:U:2979[A]:GLN:HB2	3:U:2988[A]:TRP:CD1	2.52	0.45
3:U:3024[B]:LEU:CD1	3:U:3024[B]:LEU:C	2.85	0.45
3:U:3171[B]:HIS:C	3:d:3152[B]:LYS:NZ	2.74	0.45
3:U:3180[B]:TYR:CB	3:U:3183[B]:LEU:CD2	2.90	0.45
3:U:3196[B]:THR:CB	3:U:3199[B]:GLN:OE1	2.64	0.45
3:U:3200[A]:LEU:CD2	3:U:3204[A]:LEU:CD1	2.93	0.45
3:U:3230[B]:PHE:H	3:U:3243[B]:GLY:HA3	1.79	0.45
3:U:3244[B]:THR:H	3:U:3264[B]:TYR:HE2	1.65	0.45
3:U:3273[B]:LEU:C	3:U:3275[B]:LEU:HD12	2.42	0.45
1:V:308:LEU:HG	1:V:343:ILE:HD11	1.98	0.45
2:W:2412:GLN:HG2	2:W:2422:GLU:HA	1.99	0.45
3:X:2979[A]:GLN:HB2	3:X:2988[A]:TRP:CD1	2.52	0.45
3:X:2986[A]:PRO:CB	3:X:3127[A]:TRP:CE3	3.00	0.45
3:X:3244[A]:THR:H	3:X:3264[A]:TYR:HE2	1.65	0.45
1:Y:277:ASP:OD1	1:Y:278:ASP:N	2.50	0.45
1:Y:991:LEU:HD12	1:Y:991:LEU:HA	1.69	0.45
1:Y:1473:ARG:HG3	1:Y:1479:TYR:CG	2.51	0.45
1:Y:1604:ASP:OD1	1:Y:1605:ARG:NH1	2.50	0.45
1:Y:1650:ILE:HG13	2:c:2327:GLU:HG2	1.99	0.45
2:Z:2156:ARG:HH22	2:Z:2309:GLN:HE22	1.65	0.45
2:Z:2472:ASN:N	2:Z:2473:GLY:HA2	2.31	0.45
3:a:2956[A]:LYS:O	3:a:2959[A]:SER:OG	2.33	0.45
3:a:3037[A]:TYR:C	3:a:3038[A]:ILE:HG13	2.42	0.45
3:a:3037[B]:TYR:C	3:a:3038[B]:ILE:HG13	2.42	0.45
3:a:3106[A]:THR:O	3:a:3106[A]:THR:HG23	2.16	0.45
3:a:3183[A]:LEU:H	3:a:3184[A]:ASN:CA	2.22	0.45
3:a:3200[B]:LEU:HD22	3:a:3204[B]:LEU:HD11	1.95	0.45
3:a:3204[B]:LEU:CD1	3:a:3204[B]:LEU:N	2.80	0.45
3:a:3225[B]:SER:C	3:a:3290[B]:ILE:HG23	2.39	0.45
3:a:3263[A]:LEU:N	3:a:3263[A]:LEU:CD1	2.79	0.45
1:b:452:ILE:HD11	1:b:676:PRO:O	2.16	0.45
1:b:1001:GLN:CD	1:b:1001:GLN:H	2.24	0.45
1:b:1528:ASP:N	1:b:1528:ASP:OD1	2.49	0.45
3:d:3004[A]:GLY:C	3:d:3006[A]:LYS:N	2.74	0.45
3:d:3014[B]:TRP:CG	3:d:3092[B]:ILE:CD1	2.98	0.45
3:d:3024[A]:LEU:CD1	3:d:3024[A]:LEU:C	2.85	0.45
3:d:3025[A]:VAL:CG2	3:d:3047[A]:ARG:NH1	2.73	0.45
3:d:3037[B]:TYR:C	3:d:3038[B]:ILE:HG13	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3101[B]:PRO:O	3:d:3109[B]:TYR:HD2	2.00	0.45
3:d:3116[B]:PHE:CD1	3:d:3116[B]:PHE:C	2.94	0.45
3:d:3132[A]:ALA:HB3	3:d:3197[A]:ILE:HD13	1.98	0.45
3:d:3244[A]:THR:H	3:d:3264[A]:TYR:HE2	1.65	0.45
4:q:1:NAG:H4	4:q:2:NAG:N2	2.31	0.45
1:A:19:GLN:HG2	1:A:110:PHE:CD2	2.52	0.45
1:A:470:ARG:O	1:A:472:ASP:N	2.45	0.45
1:A:729:VAL:HG22	1:A:781:ILE:O	2.17	0.45
1:A:958:PRO:O	1:A:959:PHE:HB2	2.15	0.45
2:B:2638:ARG:NH2	2:B:2706:ILE:HG13	2.32	0.45
3:C:3101[A]:PRO:O	3:C:3109[A]:TYR:HD2	2.00	0.45
3:C:3152[B]:LYS:N	3:L:3172[B]:SER:HB2	2.32	0.45
3:C:3204[A]:LEU:CD1	3:C:3204[A]:LEU:N	2.79	0.45
3:C:3209[B]:GLU:O	3:C:3310[B]:GLY:C	2.59	0.45
1:D:464:LEU:HD13	1:D:622:HIS:CD2	2.51	0.45
1:D:905:TRP:CD1	1:D:1084:PHE:HE2	2.35	0.45
3:F:2937[B]:ASN:CB	3:F:3006[B]:LYS:CE	2.85	0.45
3:F:2986[A]:PRO:CB	3:F:3127[A]:TRP:CE3	3.00	0.45
3:F:3023[B]:ILE:HA	3:F:3026[B]:THR:HG1	1.82	0.45
3:F:3087[B]:MET:HA	3:F:3090[B]:ASN:OD1	2.17	0.45
3:F:3104[A]:MET:HA	3:F:3110[A]:THR:CG2	2.17	0.45
3:F:3132[A]:ALA:HB3	3:F:3197[A]:ILE:HD13	1.98	0.45
3:F:3156[B]:MET:HG2	3:a:2979[B]:GLN:NE2	2.24	0.45
1:G:7:VAL:HG23	1:G:91:TYR:O	2.16	0.45
1:G:1604:ASP:OD1	1:G:1605:ARG:NH1	2.49	0.45
3:I:2951[A]:ASP:CG	3:I:2952[A]:ALA:N	2.74	0.45
3:I:2965[B]:LEU:CD1	3:I:2974[B]:ALA:CA	2.89	0.45
3:I:2976[A]:ALA:O	3:I:2978[A]:CYS:N	2.46	0.45
3:I:3037[A]:TYR:C	3:I:3038[A]:ILE:HG13	2.42	0.45
3:I:3150[B]:LYS:HG3	3:R:3163[B]:ASN:CB	2.46	0.45
3:I:3163[B]:ASN:HB3	3:R:3149[B]:ASN:ND2	2.30	0.45
3:I:3255[B]:PRO:CB	3:R:2959[B]:SER:C	2.69	0.45
1:J:93:ASP:HA	1:J:212:ASN:ND2	2.31	0.45
1:J:977:GLU:HG2	1:J:1021:LEU:O	2.17	0.45
1:J:1143:ALA:HA	1:J:1195:ASP:HA	1.99	0.45
2:K:2147:GLY:HA3	2:K:2437:TRP:CE3	2.51	0.45
2:K:2360:TYR:HB2	2:K:2366:TYR:CE1	2.52	0.45
3:L:2965[A]:LEU:HD13	3:L:2975[A]:PHE:O	2.16	0.45
3:L:2979[A]:GLN:HB2	3:L:2988[A]:TRP:CD1	2.52	0.45
3:L:3034[B]:HIS:HB3	3:L:3035[B]:HIS:CE1	2.50	0.45
3:L:3185[B]:TYR:CE2	3:L:3187[B]:TYR:HE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:63:PRO:HA	1:M:172:GLU:HG3	1.97	0.45
1:M:904:HIS:O	1:M:907:ARG:HB3	2.17	0.45
1:M:1260:ARG:HD3	1:M:1331:GLU:OE1	2.16	0.45
1:M:1571:TYR:HE2	1:M:1631:GLU:HB3	1.81	0.45
2:N:2128:LEU:HB3	2:N:2129:PRO:HD3	1.98	0.45
2:N:2569:TRP:O	2:N:2572:VAL:HG23	2.16	0.45
3:O:3191[A]:ASN:ND2	3:O:3191[A]:ASN:N	2.60	0.45
2:Q:2606:LEU:HD13	2:Q:2706:ILE:HG13	1.98	0.45
3:R:2989[A]:HIS:C	3:R:2991[A]:LEU:N	2.75	0.45
3:R:3037[A]:TYR:C	3:R:3038[A]:ILE:HG13	2.42	0.45
3:R:3119[B]:HIS:O	3:R:3122[B]:ASN:HB3	2.17	0.45
1:S:593:CYS:O	1:S:597:VAL:HG22	2.17	0.45
1:S:601:VAL:HG11	1:S:777:TYR:CD1	2.52	0.45
1:S:601:VAL:HG11	1:S:777:TYR:CG	2.51	0.45
1:S:897:HIS:C	1:S:899:MET:HA	2.42	0.45
1:S:1271:MET:HG2	1:S:1358:LEU:HD13	1.99	0.45
1:S:1307:MET:HE3	1:S:1307:MET:HB2	1.81	0.45
1:S:1325:LEU:HG	1:S:1516:VAL:HG11	1.99	0.45
2:T:2186:GLU:HA	2:T:2232:PHE:HE1	1.82	0.45
2:T:2561:HIS:HB3	2:T:2677:GLU:OE2	2.17	0.45
3:U:2946[A]:GLN:CD	3:U:2947[A]:ALA:N	2.72	0.45
3:U:2989[B]:HIS:C	3:U:2991[B]:LEU:N	2.75	0.45
3:U:3204[A]:LEU:CD1	3:U:3204[A]:LEU:N	2.80	0.45
1:V:495:VAL:HG12	1:V:511:VAL:HG11	1.99	0.45
1:V:1562:ILE:HD11	1:V:1645:PHE:CZ	2.52	0.45
2:W:2128:LEU:HD13	2:W:2286:HIS:CG	2.52	0.45
3:X:2985[A]:PHE:CE2	3:X:2989[A]:HIS:CD2	3.04	0.45
3:X:2985[B]:PHE:CE2	3:X:2989[B]:HIS:CD2	3.04	0.45
3:X:3200[B]:LEU:CD2	3:X:3204[B]:LEU:CD1	2.93	0.45
1:Y:53:SER:O	1:Y:55:ILE:HG13	2.17	0.45
1:Y:469:PRO:O	1:Y:673:PHE:HZ	2.00	0.45
1:Y:1423:TYR:OH	1:Y:1461:VAL:HG12	2.16	0.45
1:Y:1619:GLY:H	3:d:3190[B]:LEU:HG	1.82	0.45
2:Z:2889:ALA:HB3	2:Z:2890:VAL:C	2.41	0.45
3:a:3014[A]:TRP:CG	3:a:3092[A]:ILE:CD1	2.98	0.45
3:a:3087[A]:MET:HA	3:a:3090[A]:ASN:OD1	2.17	0.45
3:a:3087[B]:MET:HA	3:a:3090[B]:ASN:OD1	2.17	0.45
3:a:3171[A]:HIS:C	3:a:3173[A]:THR:N	2.73	0.45
3:a:3204[A]:LEU:CD1	3:a:3204[A]:LEU:N	2.80	0.45
3:a:3225[A]:SER:C	3:a:3290[A]:ILE:HG23	2.39	0.45
3:a:3244[B]:THR:H	3:a:3264[B]:TYR:HE2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:2561:HIS:HB3	2:c:2677:GLU:OE2	2.16	0.45
3:d:2932[A]:PRO:CA	3:d:2935[A]:ILE:CD1	2.85	0.45
3:d:2938[A]:LEU:O	3:d:2939[A]:ARG:C	2.58	0.45
3:d:2981[A]:GLY:N	3:d:3086[A]:GLU:OE1	2.45	0.45
3:d:2985[A]:PHE:CE2	3:d:2989[A]:HIS:CD2	3.04	0.45
3:d:3134[B]:GLN:O	3:d:3136[B]:TYR:N	2.49	0.45
3:d:3135[A]:LYS:HB2	3:d:3141[A]:TYR:CD1	2.51	0.45
3:d:3137[B]:ARG:O	3:d:3139[B]:LEU:HD22	2.16	0.45
3:d:3203[A]:HIS:O	3:d:3206[A]:LYS:HB3	2.16	0.45
3:d:3209[B]:GLU:O	3:d:3310[B]:GLY:C	2.59	0.45
3:d:3229[A]:ASN:O	3:d:3286[A]:THR:N	2.50	0.45
4:j:1:NAG:C6	4:j:2:NAG:HN2	2.01	0.45
6:r:1:NAG:C4	6:r:2:NAG:O7	2.62	0.45
1:A:163:LEU:HD21	1:A:219:LEU:HD13	1.97	0.45
1:A:407:GLN:OE1	1:A:407:GLN:N	2.39	0.45
1:A:647:LEU:O	1:A:651:ARG:HB2	2.17	0.45
2:B:2715:ASP:HB3	2:B:2778:TYR:OH	2.16	0.45
3:C:3019[A]:HIS:CD2	3:C:3020[A]:SER:H	2.35	0.45
3:C:3034[A]:HIS:HB3	3:C:3035[A]:HIS:CE1	2.50	0.45
3:C:3089[B]:HIS:C	3:L:2971[B]:ASP:HA	2.42	0.45
3:C:3134[A]:GLN:O	3:C:3136[A]:TYR:N	2.49	0.45
3:C:3153[B]:LYS:HE3	3:L:3158[B]:PHE:HB2	1.98	0.45
3:C:3174[B]:GLY:N	3:L:3154[B]:PRO:N	2.64	0.45
3:C:3242[A]:GLY:C	3:C:3243[A]:GLY:O	2.58	0.45
3:C:3264[B]:TYR:HD1	3:C:3265[B]:ASP:N	2.14	0.45
1:D:838:ARG:NH1	1:D:915:ASN:OD1	2.50	0.45
1:D:1161:ILE:HD11	1:D:1196:ILE:CD1	2.42	0.45
1:D:1493:MET:HG2	1:D:1511:SER:O	2.16	0.45
3:F:2969[A]:TYR:CD2	3:F:2970[A]:PRO:CG	3.00	0.45
3:F:2975[B]:PHE:CZ	3:a:2961[B]:HIS:CD2	3.04	0.45
3:F:2981[A]:GLY:N	3:F:3086[A]:GLU:OE1	2.45	0.45
3:F:3014[B]:TRP:CD2	3:F:3092[B]:ILE:CD1	2.98	0.45
3:F:3119[B]:HIS:O	3:F:3122[B]:ASN:HB3	2.17	0.45
3:F:3149[B]:ASN:HD22	3:a:3163[B]:ASN:C	2.25	0.45
3:F:3259[B]:ASP:H	3:a:3162[B]:ASP:CG	2.24	0.45
1:G:126:GLY:HA3	1:G:127:GLU:HA	1.72	0.45
2:H:2575:LEU:HD23	2:H:2575:LEU:HA	1.82	0.45
2:H:2870:LEU:O	1:J:1078:ARG:NH1	2.49	0.45
3:I:2965[B]:LEU:HD13	3:I:2975[B]:PHE:O	2.16	0.45
3:I:2994[A]:LYS:O	3:I:2997[A]:GLU:N	2.49	0.45
3:I:3038[B]:ILE:HG23	3:I:3040[B]:VAL:HG22	1.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3044[A]:LYS:H	3:I:3044[A]:LYS:HG2	1.65	0.45
3:I:3094[B]:SER:HG	3:I:3227[B]:ASP:CG	2.25	0.45
3:I:3132[B]:ALA:HB3	3:I:3197[B]:ILE:HD13	1.99	0.45
3:I:3148[B]:ILE:O	3:I:3148[B]:ILE:HG22	2.17	0.45
3:I:3230[A]:PHE:H	3:I:3243[A]:GLY:HA3	1.79	0.45
3:I:3251[B]:ASP:CG	3:R:3108[B]:HIS:CE1	2.94	0.45
3:I:3263[A]:LEU:CD1	3:I:3263[A]:LEU:N	2.79	0.45
1:J:906:HIS:CD2	1:J:1046:HIS:CE1	3.05	0.45
1:J:1421:VAL:HG23	1:J:1422:HIS:HD1	1.82	0.45
3:L:2952[B]:ALA:CB	3:L:2953[B]:GLY:CA	2.82	0.45
3:L:2970[B]:PRO:C	3:L:2972[B]:GLY:H	2.23	0.45
3:L:2986[A]:PRO:CB	3:L:3127[A]:TRP:CE3	3.00	0.45
3:L:3101[A]:PRO:O	3:L:3109[A]:TYR:HD2	2.00	0.45
3:L:3106[B]:THR:O	3:L:3106[B]:THR:HG23	2.17	0.45
3:L:3132[A]:ALA:HB3	3:L:3197[A]:ILE:HD13	1.99	0.45
3:L:3244[A]:THR:H	3:L:3264[A]:TYR:HE2	1.64	0.45
1:M:896:HIS:HB2	1:M:905:TRP:CD1	2.52	0.45
1:M:1378:PHE:O	1:M:1391:ARG:NH1	2.50	0.45
1:M:1627:ARG:NH2	1:M:1629:GLU:OE1	2.50	0.45
2:N:2156:ARG:HD2	2:N:2357:VAL:HG12	1.99	0.45
2:N:2275:GLY:HA3	2:N:2283:ASN:HB2	1.98	0.45
3:O:2969[A]:TYR:CD2	3:O:2970[A]:PRO:CG	3.00	0.45
3:O:3106[A]:THR:O	3:O:3106[A]:THR:HG23	2.16	0.45
3:O:3137[A]:ARG:O	3:O:3139[A]:LEU:HD22	2.16	0.45
3:O:3263[A]:LEU:N	3:O:3263[A]:LEU:CD1	2.79	0.45
3:O:3306[A]:LEU:C	3:O:3306[A]:LEU:CD1	2.85	0.45
1:P:156:LEU:O	1:P:160:LEU:HB2	2.17	0.45
1:P:613:SER:HA	1:P:805:VAL:O	2.16	0.45
2:Q:2830:GLN:H	2:Q:2863:ARG:HH22	1.64	0.45
3:R:3132[A]:ALA:HB3	3:R:3197[A]:ILE:HD13	1.99	0.45
3:R:3203[A]:HIS:O	3:R:3206[A]:LYS:HB3	2.16	0.45
3:R:3273[B]:LEU:C	3:R:3275[B]:LEU:HD12	2.42	0.45
1:S:899:MET:HE2	1:S:1012:GLU:CD	2.41	0.45
2:T:2274:LEU:HD23	2:T:2274:LEU:HA	1.78	0.45
3:U:2975[B]:PHE:CE1	3:d:3256[B]:TRP:HD1	2.19	0.45
3:U:2985[A]:PHE:CE2	3:U:2989[A]:HIS:CD2	3.04	0.45
3:U:3154[B]:PRO:HD3	3:d:3151[B]:LEU:HA	1.99	0.45
3:U:3180[A]:TYR:CA	3:U:3183[A]:LEU:CD2	2.95	0.45
3:U:3255[B]:PRO:C	3:d:2975[B]:PHE:CA	2.90	0.45
1:V:607:HIS:CE1	1:V:634:HIS:HE1	2.35	0.45
1:V:717:GLN:O	1:V:721:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:958:PRO:O	1:V:959:PHE:HB2	2.17	0.45
1:V:1166:THR:HB	1:V:1167:ASP:C	2.42	0.45
2:W:2361:LYS:HD2	2:W:2362:GLN:HG3	1.98	0.45
2:W:2564:PRO:HA	2:W:2673:GLU:HG3	1.99	0.45
3:X:2970[A]:PRO:C	3:X:2972[A]:GLY:H	2.23	0.45
3:X:3241[A]:PHE:CZ	3:X:3243[A]:GLY:O	2.70	0.45
1:Y:784:ALA:O	1:Y:788:LEU:HB2	2.16	0.45
1:Y:843:VAL:HG13	1:Y:927:PRO:HB2	1.99	0.45
1:Y:885:SER:HB3	1:Y:886:PRO:HA	1.99	0.45
1:Y:1286:ARG:HD2	1:Y:1286:ARG:HA	1.66	0.45
1:Y:1296:VAL:HG11	1:Y:1447:TYR:CE1	2.51	0.45
2:Z:2359:ASN:HB3	2:Z:2361:LYS:HZ2	1.82	0.45
3:a:2985[A]:PHE:CE2	3:a:2989[A]:HIS:CD2	3.04	0.45
3:a:3074[A]:GLU:OE2	3:a:3208[A]:GLN:HG2	2.15	0.45
3:a:3132[B]:ALA:HB3	3:a:3197[B]:ILE:HD13	1.98	0.45
1:b:266:LEU:HD12	1:b:272:LEU:HD11	1.98	0.45
1:b:999:LEU:O	1:b:1063:ARG:NH2	2.45	0.45
2:c:2251:LEU:HA	2:c:2308:TRP:HD1	1.82	0.45
3:d:2965[B]:LEU:HD13	3:d:2975[B]:PHE:O	2.16	0.45
3:d:2969[B]:TYR:CD2	3:d:2970[B]:PRO:CG	3.00	0.45
3:d:3106[A]:THR:O	3:d:3106[A]:THR:HG23	2.17	0.45
3:d:3119[B]:HIS:O	3:d:3122[B]:ASN:HB3	2.17	0.45
3:d:3132[B]:ALA:HB3	3:d:3197[B]:ILE:HD13	1.98	0.45
3:d:3134[A]:GLN:O	3:d:3136[A]:TYR:N	2.49	0.45
3:d:3242[A]:GLY:C	3:d:3243[A]:GLY:O	2.58	0.45
4:v:1:NAG:C6	4:v:2:NAG:C1	2.94	0.45
1:A:177:VAL:O	1:A:181:PRO:HD3	2.16	0.45
1:A:304:ALA:HB1	1:A:306:PHE:CE1	2.48	0.45
1:A:460:GLU:CB	1:A:465:PRO:HG2	2.44	0.45
3:C:2948[B]:ASP:CB	3:C:2949[B]:LYS:CA	2.78	0.45
3:C:2959[B]:SER:O	3:L:3255[B]:PRO:HD2	2.16	0.45
3:C:3038[B]:ILE:HG23	3:C:3040[B]:VAL:HG22	1.90	0.45
3:C:3203[B]:HIS:O	3:C:3206[B]:LYS:HB3	2.16	0.45
3:C:3241[B]:PHE:CZ	3:C:3243[B]:GLY:O	2.70	0.45
1:D:513:TYR:OH	1:D:704:ASP:OD1	2.28	0.45
1:D:953:GLU:OE2	1:D:956:PRO:HG3	2.17	0.45
1:D:1033:LEU:HA	1:D:1036:SER:HB3	1.98	0.45
1:D:1091:ASN:HA	1:D:1092:PRO:HD3	1.82	0.45
2:E:2465:LYS:HB2	2:E:2465:LYS:HE3	1.67	0.45
3:F:2965[A]:LEU:HD13	3:F:2975[A]:PHE:O	2.16	0.45
3:F:3025[A]:VAL:CG2	3:F:3047[A]:ARG:NH1	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:456:GLN:O	1:G:460:GLU:HG3	2.16	0.45
1:G:618:MET:HE2	1:G:618:MET:HB3	1.60	0.45
1:G:1019:HIS:CE1	1:G:1046:HIS:HE1	2.35	0.45
1:G:1150:GLY:N	1:G:1186:TRP:O	2.46	0.45
3:I:2976[B]:ALA:HB3	3:R:2976[B]:ALA:H	1.81	0.45
3:I:3037[B]:TYR:C	3:I:3038[B]:ILE:HG13	2.42	0.45
3:I:3101[B]:PRO:O	3:I:3109[B]:TYR:HD2	2.00	0.45
3:I:3108[B]:HIS:CE1	3:R:3252[B]:TYR:CG	3.05	0.45
3:I:3133[B]:LEU:O	3:I:3136[B]:TYR:HB3	2.17	0.45
3:I:3137[B]:ARG:HB3	3:I:3139[B]:LEU:HD21	1.97	0.45
3:I:3141[B]:TYR:CD2	3:I:3141[B]:TYR:C	2.86	0.45
3:I:3152[B]:LYS:HB2	3:R:3172[B]:SER:H	0.33	0.45
3:I:3180[A]:TYR:CA	3:I:3183[A]:LEU:CD2	2.95	0.45
1:J:193:SER:C	1:J:195:SER:H	2.25	0.45
1:J:567:LEU:HD23	1:J:571:PRO:CG	2.47	0.45
1:J:639:ARG:HB2	1:J:703:TYR:CE1	2.52	0.45
1:J:832:LYS:HA	1:J:833:PHE:HA	1.57	0.45
1:J:905:TRP:HE1	1:J:1083:PRO:HD2	1.82	0.45
1:J:1075:GLU:OE2	1:J:1076:ILE:HG13	2.17	0.45
1:J:1427:HIS:CE1	1:J:1457:HIS:HE1	2.35	0.45
1:J:1530:LEU:HD23	1:J:1530:LEU:HA	1.78	0.45
3:L:2985[B]:PHE:CE2	3:L:2989[B]:HIS:CD2	3.04	0.45
3:L:3014[A]:TRP:CG	3:L:3092[A]:ILE:CD1	2.98	0.45
3:L:3101[B]:PRO:O	3:L:3109[B]:TYR:HD2	2.00	0.45
3:L:3185[B]:TYR:HE2	3:L:3187[B]:TYR:CD2	2.35	0.45
3:L:3263[B]:LEU:N	3:L:3263[B]:LEU:CD1	2.79	0.45
1:M:2:LEU:O	1:M:275:ALA:N	2.47	0.45
1:M:294:LYS:HA	1:M:297:ARG:CD	2.46	0.45
1:M:483:GLY:HA2	1:M:773:PHE:CE1	2.52	0.45
3:O:3132[B]:ALA:HB3	3:O:3197[B]:ILE:HD13	1.99	0.45
3:O:3204[B]:LEU:CD1	3:O:3204[B]:LEU:N	2.79	0.45
3:O:3273[A]:LEU:C	3:O:3275[A]:LEU:HD12	2.42	0.45
1:P:838:ARG:NH1	1:P:915:ASN:OD1	2.31	0.45
1:P:1638:SER:C	4:6:1:NAG:H82	2.42	0.45
3:R:2986[B]:PRO:CB	3:R:3127[B]:TRP:CE3	3.00	0.45
3:R:3037[B]:TYR:C	3:R:3038[B]:ILE:HG13	2.42	0.45
3:R:3101[A]:PRO:O	3:R:3109[A]:TYR:HD2	2.00	0.45
3:R:3116[B]:PHE:CD1	3:R:3116[B]:PHE:C	2.94	0.45
3:R:3137[A]:ARG:O	3:R:3139[A]:LEU:HD22	2.16	0.45
3:R:3137[B]:ARG:HB3	3:R:3139[B]:LEU:HD21	1.97	0.45
3:R:3196[A]:THR:N	3:R:3199[A]:GLN:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3241[A]:PHE:CZ	3:R:3243[A]:GLY:O	2.70	0.45
3:R:3263[B]:LEU:N	3:R:3263[B]:LEU:CD1	2.79	0.45
3:R:3285[A]:VAL:CG2	3:R:3286[A]:THR:H	2.27	0.45
3:R:3301[A]:PRO:HB2	3:R:3302[A]:SER:H	1.33	0.45
1:S:1101:VAL:HG11	2:W:2873:HIS:HD2	1.81	0.45
1:S:1423:TYR:OH	1:S:1461:VAL:HG12	2.17	0.45
1:S:1489:MET:HA	1:S:1513:PRO:HB2	1.98	0.45
2:T:2546:LEU:N	2:T:2557:ALA:HA	2.26	0.45
3:U:3037[B]:TYR:C	3:U:3038[B]:ILE:HG13	2.42	0.45
3:U:3209[A]:GLU:O	3:U:3310[A]:GLY:C	2.59	0.45
3:U:3281[B]:PHE:HE1	3:U:3305[B]:ILE:HG21	1.81	0.45
1:V:107:HIS:O	1:V:121:ASN:ND2	2.50	0.45
1:V:1300:CYS:HB3	1:V:1494:ARG:NH1	2.32	0.45
3:X:3019[B]:HIS:CD2	3:X:3020[B]:SER:H	2.35	0.45
3:X:3023[B]:ILE:O	3:X:3026[B]:THR:OG1	2.34	0.45
3:X:3024[B]:LEU:CD1	3:X:3024[B]:LEU:C	2.85	0.45
3:X:3037[B]:TYR:C	3:X:3038[B]:ILE:HG13	2.42	0.45
3:X:3101[A]:PRO:O	3:X:3109[A]:TYR:HD2	2.00	0.45
3:X:3119[B]:HIS:O	3:X:3122[B]:ASN:HB3	2.17	0.45
3:X:3204[B]:LEU:CD1	3:X:3204[B]:LEU:N	2.80	0.45
3:X:3241[B]:PHE:CE2	3:X:3243[B]:GLY:O	2.70	0.45
3:X:3242[B]:GLY:C	3:X:3243[B]:GLY:O	2.58	0.45
3:X:3264[B]:TYR:HD1	3:X:3265[B]:ASP:N	2.14	0.45
1:Y:140:ASP:OD2	1:Y:142:ARG:NE	2.38	0.45
1:Y:490:TRP:HE1	1:Y:670:PRO:CD	2.29	0.45
2:Z:2161:GLN:NE2	2:Z:2348:THR:HG21	2.32	0.45
3:a:2956[B]:LYS:O	3:a:2959[B]:SER:OG	2.33	0.45
3:a:2981[B]:GLY:N	3:a:3086[B]:GLU:OE1	2.45	0.45
3:a:2986[A]:PRO:CB	3:a:3127[A]:TRP:CE3	3.00	0.45
3:a:3101[B]:PRO:O	3:a:3109[B]:TYR:HD2	2.00	0.45
3:a:3119[B]:HIS:O	3:a:3122[B]:ASN:HB3	2.17	0.45
3:a:3134[B]:GLN:O	3:a:3136[B]:TYR:N	2.49	0.45
3:a:3183[A]:LEU:N	3:a:3184[A]:ASN:CA	2.80	0.45
3:a:3241[A]:PHE:CZ	3:a:3243[A]:GLY:O	2.70	0.45
1:b:301:ARG:HD2	1:b:361:GLU:OE2	2.17	0.45
1:b:329:ARG:C	1:b:331:SER:H	2.24	0.45
1:b:403:TYR:HD2	1:b:658:TYR:CD1	2.35	0.45
1:b:1015:HIS:CD2	1:b:1045:HIS:HE1	2.35	0.45
1:b:1143:ALA:HB3	1:b:1235:ILE:HG23	1.99	0.45
1:b:1221:THR:OG1	1:b:1222:GLY:N	2.49	0.45
2:c:2608:ASP:O	2:c:2622:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2932[B]:PRO:CA	3:d:2935[B]:ILE:CD1	2.85	0.45
3:d:2956[A]:LYS:O	3:d:2959[A]:SER:OG	2.33	0.45
3:d:2986[A]:PRO:CB	3:d:3127[A]:TRP:CE3	3.00	0.45
3:d:3074[B]:GLU:CD	3:d:3212[B]:ARG:NH2	2.73	0.45
3:d:3204[A]:LEU:CD1	3:d:3204[A]:LEU:N	2.80	0.45
4:m:1:NAG:C3	4:m:2:NAG:HN2	2.27	0.45
1:A:192:HIS:O	1:A:193:SER:OG	2.30	0.45
1:A:389:THR:HA	2:Z:2136:THR:HB	1.99	0.45
1:A:447:MET:HA	1:A:455:TYR:CB	2.46	0.45
1:A:792:MET:HE3	1:A:822:PHE:CE2	2.52	0.45
1:A:1359:ILE:HG22	1:A:1377:PHE:HB3	1.99	0.45
3:C:2951[A]:ASP:CG	3:C:2952[A]:ALA:N	2.74	0.45
3:C:2969[B]:TYR:CE2	3:L:3120[B]:HIS:CD2	2.88	0.45
3:C:2979[A]:GLN:HB2	3:C:2988[A]:TRP:CD1	2.52	0.45
3:C:2986[B]:PRO:CB	3:C:3127[B]:TRP:CE3	3.00	0.45
3:C:3013[B]:ASP:CG	3:C:3015[B]:THR:HG1	2.24	0.45
3:C:3019[B]:HIS:CD2	3:C:3020[B]:SER:H	2.35	0.45
3:C:3047[B]:ARG:NH2	3:C:3113[B]:ASP:OD1	2.43	0.45
3:C:3135[A]:LYS:HB2	3:C:3141[A]:TYR:CD1	2.51	0.45
3:C:3172[B]:SER:CB	3:L:3152[B]:LYS:CA	2.95	0.45
3:C:3172[B]:SER:OG	3:L:3149[B]:ASN:C	2.60	0.45
3:C:3180[B]:TYR:CA	3:C:3183[B]:LEU:CD2	2.95	0.45
3:C:3241[B]:PHE:CE2	3:C:3243[B]:GLY:O	2.70	0.45
3:C:3249[B]:GLY:N	3:L:2973[B]:THR:HG22	2.32	0.45
1:D:618:MET:HE3	1:D:618:MET:HB3	1.89	0.45
1:D:638:ASP:HB3	1:D:703:TYR:OH	2.17	0.45
1:D:1300:CYS:HB3	1:D:1494:ARG:NH1	2.32	0.45
1:D:1301:PRO:O	1:D:1494:ARG:NH2	2.50	0.45
2:E:2130:PRO:HG2	2:E:2140:ARG:HD2	1.98	0.45
2:E:2213:HIS:CD2	2:E:2222:MET:HG2	2.52	0.45
3:F:2938[B]:LEU:O	3:F:2939[B]:ARG:C	2.58	0.45
3:F:3037[A]:TYR:C	3:F:3038[A]:ILE:HG13	2.42	0.45
3:F:3037[B]:TYR:C	3:F:3038[B]:ILE:HG13	2.42	0.45
3:F:3241[B]:PHE:CE2	3:F:3243[B]:GLY:O	2.70	0.45
1:G:184:TYR:CE1	1:G:386:ILE:HG12	2.52	0.45
1:G:712:SER:O	1:G:716:LEU:N	2.40	0.45
1:G:982:LYS:N	1:G:983:PRO:CD	2.80	0.45
1:G:1475:ARG:NE	1:G:1541:GLU:OE2	2.30	0.45
2:H:2825:ILE:HG23	2:H:2826:GLU:H	1.81	0.45
3:I:2932[B]:PRO:CA	3:I:2935[B]:ILE:CD1	2.85	0.45
3:I:2956[B]:LYS:O	3:I:2959[B]:SER:OG	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2977[B]:CYS:HB3	3:R:2982[B]:MET:CE	2.42	0.45
3:I:3004[A]:GLY:C	3:I:3006[A]:LYS:N	2.74	0.45
3:I:3014[B]:TRP:CG	3:I:3092[B]:ILE:CD1	2.98	0.45
3:I:3161[B]:GLU:C	3:R:3147[B]:GLU:HG2	2.29	0.45
3:I:3242[A]:GLY:C	3:I:3243[A]:GLY:O	2.58	0.45
1:J:732:GLY:HA2	1:J:777:TYR:O	2.17	0.45
2:K:2822:LYS:HG2	2:K:2831:GLU:H	1.81	0.45
3:L:2938[B]:LEU:O	3:L:2939[B]:ARG:C	2.58	0.45
3:L:2969[A]:TYR:CD2	3:L:2970[A]:PRO:CG	3.00	0.45
3:L:3114[B]:PRO:CD	3:L:3115[B]:LEU:N	2.72	0.45
3:L:3119[B]:HIS:O	3:L:3122[B]:ASN:HB3	2.17	0.45
3:L:3132[B]:ALA:HB3	3:L:3197[B]:ILE:HD13	1.99	0.45
1:M:321:LEU:HD11	1:M:377:TYR:CD1	2.52	0.45
1:M:735:LEU:HB2	1:M:773:PHE:HD2	1.82	0.45
2:N:2327:GLU:H	2:N:2327:GLU:HG3	1.40	0.45
3:O:2986[B]:PRO:CB	3:O:3127[B]:TRP:CE3	3.00	0.45
3:O:2994[A]:LYS:O	3:O:2997[A]:GLU:N	2.49	0.45
3:O:3093[B]:HIS:HD2	3:O:3248[B]:LEU:CD2	2.30	0.45
3:O:3157[B]:PRO:HA	3:X:3150[B]:LYS:CA	2.47	0.45
3:O:3182[B]:GLN:H	3:O:3182[B]:GLN:HG2	1.56	0.45
3:O:3225[A]:SER:C	3:O:3290[A]:ILE:HG23	2.39	0.45
3:O:3241[B]:PHE:CE2	3:O:3243[B]:GLY:O	2.70	0.45
3:O:3266[B]:ILE:O	3:O:3269[B]:SER:HB2	2.17	0.45
1:P:931:TRP:NE1	1:P:1048:ASN:HD22	2.15	0.45
2:Q:2451:LEU:HD11	2:Q:2462:PHE:CZ	2.51	0.45
2:Q:2500:ILE:HD11	2:Q:2776:TYR:HA	1.99	0.45
2:Q:2522:SER:O	2:Q:2526:ARG:HG2	2.16	0.45
2:Q:2791:LEU:HD23	2:Q:2791:LEU:HA	1.85	0.45
3:R:3146[A]:CYS:HA	3:R:3147[A]:GLU:HA	1.70	0.45
3:R:3171[B]:HIS:C	3:R:3173[B]:THR:N	2.73	0.45
3:R:3183[A]:LEU:N	3:R:3184[A]:ASN:CA	2.80	0.45
3:R:3200[A]:LEU:CD2	3:R:3204[A]:LEU:CD1	2.93	0.45
3:R:3241[B]:PHE:CZ	3:R:3243[B]:GLY:O	2.70	0.45
2:T:2890:VAL:HG23	2:T:2891:LEU:C	2.42	0.45
3:U:3023[B]:ILE:HA	3:U:3026[B]:THR:HG1	1.81	0.45
3:U:3027[A]:GLU:CD	3:U:3027[A]:GLU:C	2.85	0.45
3:U:3106[A]:THR:O	3:U:3106[A]:THR:HG23	2.17	0.45
3:U:3119[A]:HIS:O	3:U:3122[A]:ASN:HB3	2.17	0.45
3:U:3133[A]:LEU:O	3:U:3136[A]:TYR:HB3	2.17	0.45
3:U:3137[B]:ARG:HB3	3:U:3139[B]:LEU:HD21	1.97	0.45
3:U:3204[B]:LEU:CD1	3:U:3204[B]:LEU:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3273[A]:LEU:C	3:U:3275[A]:LEU:HD12	2.42	0.45
3:U:3301[A]:PRO:HB2	3:U:3302[A]:SER:H	1.33	0.45
1:V:901:THR:HG22	1:V:904:HIS:HB2	1.99	0.45
1:V:907:ARG:CZ	1:V:1108:TYR:HB3	2.47	0.45
2:W:2556:TYR:CE1	2:W:2844:MET:HG3	2.52	0.45
3:X:2951[A]:ASP:CG	3:X:2952[A]:ALA:N	2.74	0.45
3:X:3135[A]:LYS:HB2	3:X:3141[A]:TYR:CD1	2.51	0.45
3:X:3148[A]:ILE:O	3:X:3148[A]:ILE:HG22	2.17	0.45
1:Y:134:VAL:HG12	1:Y:135:THR:H	1.82	0.45
1:Y:142:ARG:HH22	1:Y:316:ASN:ND2	2.14	0.45
1:Y:516:TRP:CD1	1:Y:579:LEU:HB3	2.52	0.45
1:Y:684:ARG:HB3	1:Y:684:ARG:NH1	2.32	0.45
1:Y:1007:PHE:CE1	1:Y:1011:TYR:HB2	2.51	0.45
1:Y:1506:LEU:H	1:Y:1506:LEU:HG	1.39	0.45
2:Z:2181:THR:HB	2:Z:2374:ASN:H	1.82	0.45
2:Z:2278:GLU:O	2:Z:2281:SER:OG	2.32	0.45
2:Z:2739:LEU:HG	1:b:1234:VAL:O	2.17	0.45
3:a:2949[B]:LYS:NZ	3:a:2949[B]:LYS:C	2.73	0.45
3:a:2979[A]:GLN:HB2	3:a:2988[A]:TRP:CD1	2.52	0.45
3:a:2979[B]:GLN:HB2	3:a:2988[B]:TRP:CD1	2.52	0.45
3:a:3027[B]:GLU:CD	3:a:3027[B]:GLU:C	2.85	0.45
3:a:3133[B]:LEU:O	3:a:3136[B]:TYR:HB3	2.17	0.45
3:a:3180[A]:TYR:CA	3:a:3183[A]:LEU:CD2	2.95	0.45
3:a:3185[A]:TYR:HE2	3:a:3187[A]:TYR:CD2	2.35	0.45
3:a:3242[B]:GLY:C	3:a:3243[B]:GLY:O	2.58	0.45
1:b:108:PRO:HA	1:b:124:TYR:CG	2.52	0.45
1:b:810:LEU:HD12	1:b:810:LEU:HA	1.88	0.45
1:b:836:GLN:H	1:b:836:GLN:HG3	1.60	0.45
1:b:987:LYS:HE2	1:b:987:LYS:N	2.31	0.45
1:b:1059:LEU:HD13	1:b:1063:ARG:HH21	1.82	0.45
3:d:3019[B]:HIS:CD2	3:d:3020[B]:SER:H	2.35	0.45
3:d:3038[A]:ILE:HG23	3:d:3040[A]:VAL:HG22	1.90	0.45
3:d:3093[A]:HIS:HD2	3:d:3248[A]:LEU:CD2	2.30	0.45
3:d:3101[A]:PRO:O	3:d:3109[A]:TYR:HD2	2.00	0.45
3:d:3180[B]:TYR:CA	3:d:3183[B]:LEU:CD2	2.95	0.45
3:d:3196[A]:THR:N	3:d:3199[A]:GLN:CB	2.65	0.45
3:d:3241[A]:PHE:CE2	3:d:3243[A]:GLY:O	2.70	0.45
3:d:3244[B]:THR:H	3:d:3264[B]:TYR:HE2	1.65	0.45
2:B:2370:MET:HE1	2:E:2094:ARG:NH1	2.32	0.44
2:B:2448:THR:OG1	2:B:2449:ASP:N	2.49	0.44
2:B:2630:LYS:HA	2:B:2630:LYS:HD2	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2901:LEU:H	1:D:1075:GLU:HG3	1.81	0.44
3:C:2938[B]:LEU:O	3:C:2939[B]:ARG:C	2.58	0.44
3:C:2961[B]:HIS:HB2	3:C:2992[B]:TYR:HE2	1.80	0.44
3:C:2986[A]:PRO:CB	3:C:3127[A]:TRP:CE3	3.00	0.44
3:C:2989[A]:HIS:CD2	9:L:3401[A]:CUO:O1	2.70	0.44
3:C:3087[A]:MET:HA	3:C:3090[A]:ASN:OD1	2.17	0.44
3:C:3119[A]:HIS:O	3:C:3122[A]:ASN:HB3	2.17	0.44
3:C:3225[B]:SER:C	3:C:3290[B]:ILE:HG23	2.39	0.44
3:C:3229[A]:ASN:O	3:C:3286[A]:THR:N	2.50	0.44
3:C:3255[B]:PRO:HD3	3:L:2961[B]:HIS:C	2.42	0.44
1:D:901:THR:HG22	1:D:904:HIS:HD2	1.82	0.44
1:D:905:TRP:HZ2	1:D:1083:PRO:HG2	1.82	0.44
1:D:906:HIS:HD2	1:D:1046:HIS:CD2	2.35	0.44
1:D:1393:THR:HG22	1:D:1434:LEU:HD12	1.99	0.44
2:E:2128:LEU:HD23	2:E:2216:PHE:HZ	1.80	0.44
3:F:3027[A]:GLU:CD	3:F:3027[A]:GLU:C	2.85	0.44
3:F:3204[A]:LEU:CD1	3:F:3204[A]:LEU:N	2.80	0.44
3:F:3241[B]:PHE:CZ	3:F:3243[B]:GLY:O	2.70	0.44
3:F:3253[B]:GLU:HA	3:a:2976[B]:ALA:H	1.74	0.44
1:G:411:ASP:OD1	1:G:411:ASP:N	2.49	0.44
1:G:1075:GLU:H	1:G:1075:GLU:HG3	1.38	0.44
1:G:1302:SER:H	1:G:1494:ARG:HH22	1.64	0.44
2:H:2854:MET:HE3	2:H:2854:MET:HB2	1.94	0.44
3:I:2932[A]:PRO:CA	3:I:2935[A]:ILE:CD1	2.85	0.44
3:I:3106[A]:THR:O	3:I:3106[A]:THR:HG23	2.16	0.44
3:I:3137[A]:ARG:O	3:I:3139[A]:LEU:HD22	2.16	0.44
3:I:3150[B]:LYS:O	3:R:3172[B]:SER:HB2	2.15	0.44
3:I:3150[B]:LYS:HD3	3:R:3160[B]:SER:N	1.89	0.44
3:I:3162[B]:ASP:OD1	3:R:2983[B]:VAL:HG22	2.17	0.44
3:I:3241[B]:PHE:CZ	3:I:3243[B]:GLY:O	2.70	0.44
3:I:3244[B]:THR:H	3:I:3264[B]:TYR:HE2	1.65	0.44
3:I:3253[B]:GLU:HA	3:R:3252[B]:TYR:O	2.17	0.44
3:I:3266[B]:ILE:O	3:I:3269[B]:SER:HB2	2.17	0.44
1:J:23:ARG:HD3	1:J:120:LYS:HD3	1.99	0.44
1:J:452:ILE:HD11	1:J:679:ASN:HD21	1.82	0.44
1:J:957:ASN:N	1:J:958:PRO:HA	2.32	0.44
1:J:1321:HIS:CD2	1:J:1465:TRP:HH2	2.35	0.44
2:K:2541:GLY:O	2:K:2545:SER:OG	2.28	0.44
3:L:2951[B]:ASP:CG	3:L:2952[B]:ALA:N	2.74	0.44
3:L:2986[B]:PRO:CB	3:L:3127[B]:TRP:CE3	3.00	0.44
3:L:2989[B]:HIS:O	3:L:2990[B]:ARG:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3004[A]:GLY:O	3:L:3006[A]:LYS:N	2.44	0.44
3:L:3023[A]:ILE:HA	3:L:3026[A]:THR:HG1	1.82	0.44
3:L:3196[A]:THR:CB	3:L:3199[A]:GLN:OE1	2.64	0.44
3:L:3273[B]:LEU:C	3:L:3275[B]:LEU:HD12	2.42	0.44
1:M:148:GLN:O	1:M:149:GLU:HG2	2.17	0.44
1:M:1636:ASN:OD1	4:1:1:NAG:H82	2.17	0.44
3:O:2949[B]:LYS:NZ	3:O:2949[B]:LYS:C	2.73	0.44
3:O:2985[A]:PHE:CE2	3:O:2989[A]:HIS:CD2	3.04	0.44
3:O:3019[B]:HIS:CD2	3:O:3020[B]:SER:H	2.35	0.44
3:O:3106[B]:THR:O	3:O:3106[B]:THR:HG23	2.16	0.44
3:O:3133[A]:LEU:O	3:O:3136[A]:TYR:HB3	2.17	0.44
3:O:3134[A]:GLN:O	3:O:3136[A]:TYR:N	2.49	0.44
3:O:3137[B]:ARG:HA	3:O:3137[B]:ARG:HD3	1.71	0.44
3:O:3157[B]:PRO:CA	3:X:3152[B]:LYS:N	2.80	0.44
3:O:3241[B]:PHE:CZ	3:O:3243[B]:GLY:O	2.70	0.44
3:O:3273[B]:LEU:C	3:O:3275[B]:LEU:HD12	2.42	0.44
1:P:300:ALA:HB2	1:P:406:PRO:HD3	2.00	0.44
1:P:1149:GLU:HG3	1:P:1187:LYS:HE2	2.00	0.44
1:P:1321:HIS:CD2	1:P:1465:TRP:CH2	3.01	0.44
3:R:2979[B]:GLN:HB2	3:R:2988[B]:TRP:CD1	2.52	0.44
3:R:3038[A]:ILE:HG23	3:R:3040[A]:VAL:HG22	1.90	0.44
3:R:3241[A]:PHE:CE2	3:R:3243[A]:GLY:O	2.70	0.44
3:R:3266[B]:ILE:O	3:R:3269[B]:SER:HB2	2.18	0.44
1:S:472:ASP:HA	1:S:473:ALA:HA	1.69	0.44
1:S:957:ASN:N	1:S:958:PRO:HA	2.33	0.44
2:T:2252:GLU:HA	2:T:2385:ILE:HD13	1.99	0.44
2:T:2884:LYS:HB3	2:T:2889:ALA:O	2.17	0.44
3:U:2938[A]:LEU:O	3:U:2939[A]:ARG:C	2.58	0.44
3:U:3185[A]:TYR:HE2	3:U:3187[A]:TYR:CD2	2.35	0.44
3:U:3299[A]:LEU:O	3:U:3300[A]:LEU:C	2.60	0.44
2:W:2823:ILE:HG13	2:W:2830:GLN:NE2	2.23	0.44
3:X:2989[A]:HIS:C	3:X:2991[A]:LEU:N	2.75	0.44
3:X:2989[B]:HIS:CD2	9:X:3401[B]:CUO:O1	2.70	0.44
3:X:2994[B]:LYS:O	3:X:2997[B]:GLU:N	2.49	0.44
3:X:3019[A]:HIS:CD2	3:X:3020[A]:SER:H	2.35	0.44
3:X:3087[A]:MET:HA	3:X:3090[A]:ASN:OD1	2.17	0.44
3:X:3093[A]:HIS:HD2	3:X:3248[A]:LEU:CD2	2.31	0.44
3:X:3116[A]:PHE:CD1	3:X:3116[A]:PHE:C	2.94	0.44
3:X:3182[A]:GLN:C	3:X:3183[A]:LEU:CD1	2.91	0.44
3:X:3229[B]:ASN:O	3:X:3286[B]:THR:N	2.50	0.44
3:X:3241[A]:PHE:CE2	3:X:3243[A]:GLY:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1156:LEU:HB2	1:Y:1176:TYR:CE1	2.52	0.44
1:Y:1349:VAL:HG13	1:Y:1404:TYR:HA	2.00	0.44
2:Z:2340:ALA:HB1	2:Z:2341:PRO:CD	2.47	0.44
2:Z:2739:LEU:HD11	1:b:1236:TYR:HB2	1.98	0.44
3:a:2951[B]:ASP:CG	3:a:2952[B]:ALA:N	2.74	0.44
3:a:3101[A]:PRO:O	3:a:3109[A]:TYR:HD2	2.00	0.44
3:a:3137[A]:ARG:HD3	3:a:3137[A]:ARG:HA	1.71	0.44
3:a:3273[B]:LEU:C	3:a:3275[B]:LEU:HD12	2.42	0.44
3:a:3281[A]:PHE:HE1	3:a:3305[A]:ILE:HG21	1.81	0.44
1:b:38:SER:HB3	1:b:202:TYR:CD1	2.52	0.44
3:d:2970[A]:PRO:C	3:d:2972[A]:GLY:N	2.72	0.44
3:d:2979[B]:GLN:HB2	3:d:2988[B]:TRP:CD1	2.52	0.44
3:d:3185[B]:TYR:HE2	3:d:3187[B]:TYR:CD2	2.35	0.44
3:d:3200[B]:LEU:CD2	3:d:3204[B]:LEU:HD11	2.48	0.44
3:d:3273[B]:LEU:C	3:d:3275[B]:LEU:HD12	2.42	0.44
1:A:17:ASN:OD1	1:A:18:LEU:N	2.50	0.44
1:A:133:LYS:HG3	1:A:134:VAL:N	2.32	0.44
1:A:593:CYS:O	1:A:597:VAL:HG23	2.17	0.44
2:B:2135:PRO:HG3	2:B:2342:TYR:CE2	2.52	0.44
3:C:2988[B]:TRP:CD1	3:C:3158[B]:PHE:CE2	3.06	0.44
3:C:3014[A]:TRP:CH2	3:C:3123[A]:THR:HG23	2.53	0.44
3:C:3133[B]:LEU:O	3:C:3136[B]:TYR:HB3	2.17	0.44
3:C:3200[A]:LEU:CD2	3:C:3204[A]:LEU:CD1	2.93	0.44
3:C:3241[A]:PHE:CZ	3:C:3243[A]:GLY:O	2.70	0.44
3:C:3252[B]:TYR:HB3	3:L:3253[B]:GLU:CG	2.47	0.44
3:C:3256[B]:TRP:CZ2	3:L:2965[B]:LEU:HG	2.49	0.44
3:C:3266[A]:ILE:O	3:C:3269[A]:SER:HB2	2.17	0.44
1:D:170:HIS:O	1:D:173:VAL:HG22	2.17	0.44
1:D:748:VAL:HG22	1:D:781:ILE:HD11	1.99	0.44
1:D:957:ASN:CB	1:D:960:PHE:HB2	2.47	0.44
3:F:2964[B]:PRO:CB	3:a:3255[B]:PRO:HB3	2.39	0.44
3:F:2989[B]:HIS:O	3:F:2990[B]:ARG:C	2.61	0.44
3:F:3014[B]:TRP:CH2	3:F:3123[B]:THR:HG23	2.53	0.44
3:F:3019[B]:HIS:CD2	3:F:3020[B]:SER:H	2.36	0.44
3:F:3156[B]:MET:O	3:a:3153[B]:LYS:NZ	2.50	0.44
3:F:3241[A]:PHE:CE2	3:F:3243[A]:GLY:O	2.70	0.44
3:F:3241[A]:PHE:CZ	3:F:3243[A]:GLY:O	2.70	0.44
3:F:3273[A]:LEU:C	3:F:3275[A]:LEU:HD12	2.42	0.44
3:F:3293[A]:LYS:HB2	3:F:3294[A]:SER:CA	2.41	0.44
1:G:1000:GLU:OE1	1:G:1141:ARG:NH2	2.50	0.44
1:G:1324:ARG:NH1	1:G:1516:VAL:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2970[A]:PRO:C	3:I:2972[A]:GLY:N	2.72	0.44
3:I:2992[B]:TYR:CE2	3:R:2969[B]:TYR:CE1	3.05	0.44
3:I:3027[B]:GLU:CD	3:I:3027[B]:GLU:C	2.86	0.44
3:I:3183[A]:LEU:N	3:I:3184[A]:ASN:HA	2.12	0.44
3:I:3229[B]:ASN:O	3:I:3286[B]:THR:N	2.50	0.44
1:J:247:PHE:O	1:J:252:ASN:ND2	2.37	0.44
1:J:906:HIS:HA	1:J:909:ILE:HG22	1.99	0.44
1:J:932:THR:O	1:J:989:THR:OG1	2.32	0.44
1:J:1160:PHE:HB3	1:J:1171:LYS:HA	1.98	0.44
3:L:2994[A]:LYS:O	3:L:2997[A]:GLU:N	2.49	0.44
3:L:3004[A]:GLY:C	3:L:3006[A]:LYS:N	2.74	0.44
3:L:3087[A]:MET:HA	3:L:3090[A]:ASN:OD1	2.17	0.44
3:L:3135[A]:LYS:HB2	3:L:3141[A]:TYR:CD1	2.51	0.44
3:L:3200[A]:LEU:CD2	3:L:3204[A]:LEU:HD11	2.48	0.44
3:L:3204[B]:LEU:CD1	3:L:3204[B]:LEU:N	2.80	0.44
1:M:956:PRO:HD2	1:M:957:ASN:O	2.17	0.44
1:M:1240:ILE:HD12	1:M:1247:ARG:HG3	2.00	0.44
2:N:2502:LEU:HB3	2:Q:2168:ARG:HA	1.99	0.44
3:O:2963[B]:MET:CE	3:X:2969[B]:TYR:N	2.81	0.44
3:O:2967[B]:CYS:CB	3:X:3155[B]:MET:CG	2.82	0.44
3:O:2974[B]:ALA:N	3:X:2977[B]:CYS:O	2.46	0.44
3:O:2989[A]:HIS:CD2	9:O:3401[A]:CUO:O1	2.71	0.44
3:O:2989[B]:HIS:CD2	9:O:3401[B]:CUO:O1	2.70	0.44
3:O:3087[B]:MET:HA	3:O:3090[B]:ASN:OD1	2.17	0.44
3:O:3132[A]:ALA:HB3	3:O:3197[A]:ILE:HD13	1.99	0.44
3:O:3180[A]:TYR:CB	3:O:3183[A]:LEU:CD2	2.89	0.44
3:O:3298[A]:ASN:CA	3:O:3299[A]:LEU:HB2	2.44	0.44
1:P:842:ASN:HB3	1:P:928:TYR:CE1	2.52	0.44
2:Q:2270:ILE:HB	2:Q:2297:HIS:CD2	2.53	0.44
2:Q:2635:TYR:HB2	1:S:109:LEU:HD21	1.99	0.44
2:Q:2765:PRO:HA	2:Q:2768:LEU:HD12	1.98	0.44
3:R:2979[A]:GLN:HB2	3:R:2988[A]:TRP:CD1	2.52	0.44
3:R:3014[B]:TRP:CG	3:R:3092[B]:ILE:CD1	2.98	0.44
3:R:3027[A]:GLU:CD	3:R:3027[A]:GLU:C	2.85	0.44
3:R:3093[A]:HIS:HB2	3:R:3248[A]:LEU:CD1	2.48	0.44
3:R:3180[B]:TYR:CA	3:R:3183[B]:LEU:CD2	2.95	0.44
3:R:3182[A]:GLN:C	3:R:3183[A]:LEU:CD1	2.91	0.44
3:R:3200[B]:LEU:CD2	3:R:3204[B]:LEU:CD1	2.93	0.44
1:S:7:VAL:HG23	1:S:91:TYR:C	2.43	0.44
1:S:385:ALA:HB2	1:S:391:MET:SD	2.57	0.44
1:S:1315:GLY:HA3	1:S:1601:TRP:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:2571:ARG:NH1	2:T:2771:TYR:HB3	2.32	0.44
3:U:2956[B]:LYS:O	3:U:2959[B]:SER:OG	2.33	0.44
3:U:2961[B]:HIS:HB2	3:U:2992[B]:TYR:HE2	1.81	0.44
3:U:3037[A]:TYR:C	3:U:3038[A]:ILE:HG13	2.42	0.44
3:U:3163[B]:ASN:HB3	3:d:3147[B]:GLU:OE2	2.17	0.44
3:U:3171[A]:HIS:C	3:U:3173[A]:THR:N	2.73	0.44
3:U:3229[A]:ASN:O	3:U:3286[A]:THR:N	2.50	0.44
1:V:71:LEU:HD22	1:V:266:LEU:HD21	1.99	0.44
1:V:991:LEU:O	1:V:995:ILE:HG13	2.18	0.44
2:W:2644:LEU:HD22	2:W:2687:ILE:HG22	1.99	0.44
3:X:3148[B]:ILE:HG22	3:X:3148[B]:ILE:O	2.17	0.44
3:X:3149[B]:ASN:N	3:X:3149[B]:ASN:OD1	2.51	0.44
3:X:3161[B]:GLU:CD	3:X:3161[B]:GLU:H	2.19	0.44
3:X:3182[B]:GLN:C	3:X:3183[B]:LEU:CD1	2.91	0.44
3:X:3244[B]:THR:H	3:X:3264[B]:TYR:HE2	1.65	0.44
3:X:3266[B]:ILE:O	3:X:3269[B]:SER:HB2	2.17	0.44
1:Y:183:HIS:O	1:Y:195:SER:HA	2.17	0.44
1:Y:1134:ASN:HB2	1:Y:1253:ILE:HD12	2.00	0.44
1:Y:1290:ILE:HD13	1:Y:1329:LEU:HG	1.99	0.44
3:a:2981[A]:GLY:N	3:a:3086[A]:GLU:OE1	2.45	0.44
3:a:3104[B]:MET:SD	3:a:3110[B]:THR:CG2	3.06	0.44
3:a:3149[A]:ASN:OD1	3:a:3149[A]:ASN:N	2.51	0.44
3:a:3229[B]:ASN:O	3:a:3286[B]:THR:N	2.50	0.44
3:a:3241[B]:PHE:CE2	3:a:3243[B]:GLY:O	2.70	0.44
3:a:3273[A]:LEU:C	3:a:3275[A]:LEU:HD12	2.42	0.44
3:a:3284[B]:LYS:HD3	3:a:3285[B]:VAL:O	2.16	0.44
1:b:40:TYR:CD1	1:b:246:PRO:HG2	2.52	0.44
2:c:2345:ASN:HB3	2:c:2348:THR:HB	1.98	0.44
2:c:2723:GLU:HG2	2:c:2788:ILE:CD1	2.47	0.44
3:d:2986[B]:PRO:CB	3:d:3127[B]:TRP:CE3	3.00	0.44
3:d:3027[A]:GLU:CD	3:d:3027[A]:GLU:C	2.85	0.44
3:d:3037[A]:TYR:C	3:d:3038[A]:ILE:HG13	2.42	0.44
3:d:3093[A]:HIS:HB2	3:d:3248[A]:LEU:CD1	2.48	0.44
3:d:3182[B]:GLN:C	3:d:3183[B]:LEU:CD1	2.90	0.44
3:d:3241[B]:PHE:CE2	3:d:3243[B]:GLY:O	2.70	0.44
3:d:3273[A]:LEU:C	3:d:3275[A]:LEU:HD12	2.42	0.44
3:d:3284[B]:LYS:CD	3:d:3284[B]:LYS:C	2.86	0.44
1:A:40:TYR:CG	1:A:246:PRO:HG2	2.52	0.44
1:A:117:LYS:H	1:A:117:LYS:HG2	1.33	0.44
1:A:173:VAL:HG12	1:A:354:PHE:CD1	2.53	0.44
1:A:1209:ASP:HA	2:E:2743:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:TYR:OH	2:E:2739:LEU:HB2	2.18	0.44
1:A:1305:GLY:HA3	1:A:1306:THR:HA	1.60	0.44
2:B:2244:PHE:HD1	2:B:2373:MET:HE2	1.81	0.44
3:C:2982[B]:MET:HB2	3:L:3156[B]:MET:CB	2.09	0.44
3:C:3037[B]:TYR:C	3:C:3038[B]:ILE:HG13	2.42	0.44
3:C:3132[B]:ALA:HB3	3:C:3197[B]:ILE:HD13	1.99	0.44
3:C:3133[A]:LEU:O	3:C:3136[A]:TYR:HB3	2.17	0.44
3:C:3154[B]:PRO:O	3:L:3155[B]:MET:CE	2.64	0.44
3:C:3182[A]:GLN:C	3:C:3183[A]:LEU:CD1	2.90	0.44
1:D:670:PRO:HD2	1:D:671:PHE:CD1	2.53	0.44
2:E:2147:GLY:N	2:E:2264:GLU:OE2	2.48	0.44
2:E:2573:TYR:CE2	2:E:2707:PHE:HE2	2.33	0.44
3:F:3180[A]:TYR:CB	3:F:3183[A]:LEU:CD2	2.90	0.44
3:F:3182[B]:GLN:C	3:F:3183[B]:LEU:CD1	2.90	0.44
3:F:3191[B]:ASN:ND2	3:F:3191[B]:ASN:N	2.60	0.44
3:F:3229[A]:ASN:O	3:F:3286[A]:THR:N	2.50	0.44
3:F:3232[A]:VAL:HG21	3:F:3273[A]:LEU:HD11	2.00	0.44
3:F:3252[B]:TYR:C	3:a:3252[B]:TYR:O	2.60	0.44
1:G:562:GLN:HG2	1:G:563:ILE:N	2.33	0.44
1:G:784:ALA:O	1:G:788:LEU:HB2	2.17	0.44
1:G:1581:GLU:HG3	1:G:1582:ASN:N	2.31	0.44
2:H:2286:HIS:CD2	2:H:2433:THR:HG22	2.51	0.44
2:H:2450:ILE:O	2:H:2454:MET:HG3	2.17	0.44
3:I:2938[A]:LEU:O	3:I:2939[A]:ARG:C	2.58	0.44
3:I:2981[B]:GLY:CA	3:R:2966[B]:SER:O	2.65	0.44
3:I:2986[A]:PRO:CB	3:I:3127[A]:TRP:CE3	3.00	0.44
3:I:3074[A]:GLU:CD	3:I:3212[A]:ARG:NH2	2.73	0.44
3:I:3074[B]:GLU:CD	3:I:3212[B]:ARG:NH2	2.73	0.44
3:I:3116[B]:PHE:C	3:I:3116[B]:PHE:CD1	2.94	0.44
3:I:3137[A]:ARG:HA	3:I:3137[A]:ARG:HD3	1.72	0.44
3:I:3150[B]:LYS:HB2	3:R:3169[B]:LYS:HE3	1.99	0.44
3:I:3174[B]:GLY:H	3:R:3154[B]:PRO:CB	2.02	0.44
1:J:876:PHE:H	1:J:876:PHE:HD1	1.65	0.44
1:J:1315:GLY:HA3	1:J:1601:TRP:CG	2.53	0.44
2:K:2821:LEU:HD11	2:K:2879:LEU:HD23	1.98	0.44
3:L:2989[B]:HIS:C	3:L:2991[B]:LEU:N	2.75	0.44
3:L:2991[B]:LEU:HD23	3:L:3158[B]:PHE:CE1	2.47	0.44
3:L:3013[B]:ASP:CG	3:L:3015[B]:THR:HG1	2.23	0.44
3:L:3019[B]:HIS:CD2	3:L:3020[B]:SER:H	2.35	0.44
3:L:3087[B]:MET:HA	3:L:3090[B]:ASN:OD1	2.17	0.44
3:L:3171[A]:HIS:C	3:L:3173[A]:THR:N	2.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:883:CYS:HB3	1:M:884:PRO:CD	2.47	0.44
1:M:1240:ILE:HG22	1:M:1250:ILE:HG21	1.99	0.44
1:M:1348:TRP:CG	1:M:1430:ILE:HD11	2.51	0.44
2:N:2161:GLN:NE2	2:N:2348:THR:HG21	2.33	0.44
3:O:2969[B]:TYR:CA	3:X:2991[B]:LEU:HD22	2.36	0.44
3:O:3024[A]:LEU:CD1	3:O:3024[A]:LEU:C	2.85	0.44
3:O:3101[A]:PRO:O	3:O:3109[A]:TYR:HD2	2.00	0.44
3:O:3157[B]:PRO:O	3:X:3149[B]:ASN:CA	2.57	0.44
3:O:3159[B]:SER:HB2	3:X:3152[B]:LYS:HG2	1.12	0.44
3:O:3241[A]:PHE:CZ	3:O:3243[A]:GLY:O	2.70	0.44
3:O:3255[B]:PRO:CB	3:X:3161[B]:GLU:HA	2.48	0.44
1:P:450:LYS:CE	1:P:451:SER:H	2.30	0.44
1:P:729:VAL:HG11	1:P:785:LEU:HD12	1.99	0.44
1:P:1209:ASP:O	1:P:1211:TYR:HD2	2.00	0.44
3:R:2961[A]:HIS:CD2	3:R:2988[A]:TRP:CZ3	2.96	0.44
3:R:2986[A]:PRO:CB	3:R:3127[A]:TRP:CE3	3.00	0.44
3:R:3019[B]:HIS:CD2	3:R:3020[B]:SER:H	2.35	0.44
3:R:3024[A]:LEU:CD1	3:R:3024[A]:LEU:C	2.85	0.44
3:R:3218[B]:LEU:HD12	3:R:3218[B]:LEU:HA	1.78	0.44
1:S:729:VAL:HG23	1:S:820:VAL:HG13	1.99	0.44
1:S:899:MET:HE2	1:S:1012:GLU:OE2	2.17	0.44
1:S:1575:PRO:HA	1:S:1581:GLU:O	2.18	0.44
2:T:2161:GLN:NE2	2:T:2348:THR:HG21	2.32	0.44
2:T:2317:LEU:HB3	2:T:2318:PRO:HD2	2.00	0.44
3:U:3024[A]:LEU:CD1	3:U:3024[A]:LEU:C	2.85	0.44
3:U:3087[A]:MET:HA	3:U:3090[A]:ASN:OD1	2.17	0.44
3:U:3132[A]:ALA:HB3	3:U:3197[A]:ILE:HD13	1.98	0.44
3:U:3133[B]:LEU:O	3:U:3136[B]:TYR:HB3	2.17	0.44
3:U:3137[B]:ARG:O	3:U:3139[B]:LEU:HD22	2.16	0.44
3:U:3230[B]:PHE:CB	3:U:3242[B]:GLY:C	2.91	0.44
3:U:3241[A]:PHE:CZ	3:U:3243[A]:GLY:O	2.70	0.44
3:U:3241[B]:PHE:CZ	3:U:3243[B]:GLY:O	2.70	0.44
3:U:3242[B]:GLY:C	3:U:3243[B]:GLY:O	2.58	0.44
3:U:3254[B]:MET:CB	3:d:3254[B]:MET:HB3	2.25	0.44
3:U:3301[B]:PRO:HB2	3:U:3302[B]:SER:H	1.33	0.44
1:V:111:ILE:HG23	2:Z:2637:VAL:HG11	1.99	0.44
1:V:1086:LEU:HD13	1:V:1090:ILE:HG21	1.98	0.44
2:W:2722:GLN:NE2	2:W:2769:PHE:O	2.33	0.44
3:X:2969[A]:TYR:CD2	3:X:2970[A]:PRO:CG	3.00	0.44
3:X:2986[B]:PRO:CB	3:X:3127[B]:TRP:CE3	3.00	0.44
3:X:3027[B]:GLU:CD	3:X:3027[B]:GLU:C	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3037[A]:TYR:C	3:X:3038[A]:ILE:HG13	2.42	0.44
3:X:3133[A]:LEU:O	3:X:3136[A]:TYR:HB3	2.17	0.44
3:X:3200[B]:LEU:CD2	3:X:3204[B]:LEU:HD11	2.47	0.44
1:Y:654:PRO:HB2	1:Y:658:TYR:HE2	1.82	0.44
1:Y:1156:LEU:HB2	1:Y:1176:TYR:HE1	1.83	0.44
1:Y:1616:LYS:HG2	3:d:3186[B]:GLU:HB3	1.66	0.44
2:Z:2142:ALA:HB3	2:Z:2434:GLU:HA	1.99	0.44
2:Z:2627:GLY:HA3	2:Z:2703:PHE:O	2.17	0.44
2:Z:2782:ASN:HB2	2:Z:2786:MET:O	2.17	0.44
2:Z:2866:PRO:HB3	3:a:2933[A]:SER:CB	2.47	0.44
3:a:2969[A]:TYR:CD2	3:a:2970[A]:PRO:CG	3.00	0.44
3:a:2986[B]:PRO:CB	3:a:3127[B]:TRP:CE3	3.00	0.44
3:a:3028[B]:PRO:HG2	3:a:3029[B]:LYS:HG3	2.00	0.44
3:a:3093[B]:HIS:HB2	3:a:3248[B]:LEU:CD1	2.48	0.44
3:a:3093[B]:HIS:HD2	3:a:3248[B]:LEU:CD2	2.31	0.44
3:a:3283[A]:ILE:C	3:a:3283[A]:ILE:CD1	2.85	0.44
3:a:3298[B]:ASN:CA	3:a:3299[B]:LEU:HB2	2.44	0.44
1:b:953:GLU:HG2	1:b:954:ALA:N	2.32	0.44
3:d:2989[B]:HIS:O	3:d:2990[B]:ARG:C	2.61	0.44
3:d:3093[B]:HIS:HB2	3:d:3248[B]:LEU:CD1	2.47	0.44
3:d:3182[A]:GLN:C	3:d:3183[A]:LEU:CD1	2.91	0.44
1:A:903:PRO:HG2	1:A:904:HIS:CD2	2.53	0.44
1:A:974:ALA:HB1	1:A:1022:VAL:HG22	2.00	0.44
2:B:2155:HIS:CD2	2:B:2298:HIS:CE1	3.05	0.44
2:B:2739:LEU:HD12	1:D:1211:TYR:OH	2.17	0.44
3:C:2951[B]:ASP:CG	3:C:2952[B]:ALA:N	2.74	0.44
3:C:2965[B]:LEU:HB2	3:L:3222[B]:ILE:N	2.31	0.44
3:C:3074[B]:GLU:CD	3:C:3212[B]:ARG:NH2	2.73	0.44
3:C:3137[A]:ARG:O	3:C:3139[A]:LEU:HD22	2.16	0.44
3:C:3146[B]:CYS:HA	3:C:3147[B]:GLU:HA	1.70	0.44
3:C:3161[B]:GLU:N	3:L:2983[B]:VAL:CG2	2.41	0.44
3:C:3182[B]:GLN:C	3:C:3183[B]:LEU:CD1	2.91	0.44
3:C:3200[A]:LEU:CD2	3:C:3204[A]:LEU:HD11	2.48	0.44
3:C:3241[A]:PHE:CE2	3:C:3243[A]:GLY:O	2.70	0.44
3:C:3242[B]:GLY:C	3:C:3243[B]:GLY:O	2.58	0.44
1:D:350:MET:O	1:D:352:TRP:HD1	2.00	0.44
1:D:516:TRP:CD1	1:D:579:LEU:HD13	2.53	0.44
1:D:1494:ARG:HH11	1:D:1494:ARG:CG	2.16	0.44
2:E:2631:TYR:HD1	2:E:2631:TYR:H	1.64	0.44
3:F:3023[B]:ILE:O	3:F:3026[B]:THR:OG1	2.34	0.44
3:F:3087[A]:MET:HA	3:F:3090[A]:ASN:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3104[B]:MET:HA	3:F:3110[B]:THR:CG2	2.17	0.44
3:F:3133[B]:LEU:O	3:F:3136[B]:TYR:HB3	2.17	0.44
3:F:3157[B]:PRO:HD2	3:a:3153[B]:LYS:HZ2	1.81	0.44
3:F:3200[A]:LEU:CD2	3:F:3204[A]:LEU:CD1	2.93	0.44
3:F:3218[B]:LEU:HD12	3:F:3218[B]:LEU:HA	1.78	0.44
3:F:3225[B]:SER:C	3:F:3290[B]:ILE:HG23	2.39	0.44
3:F:3273[B]:LEU:C	3:F:3275[B]:LEU:HD12	2.42	0.44
1:G:1055:THR:HA	1:G:1119:LEU:HD13	1.99	0.44
2:H:2424:SER:HB3	2:H:2445:MET:HG2	1.99	0.44
2:H:2527:LEU:HD22	2:H:2581:MET:HG3	2.00	0.44
2:H:2680:HIS:CD2	2:H:2684:HIS:HD2	2.36	0.44
3:I:2946[A]:GLN:CD	3:I:2947[A]:ALA:N	2.72	0.44
3:I:2989[A]:HIS:O	3:I:2990[A]:ARG:C	2.61	0.44
3:I:3014[A]:TRP:CG	3:I:3092[A]:ILE:CD1	2.98	0.44
3:I:3014[A]:TRP:CH2	3:I:3123[A]:THR:HG23	2.53	0.44
3:I:3023[B]:ILE:HA	3:I:3026[B]:THR:HG1	1.83	0.44
3:I:3137[A]:ARG:HB3	3:I:3139[A]:LEU:HD21	1.97	0.44
3:I:3147[B]:GLU:CD	3:R:3163[B]:ASN:O	2.61	0.44
3:I:3169[B]:LYS:O	3:R:3152[B]:LYS:CA	2.62	0.44
3:I:3180[B]:TYR:CB	3:I:3183[B]:LEU:CD2	2.89	0.44
3:I:3185[A]:TYR:HE2	3:I:3187[A]:TYR:CD2	2.35	0.44
3:I:3191[B]:ASN:C	3:I:3192[B]:PHE:O	2.52	0.44
3:I:3196[A]:THR:CB	3:I:3199[A]:GLN:OE1	2.64	0.44
3:I:3200[A]:LEU:CD2	3:I:3204[A]:LEU:CD1	2.93	0.44
1:J:119:LYS:HB2	1:J:120:LYS:CA	2.48	0.44
1:J:931:TRP:CD1	1:J:1048:ASN:HD22	2.36	0.44
1:J:1629:GLU:HG3	1:J:1630:MET:N	2.33	0.44
2:K:2390:GLN:O	2:K:2491:PRO:HB3	2.18	0.44
2:K:2602:LEU:HG	2:K:2603:PRO:HD2	2.00	0.44
3:L:2949[A]:LYS:NZ	3:L:2949[A]:LYS:C	2.73	0.44
3:L:2988[B]:TRP:CD1	3:L:3158[B]:PHE:CE2	3.06	0.44
3:L:3074[A]:GLU:CD	3:L:3212[A]:ARG:NH2	2.73	0.44
3:L:3230[A]:PHE:CB	3:L:3242[A]:GLY:C	2.91	0.44
3:L:3266[A]:ILE:O	3:L:3269[A]:SER:HB2	2.17	0.44
3:L:3273[A]:LEU:C	3:L:3275[A]:LEU:HD12	2.42	0.44
1:M:930:ASP:OD1	1:M:1051:ARG:NH2	2.51	0.44
1:M:1649:THR:HA	2:Q:2327:GLU:HG2	2.00	0.44
2:N:2797:LYS:HA	2:N:2800:LYS:HD3	1.98	0.44
3:O:2956[B]:LYS:O	3:O:2959[B]:SER:OG	2.33	0.44
3:O:3093[A]:HIS:HD2	3:O:3248[A]:LEU:CD2	2.30	0.44
3:O:3135[B]:LYS:HB2	3:O:3141[B]:TYR:CD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3230[B]:PHE:CB	3:O:3242[B]:GLY:C	2.91	0.44
3:O:3300[A]:LEU:HD23	3:O:3300[A]:LEU:H	1.83	0.44
1:P:567:LEU:HB2	1:P:571:PRO:CA	2.46	0.44
1:P:745:ASP:HB2	1:P:801:ASP:OD1	2.16	0.44
1:P:962:GLY:HA2	1:P:971:THR:HB	1.99	0.44
1:P:1013:ILE:HG21	1:P:1192:TYR:CD1	2.53	0.44
3:R:2988[B]:TRP:CD1	3:R:3158[B]:PHE:CE2	3.06	0.44
3:R:3031[B]:ASN:HA	3:R:3032[B]:PRO:HD2	1.87	0.44
3:R:3047[A]:ARG:NH2	3:R:3113[A]:ASP:OD1	2.43	0.44
3:R:3106[A]:THR:O	3:R:3106[A]:THR:HG23	2.16	0.44
3:R:3182[B]:GLN:C	3:R:3183[B]:LEU:CD1	2.91	0.44
3:R:3284[A]:LYS:CE	3:R:3285[A]:VAL:H	2.29	0.44
1:S:400:ILE:HG23	1:S:663:GLU:HG2	1.99	0.44
1:S:739:GLN:OE1	1:S:739:GLN:N	2.51	0.44
1:S:1485:ALA:O	1:S:1489:MET:HG2	2.18	0.44
2:T:2132:CYS:HB2	2:T:2142:ALA:HB1	1.99	0.44
2:T:2550:THR:O	2:T:2553:ALA:N	2.27	0.44
2:T:2799:LYS:HA	2:T:2803:ARG:NH1	2.32	0.44
3:U:2938[B]:LEU:O	3:U:2939[B]:ARG:C	2.58	0.44
3:U:2980[B]:HIS:HB2	3:d:2969[B]:TYR:OH	2.17	0.44
3:U:2988[B]:TRP:CD1	3:U:3158[B]:PHE:CE2	3.06	0.44
3:U:3004[A]:GLY:C	3:U:3006[A]:LYS:N	2.74	0.44
3:U:3200[A]:LEU:CD2	3:U:3204[A]:LEU:HD11	2.48	0.44
3:U:3225[A]:SER:C	3:U:3290[A]:ILE:HG23	2.39	0.44
1:V:639:ARG:HB2	1:V:703:TYR:CE1	2.52	0.44
2:W:2124:SER:HB2	2:W:2129:PRO:HG2	2.00	0.44
2:W:2745:PRO:HA	2:W:2764:THR:HA	1.99	0.44
3:X:2931[A]:THR:O	3:X:2934[A]:GLU:HG3	2.18	0.44
3:X:3093[A]:HIS:HB2	3:X:3248[A]:LEU:CD1	2.48	0.44
3:X:3171[B]:HIS:C	3:X:3173[B]:THR:N	2.73	0.44
3:X:3183[A]:LEU:H	3:X:3184[A]:ASN:CA	2.21	0.44
3:X:3222[B]:ILE:CD1	3:X:3223[B]:GLY:N	2.73	0.44
3:X:3293[B]:LYS:HB2	3:X:3294[B]:SER:CA	2.41	0.44
1:Y:638:ASP:O	1:Y:641:TRP:HB3	2.18	0.44
1:Y:999:LEU:HB3	1:Y:1133:ILE:HD11	2.00	0.44
2:Z:2234:GLN:HG3	2:Z:2235:PRO:HD2	1.99	0.44
2:Z:2866:PRO:CG	3:a:2933[A]:SER:OG	2.65	0.44
3:a:2989[A]:HIS:O	3:a:2990[A]:ARG:C	2.61	0.44
3:a:3014[A]:TRP:CH2	3:a:3123[A]:THR:HG23	2.53	0.44
3:a:3019[A]:HIS:CD2	3:a:3020[A]:SER:H	2.35	0.44
3:a:3019[B]:HIS:CD2	3:a:3020[B]:SER:H	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3093[A]:HIS:HD2	3:a:3248[A]:LEU:CD2	2.30	0.44
3:a:3104[A]:MET:SD	3:a:3110[A]:THR:CG2	3.06	0.44
3:a:3137[B]:ARG:HD3	3:a:3137[B]:ARG:HA	1.72	0.44
3:a:3182[B]:GLN:C	3:a:3183[B]:LEU:CD1	2.91	0.44
3:a:3218[A]:LEU:HD12	3:a:3218[A]:LEU:HA	1.78	0.44
3:a:3229[A]:ASN:O	3:a:3286[A]:THR:N	2.50	0.44
3:a:3299[A]:LEU:O	3:a:3300[A]:LEU:C	2.60	0.44
1:b:1427:HIS:NE2	1:b:1431:HIS:CD2	2.84	0.44
3:d:2951[A]:ASP:CG	3:d:2952[A]:ALA:N	2.74	0.44
3:d:2961[A]:HIS:HB2	3:d:2992[A]:TYR:HE2	1.80	0.44
3:d:3014[B]:TRP:CH2	3:d:3123[B]:THR:HG23	2.53	0.44
3:d:3019[A]:HIS:CD2	3:d:3020[A]:SER:H	2.35	0.44
3:d:3116[A]:PHE:CD1	3:d:3116[A]:PHE:C	2.94	0.44
3:d:3119[A]:HIS:O	3:d:3122[A]:ASN:HB3	2.17	0.44
3:d:3230[B]:PHE:CB	3:d:3242[B]:GLY:C	2.91	0.44
3:d:3283[A]:ILE:C	3:d:3283[A]:ILE:CD1	2.85	0.44
3:d:3293[B]:LYS:HB2	3:d:3294[B]:SER:CA	2.41	0.44
1:A:1145:THR:HB	1:A:1191:PRO:CB	2.47	0.44
1:A:1260:ARG:HD3	1:A:1331:GLU:OE1	2.17	0.44
1:A:1622:GLN:HG2	1:A:1652:PHE:CD1	2.53	0.44
2:B:2814:LYS:HE3	2:B:2843:GLU:HB3	1.99	0.44
3:C:2931[B]:THR:O	3:C:2934[B]:GLU:HG3	2.18	0.44
3:C:2989[A]:HIS:C	3:C:2991[A]:LEU:N	2.75	0.44
3:C:3025[B]:VAL:CG2	3:C:3047[B]:ARG:NH1	2.73	0.44
3:C:3171[A]:HIS:C	3:C:3173[A]:THR:N	2.73	0.44
3:C:3218[A]:LEU:HD12	3:C:3218[A]:LEU:HA	1.78	0.44
3:C:3229[B]:ASN:O	3:C:3286[B]:THR:N	2.50	0.44
3:C:3244[A]:THR:H	3:C:3264[A]:TYR:HE2	1.65	0.44
3:C:3254[B]:MET:HE2	3:L:2977[B]:CYS:HB3	1.02	0.44
1:D:464:LEU:HD13	1:D:622:HIS:CG	2.52	0.44
1:D:999:LEU:HD12	1:D:1056:TRP:HD1	1.82	0.44
2:E:2329:MET:HA	2:E:2354:PRO:HG2	2.00	0.44
2:E:2389:ARG:HG2	2:E:2393:ARG:HH22	1.82	0.44
3:F:2979[B]:GLN:HB2	3:F:2988[B]:TRP:CD1	2.52	0.44
3:F:2989[A]:HIS:CD2	9:a:3401[A]:CUO:O1	2.71	0.44
3:F:3242[A]:GLY:C	3:F:3243[A]:GLY:O	2.58	0.44
3:F:3248[B]:LEU:HB3	3:a:2973[B]:THR:C	2.24	0.44
3:F:3266[A]:ILE:O	3:F:3269[A]:SER:HB2	2.17	0.44
1:G:946:GLU:HG2	1:G:955:LYS:HB3	1.99	0.44
1:G:961:SER:HB3	1:G:974:ALA:HB3	2.00	0.44
1:G:1245:GLU:N	1:G:1245:GLU:OE1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2989[A]:HIS:CD2	9:R:3401[A]:CUO:O1	2.71	0.44
3:I:3019[A]:HIS:CD2	3:I:3020[A]:SER:H	2.35	0.44
3:I:3101[A]:PRO:O	3:I:3109[A]:TYR:HD2	2.00	0.44
3:I:3106[B]:THR:O	3:I:3106[B]:THR:HG23	2.17	0.44
3:I:3160[B]:SER:O	3:R:3147[B]:GLU:HG3	2.18	0.44
3:I:3163[B]:ASN:HD22	3:R:3150[B]:LYS:HG3	0.59	0.44
3:I:3241[B]:PHE:CE2	3:I:3243[B]:GLY:O	2.70	0.44
2:K:2114:ARG:HA	2:K:2114:ARG:HD3	1.82	0.44
3:L:3013[A]:ASP:CG	3:L:3015[A]:THR:HG1	2.24	0.44
3:L:3106[A]:THR:O	3:L:3106[A]:THR:HG23	2.16	0.44
3:L:3182[A]:GLN:C	3:L:3183[A]:LEU:CD1	2.90	0.44
3:L:3182[B]:GLN:C	3:L:3183[B]:LEU:CD1	2.91	0.44
3:L:3241[A]:PHE:CE2	3:L:3243[A]:GLY:O	2.70	0.44
3:L:3241[B]:PHE:CZ	3:L:3243[B]:GLY:O	2.70	0.44
3:L:3293[A]:LYS:HB2	3:L:3294[A]:SER:CA	2.41	0.44
1:M:669:LYS:HA	1:M:669:LYS:HD2	1.63	0.44
2:N:2361:LYS:HD2	2:N:2362:GLN:N	2.32	0.44
2:N:2472:ASN:N	2:N:2473:GLY:HA2	2.33	0.44
3:O:2972[B]:GLY:HA3	3:X:2985[B]:PHE:O	2.18	0.44
3:O:3104[A]:MET:SD	3:O:3110[A]:THR:CG2	3.06	0.44
3:O:3180[B]:TYR:CA	3:O:3183[B]:LEU:CD2	2.95	0.44
3:O:3230[A]:PHE:CB	3:O:3242[A]:GLY:C	2.91	0.44
3:O:3285[B]:VAL:CG2	3:O:3286[B]:THR:H	2.27	0.44
1:P:788:LEU:HB3	1:P:790:VAL:HG23	1.99	0.44
1:P:1091:ASN:HA	1:P:1092:PRO:HD3	1.61	0.44
1:P:1279:LYS:HE3	1:P:1376:PRO:HG3	2.00	0.44
1:P:1528:ASP:OD1	1:P:1528:ASP:N	2.48	0.44
2:Q:2800:LYS:HB3	3:R:3023[A]:ILE:HD13	1.99	0.44
3:R:2940[A]:ASN:O	3:R:2943[A]:ALA:HB3	2.18	0.44
3:R:3014[A]:TRP:CH2	3:R:3123[A]:THR:HG23	2.53	0.44
3:R:3019[A]:HIS:CD2	3:R:3020[A]:SER:H	2.35	0.44
3:R:3093[A]:HIS:HD2	3:R:3248[A]:LEU:CD2	2.30	0.44
3:R:3093[B]:HIS:HD2	3:R:3248[B]:LEU:CD2	2.31	0.44
3:R:3133[B]:LEU:O	3:R:3136[B]:TYR:HB3	2.18	0.44
3:R:3204[A]:LEU:CD1	3:R:3204[A]:LEU:N	2.80	0.44
3:R:3230[B]:PHE:CB	3:R:3242[B]:GLY:C	2.91	0.44
3:R:3244[A]:THR:H	3:R:3264[A]:TYR:HE2	1.65	0.44
3:R:3266[A]:ILE:O	3:R:3269[A]:SER:HB2	2.17	0.44
1:S:22:LEU:HD12	1:S:25:MET:HG2	1.98	0.44
1:S:633:HIS:C	1:S:633:HIS:ND1	2.75	0.44
1:S:903:PRO:HG3	1:S:1004:PHE:HZ	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1195:ASP:HA	1:S:1196:ILE:HG22	1.98	0.44
1:S:1335:LEU:HD23	1:S:1339:SER:HA	1.99	0.44
1:S:1634:ALA:HB2	1:S:1639:LYS:NZ	2.33	0.44
2:T:2873:HIS:ND1	1:V:1101:VAL:HG21	2.32	0.44
3:U:2963[B]:MET:SD	3:U:2963[B]:MET:C	3.01	0.44
3:U:2975[B]:PHE:CG	3:d:3256[B]:TRP:CB	3.00	0.44
3:U:2979[B]:GLN:HB2	3:U:2988[B]:TRP:CD1	2.52	0.44
3:U:2986[A]:PRO:CB	3:U:3127[A]:TRP:CE3	3.00	0.44
3:U:3023[B]:ILE:O	3:U:3026[B]:THR:OG1	2.34	0.44
3:U:3148[A]:ILE:O	3:U:3148[A]:ILE:HG22	2.17	0.44
3:U:3182[B]:GLN:C	3:U:3183[B]:LEU:CD1	2.91	0.44
3:U:3230[A]:PHE:CB	3:U:3242[A]:GLY:C	2.91	0.44
1:V:1324:ARG:NH1	1:V:1516:VAL:O	2.50	0.44
1:V:1587:ALA:HA	1:V:1614:GLU:HG2	1.99	0.44
3:X:2956[B]:LYS:O	3:X:2959[B]:SER:OG	2.33	0.44
3:X:3028[B]:PRO:HG2	3:X:3029[B]:LYS:HG3	2.00	0.44
3:X:3146[A]:CYS:HA	3:X:3147[A]:GLU:HA	1.70	0.44
3:X:3146[B]:CYS:HA	3:X:3147[B]:GLU:HA	1.70	0.44
3:X:3196[B]:THR:CB	3:X:3199[B]:GLN:OE1	2.64	0.44
3:X:3200[A]:LEU:CD2	3:X:3204[A]:LEU:HD11	2.48	0.44
1:Y:1158:GLU:HB2	1:Y:1171:LYS:HE3	2.00	0.44
2:Z:2107:LEU:HA	2:Z:2110:MET:HG2	1.98	0.44
2:Z:2244:PHE:HA	2:Z:2373:MET:HE1	1.99	0.44
2:Z:2310:GLU:HG3	2:Z:2371:LEU:HD13	1.99	0.44
2:Z:2824:CYS:HB3	2:Z:2826:GLU:O	2.17	0.44
3:a:2979[A]:GLN:HG2	3:a:3155[A]:MET:HE2	1.85	0.44
3:a:2988[B]:TRP:CD1	3:a:3158[B]:PHE:CE2	3.06	0.44
3:a:2989[A]:HIS:C	3:a:2991[A]:LEU:N	2.75	0.44
3:a:3038[B]:ILE:HG23	3:a:3040[B]:VAL:HG22	1.90	0.44
3:a:3074[A]:GLU:CD	3:a:3212[A]:ARG:NH2	2.73	0.44
3:a:3244[A]:THR:H	3:a:3264[A]:TYR:HE2	1.65	0.44
3:a:3266[A]:ILE:O	3:a:3269[A]:SER:HB2	2.17	0.44
2:c:2361:LYS:H	2:c:2361:LYS:HG3	1.53	0.44
2:c:2539:ILE:O	2:c:2573:TYR:OH	2.21	0.44
3:d:2952[A]:ALA:CB	3:d:2953[A]:GLY:CA	2.82	0.44
3:d:2963[B]:MET:SD	3:d:2963[B]:MET:C	3.01	0.44
3:d:3133[A]:LEU:O	3:d:3136[A]:TYR:HB3	2.17	0.44
3:d:3137[A]:ARG:O	3:d:3139[A]:LEU:HD22	2.16	0.44
3:d:3204[B]:LEU:CD1	3:d:3204[B]:LEU:N	2.80	0.44
3:d:3241[A]:PHE:CZ	3:d:3243[A]:GLY:O	2.70	0.44
3:d:3242[B]:GLY:C	3:d:3243[B]:GLY:O	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3266[B]:ILE:O	3:d:3269[B]:SER:HB2	2.17	0.44
2:B:2089:ARG:HB3	2:B:2175:VAL:O	2.18	0.44
2:B:2745:PRO:HB2	2:B:2750:ILE:HD12	1.99	0.44
2:B:2791:LEU:HD23	2:B:2791:LEU:HA	1.84	0.44
3:C:3087[B]:MET:HA	3:C:3090[B]:ASN:OD1	2.17	0.44
3:C:3106[A]:THR:O	3:C:3106[A]:THR:HG23	2.17	0.44
3:C:3137[B]:ARG:O	3:C:3139[B]:LEU:HD22	2.16	0.44
3:C:3230[B]:PHE:CB	3:C:3242[B]:GLY:C	2.91	0.44
3:C:3273[A]:LEU:C	3:C:3275[A]:LEU:HD12	2.42	0.44
3:C:3299[A]:LEU:HB3	3:C:3300[A]:LEU:H	1.54	0.44
3:C:3300[B]:LEU:HD23	3:C:3300[B]:LEU:H	1.83	0.44
9:C:3401[A]:CUO:O1	3:L:2989[A]:HIS:CD2	2.70	0.44
1:D:737:GLY:HA2	1:D:771:TRP:CZ2	2.52	0.44
1:D:991:LEU:HD22	1:D:991:LEU:H	1.82	0.44
2:E:2554:PRO:HA	2:E:2555:GLU:HB3	1.98	0.44
3:F:2986[B]:PRO:CB	3:F:3127[B]:TRP:CE3	3.00	0.44
3:F:3093[B]:HIS:HB2	3:F:3248[B]:LEU:CD1	2.48	0.44
3:F:3185[B]:TYR:HE2	3:F:3187[B]:TYR:CD2	2.35	0.44
3:F:3252[B]:TYR:CG	3:a:3108[B]:HIS:CE1	3.06	0.44
3:F:3300[B]:LEU:HD23	3:F:3300[B]:LEU:H	1.83	0.44
1:G:392:PRO:O	1:G:395:THR:OG1	2.31	0.44
1:G:1172:ALA:CB	1:G:1196:ILE:HG13	2.48	0.44
1:G:1470:GLU:HG2	1:G:1537:ILE:CD1	2.46	0.44
2:H:2107:LEU:O	2:H:2111:GLN:HB2	2.18	0.44
2:H:2133:PRO:HG2	2:H:2140:ARG:HA	1.99	0.44
2:H:2849:ASP:HB3	2:H:2850:ARG:NH1	2.33	0.44
3:I:2969[A]:TYR:CD2	3:I:2970[A]:PRO:CG	3.00	0.44
3:I:3241[A]:PHE:CZ	3:I:3243[A]:GLY:O	2.70	0.44
3:I:3273[A]:LEU:C	3:I:3275[A]:LEU:HD12	2.42	0.44
3:I:3273[B]:LEU:C	3:I:3275[B]:LEU:HD12	2.42	0.44
1:J:270:GLU:OE1	1:J:270:GLU:N	2.47	0.44
1:J:464:LEU:HD22	1:J:622:HIS:CG	2.52	0.44
1:J:875:ALA:HA	1:J:1038:PHE:CZ	2.52	0.44
1:J:1315:GLY:HA3	1:J:1601:TRP:CB	2.48	0.44
2:K:2327:GLU:H	2:K:2327:GLU:HG3	1.45	0.44
2:K:2663:MET:HG3	2:K:2675:GLN:HB2	1.98	0.44
3:L:2979[B]:GLN:HB2	3:L:2988[B]:TRP:CD1	2.52	0.44
3:L:2988[A]:TRP:CD1	3:L:3158[A]:PHE:CE2	3.06	0.44
3:L:2989[A]:HIS:O	3:L:2990[A]:ARG:C	2.61	0.44
3:L:3019[A]:HIS:CD2	3:L:3020[A]:SER:H	2.36	0.44
3:L:3104[A]:MET:SD	3:L:3110[A]:THR:CG2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3104[B]:MET:SD	3:L:3110[B]:THR:CG2	3.06	0.44
3:L:3148[A]:ILE:O	3:L:3148[A]:ILE:HG22	2.17	0.44
3:L:3241[A]:PHE:CZ	3:L:3243[A]:GLY:O	2.70	0.44
1:M:108:PRO:HA	1:M:124:TYR:CG	2.52	0.44
1:M:472:ASP:HA	1:M:473:ALA:HA	1.70	0.44
2:N:2562:GLY:H	2:N:2846:TRP:CB	2.30	0.44
3:O:2938[A]:LEU:O	3:O:2939[A]:ARG:C	2.58	0.44
3:O:2951[B]:ASP:CG	3:O:2952[B]:ALA:N	2.74	0.44
3:O:2979[B]:GLN:HB2	3:O:2988[B]:TRP:CD1	2.52	0.44
3:O:3027[A]:GLU:CD	3:O:3027[A]:GLU:C	2.85	0.44
3:O:3093[B]:HIS:HB2	3:O:3248[B]:LEU:CD1	2.48	0.44
3:O:3094[B]:SER:HG	3:O:3227[B]:ASP:CG	2.25	0.44
3:O:3156[B]:MET:SD	3:X:3173[B]:THR:HG22	2.57	0.44
3:O:3244[B]:THR:H	3:O:3264[B]:TYR:HE2	1.65	0.44
1:P:140:ASP:OD1	1:P:142:ARG:NE	2.34	0.44
1:P:448:SER:O	1:P:450:LYS:HG2	2.18	0.44
1:P:587:PHE:HA	1:P:644:TRP:HD1	1.83	0.44
1:P:736:MET:HG2	1:P:772:ARG:HD2	2.00	0.44
1:P:1156:LEU:HB2	1:P:1176:TYR:CE1	2.53	0.44
1:P:1411:PHE:HB3	1:P:1544:LEU:HD21	1.99	0.44
2:Q:2879:LEU:HA	2:Q:2879:LEU:HD12	1.77	0.44
3:R:2946[A]:GLN:CD	3:R:2947[A]:ALA:N	2.72	0.44
3:R:2948[B]:ASP:CB	3:R:2949[B]:LYS:CA	2.78	0.44
3:R:2969[A]:TYR:CD2	3:R:2970[A]:PRO:CG	3.00	0.44
3:R:3023[B]:ILE:HA	3:R:3026[B]:THR:HG1	1.82	0.44
3:R:3027[B]:GLU:CD	3:R:3027[B]:GLU:C	2.85	0.44
3:R:3087[A]:MET:HA	3:R:3090[A]:ASN:OD1	2.17	0.44
3:R:3133[A]:LEU:O	3:R:3136[A]:TYR:HB3	2.18	0.44
3:R:3241[B]:PHE:CE2	3:R:3243[B]:GLY:O	2.71	0.44
1:S:7:VAL:HG21	1:S:208:LEU:HD23	2.00	0.44
1:S:627:ASP:HA	1:S:628:PRO:HD3	1.86	0.44
1:S:858:MET:HE1	1:S:870:TYR:CE1	2.52	0.44
1:S:1236:TYR:HB3	2:W:2736:TYR:HB3	1.99	0.44
2:T:2128:LEU:O	2:T:2130:PRO:HD3	2.18	0.44
2:T:2186:GLU:HA	2:T:2232:PHE:CE1	2.53	0.44
2:T:2526:ARG:HE	2:W:2114:ARG:HG3	1.82	0.44
2:T:2840:GLY:O	2:T:2843:GLU:HB2	2.17	0.44
3:U:2969[B]:TYR:CD2	3:U:2970[B]:PRO:CG	3.00	0.44
3:U:2975[B]:PHE:HA	3:d:3255[B]:PRO:HA	1.33	0.44
3:U:2976[B]:ALA:O	3:U:2978[B]:CYS:N	2.46	0.44
3:U:2989[B]:HIS:O	3:U:2990[B]:ARG:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3028[B]:PRO:HG2	3:U:3029[B]:LYS:HG3	2.00	0.44
3:U:3093[A]:HIS:HB2	3:U:3248[A]:LEU:CD1	2.48	0.44
3:U:3101[A]:PRO:O	3:U:3109[A]:TYR:HD2	2.00	0.44
3:U:3101[B]:PRO:O	3:U:3109[B]:TYR:HD2	2.00	0.44
3:U:3171[B]:HIS:C	3:U:3173[B]:THR:N	2.73	0.44
3:U:3182[A]:GLN:C	3:U:3183[A]:LEU:CD1	2.91	0.44
3:U:3254[B]:MET:HB3	3:d:3255[B]:PRO:N	2.31	0.44
3:U:3306[A]:LEU:C	3:U:3306[A]:LEU:CD1	2.86	0.44
1:V:437:TYR:CE1	1:V:535:PRO:HD2	2.53	0.44
1:V:931:TRP:CB	1:V:1018:ILE:HD11	2.47	0.44
1:V:956:PRO:HD2	1:V:957:ASN:O	2.18	0.44
2:W:2286:HIS:NE2	2:W:2433:THR:HG22	2.32	0.44
2:W:2373:MET:HB3	2:W:2381:LEU:HD11	2.00	0.44
3:X:2938[A]:LEU:O	3:X:2939[A]:ARG:C	2.58	0.44
3:X:2989[A]:HIS:O	3:X:2990[A]:ARG:C	2.61	0.44
3:X:3004[B]:GLY:C	3:X:3006[B]:LYS:N	2.73	0.44
3:X:3241[B]:PHE:CZ	3:X:3243[B]:GLY:O	2.70	0.44
3:X:3273[A]:LEU:C	3:X:3275[A]:LEU:HD12	2.42	0.44
1:Y:147:SER:O	1:Y:149:GLU:N	2.49	0.44
1:Y:262:LYS:NZ	1:Y:795:GLU:OE1	2.50	0.44
1:Y:492:ARG:NH2	1:Y:641:TRP:CE2	2.85	0.44
1:Y:817:PRO:HA	1:Y:818:PRO:HD3	1.87	0.44
1:Y:987:LYS:H	1:Y:987:LYS:HG2	1.51	0.44
1:Y:1655:SER:CB	3:d:3007[B]:ILE:HG23	2.34	0.44
3:a:2951[A]:ASP:CG	3:a:2952[A]:ALA:N	2.74	0.44
3:a:2963[A]:MET:SD	3:a:2963[A]:MET:C	3.01	0.44
3:a:2991[A]:LEU:HD23	3:a:3158[A]:PHE:CE1	2.48	0.44
3:a:3034[A]:HIS:HB3	3:a:3035[A]:HIS:CE1	2.50	0.44
3:a:3132[A]:ALA:HB3	3:a:3197[A]:ILE:HD13	1.99	0.44
3:a:3135[B]:LYS:HB2	3:a:3141[B]:TYR:CD1	2.51	0.44
3:a:3161[A]:GLU:H	3:a:3161[A]:GLU:CD	2.19	0.44
3:a:3230[A]:PHE:CB	3:a:3242[A]:GLY:C	2.91	0.44
3:a:3264[B]:TYR:HD1	3:a:3265[B]:ASP:N	2.14	0.44
3:a:3300[A]:LEU:HD23	3:a:3300[A]:LEU:H	1.83	0.44
1:b:725:SER:HB2	1:b:827:ALA:HB2	1.98	0.44
3:d:2931[A]:THR:O	3:d:2934[A]:GLU:HG3	2.18	0.44
3:d:2949[B]:LYS:NZ	3:d:2949[B]:LYS:C	2.73	0.44
3:d:2952[B]:ALA:CA	3:d:2956[B]:LYS:CB	2.89	0.44
3:d:2969[A]:TYR:CD2	3:d:2970[A]:PRO:CG	3.00	0.44
3:d:2985[B]:PHE:CE2	3:d:2989[B]:HIS:CD2	3.04	0.44
3:d:2989[B]:HIS:C	3:d:2991[B]:LEU:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3180[A]:TYR:CA	3:d:3183[A]:LEU:CD2	2.95	0.44
3:d:3180[A]:TYR:CB	3:d:3183[A]:LEU:CD2	2.90	0.44
6:NA:1:NAG:H61	6:NA:2:NAG:N2	2.24	0.44
1:A:76:PHE:HD2	1:A:89:ILE:HD13	1.83	0.44
1:A:457:ALA:O	1:A:460:GLU:HB2	2.17	0.44
1:A:855:ARG:HH21	1:A:941:LEU:HA	1.83	0.44
1:A:1026:GLU:C	1:A:1028:VAL:H	2.26	0.44
1:A:1163:ALA:HB2	1:A:1205:LEU:HD21	1.99	0.44
1:A:1315:GLY:HA3	1:A:1601:TRP:CB	2.48	0.44
1:A:1643:LYS:HA	1:A:1643:LYS:HD2	1.76	0.44
2:B:2782:ASN:HB2	2:B:2786:MET:O	2.18	0.44
2:B:2907:LYS:HB3	2:B:2907:LYS:HE2	1.66	0.44
3:C:2974[B]:ALA:O	3:L:3249[B]:GLY:HA2	2.18	0.44
3:C:3014[B]:TRP:CH2	3:C:3123[B]:THR:HG23	2.53	0.44
3:C:3101[B]:PRO:O	3:C:3109[B]:TYR:HD2	2.00	0.44
3:C:3293[A]:LYS:CB	3:C:3294[A]:SER:CA	2.96	0.44
1:D:120:LYS:HA	1:D:120:LYS:HD2	1.72	0.44
1:D:610:THR:HB	1:D:629:MET:HE1	1.99	0.44
1:D:1166:THR:CB	1:D:1168:GLN:HG3	2.48	0.44
2:E:2651:GLN:NE2	2:E:2652:LYS:HG3	2.33	0.44
3:F:2931[A]:THR:O	3:F:2934[A]:GLU:HG3	2.18	0.44
3:F:2931[B]:THR:O	3:F:2934[B]:GLU:HG3	2.18	0.44
3:F:2963[B]:MET:SD	3:F:2963[B]:MET:C	3.01	0.44
3:F:2989[A]:HIS:C	3:F:2991[A]:LEU:N	2.75	0.44
3:F:3023[A]:ILE:O	3:F:3026[A]:THR:OG1	2.34	0.44
3:F:3093[B]:HIS:HD2	3:F:3248[B]:LEU:CD2	2.31	0.44
3:F:3106[B]:THR:O	3:F:3106[B]:THR:HG23	2.16	0.44
3:F:3135[A]:LYS:HB2	3:F:3141[A]:TYR:CD1	2.52	0.44
3:F:3200[B]:LEU:CD2	3:F:3204[B]:LEU:HD11	2.47	0.44
1:G:127:GLU:HG2	1:G:135:THR:N	2.31	0.44
2:H:2132:CYS:O	2:H:2334:LYS:HD3	2.18	0.44
2:H:2133:PRO:HG3	2:H:2141:HIS:CE1	2.53	0.44
3:I:2940[A]:ASN:O	3:I:2943[A]:ALA:HB3	2.18	0.44
3:I:2963[A]:MET:SD	3:I:2963[A]:MET:C	3.01	0.44
3:I:2979[B]:GLN:HB2	3:I:2988[B]:TRP:CD1	2.52	0.44
3:I:2989[A]:HIS:C	3:I:2991[A]:LEU:N	2.75	0.44
3:I:3104[A]:MET:SD	3:I:3110[A]:THR:CG2	3.06	0.44
3:I:3204[B]:LEU:CD1	3:I:3204[B]:LEU:N	2.80	0.44
3:I:3230[A]:PHE:CB	3:I:3242[A]:GLY:C	2.91	0.44
3:I:3284[B]:LYS:CD	3:I:3284[B]:LYS:C	2.86	0.44
3:I:3298[B]:ASN:CA	3:I:3299[B]:LEU:HB2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1498:ASN:ND2	1:J:1500:THR:O	2.51	0.44
2:K:2158:TYR:HE2	2:K:2294:PHE:CE1	2.35	0.44
2:K:2265:ILE:HD12	2:K:2443:TYR:CG	2.53	0.44
2:K:2283:ASN:O	2:K:2283:ASN:ND2	2.51	0.44
3:L:2963[B]:MET:SD	3:L:2963[B]:MET:C	3.01	0.44
3:L:3028[B]:PRO:HG2	3:L:3029[B]:LYS:HG3	2.00	0.44
3:L:3093[A]:HIS:HB2	3:L:3248[A]:LEU:CD1	2.48	0.44
3:L:3133[A]:LEU:O	3:L:3136[A]:TYR:HB3	2.17	0.44
3:L:3148[B]:ILE:O	3:L:3148[B]:ILE:HG22	2.17	0.44
3:L:3180[A]:TYR:CA	3:L:3183[A]:LEU:CD2	2.95	0.44
3:L:3266[B]:ILE:O	3:L:3269[B]:SER:HB2	2.18	0.44
3:L:3293[B]:LYS:CD	3:L:3293[B]:LYS:C	2.86	0.44
1:M:567:LEU:HD12	1:M:567:LEU:HA	1.89	0.44
1:M:1614:GLU:OE1	1:M:1614:GLU:N	2.50	0.44
2:N:2504:ARG:HD3	2:N:2775:GLY:O	2.17	0.44
3:O:2963[B]:MET:SD	3:O:2963[B]:MET:C	3.01	0.44
3:O:2971[B]:ASP:OD2	3:X:3158[B]:PHE:HZ	2.00	0.44
3:O:2977[B]:CYS:SG	3:X:3154[B]:PRO:O	2.67	0.44
3:O:3027[B]:GLU:CD	3:O:3027[B]:GLU:C	2.85	0.44
3:O:3119[A]:HIS:O	3:O:3122[A]:ASN:HB3	2.17	0.44
3:O:3229[B]:ASN:O	3:O:3286[B]:THR:N	2.50	0.44
3:O:3300[B]:LEU:HD23	3:O:3300[B]:LEU:H	1.83	0.44
1:P:746:LEU:HD21	1:P:781:ILE:HD11	1.99	0.44
1:P:1073:ALA:O	1:P:1077:LEU:HB2	2.18	0.44
1:P:1078:ARG:HB2	1:P:1078:ARG:HH11	1.82	0.44
2:Q:2107:LEU:HD22	2:Q:2209:PHE:CE2	2.53	0.44
2:Q:2568:HIS:HD2	2:Q:2718:TRP:CH2	2.35	0.44
3:R:2931[A]:THR:O	3:R:2934[A]:GLU:HG3	2.18	0.44
3:R:2951[B]:ASP:OD2	3:R:2952[B]:ALA:CB	2.66	0.44
3:R:2963[A]:MET:SD	3:R:2963[A]:MET:C	3.01	0.44
3:R:2989[A]:HIS:O	3:R:2990[A]:ARG:C	2.61	0.44
3:R:3135[A]:LYS:HB2	3:R:3141[A]:TYR:CD1	2.52	0.44
3:R:3148[A]:ILE:O	3:R:3148[A]:ILE:HG22	2.17	0.44
3:R:3200[A]:LEU:CD2	3:R:3204[A]:LEU:HD11	2.48	0.44
3:R:3229[B]:ASN:O	3:R:3286[B]:THR:N	2.50	0.44
3:R:3230[A]:PHE:CB	3:R:3242[A]:GLY:C	2.91	0.44
3:R:3293[A]:LYS:CB	3:R:3294[A]:SER:CA	2.96	0.44
1:S:1082:SER:O	1:S:1086:LEU:HD23	2.18	0.44
3:U:2937[B]:ASN:CB	3:U:3006[B]:LYS:CE	2.86	0.44
3:U:2986[B]:PRO:CB	3:U:3127[B]:TRP:CE3	3.00	0.44
3:U:2988[A]:TRP:CD1	3:U:3158[A]:PHE:CE2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3014[A]:TRP:CH2	3:U:3123[A]:THR:HG23	2.53	0.44
3:U:3027[B]:GLU:CD	3:U:3027[B]:GLU:C	2.85	0.44
3:U:3241[A]:PHE:CE2	3:U:3243[A]:GLY:O	2.70	0.44
3:U:3266[A]:ILE:O	3:U:3269[A]:SER:HB2	2.18	0.44
3:U:3266[B]:ILE:O	3:U:3269[B]:SER:HB2	2.17	0.44
1:V:329:ARG:NH2	1:Y:1584:GLY:HA2	2.33	0.44
1:V:1249:TRP:CZ2	1:V:1537:ILE:HD12	2.53	0.44
2:W:2446:GLU:HG2	2:W:2448:THR:HG23	2.00	0.44
2:W:2854:MET:HE3	2:W:2854:MET:HB2	1.84	0.44
3:X:2938[B]:LEU:O	3:X:2939[B]:ARG:C	2.58	0.44
3:X:2988[A]:TRP:CD1	3:X:3158[A]:PHE:CE2	3.06	0.44
3:X:3014[B]:TRP:CH2	3:X:3123[B]:THR:HG23	2.53	0.44
3:X:3306[A]:LEU:C	3:X:3306[A]:LEU:CD1	2.86	0.44
1:Y:490:TRP:HE1	1:Y:670:PRO:HD2	1.82	0.44
1:Y:1325:LEU:HD11	1:Y:1511:SER:HA	2.00	0.44
1:Y:1636:ASN:HB3	1:Y:1638:SER:O	2.16	0.44
3:a:2948[B]:ASP:HB3	3:a:2949[B]:LYS:C	2.43	0.44
3:a:2963[B]:MET:C	3:a:2963[B]:MET:SD	3.01	0.44
3:a:3119[A]:HIS:O	3:a:3122[A]:ASN:HB3	2.17	0.44
3:a:3182[A]:GLN:C	3:a:3183[A]:LEU:CD1	2.91	0.44
3:a:3200[A]:LEU:CD2	3:a:3204[A]:LEU:HD11	2.48	0.44
3:a:3200[B]:LEU:CD2	3:a:3204[B]:LEU:HD11	2.48	0.44
3:a:3232[B]:VAL:HG21	3:a:3273[B]:LEU:HD11	2.00	0.44
1:b:238:ASN:OD1	1:b:238:ASN:N	2.38	0.44
1:b:832:LYS:HD2	1:b:832:LYS:HA	1.67	0.44
2:c:2431:GLY:O	2:c:2434:GLU:HG2	2.16	0.44
2:c:2640:ILE:H	2:c:2640:ILE:HG12	1.55	0.44
2:c:2716:ARG:HB2	2:c:2778:TYR:CE1	2.52	0.44
3:d:2979[A]:GLN:HB2	3:d:2988[A]:TRP:CD1	2.52	0.44
3:d:2989[B]:HIS:CD2	9:d:3401[B]:CUO:O1	2.70	0.44
3:d:3013[A]:ASP:CG	3:d:3015[A]:THR:HG1	2.24	0.44
3:d:3028[A]:PRO:HG2	3:d:3029[A]:LYS:HG3	2.00	0.44
3:d:3185[B]:TYR:CE2	3:d:3187[B]:TYR:HE2	2.31	0.44
3:d:3196[B]:THR:N	3:d:3199[B]:GLN:CB	2.65	0.44
3:d:3241[B]:PHE:CZ	3:d:3243[B]:GLY:O	2.70	0.44
1:A:643:ILE:HD13	1:A:708:PHE:HB2	1.99	0.44
1:A:817:PRO:HA	1:A:818:PRO:HD3	1.78	0.44
1:A:1412:GLU:OE2	1:A:1552:ARG:NH1	2.51	0.44
2:B:2780:HIS:HD2	2:B:2782:ASN:ND2	2.15	0.44
3:C:2931[A]:THR:O	3:C:2934[A]:GLU:HG3	2.18	0.44
3:C:2969[A]:TYR:CD2	3:C:2970[A]:PRO:CG	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2988[A]:TRP:CD1	3:C:3158[A]:PHE:CE2	3.06	0.44
3:C:3093[A]:HIS:HB2	3:C:3248[A]:LEU:CD1	2.48	0.44
3:C:3133[B]:LEU:HD12	3:C:3133[B]:LEU:HA	1.86	0.44
3:C:3230[A]:PHE:CB	3:C:3242[A]:GLY:C	2.91	0.44
3:C:3244[B]:THR:H	3:C:3264[B]:TYR:HE2	1.65	0.44
1:D:23:ARG:HD3	1:D:120:LYS:HG2	2.00	0.44
1:D:320:LYS:HD3	1:D:337:ASP:HB3	2.00	0.44
1:D:1231:VAL:HG22	1:D:1231:VAL:O	2.18	0.44
1:D:1286:ARG:NH2	1:D:1333:GLU:OE2	2.49	0.44
2:E:2180:TRP:CD1	2:E:2247:ILE:HD11	2.53	0.44
2:E:2345:ASN:HA	2:E:2346:PRO:HD2	1.86	0.44
2:E:2680:HIS:CD2	2:E:2684:HIS:HD2	2.35	0.44
2:E:2723:GLU:HG2	2:E:2788:ILE:CD1	2.47	0.44
3:F:2933[A]:SER:CA	3:F:2936[A]:GLU:HB3	2.48	0.44
3:F:2964[B]:PRO:CA	3:a:3221[B]:ALA:HB3	2.48	0.44
3:F:2979[A]:GLN:HB2	3:F:2988[A]:TRP:CD1	2.52	0.44
3:F:3047[A]:ARG:NH2	3:F:3113[A]:ASP:OD1	2.43	0.44
3:F:3074[A]:GLU:CD	3:F:3212[A]:ARG:NH2	2.73	0.44
3:F:3101[A]:PRO:O	3:F:3109[A]:TYR:HD2	2.00	0.44
3:F:3133[A]:LEU:O	3:F:3136[A]:TYR:HB3	2.17	0.44
3:F:3204[B]:LEU:CD1	3:F:3204[B]:LEU:N	2.80	0.44
3:F:3222[B]:ILE:CD1	3:F:3223[B]:GLY:N	2.73	0.44
3:F:3230[A]:PHE:CB	3:F:3242[A]:GLY:C	2.91	0.44
3:F:3281[A]:PHE:HE1	3:F:3305[A]:ILE:HG21	1.81	0.44
9:F:3401[A]:CUO:O1	3:a:2989[A]:HIS:CD2	2.70	0.44
1:G:62:MET:HE2	1:G:62:MET:HB3	1.88	0.44
1:G:470:ARG:HD2	1:G:470:ARG:HA	1.80	0.44
1:G:566:ARG:HA	1:G:567:LEU:HB2	2.00	0.44
1:G:710:GLY:H	1:G:711:LEU:HD12	1.82	0.44
1:G:1145:THR:HB	1:G:1191:PRO:HB2	1.99	0.44
1:G:1324:ARG:NE	1:G:1462:ASP:OD1	2.42	0.44
1:G:1536:SER:O	1:G:1539:GLN:HG2	2.18	0.44
3:I:2931[A]:THR:O	3:I:2934[A]:GLU:HG3	2.18	0.44
3:I:2973[B]:THR:HG21	3:R:3106[B]:THR:O	2.18	0.44
3:I:2988[A]:TRP:CD1	3:I:3158[A]:PHE:CE2	3.06	0.44
3:I:3182[A]:GLN:C	3:I:3183[A]:LEU:CD1	2.91	0.44
3:I:3230[B]:PHE:CB	3:I:3242[B]:GLY:C	2.91	0.44
3:I:3241[A]:PHE:CE2	3:I:3243[A]:GLY:O	2.71	0.44
3:I:3281[B]:PHE:HE1	3:I:3305[B]:ILE:HG21	1.81	0.44
1:J:2:LEU:HD12	1:J:2:LEU:HA	1.88	0.44
1:J:1552:ARG:HB2	1:J:1653:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2574:LEU:HD12	2:K:2574:LEU:HA	1.85	0.44
3:L:2937[B]:ASN:CB	3:L:3006[B]:LYS:CE	2.86	0.44
3:L:2940[A]:ASN:O	3:L:2943[A]:ALA:HB3	2.18	0.44
3:L:3014[A]:TRP:CH2	3:L:3123[A]:THR:HG23	2.53	0.44
3:L:3014[B]:TRP:CH2	3:L:3123[B]:THR:HG23	2.53	0.44
3:L:3034[A]:HIS:HB3	3:L:3035[A]:HIS:CE1	2.50	0.44
3:L:3200[B]:LEU:CD2	3:L:3204[B]:LEU:HD11	2.48	0.44
1:M:173:VAL:HG23	1:M:174:GLN:HG2	1.99	0.44
1:M:1030:MET:HA	1:M:1036:SER:HA	2.00	0.44
1:M:1093:ASP:HB2	1:M:1096:THR:OG1	2.17	0.44
1:M:1331:GLU:HB2	1:M:1343:VAL:HG23	1.99	0.44
2:N:2263:PHE:HE1	2:N:2304:LEU:HB3	1.82	0.44
2:N:2554:PRO:HA	2:N:2555:GLU:HB3	2.00	0.44
2:N:2627:GLY:HA3	2:N:2703:PHE:O	2.18	0.44
3:O:2931[B]:THR:O	3:O:2934[B]:GLU:HG3	2.18	0.44
3:O:2974[B]:ALA:HA	3:X:2979[B]:GLN:OE1	2.17	0.44
3:O:2988[A]:TRP:CD1	3:O:3158[A]:PHE:CE2	3.06	0.44
3:O:3133[B]:LEU:O	3:O:3136[B]:TYR:HB3	2.17	0.44
3:O:3161[A]:GLU:H	3:O:3161[A]:GLU:CD	2.19	0.44
3:O:3200[B]:LEU:CD2	3:O:3204[B]:LEU:HD11	2.48	0.44
3:O:3266[A]:ILE:O	3:O:3269[A]:SER:HB2	2.18	0.44
1:P:781:ILE:HG22	1:P:781:ILE:O	2.18	0.44
1:P:870:TYR:OH	1:P:963:ALA:HB1	2.18	0.44
1:P:1274:LEU:HD21	1:P:1344:PRO:HD3	1.99	0.44
2:Q:2327:GLU:H	2:Q:2327:GLU:HG3	1.44	0.44
2:Q:2799:LYS:HA	2:Q:2803:ARG:NH1	2.33	0.44
3:R:2987[B]:HIS:O	3:R:2991[B]:LEU:HB2	2.16	0.44
3:R:3101[B]:PRO:O	3:R:3109[B]:TYR:HD2	2.00	0.44
1:S:516:TRP:HH2	1:S:637:VAL:HG22	1.82	0.44
1:S:905:TRP:CZ3	1:S:909:ILE:HG13	2.53	0.44
1:S:980:TYR:CE2	1:S:1021:LEU:HD13	2.53	0.44
2:T:2873:HIS:CD2	2:T:2873:HIS:H	2.36	0.44
3:U:2951[A]:ASP:CG	3:U:2952[A]:ALA:N	2.74	0.44
3:U:2989[A]:HIS:O	3:U:2990[A]:ARG:C	2.61	0.44
3:U:3019[B]:HIS:CD2	3:U:3020[B]:SER:H	2.35	0.44
1:V:282:ASN:OD1	1:V:282:ASN:N	2.49	0.44
3:X:2933[A]:SER:CA	3:X:2936[A]:GLU:HB3	2.48	0.44
3:X:2985[B]:PHE:HE2	3:X:2989[B]:HIS:HE2	1.66	0.44
3:X:3044[A]:LYS:H	3:X:3044[A]:LYS:HG2	1.64	0.44
2:Z:2134:ASN:ND2	2:Z:2137:ALA:HB2	2.33	0.44
2:Z:2539:ILE:O	2:Z:2573:TYR:OH	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:2695:MET:HE1	2:Z:2707:PHE:HB2	2.00	0.44
2:Z:2844:MET:O	2:Z:2846:TRP:HD1	2.01	0.44
3:a:2988[A]:TRP:HE3	3:a:2989[A]:HIS:CE1	2.25	0.44
3:a:2988[A]:TRP:CD1	3:a:3158[A]:PHE:CE2	3.06	0.44
3:a:3133[A]:LEU:O	3:a:3136[A]:TYR:HB3	2.17	0.44
3:a:3137[A]:ARG:O	3:a:3139[A]:LEU:HD22	2.16	0.44
1:b:139:VAL:HG11	1:b:144:TYR:OH	2.18	0.44
1:b:597:VAL:HG12	1:b:773:PHE:CD1	2.52	0.44
1:b:668:MET:HE2	1:b:668:MET:HA	2.00	0.44
2:c:2286:HIS:CD2	2:c:2433:THR:HG22	2.53	0.44
3:d:2931[B]:THR:O	3:d:2934[B]:GLU:HG3	2.18	0.44
3:d:2981[B]:GLY:N	3:d:3086[B]:GLU:OE1	2.45	0.44
3:d:3133[B]:LEU:O	3:d:3136[B]:TYR:HB3	2.17	0.44
3:d:3137[A]:ARG:HB3	3:d:3139[A]:LEU:HD21	1.97	0.44
3:d:3299[B]:LEU:O	3:d:3300[B]:LEU:C	2.60	0.44
1:A:282:ASN:N	1:A:282:ASN:OD1	2.51	0.44
1:A:1258:ARG:NH2	1:A:1332:ASP:OD1	2.50	0.44
1:A:1482:ALA:HB2	1:A:1517:PHE:HZ	1.83	0.44
3:C:2948[A]:ASP:HB3	3:C:2949[A]:LYS:C	2.43	0.44
3:C:2951[A]:ASP:OD2	3:C:2952[A]:ALA:CB	2.66	0.44
3:C:2989[A]:HIS:O	3:C:2990[A]:ARG:C	2.61	0.44
3:C:3023[A]:ILE:O	3:C:3026[A]:THR:OG1	2.34	0.44
3:C:3132[A]:ALA:HB3	3:C:3197[A]:ILE:HD13	1.99	0.44
3:C:3147[A]:GLU:CG	3:C:3149[A]:ASN:ND2	2.73	0.44
3:C:3155[B]:MET:HG2	3:L:3153[B]:LYS:O	2.15	0.44
3:C:3161[A]:GLU:N	3:C:3161[A]:GLU:CD	2.73	0.44
3:C:3172[B]:SER:OG	3:L:3150[B]:LYS:N	2.49	0.44
3:C:3293[A]:LYS:CD	3:C:3293[A]:LYS:C	2.86	0.44
1:D:35:GLN:HG3	1:D:129:LYS:HB2	2.00	0.44
1:D:226:HIS:HA	1:D:227:ARG:HA	1.55	0.44
1:D:353:ASN:HD22	1:D:772:ARG:HH22	1.66	0.44
1:D:446:PHE:CZ	1:D:455:TYR:HA	2.53	0.44
1:D:527:LEU:O	1:D:561:ARG:NH1	2.51	0.44
1:D:836:GLN:O	1:D:1113:HIS:HB3	2.18	0.44
1:D:843:VAL:HG22	1:D:928:TYR:O	2.18	0.44
1:D:995:ILE:O	1:D:999:LEU:HD22	2.18	0.44
2:E:2415:PRO:HD2	2:E:2418:GLY:O	2.17	0.44
2:E:2663:MET:HE1	2:E:2717:LEU:HD13	2.00	0.44
3:F:2937[A]:ASN:CG	3:F:3006[A]:LYS:HD3	2.43	0.44
3:F:2965[B]:LEU:O	3:a:3221[B]:ALA:CB	2.53	0.44
3:F:2977[B]:CYS:SG	3:a:2982[B]:MET:CE	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2995[B]:GLN:CG	3:F:3168[B]:THR:HG21	2.48	0.44
3:F:3034[B]:HIS:HB3	3:F:3035[B]:HIS:CE1	2.50	0.44
3:F:3137[B]:ARG:HD3	3:F:3137[B]:ARG:HA	1.72	0.44
3:F:3149[B]:ASN:HD22	3:a:3163[B]:ASN:CA	2.29	0.44
3:F:3182[A]:GLN:C	3:F:3183[A]:LEU:CD1	2.91	0.44
3:F:3223[B]:GLY:N	3:a:2963[B]:MET:HE1	2.32	0.44
3:F:3230[B]:PHE:CB	3:F:3242[B]:GLY:C	2.91	0.44
3:F:3251[B]:ASP:C	3:a:3251[B]:ASP:CB	2.76	0.44
1:G:105:VAL:HB	1:G:137:ARG:NH1	2.32	0.44
1:G:434:GLU:H	1:G:434:GLU:HG3	1.55	0.44
1:G:949:ASP:HB2	1:G:953:GLU:HB2	2.00	0.44
2:H:2128:LEU:O	2:H:2130:PRO:HD3	2.18	0.44
3:I:2938[B]:LEU:O	3:I:2939[B]:ARG:C	2.58	0.44
3:I:2970[B]:PRO:C	3:I:2972[B]:GLY:N	2.72	0.44
3:I:2971[B]:ASP:O	3:R:3090[B]:ASN:CB	2.66	0.44
3:I:3093[A]:HIS:HB2	3:I:3248[A]:LEU:CD1	2.48	0.44
3:I:3093[A]:HIS:HD2	3:I:3248[A]:LEU:CD2	2.30	0.44
3:I:3155[B]:MET:CB	3:R:3153[B]:LYS:HB3	2.47	0.44
3:I:3163[B]:ASN:O	3:R:3147[B]:GLU:OE2	2.36	0.44
3:I:3171[A]:HIS:C	3:I:3173[A]:THR:N	2.73	0.44
3:I:3200[B]:LEU:CD2	3:I:3204[B]:LEU:HD11	2.48	0.44
3:I:3266[A]:ILE:O	3:I:3269[A]:SER:HB2	2.18	0.44
9:I:3401[A]:CUO:O1	3:R:2989[A]:HIS:CD2	2.70	0.44
1:J:293:LEU:O	1:J:296:ARG:HG2	2.18	0.44
1:J:590:ASP:CG	1:J:653:LYS:HZ1	2.26	0.44
1:J:840:ARG:HD3	1:J:926:LEU:O	2.17	0.44
1:J:1347:ASP:HA	1:J:1460:ASN:ND2	2.33	0.44
3:L:3025[A]:VAL:CG2	3:L:3047[A]:ARG:NH1	2.73	0.44
3:L:3027[A]:GLU:CD	3:L:3027[A]:GLU:C	2.85	0.44
3:L:3037[B]:TYR:C	3:L:3038[B]:ILE:HG13	2.42	0.44
3:L:3241[B]:PHE:CE2	3:L:3243[B]:GLY:O	2.70	0.44
1:M:873:VAL:HA	1:M:876:PHE:HE1	1.80	0.44
1:M:1212:HIS:CD2	1:M:1212:HIS:N	2.86	0.44
3:O:2933[B]:SER:CA	3:O:2936[B]:GLU:HB3	2.48	0.44
3:O:2940[A]:ASN:O	3:O:2943[A]:ALA:HB3	2.18	0.44
3:O:2951[B]:ASP:OD2	3:O:2952[B]:ALA:CB	2.66	0.44
3:O:3148[A]:ILE:O	3:O:3148[A]:ILE:HG22	2.17	0.44
3:O:3148[B]:ILE:O	3:O:3148[B]:ILE:HG22	2.17	0.44
3:O:3182[A]:GLN:C	3:O:3183[A]:LEU:CD1	2.91	0.44
1:P:979:LEU:HD23	1:P:980:TYR:CD1	2.52	0.44
1:P:1639:LYS:HD2	1:S:472:ASP:CB	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:2830:GLN:H	2:Q:2863:ARG:NH2	2.15	0.44
3:R:2963[B]:MET:C	3:R:2963[B]:MET:SD	3.01	0.44
3:R:2988[A]:TRP:CD1	3:R:3158[A]:PHE:CE2	3.06	0.44
3:R:3013[B]:ASP:CG	3:R:3015[B]:THR:HG1	2.24	0.44
3:R:3023[A]:ILE:HA	3:R:3026[A]:THR:HG1	1.82	0.44
3:R:3149[B]:ASN:OD1	3:R:3149[B]:ASN:N	2.51	0.44
3:R:3273[A]:LEU:C	3:R:3275[A]:LEU:HD12	2.42	0.44
3:R:3284[A]:LYS:CD	3:R:3284[A]:LYS:C	2.86	0.44
1:S:318:ARG:HB2	1:S:382:GLU:HB2	1.98	0.44
1:S:464:LEU:HD22	1:S:622:HIS:CG	2.53	0.44
1:S:1160:PHE:HB3	1:S:1171:LYS:HA	2.00	0.44
1:S:1390:ASP:HB2	1:S:1438:ASP:OD2	2.17	0.44
1:S:1622:GLN:H	1:S:1622:GLN:HG3	1.47	0.44
2:T:2239:LYS:HG2	2:T:2240:GLN:N	2.33	0.44
2:T:2877:ILE:HB	1:V:1078:ARG:HH21	1.82	0.44
3:U:2969[A]:TYR:CD2	3:U:2970[A]:PRO:CG	3.00	0.44
3:U:3014[B]:TRP:CH2	3:U:3123[B]:THR:HG23	2.53	0.44
3:U:3093[A]:HIS:HD2	3:U:3248[A]:LEU:CD2	2.31	0.44
3:U:3104[B]:MET:SD	3:U:3110[B]:THR:CG2	3.06	0.44
3:U:3148[B]:ILE:O	3:U:3148[B]:ILE:HG22	2.17	0.44
3:U:3183[A]:LEU:N	3:U:3184[A]:ASN:CA	2.80	0.44
3:U:3217[B]:PHE:CD2	3:U:3300[B]:LEU:HD12	2.53	0.44
3:U:3281[A]:PHE:HE1	3:U:3305[A]:ILE:HG21	1.81	0.44
3:U:3284[B]:LYS:CE	3:U:3284[B]:LYS:CA	2.85	0.44
3:U:3298[B]:ASN:CA	3:U:3299[B]:LEU:HB2	2.44	0.44
1:V:464:LEU:HG	1:V:465:PRO:HA	1.99	0.44
2:W:2765:PRO:HA	2:W:2768:LEU:HD11	2.00	0.44
2:W:2868:GLU:CD	3:X:2932[A]:PRO:O	2.61	0.44
3:X:2989[A]:HIS:CD2	9:X:3401[A]:CUO:O1	2.70	0.44
3:X:3001[B]:LYS:H	3:X:3003[B]:LYS:HG3	1.83	0.44
3:X:3093[B]:HIS:HB2	3:X:3248[B]:LEU:CD1	2.47	0.44
3:X:3141[B]:TYR:CD2	3:X:3141[B]:TYR:C	2.86	0.44
3:X:3229[A]:ASN:O	3:X:3286[A]:THR:N	2.50	0.44
3:X:3273[B]:LEU:C	3:X:3275[B]:LEU:HD12	2.42	0.44
1:Y:114:THR:O	1:Y:116:LYS:HG3	2.18	0.44
2:Z:2803:ARG:HH21	2:Z:2805:PHE:HZ	1.66	0.44
2:Z:2867:PRO:CD	3:a:2932[A]:PRO:HB2	2.46	0.44
3:a:3241[A]:PHE:CE2	3:a:3243[A]:GLY:O	2.71	0.44
1:b:376:ASN:HB2	1:b:665:TYR:CG	2.52	0.44
1:b:480:CYS:SG	1:b:621:LEU:HD11	2.58	0.44
1:b:905:TRP:CD1	1:b:1084:PHE:HE2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2963[A]:MET:SD	3:d:2963[A]:MET:C	3.01	0.44
3:d:2965[B]:LEU:CG	3:d:2974[B]:ALA:CB	2.85	0.44
3:d:3027[B]:GLU:CD	3:d:3027[B]:GLU:C	2.85	0.44
3:d:3028[B]:PRO:HG2	3:d:3029[B]:LYS:HG3	2.00	0.44
2:B:2549:PRO:HA	2:B:2550:THR:HG23	1.99	0.43
2:B:2680:HIS:CD2	2:B:2684:HIS:CD2	3.06	0.43
3:C:2937[B]:ASN:CG	3:C:3006[B]:LYS:HD3	2.43	0.43
3:C:2975[B]:PHE:CA	3:L:3253[B]:GLU:HB2	2.46	0.43
3:C:2989[B]:HIS:C	3:C:2991[B]:LEU:N	2.75	0.43
3:C:3028[B]:PRO:HG2	3:C:3029[B]:LYS:HG3	2.00	0.43
3:C:3194[A]:GLY:C	3:C:3195[A]:MET:CG	2.90	0.43
3:C:3217[A]:PHE:CD2	3:C:3300[A]:LEU:HD12	2.53	0.43
3:C:3273[B]:LEU:C	3:C:3275[B]:LEU:HD12	2.42	0.43
1:D:717:GLN:O	1:D:720:VAL:HG22	2.18	0.43
1:D:997:SER:O	1:D:1000:GLU:HB2	2.18	0.43
1:D:1390:ASP:HB3	1:G:1372:ILE:CD1	2.49	0.43
3:F:2981[B]:GLY:HA3	3:a:2967[B]:CYS:HA	1.36	0.43
3:F:2982[B]:MET:CG	3:a:3156[B]:MET:CB	2.93	0.43
3:F:3019[A]:HIS:CD2	3:F:3020[A]:SER:H	2.35	0.43
3:F:3093[A]:HIS:HD2	3:F:3248[A]:LEU:CD2	2.31	0.43
3:F:3094[B]:SER:HG	3:F:3227[B]:ASP:CG	2.25	0.43
3:F:3101[B]:PRO:O	3:F:3109[B]:TYR:HD2	2.00	0.43
3:F:3150[B]:LYS:CE	3:a:3163[B]:ASN:HB2	2.23	0.43
3:F:3156[B]:MET:CG	3:a:2982[B]:MET:HG3	2.48	0.43
3:F:3276[B]:ASP:C	3:F:3278[B]:HIS:N	2.75	0.43
1:G:387:ASN:HD21	4:o:1:NAG:C6	2.31	0.43
1:G:419:THR:HA	1:G:420:SER:HA	1.65	0.43
1:G:464:LEU:HD22	1:G:622:HIS:HB3	1.99	0.43
1:G:494:VAL:HG13	1:G:631:TRP:HZ3	1.82	0.43
1:G:704:ASP:N	1:G:704:ASP:OD1	2.50	0.43
1:G:717:GLN:HA	1:G:720:VAL:HG22	1.99	0.43
1:G:939:PRO:O	1:G:943:LEU:HG	2.17	0.43
1:G:979:LEU:HB3	1:G:980:TYR:CG	2.52	0.43
2:H:2339:GLY:HA2	2:H:2349:THR:HG21	2.00	0.43
2:H:2370:MET:HE3	2:H:2370:MET:HB2	1.78	0.43
2:H:2780:HIS:CE1	2:H:2782:ASN:HD21	2.35	0.43
3:I:2931[B]:THR:O	3:I:2934[B]:GLU:HG3	2.18	0.43
3:I:2986[B]:PRO:CB	3:I:3127[B]:TRP:CE3	3.00	0.43
3:I:3019[B]:HIS:CD2	3:I:3020[B]:SER:H	2.35	0.43
3:I:3047[A]:ARG:NH2	3:I:3113[A]:ASP:OD1	2.43	0.43
3:I:3133[A]:LEU:O	3:I:3136[A]:TYR:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3232[A]:VAL:HG21	3:I:3273[A]:LEU:HD11	2.00	0.43
2:K:2130:PRO:HB2	2:K:2142:ALA:HB3	2.00	0.43
3:L:2933[A]:SER:CA	3:L:2936[A]:GLU:HB3	2.48	0.43
3:L:2963[A]:MET:SD	3:L:2963[A]:MET:C	3.01	0.43
3:L:3229[A]:ASN:O	3:L:3286[A]:THR:N	2.50	0.43
1:M:882:TRP:HE1	1:M:1090:ILE:HD13	1.83	0.43
2:N:2628:HIS:HB2	2:N:2635:TYR:CE2	2.53	0.43
2:N:2866:PRO:HB2	2:N:2868:GLU:OE2	2.18	0.43
3:O:2951[A]:ASP:OD2	3:O:2952[A]:ALA:CB	2.66	0.43
3:O:2963[A]:MET:C	3:O:2963[A]:MET:SD	3.01	0.43
3:O:2968[B]:GLN:HB3	3:X:2979[B]:GLN:CG	2.48	0.43
3:O:2975[B]:PHE:HD1	3:X:3156[B]:MET:O	2.00	0.43
3:O:2979[A]:GLN:HB2	3:O:2988[A]:TRP:CD1	2.52	0.43
3:O:3014[B]:TRP:CH2	3:O:3123[B]:THR:HG23	2.53	0.43
3:O:3217[B]:PHE:CD2	3:O:3300[B]:LEU:HD12	2.53	0.43
1:P:728:ARG:HD2	1:P:780:GLU:OE2	2.18	0.43
1:P:733:PHE:CZ	1:P:746:LEU:HD22	2.53	0.43
1:P:899:MET:HB3	1:P:1012:GLU:OE1	2.18	0.43
3:R:3044[A]:LYS:H	3:R:3044[A]:LYS:HG2	1.65	0.43
3:R:3104[B]:MET:SD	3:R:3110[B]:THR:CG2	3.06	0.43
3:R:3141[B]:TYR:CD2	3:R:3141[B]:TYR:C	2.85	0.43
3:R:3200[B]:LEU:CD2	3:R:3204[B]:LEU:HD11	2.48	0.43
1:S:21:SER:HB2	1:S:83:HIS:O	2.18	0.43
1:S:482:HIS:CE1	1:S:621:LEU:HD11	2.53	0.43
2:T:2644:LEU:HD22	2:T:2687:ILE:HG22	2.00	0.43
3:U:3160[B]:SER:O	3:d:3147[B]:GLU:CG	2.38	0.43
3:U:3241[B]:PHE:CE2	3:U:3243[B]:GLY:O	2.70	0.43
1:V:988:TYR:O	1:V:992:ALA:HB3	2.18	0.43
2:W:2156:ARG:HD2	2:W:2357:VAL:HG12	1.99	0.43
2:W:2267:HIS:CD2	2:W:2297:HIS:HE1	2.29	0.43
2:W:2472:ASN:N	2:W:2472:ASN:OD1	2.48	0.43
2:W:2746:MET:HE2	2:W:2746:MET:HB2	1.91	0.43
2:W:2870:LEU:HA	2:W:2877:ILE:HD11	1.99	0.43
3:X:2940[A]:ASN:O	3:X:2943[A]:ALA:HB3	2.18	0.43
3:X:2948[A]:ASP:HB3	3:X:2949[A]:LYS:C	2.43	0.43
3:X:2963[A]:MET:SD	3:X:2963[A]:MET:C	3.01	0.43
3:X:2965[A]:LEU:CG	3:X:2974[A]:ALA:CB	2.85	0.43
3:X:3027[A]:GLU:CD	3:X:3027[A]:GLU:C	2.85	0.43
3:X:3028[A]:PRO:HG2	3:X:3029[A]:LYS:HG3	2.00	0.43
3:X:3133[B]:LEU:O	3:X:3136[B]:TYR:HB3	2.17	0.43
3:X:3180[A]:TYR:CA	3:X:3183[A]:LEU:CD2	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3183[A]:LEU:N	3:X:3184[A]:ASN:CA	2.80	0.43
3:X:3230[A]:PHE:CB	3:X:3242[A]:GLY:C	2.91	0.43
3:X:3299[B]:LEU:O	3:X:3300[B]:LEU:C	2.60	0.43
1:Y:567:LEU:N	1:Y:568:PHE:CA	2.77	0.43
1:Y:1171:LYS:HG2	1:Y:1173:GLY:H	1.83	0.43
2:Z:2303:ARG:NH2	2:Z:2372:GLU:O	2.51	0.43
2:Z:2551:PRO:HA	2:Z:2552:GLU:HA	1.49	0.43
3:a:3194[B]:GLY:C	3:a:3195[B]:MET:CG	2.91	0.43
3:a:3217[A]:PHE:CD2	3:a:3300[A]:LEU:HD12	2.53	0.43
3:a:3293[A]:LYS:CD	3:a:3293[A]:LYS:C	2.86	0.43
2:c:2469:VAL:HG12	2:c:2475:GLU:HA	2.00	0.43
3:d:2940[B]:ASN:O	3:d:2943[B]:ALA:HB3	2.18	0.43
3:d:3047[B]:ARG:NH2	3:d:3113[B]:ASP:OD1	2.43	0.43
1:A:1210:LYS:HG2	2:E:2744:PHE:CD2	2.53	0.43
3:C:3024[A]:LEU:CD1	3:C:3024[A]:LEU:C	2.85	0.43
3:C:3185[A]:TYR:HE2	3:C:3187[A]:TYR:CD2	2.35	0.43
3:C:3200[B]:LEU:CD2	3:C:3204[B]:LEU:HD11	2.48	0.43
3:C:3253[B]:GLU:OE1	3:L:2975[B]:PHE:C	2.61	0.43
3:C:3266[B]:ILE:O	3:C:3269[B]:SER:HB2	2.17	0.43
1:D:480:CYS:SG	1:D:621:LEU:HD11	2.58	0.43
1:D:572:SER:HA	1:D:573:LYS:HA	1.42	0.43
1:D:588:GLU:HG3	1:D:724:LYS:HD2	1.99	0.43
1:D:893:ALA:HB2	1:D:1182:ASN:HB2	1.99	0.43
3:F:2951[A]:ASP:OD2	3:F:2952[A]:ALA:CB	2.66	0.43
3:F:2970[B]:PRO:HD2	3:a:2989[B]:HIS:CE1	2.43	0.43
3:F:2976[A]:ALA:O	3:F:2978[A]:CYS:N	2.46	0.43
3:F:2991[A]:LEU:HD23	3:F:3158[A]:PHE:CE1	2.48	0.43
3:F:3014[A]:TRP:CH2	3:F:3123[A]:THR:HG23	2.53	0.43
3:F:3027[B]:GLU:CD	3:F:3027[B]:GLU:C	2.85	0.43
3:F:3093[A]:HIS:HB2	3:F:3248[A]:LEU:CD1	2.48	0.43
3:F:3131[B]:GLN:HE21	3:F:3131[B]:GLN:HB3	1.66	0.43
3:F:3217[A]:PHE:CD2	3:F:3300[A]:LEU:HD12	2.53	0.43
3:F:3266[B]:ILE:O	3:F:3269[B]:SER:HB2	2.18	0.43
1:G:22:LEU:HD23	1:G:123:PHE:HE1	1.83	0.43
1:G:84:GLY:HA2	1:G:85:SER:C	2.43	0.43
1:G:125:SER:OG	1:G:125:SER:O	2.31	0.43
1:G:1262:ASN:OD1	1:G:1263:LEU:N	2.52	0.43
1:G:1346:TRP:O	1:G:1460:ASN:ND2	2.51	0.43
2:H:2381:LEU:HD23	2:H:2381:LEU:HA	1.84	0.43
2:H:2679:ILE:O	2:H:2682:SER:HB3	2.18	0.43
3:I:2963[B]:MET:SD	3:I:2963[B]:MET:C	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2988[B]:TRP:CD1	3:I:3158[B]:PHE:CE2	3.06	0.43
3:I:3086[B]:GLU:HG3	3:R:2968[B]:GLN:HG3	1.47	0.43
3:I:3093[B]:HIS:HB2	3:I:3248[B]:LEU:CD1	2.48	0.43
3:I:3104[B]:MET:SD	3:I:3110[B]:THR:CG2	3.06	0.43
3:I:3132[A]:ALA:HB3	3:I:3197[A]:ILE:HD13	1.98	0.43
3:I:3200[A]:LEU:CD2	3:I:3204[A]:LEU:HD11	2.48	0.43
3:I:3223[B]:GLY:CA	3:R:2963[B]:MET:CE	2.80	0.43
3:I:3293[A]:LYS:CB	3:I:3294[A]:SER:CA	2.96	0.43
1:J:98:MET:O	1:J:144:TYR:HB3	2.18	0.43
1:J:237:LEU:HB2	1:J:820:VAL:HB	2.00	0.43
1:J:918:ARG:HD3	1:J:924:GLY:O	2.18	0.43
1:J:1230:LEU:H	1:J:1230:LEU:HD23	1.83	0.43
1:J:1390:ASP:HB2	1:J:1438:ASP:OD2	2.18	0.43
1:J:1438:ASP:OD1	1:J:1439:VAL:N	2.50	0.43
1:J:1519:TYR:OH	1:J:1530:LEU:HD11	2.18	0.43
2:K:2089:ARG:HD2	2:K:2175:VAL:O	2.18	0.43
2:K:2198:ASP:O	2:K:2202:GLY:N	2.50	0.43
2:K:2403:PHE:CD2	2:K:2476:LEU:HD13	2.52	0.43
2:K:2826:GLU:HB3	2:K:2827:ALA:H	1.51	0.43
3:L:2937[B]:ASN:CG	3:L:3006[B]:LYS:HD3	2.43	0.43
3:L:2991[A]:LEU:HD23	3:L:3158[A]:PHE:CE1	2.48	0.43
3:L:3217[B]:PHE:CD2	3:L:3300[B]:LEU:HD12	2.53	0.43
3:L:3285[B]:VAL:CG2	3:L:3286[B]:THR:H	2.27	0.43
1:M:935:ILE:HD11	1:M:980:TYR:CD2	2.53	0.43
1:M:1161:ILE:O	1:M:1203:MET:HE1	2.18	0.43
1:M:1427:HIS:CE1	1:M:1457:HIS:HE1	2.35	0.43
3:O:2971[B]:ASP:C	3:X:2988[B]:TRP:CE3	2.96	0.43
3:O:2995[A]:GLN:CG	3:O:3168[A]:THR:HG21	2.48	0.43
3:O:3034[B]:HIS:HB3	3:O:3035[B]:HIS:CE1	2.50	0.43
3:O:3093[A]:HIS:HB2	3:O:3248[A]:LEU:CD1	2.48	0.43
3:O:3182[B]:GLN:C	3:O:3183[B]:LEU:CD1	2.91	0.43
1:P:387:ASN:ND2	6:3:1:NAG:C7	2.79	0.43
1:P:977:GLU:HG3	1:P:978:ALA:H	1.83	0.43
1:P:1271:MET:HE1	1:P:1357:ARG:NH1	2.32	0.43
1:P:1578:ILE:HA	1:P:1579:GLY:HA2	1.58	0.43
2:Q:2370:MET:HB2	2:Q:2370:MET:HE3	1.60	0.43
3:R:2952[A]:ALA:CA	3:R:2956[A]:LYS:CB	2.89	0.43
3:R:3001[B]:LYS:H	3:R:3003[B]:LYS:HG3	1.83	0.43
3:R:3013[A]:ASP:CG	3:R:3015[A]:THR:HG1	2.25	0.43
3:R:3149[A]:ASN:OD1	3:R:3149[A]:ASN:N	2.51	0.43
1:S:1296:VAL:HG13	1:S:1384:PHE:HZ	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:2572:VAL:HG13	2:T:2768:LEU:HD23	1.99	0.43
2:T:2627:GLY:HA3	2:T:2703:PHE:O	2.18	0.43
3:U:2931[A]:THR:O	3:U:2934[A]:GLU:HG3	2.18	0.43
3:U:2973[B]:THR:CG2	3:d:3222[B]:ILE:O	2.65	0.43
3:U:2989[A]:HIS:CD2	9:U:3401[A]:CUO:O1	2.71	0.43
3:U:2989[A]:HIS:C	3:U:2991[A]:LEU:N	2.75	0.43
3:U:2989[B]:HIS:CD2	9:U:3401[B]:CUO:O1	2.71	0.43
3:U:3096[B]:VAL:CG1	3:U:3115[B]:LEU:CD1	2.86	0.43
3:U:3149[B]:ASN:OD1	3:U:3149[B]:ASN:N	2.51	0.43
3:U:3217[A]:PHE:CD2	3:U:3300[A]:LEU:HD12	2.53	0.43
3:U:3242[A]:GLY:C	3:U:3243[A]:GLY:O	2.58	0.43
1:V:385:ALA:HB2	1:V:391:MET:SD	2.58	0.43
1:V:447:MET:HE2	1:V:447:MET:HB3	1.90	0.43
1:V:1286:ARG:HD2	1:V:1286:ARG:HA	1.74	0.43
2:W:2237:LEU:H	2:W:2237:LEU:HD13	1.82	0.43
3:X:2963[B]:MET:SD	3:X:2963[B]:MET:C	3.01	0.43
3:X:2979[B]:GLN:HB2	3:X:2988[B]:TRP:CD1	2.52	0.43
3:X:3096[A]:VAL:CG1	3:X:3115[A]:LEU:CD1	2.86	0.43
3:X:3101[B]:PRO:O	3:X:3109[B]:TYR:HD2	2.00	0.43
3:X:3104[A]:MET:SD	3:X:3110[A]:THR:CG2	3.06	0.43
3:X:3104[B]:MET:SD	3:X:3110[B]:THR:CG2	3.06	0.43
3:X:3132[A]:ALA:HB3	3:X:3197[A]:ILE:HD13	1.99	0.43
2:Z:2226:GLU:OE1	2:Z:2277:LYS:HG2	2.17	0.43
3:a:3094[B]:SER:HG	3:a:3227[B]:ASP:CG	2.25	0.43
1:b:464:LEU:HD22	1:b:622:HIS:CD2	2.54	0.43
1:b:1005:CYS:O	1:b:1009:VAL:HG23	2.18	0.43
1:b:1317:PRO:HA	1:b:1420:GLU:HG3	2.01	0.43
2:c:2369:ASP:OD1	2:c:2370:MET:N	2.51	0.43
3:d:2940[A]:ASN:O	3:d:2943[A]:ALA:HB3	2.18	0.43
3:d:2989[A]:HIS:CD2	9:d:3401[A]:CUO:O1	2.70	0.43
3:d:3104[A]:MET:SD	3:d:3110[A]:THR:CG2	3.06	0.43
3:d:3306[A]:LEU:C	3:d:3306[A]:LEU:CD1	2.86	0.43
1:A:206:PHE:HE1	9:A:5001:CUO:O2	2.01	0.43
1:A:806:ASN:OD1	1:A:807:GLY:N	2.51	0.43
1:A:1161:ILE:HB	1:A:1203:MET:HE3	1.99	0.43
1:A:1325:LEU:O	1:A:1328:SER:HB3	2.17	0.43
2:B:2553:ALA:N	2:B:2554:PRO:CD	2.81	0.43
3:C:2940[A]:ASN:O	3:C:2943[A]:ALA:HB3	2.18	0.43
3:C:2948[A]:ASP:CB	3:C:2949[A]:LYS:CA	2.78	0.43
3:C:2963[A]:MET:SD	3:C:2963[A]:MET:C	3.01	0.43
3:C:2963[B]:MET:C	3:C:2963[B]:MET:SD	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3104[A]:MET:SD	3:C:3110[A]:THR:CG2	3.06	0.43
1:D:322:CYS:HA	1:D:333:ASN:O	2.18	0.43
1:D:456:GLN:HG2	1:D:551:GLU:CB	2.48	0.43
1:D:816:PRO:HA	1:D:817:PRO:HD3	1.89	0.43
1:D:975:PRO:HB2	1:D:1024:GLY:HA3	2.00	0.43
2:E:2370:MET:HE3	2:E:2370:MET:HB2	1.76	0.43
3:F:2946[A]:GLN:CD	3:F:2947[A]:ALA:N	2.72	0.43
3:F:2949[A]:LYS:C	3:F:2949[A]:LYS:HZ3	2.14	0.43
3:F:2951[A]:ASP:CG	3:F:2952[A]:ALA:N	2.74	0.43
3:F:2988[A]:TRP:CD1	3:F:3158[A]:PHE:CE2	3.06	0.43
3:F:2988[B]:TRP:CD1	3:F:3158[B]:PHE:CE2	3.06	0.43
3:F:3107[B]:LEU:HD21	3:a:2975[B]:PHE:HA	1.99	0.43
3:F:3148[B]:ILE:HG22	3:F:3152[B]:LYS:HE3	2.01	0.43
3:F:3180[A]:TYR:CA	3:F:3183[A]:LEU:CD2	2.95	0.43
3:F:3200[A]:LEU:CD2	3:F:3204[A]:LEU:HD11	2.48	0.43
3:F:3232[B]:VAL:HG21	3:F:3273[B]:LEU:HD11	2.00	0.43
3:F:3276[A]:ASP:C	3:F:3278[A]:HIS:N	2.75	0.43
1:G:14:GLU:O	1:G:17:ASN:ND2	2.48	0.43
1:G:353:ASN:HB3	1:G:772:ARG:NH2	2.33	0.43
1:G:630:PHE:CE2	1:G:634:HIS:CE1	3.06	0.43
1:G:1148:LEU:HB2	1:G:1188:PHE:HD2	1.83	0.43
2:H:2666:GLN:HG3	2:H:2671:ASP:O	2.18	0.43
3:I:2937[B]:ASN:CG	3:I:3006[B]:LYS:HD3	2.43	0.43
3:I:2960[B]:PHE:C	3:R:3255[B]:PRO:CD	2.88	0.43
3:I:2965[B]:LEU:HG	3:R:3249[B]:GLY:HA3	1.98	0.43
3:I:3023[A]:ILE:O	3:I:3026[A]:THR:OG1	2.34	0.43
3:I:3034[B]:HIS:HB3	3:I:3035[B]:HIS:CE1	2.50	0.43
3:I:3148[A]:ILE:O	3:I:3148[A]:ILE:HG22	2.17	0.43
3:I:3152[B]:LYS:O	3:R:3171[B]:HIS:C	2.59	0.43
3:I:3182[B]:GLN:C	3:I:3183[B]:LEU:CD1	2.91	0.43
3:I:3217[B]:PHE:CD2	3:I:3300[B]:LEU:HD12	2.53	0.43
3:I:3232[B]:VAL:HG21	3:I:3273[B]:LEU:HD11	2.00	0.43
1:J:954:ALA:O	1:J:956:PRO:HD3	2.18	0.43
1:J:1010:GLN:HE22	1:J:1193:LYS:H	1.66	0.43
2:K:2341:PRO:HG2	2:K:2342:TYR:CD2	2.53	0.43
3:L:3229[B]:ASN:O	3:L:3286[B]:THR:N	2.50	0.43
3:L:3232[B]:VAL:HG21	3:L:3273[B]:LEU:HD11	2.00	0.43
1:M:187:GLY:HA3	1:M:195:SER:HB3	1.99	0.43
1:M:891:LYS:HB2	1:M:892:TYR:CD2	2.53	0.43
1:M:906:HIS:HA	1:M:909:ILE:HB	2.00	0.43
2:N:2168:ARG:O	2:Q:2503:ASN:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2940[B]:ASN:O	3:O:2943[B]:ALA:HB3	2.18	0.43
3:O:2968[B]:GLN:CD	3:X:2984[B]:THR:CB	2.91	0.43
3:O:2986[A]:PRO:CB	3:O:3127[A]:TRP:CE3	3.00	0.43
3:O:2995[B]:GLN:CG	3:O:3168[B]:THR:HG21	2.48	0.43
3:O:3019[A]:HIS:CD2	3:O:3020[A]:SER:H	2.35	0.43
3:O:3028[B]:PRO:HG2	3:O:3029[B]:LYS:HG3	2.00	0.43
3:O:3037[B]:TYR:C	3:O:3038[B]:ILE:HG13	2.42	0.43
3:O:3217[A]:PHE:CD2	3:O:3300[A]:LEU:HD12	2.53	0.43
1:P:415:VAL:HB	1:P:697:ALA:HB2	1.99	0.43
1:P:568:PHE:CD1	1:P:568:PHE:N	2.85	0.43
1:P:1427:HIS:CD2	1:P:1457:HIS:HE1	2.37	0.43
2:Q:2249:LEU:HD11	2:Q:2395:PHE:HE2	1.83	0.43
2:Q:2561:HIS:HB3	2:Q:2677:GLU:OE2	2.18	0.43
3:R:3025[B]:VAL:CG2	3:R:3047[B]:ARG:NH1	2.73	0.43
3:R:3298[A]:ASN:CB	3:R:3300[A]:LEU:CD2	2.61	0.43
3:R:3306[A]:LEU:C	3:R:3306[A]:LEU:CD1	2.86	0.43
1:S:515:ASP:O	1:S:518:LYS:HG2	2.17	0.43
1:S:1074:ILE:O	1:S:1078:ARG:HG2	2.18	0.43
1:S:1195:ASP:HA	1:S:1196:ILE:CG2	2.49	0.43
3:U:2948[A]:ASP:HB3	3:U:2949[A]:LYS:C	2.43	0.43
3:U:2956[A]:LYS:O	3:U:2959[A]:SER:OG	2.33	0.43
3:U:2991[A]:LEU:HD23	3:U:3158[A]:PHE:CE1	2.47	0.43
3:U:3148[A]:ILE:HG22	3:U:3152[A]:LYS:HE3	2.01	0.43
3:U:3169[B]:LYS:HD3	3:d:3145[B]:ASN:O	2.18	0.43
3:U:3194[A]:GLY:C	3:U:3195[A]:MET:CG	2.91	0.43
3:U:3200[B]:LEU:CD2	3:U:3204[B]:LEU:HD11	2.48	0.43
1:V:452:ILE:HD12	1:V:1367:SER:CB	2.48	0.43
1:V:1156:LEU:HD11	1:V:1174:GLU:HG3	2.00	0.43
1:V:1512:ARG:HA	1:V:1513:PRO:HD3	1.86	0.43
2:W:2345:ASN:HA	2:W:2346:PRO:HD2	1.71	0.43
3:X:3014[A]:TRP:CH2	3:X:3123[A]:THR:HG23	2.52	0.43
3:X:3093[B]:HIS:HD2	3:X:3248[B]:LEU:CD2	2.31	0.43
3:X:3106[A]:THR:O	3:X:3106[A]:THR:HG23	2.17	0.43
3:X:3276[B]:ASP:C	3:X:3278[B]:HIS:N	2.75	0.43
1:Y:603:HIS:O	1:Y:606:ILE:HG22	2.19	0.43
2:Z:2500:ILE:HD11	2:Z:2776:TYR:HA	1.99	0.43
3:a:2971[B]:ASP:CG	9:a:3401[B]:CUO:O2	2.61	0.43
3:a:2989[B]:HIS:O	3:a:2990[B]:ARG:C	2.61	0.43
3:a:3137[A]:ARG:HB3	3:a:3139[A]:LEU:HD21	1.97	0.43
3:a:3242[A]:GLY:C	3:a:3243[A]:GLY:O	2.58	0.43
3:a:3299[A]:LEU:HB3	3:a:3300[A]:LEU:H	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:119:LYS:HB2	1:b:120:LYS:CA	2.48	0.43
1:b:157:GLU:OE2	1:b:296:ARG:NH2	2.51	0.43
1:b:322:CYS:HA	1:b:333:ASN:O	2.18	0.43
1:b:419:THR:N	1:b:420:SER:HA	2.33	0.43
1:b:1156:LEU:HD11	1:b:1174:GLU:HB2	2.00	0.43
3:d:2933[A]:SER:CA	3:d:2936[A]:GLU:HB3	2.48	0.43
3:d:2933[B]:SER:CA	3:d:2936[B]:GLU:HB3	2.48	0.43
3:d:3131[A]:GLN:HE21	3:d:3131[A]:GLN:HB3	1.66	0.43
3:d:3191[B]:ASN:ND2	3:d:3191[B]:ASN:N	2.60	0.43
5:FA:3:BMA:O4	5:FA:4:MAN:H2	2.17	0.43
1:A:229:LEU:HB3	1:A:230:PRO:HD2	1.99	0.43
2:B:2163:GLU:HG3	2:B:2175:VAL:HG23	2.00	0.43
3:C:2989[B]:HIS:O	3:C:2990[B]:ARG:C	2.61	0.43
3:C:3001[B]:LYS:N	3:C:3003[B]:LYS:HG3	2.34	0.43
3:C:3028[A]:PRO:HG2	3:C:3029[A]:LYS:HG3	2.00	0.43
3:C:3093[B]:HIS:HB2	3:C:3248[B]:LEU:CD1	2.48	0.43
3:C:3104[B]:MET:SD	3:C:3110[B]:THR:CG2	3.06	0.43
3:C:3149[A]:ASN:OD1	3:C:3149[A]:ASN:N	2.51	0.43
3:C:3163[B]:ASN:HD22	3:L:3149[B]:ASN:HB2	1.48	0.43
1:D:45:ALA:HB1	1:D:55:ILE:C	2.43	0.43
1:D:71:LEU:HD22	1:D:266:LEU:HD21	1.99	0.43
1:D:547:LYS:HD2	1:D:558:HIS:HB3	1.99	0.43
1:D:564:ASP:OD1	1:D:564:ASP:N	2.49	0.43
1:D:1060:GLN:OE1	1:D:1063:ARG:NH1	2.51	0.43
1:D:1210:LYS:O	1:D:1210:LYS:HD2	2.18	0.43
3:F:2940[A]:ASN:O	3:F:2943[A]:ALA:HB3	2.18	0.43
3:F:2940[B]:ASN:O	3:F:2943[B]:ALA:HB3	2.18	0.43
3:F:2989[A]:HIS:O	3:F:2990[A]:ARG:C	2.61	0.43
3:F:3001[B]:LYS:H	3:F:3003[B]:LYS:HG3	1.83	0.43
3:F:3001[B]:LYS:N	3:F:3003[B]:LYS:HG3	2.34	0.43
3:F:3149[A]:ASN:OD1	3:F:3149[A]:ASN:N	2.51	0.43
3:F:3185[B]:TYR:CE2	3:F:3187[B]:TYR:HE2	2.31	0.43
3:F:3217[B]:PHE:CD2	3:F:3300[B]:LEU:HD12	2.53	0.43
1:G:1356:PRO:HD2	1:G:1359:ILE:HD11	2.01	0.43
2:H:2156:ARG:O	2:H:2160:VAL:HG13	2.17	0.43
3:I:2933[B]:SER:CA	3:I:2936[B]:GLU:HB3	2.48	0.43
3:I:3013[B]:ASP:CG	3:I:3015[B]:THR:HG1	2.24	0.43
3:I:3014[B]:TRP:CH2	3:I:3123[B]:THR:HG23	2.53	0.43
3:I:3120[B]:HIS:HD2	3:R:2969[B]:TYR:CE2	2.21	0.43
3:I:3161[B]:GLU:C	3:R:3147[B]:GLU:CG	2.60	0.43
3:I:3244[A]:THR:H	3:I:3264[A]:TYR:HE2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3251[B]:ASP:CG	3:R:3108[B]:HIS:HE1	2.26	0.43
3:I:3255[B]:PRO:CB	3:R:2964[B]:PRO:CA	2.95	0.43
3:I:3299[A]:LEU:O	3:I:3300[A]:LEU:C	2.60	0.43
1:J:108:PRO:HB3	1:J:124:TYR:CE2	2.53	0.43
1:J:462:HIS:HA	1:J:490:TRP:CH2	2.52	0.43
1:J:638:ASP:HB3	1:J:703:TYR:OH	2.18	0.43
1:J:979:LEU:HD12	1:J:1021:LEU:HD22	2.01	0.43
1:J:1271:MET:HG2	1:J:1358:LEU:HD13	2.00	0.43
3:L:2931[B]:THR:O	3:L:2934[B]:GLU:HG3	2.18	0.43
3:L:2933[B]:SER:CA	3:L:2936[B]:GLU:HB3	2.48	0.43
3:L:3027[B]:GLU:CD	3:L:3027[B]:GLU:C	2.85	0.43
3:L:3133[B]:LEU:O	3:L:3136[B]:TYR:HB3	2.17	0.43
3:L:3161[A]:GLU:H	3:L:3161[A]:GLU:CD	2.19	0.43
3:L:3230[B]:PHE:CB	3:L:3242[B]:GLY:C	2.91	0.43
3:L:3232[A]:VAL:HG21	3:L:3273[A]:LEU:HD11	2.00	0.43
3:L:3267[B]:SER:H	3:L:3267[B]:SER:HG	1.32	0.43
3:L:3298[A]:ASN:CA	3:L:3299[A]:LEU:HB2	2.44	0.43
1:M:450:LYS:HD3	1:M:1338:GLY:O	2.18	0.43
1:M:1250:ILE:O	1:M:1473:ARG:NH2	2.51	0.43
2:N:2132:CYS:HB2	2:N:2142:ALA:HB1	2.00	0.43
2:N:2247:ILE:HG12	2:N:2266:VAL:HG11	1.99	0.43
2:N:2462:PHE:CE2	2:N:2486:ILE:HD13	2.53	0.43
3:O:3104[B]:MET:SD	3:O:3110[B]:THR:CG2	3.06	0.43
3:O:3183[B]:LEU:N	3:O:3184[B]:ASN:CA	2.80	0.43
3:O:3241[A]:PHE:CE2	3:O:3243[A]:GLY:O	2.70	0.43
3:O:3245[A]:PHE:CD1	3:O:3245[A]:PHE:C	2.97	0.43
3:O:3252[B]:TYR:HB3	3:X:3156[B]:MET:CG	2.49	0.43
1:P:603:HIS:O	1:P:606:ILE:HG22	2.19	0.43
2:Q:2156:ARG:O	2:Q:2160:VAL:HG13	2.18	0.43
2:Q:2545:SER:HB2	2:Q:2547:MET:HG2	1.99	0.43
2:Q:2549:PRO:HA	2:Q:2550:THR:HA	1.49	0.43
2:Q:2567:MET:HE3	2:Q:2718:TRP:HB2	1.99	0.43
3:R:2949[B]:LYS:NZ	3:R:2949[B]:LYS:C	2.73	0.43
3:R:2961[A]:HIS:HB2	3:R:2992[A]:TYR:HE2	1.81	0.43
3:R:3001[B]:LYS:N	3:R:3003[B]:LYS:HG3	2.34	0.43
3:R:3180[A]:TYR:CA	3:R:3183[A]:LEU:CD2	2.95	0.43
3:R:3222[B]:ILE:CD1	3:R:3223[B]:GLY:N	2.73	0.43
3:R:3242[A]:GLY:C	3:R:3243[A]:GLY:O	2.58	0.43
3:R:3244[B]:THR:H	3:R:3264[B]:TYR:HE2	1.65	0.43
3:R:3293[B]:LYS:CB	3:R:3294[B]:SER:CA	2.96	0.43
1:S:450:LYS:HE2	1:S:450:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1380:GLY:HA3	1:S:1450:TYR:O	2.19	0.43
1:S:1422:HIS:NE2	1:S:1608:ARG:HB2	2.34	0.43
2:T:2488:ARG:O	1:V:1483:ASN:HB3	2.18	0.43
3:U:2940[B]:ASN:O	3:U:2943[B]:ALA:HB3	2.18	0.43
3:U:3152[B]:LYS:CD	3:d:3173[B]:THR:OG1	2.61	0.43
3:U:3180[B]:TYR:CA	3:U:3183[B]:LEU:CD2	2.95	0.43
3:U:3196[B]:THR:N	3:U:3199[B]:GLN:CB	2.64	0.43
3:U:3285[A]:VAL:CG2	3:U:3286[A]:THR:H	2.27	0.43
1:V:499:GLU:HG3	1:V:511:VAL:H	1.83	0.43
2:W:2799:LYS:HA	2:W:2803:ARG:NH1	2.34	0.43
3:X:2940[B]:ASN:O	3:X:2943[B]:ALA:HB3	2.18	0.43
3:X:2951[A]:ASP:OD2	3:X:2952[A]:ALA:CB	2.66	0.43
3:X:3132[B]:ALA:HB3	3:X:3197[B]:ILE:HD13	1.99	0.43
3:X:3141[A]:TYR:CD2	3:X:3141[A]:TYR:C	2.85	0.43
3:X:3266[A]:ILE:O	3:X:3269[A]:SER:HB2	2.18	0.43
1:Y:797:THR:HG22	1:Y:798:LEU:H	1.83	0.43
1:Y:961:SER:HB2	1:Y:972:SER:O	2.18	0.43
2:Z:2129:PRO:O	2:Z:2131:LEU:HD23	2.18	0.43
2:Z:2156:ARG:O	2:Z:2160:VAL:HG13	2.18	0.43
3:a:2932[B]:PRO:CA	3:a:2935[B]:ILE:CD1	2.85	0.43
3:a:2940[A]:ASN:O	3:a:2943[A]:ALA:HB3	2.18	0.43
3:a:2991[B]:LEU:HD23	3:a:3158[B]:PHE:CE1	2.47	0.43
3:a:3106[B]:THR:O	3:a:3106[B]:THR:HG23	2.17	0.43
3:a:3196[B]:THR:N	3:a:3199[B]:GLN:CB	2.64	0.43
3:a:3241[B]:PHE:CZ	3:a:3243[B]:GLY:O	2.70	0.43
3:a:3266[B]:ILE:O	3:a:3269[B]:SER:HB2	2.17	0.43
3:a:3293[B]:LYS:CB	3:a:3294[B]:SER:CA	2.96	0.43
1:b:497:GLN:NE2	1:b:683:THR:OG1	2.50	0.43
1:b:991:LEU:HD21	1:b:1017:HIS:CG	2.54	0.43
1:b:1004:PHE:HE1	1:b:1053:TRP:CZ3	2.37	0.43
1:b:1067:TYR:N	1:b:1067:TYR:CD1	2.84	0.43
3:d:2937[A]:ASN:CG	3:d:3006[A]:LYS:HD3	2.44	0.43
3:d:2988[A]:TRP:CD1	3:d:3158[A]:PHE:CE2	3.06	0.43
3:d:3183[A]:LEU:N	3:d:3184[A]:ASN:CA	2.80	0.43
1:A:329:ARG:HA	1:b:1584:GLY:H	1.83	0.43
1:A:451:SER:HB3	1:A:1273:SER:HA	1.99	0.43
1:A:695:TYR:N	1:A:695:TYR:CD1	2.87	0.43
1:A:732:GLY:HA2	1:A:777:TYR:O	2.18	0.43
2:B:2522:SER:O	2:B:2526:ARG:HG2	2.18	0.43
2:B:2799:LYS:HA	2:B:2803:ARG:HH12	1.83	0.43
2:B:2823:ILE:HG22	2:B:2879:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2940[B]:ASN:O	3:C:2943[B]:ALA:HB3	2.18	0.43
3:C:2963[B]:MET:CE	3:L:3223[B]:GLY:H	2.08	0.43
3:C:2979[B]:GLN:HB2	3:C:2988[B]:TRP:CD1	2.52	0.43
3:C:3001[A]:LYS:N	3:C:3003[A]:LYS:HG3	2.34	0.43
3:C:3027[B]:GLU:CD	3:C:3027[B]:GLU:C	2.85	0.43
3:C:3135[B]:LYS:HB2	3:C:3141[B]:TYR:CD1	2.52	0.43
3:C:3148[B]:ILE:HG22	3:C:3152[B]:LYS:HE3	2.01	0.43
3:C:3153[B]:LYS:HZ3	3:L:2988[B]:TRP:HD1	1.44	0.43
3:C:3161[B]:GLU:OE1	3:L:3079[B]:CYS:HA	2.18	0.43
3:C:3249[B]:GLY:C	3:L:3252[B]:TYR:CD2	2.62	0.43
1:D:138:ALA:O	1:D:188:GLY:HA3	2.19	0.43
1:D:563:ILE:HD12	1:D:613:SER:OG	2.18	0.43
1:D:957:ASN:HB3	1:D:960:PHE:HB2	2.00	0.43
1:D:987:LYS:HB3	1:D:988:TYR:HD1	1.84	0.43
2:E:2546:LEU:HG	2:E:2842:THR:HG21	2.00	0.43
3:F:2951[B]:ASP:OD2	3:F:2952[B]:ALA:CB	2.66	0.43
3:F:2971[A]:ASP:CG	3:F:2973[A]:THR:HG1	2.14	0.43
3:F:3001[A]:LYS:N	3:F:3003[A]:LYS:HG3	2.34	0.43
3:F:3023[A]:ILE:HA	3:F:3026[A]:THR:HG1	1.84	0.43
3:F:3132[B]:ALA:HB3	3:F:3197[B]:ILE:HD13	1.98	0.43
3:F:3135[B]:LYS:HB2	3:F:3141[B]:TYR:CD1	2.52	0.43
3:F:3228[A]:VAL:CG2	3:F:3245[A]:PHE:CD2	3.02	0.43
3:F:3259[B]:ASP:N	3:a:3162[B]:ASP:HB3	2.33	0.43
3:F:3299[B]:LEU:O	3:F:3300[B]:LEU:C	2.60	0.43
1:G:226:HIS:HA	1:G:227:ARG:HB2	2.00	0.43
1:G:732:GLY:HA2	1:G:777:TYR:O	2.18	0.43
2:H:2179:ASP:HB3	2:H:2303:ARG:NH1	2.33	0.43
3:I:2995[A]:GLN:CG	3:I:3168[A]:THR:HG21	2.48	0.43
3:I:3001[B]:LYS:H	3:I:3003[B]:LYS:HG3	1.83	0.43
3:I:3027[A]:GLU:CD	3:I:3027[A]:GLU:C	2.85	0.43
3:I:3148[A]:ILE:HG22	3:I:3152[A]:LYS:HE3	2.01	0.43
3:I:3293[A]:LYS:CD	3:I:3293[A]:LYS:C	2.86	0.43
1:J:206:PHE:O	1:J:209:HIS:HB3	2.19	0.43
1:J:294:LYS:HA	1:J:297:ARG:HD2	2.00	0.43
2:K:2644:LEU:H	2:K:2644:LEU:HD23	1.84	0.43
3:L:3001[B]:LYS:N	3:L:3003[B]:LYS:HG3	2.34	0.43
3:L:3028[A]:PRO:HG2	3:L:3029[A]:LYS:HG3	2.00	0.43
3:L:3245[B]:PHE:CD1	3:L:3245[B]:PHE:C	2.97	0.43
1:M:293:LEU:O	1:M:297:ARG:HG3	2.18	0.43
1:M:480:CYS:HA	1:M:490:TRP:CE2	2.53	0.43
1:M:566:ARG:O	1:M:609:TRP:NE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1247:ARG:HD3	1:M:1247:ARG:HA	1.78	0.43
1:M:1621:ASN:HB3	1:M:1624:SER:H	1.83	0.43
3:O:2989[B]:HIS:C	3:O:2991[B]:LEU:N	2.75	0.43
3:O:3001[B]:LYS:N	3:O:3003[B]:LYS:HG3	2.34	0.43
3:O:3047[A]:ARG:NH2	3:O:3113[A]:ASP:OD1	2.43	0.43
3:O:3192[A]:PHE:HD2	3:O:3192[A]:PHE:HA	1.77	0.43
3:O:3218[B]:LEU:HD13	3:O:3261[B]:LEU:HD23	2.01	0.43
1:P:17:ASN:OD1	1:P:85:SER:N	2.52	0.43
1:P:947:TYR:HE1	1:P:956:PRO:HG2	1.83	0.43
1:P:1427:HIS:HD2	1:P:1457:HIS:CE1	2.36	0.43
2:Q:2089:ARG:HB2	2:Q:2368:TYR:CD1	2.54	0.43
3:R:2931[B]:THR:O	3:R:2934[B]:GLU:HG3	2.18	0.43
3:R:2995[B]:GLN:CG	3:R:3168[B]:THR:HG21	2.48	0.43
3:R:3001[A]:LYS:N	3:R:3003[A]:LYS:HG3	2.34	0.43
3:R:3194[B]:GLY:C	3:R:3195[B]:MET:CG	2.90	0.43
3:R:3228[A]:VAL:CG2	3:R:3245[A]:PHE:CD2	3.02	0.43
3:R:3229[A]:ASN:O	3:R:3286[A]:THR:N	2.50	0.43
1:S:89:ILE:H	1:S:89:ILE:HG12	1.63	0.43
1:S:1075:GLU:HG2	2:W:2900:SER:HA	2.01	0.43
2:T:2207:ASN:HA	2:T:2208:PRO:HD2	1.84	0.43
2:T:2525:LYS:HE3	2:T:2526:ARG:HH12	1.83	0.43
3:U:2940[A]:ASN:O	3:U:2943[A]:ALA:HB3	2.18	0.43
3:U:2972[B]:GLY:C	3:d:3247[B]:VAL:HG11	2.40	0.43
3:U:3001[B]:LYS:H	3:U:3003[B]:LYS:HG3	1.83	0.43
3:U:3019[A]:HIS:CD2	3:U:3020[A]:SER:H	2.35	0.43
3:U:3162[B]:ASP:OD1	3:d:3260[B]:ARG:CD	2.66	0.43
3:U:3293[B]:LYS:CB	3:U:3294[B]:SER:CA	2.96	0.43
1:V:376:ASN:HB3	1:V:665:TYR:CE1	2.52	0.43
1:V:1171:LYS:HG2	1:V:1173:GLY:H	1.83	0.43
1:V:1397:LEU:HA	1:V:1433:TRP:HD1	1.84	0.43
1:V:1467:ILE:HD13	1:V:1532:PHE:HB2	2.00	0.43
2:W:2480:LEU:HD21	4:HA:2:NAG:H83	2.00	0.43
2:W:2641:GLN:HB3	2:W:2643:GLU:OE1	2.18	0.43
2:W:2726:LYS:HB2	2:W:2726:LYS:HE3	1.64	0.43
3:X:2937[A]:ASN:CG	3:X:3006[A]:LYS:HD3	2.43	0.43
3:X:2948[B]:ASP:HB3	3:X:2949[B]:LYS:C	2.43	0.43
3:X:2989[B]:HIS:O	3:X:2990[B]:ARG:C	2.61	0.43
3:X:3074[B]:GLU:CD	3:X:3212[B]:ARG:NH2	2.73	0.43
3:X:3218[B]:LEU:HD13	3:X:3261[B]:LEU:HD23	2.01	0.43
1:Y:7:VAL:HG21	1:Y:208:LEU:HD23	1.99	0.43
1:Y:26:GLN:CD	1:Y:122:VAL:HG13	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:357:PRO:HB3	1:Y:774:ASP:HB2	2.00	0.43
1:Y:448:SER:HA	1:Y:449:ASP:HA	1.54	0.43
1:Y:641:TRP:CD1	1:Y:641:TRP:C	2.97	0.43
2:Z:2327:GLU:HG2	1:b:1650:ILE:H	1.84	0.43
2:Z:2472:ASN:CG	4:MA:1:NAG:H82	2.42	0.43
2:Z:2549:PRO:HA	2:Z:2550:THR:HA	1.41	0.43
2:Z:2734:LYS:HG2	2:Z:2735:ALA:H	1.82	0.43
3:a:2931[A]:THR:O	3:a:2934[A]:GLU:HG3	2.18	0.43
3:a:2946[B]:GLN:CD	3:a:2947[B]:ALA:N	2.72	0.43
3:a:3001[A]:LYS:H	3:a:3003[A]:LYS:HG3	1.83	0.43
3:a:3001[B]:LYS:N	3:a:3003[B]:LYS:HG3	2.34	0.43
3:a:3027[A]:GLU:CD	3:a:3027[A]:GLU:C	2.86	0.43
3:a:3228[A]:VAL:CG2	3:a:3245[A]:PHE:CD2	3.02	0.43
3:a:3228[B]:VAL:CG2	3:a:3245[B]:PHE:CD2	3.02	0.43
3:a:3276[B]:ASP:C	3:a:3278[B]:HIS:N	2.75	0.43
1:b:197:LEU:HB3	1:b:344:LEU:HD21	2.01	0.43
1:b:450:LYS:HD2	1:b:450:LYS:HA	1.72	0.43
1:b:905:TRP:HZ2	1:b:1083:PRO:HG2	1.84	0.43
2:c:2267:HIS:HD2	2:c:2297:HIS:CE1	2.18	0.43
3:d:2988[B]:TRP:CD1	3:d:3158[B]:PHE:CE2	3.06	0.43
3:d:3183[B]:LEU:H	3:d:3184[B]:ASN:CA	2.21	0.43
1:A:1303:GLU:H	1:A:1303:GLU:CD	2.17	0.43
2:B:2446:GLU:HG2	2:B:2448:THR:HG23	2.01	0.43
2:B:2502:LEU:O	2:B:2505:ILE:HG12	2.19	0.43
3:C:3106[B]:THR:O	3:C:3106[B]:THR:HG23	2.17	0.43
3:C:3228[A]:VAL:CG2	3:C:3245[A]:PHE:CD2	3.02	0.43
3:C:3256[B]:TRP:HZ2	3:L:2965[B]:LEU:HG	1.81	0.43
1:D:270:GLU:N	1:D:270:GLU:OE1	2.51	0.43
1:D:1296:VAL:HG11	1:D:1447:TYR:CE1	2.53	0.43
3:F:2980[B]:HIS:CB	3:a:2968[B]:GLN:CG	2.50	0.43
3:F:3028[B]:PRO:HG2	3:F:3029[B]:LYS:HG3	2.00	0.43
3:F:3104[B]:MET:SD	3:F:3110[B]:THR:CG2	3.06	0.43
3:F:3150[B]:LYS:HA	3:a:3172[B]:SER:HB3	2.01	0.43
3:F:3163[B]:ASN:HB3	3:a:3149[B]:ASN:ND2	2.33	0.43
3:F:3218[B]:LEU:HD13	3:F:3261[B]:LEU:HD23	2.01	0.43
3:F:3299[A]:LEU:O	3:F:3300[A]:LEU:C	2.60	0.43
1:G:122:VAL:HG23	1:G:123:PHE:CD1	2.54	0.43
1:G:728:ARG:HD2	1:G:780:GLU:OE2	2.17	0.43
1:G:1411:PHE:HB3	1:G:1544:LEU:HD21	2.00	0.43
2:H:2549:PRO:HA	2:H:2550:THR:HA	1.39	0.43
2:H:2803:ARG:HE	2:H:2805:PHE:HZ	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2814:LYS:HD2	2:H:2814:LYS:HA	1.87	0.43
3:I:2949[A]:LYS:C	3:I:2949[A]:LYS:HZ3	2.15	0.43
3:I:2965[B]:LEU:CA	3:R:3221[B]:ALA:CB	2.86	0.43
3:I:2979[B]:GLN:NE2	3:I:3155[B]:MET:HE3	2.19	0.43
3:I:2985[B]:PHE:HE2	3:R:2968[B]:GLN:C	2.26	0.43
3:I:2989[B]:HIS:O	3:I:2990[B]:ARG:C	2.61	0.43
3:I:3028[A]:PRO:HG2	3:I:3029[A]:LYS:HG3	2.00	0.43
3:I:3083[B]:ILE:HD11	3:I:3260[B]:ARG:CG	2.49	0.43
3:I:3108[B]:HIS:CE1	3:R:3252[B]:TYR:CD1	3.06	0.43
3:I:3120[B]:HIS:HA	3:I:3123[B]:THR:HG1	1.82	0.43
3:I:3131[A]:GLN:HE21	3:I:3131[A]:GLN:HB3	1.66	0.43
3:I:3148[B]:ILE:HG22	3:I:3152[B]:LYS:HE3	2.01	0.43
3:I:3159[B]:SER:C	3:R:3150[B]:LYS:CG	2.90	0.43
3:I:3242[B]:GLY:C	3:I:3243[B]:GLY:O	2.58	0.43
1:J:66:PRO:O	1:J:70:ARG:HB3	2.18	0.43
1:J:159:VAL:HG11	1:J:216:HIS:CE1	2.54	0.43
1:J:1622:GLN:HG2	1:J:1652:PHE:CD1	2.54	0.43
3:L:2961[A]:HIS:HB2	3:L:2992[A]:TYR:HE2	1.81	0.43
3:L:3183[A]:LEU:N	3:L:3184[A]:ASN:CA	2.80	0.43
3:L:3293[A]:LYS:CB	3:L:3294[A]:SER:CA	2.96	0.43
1:M:956:PRO:HB2	1:M:957:ASN:C	2.43	0.43
2:N:2089:ARG:HB3	2:N:2175:VAL:O	2.19	0.43
3:O:2965[B]:LEU:HD23	3:X:3156[B]:MET:HE3	2.00	0.43
3:O:2972[B]:GLY:C	3:X:2979[B]:GLN:HB3	2.40	0.43
3:O:3014[A]:TRP:CH2	3:O:3123[A]:THR:HG23	2.53	0.43
3:O:3023[A]:ILE:O	3:O:3026[A]:THR:OG1	2.34	0.43
3:O:3023[B]:ILE:HA	3:O:3026[B]:THR:HG1	1.82	0.43
3:O:3180[B]:TYR:CB	3:O:3183[B]:LEU:CD2	2.90	0.43
3:O:3183[A]:LEU:N	3:O:3184[A]:ASN:CA	2.80	0.43
1:P:321:LEU:HD11	1:P:377:TYR:CD2	2.54	0.43
1:P:729:VAL:O	1:P:780:GLU:O	2.36	0.43
3:R:2956[A]:LYS:O	3:R:2959[A]:SER:OG	2.33	0.43
3:R:3028[A]:PRO:HG2	3:R:3029[A]:LYS:HG3	2.00	0.43
3:R:3242[B]:GLY:C	3:R:3243[B]:GLY:O	2.58	0.43
3:R:3276[B]:ASP:C	3:R:3278[B]:HIS:N	2.75	0.43
1:S:1248:ARG:O	1:S:1250:ILE:HG13	2.19	0.43
2:T:2271:HIS:O	2:T:2283:ASN:HB3	2.19	0.43
2:T:2858:ASP:O	2:T:2862:LYS:HG2	2.18	0.43
3:U:2931[B]:THR:O	3:U:2934[B]:GLU:HG3	2.18	0.43
3:U:2951[B]:ASP:CG	3:U:2952[B]:ALA:N	2.74	0.43
3:U:2952[B]:ALA:CB	3:U:2953[B]:GLY:CA	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2969[B]:TYR:CE1	3:d:2980[B]:HIS:ND1	2.86	0.43
3:U:2970[B]:PRO:CA	3:d:3086[B]:GLU:HG2	2.48	0.43
3:U:3093[B]:HIS:HD2	3:U:3248[B]:LEU:CD2	2.31	0.43
3:U:3267[B]:SER:H	3:U:3267[B]:SER:HG	1.26	0.43
1:V:883:CYS:HA	1:V:884:PRO:HA	1.70	0.43
1:V:1455:PHE:CE1	1:V:1456:LEU:HD12	2.53	0.43
2:W:2161:GLN:NE2	2:W:2348:THR:HG21	2.33	0.43
3:X:2951[B]:ASP:CG	3:X:2952[B]:ALA:N	2.74	0.43
3:X:3001[B]:LYS:N	3:X:3003[B]:LYS:HG3	2.34	0.43
3:X:3183[B]:LEU:H	3:X:3184[B]:ASN:CA	2.22	0.43
3:X:3185[A]:TYR:HE2	3:X:3187[A]:TYR:CD2	2.35	0.43
3:X:3217[A]:PHE:CD2	3:X:3300[A]:LEU:HD12	2.53	0.43
3:X:3218[A]:LEU:HD13	3:X:3261[A]:LEU:HD23	2.01	0.43
1:Y:100:GLN:NE2	1:Y:103:GLU:OE1	2.47	0.43
1:Y:308:LEU:O	1:Y:772:ARG:NH2	2.51	0.43
1:Y:708:PHE:HB3	1:Y:716:LEU:HD22	2.01	0.43
1:Y:999:LEU:HD12	1:Y:1056:TRP:HD1	1.82	0.43
1:Y:1179:GLY:HA2	1:Y:1183:GLU:OE1	2.19	0.43
2:Z:2470:ALA:HB2	2:Z:2476:LEU:HD21	2.00	0.43
2:Z:2738:ALA:HA	1:b:1234:VAL:H	1.82	0.43
3:a:2937[A]:ASN:CG	3:a:3006[A]:LYS:HD3	2.43	0.43
3:a:2940[B]:ASN:O	3:a:2943[B]:ALA:HB3	2.18	0.43
3:a:2961[A]:HIS:HB2	3:a:2992[A]:TYR:HE2	1.81	0.43
3:a:2961[B]:HIS:HB2	3:a:2992[B]:TYR:HE2	1.81	0.43
3:a:2988[B]:TRP:CZ3	3:a:2989[B]:HIS:CE1	3.07	0.43
3:a:3183[B]:LEU:N	3:a:3184[B]:ASN:CA	2.80	0.43
3:a:3217[B]:PHE:CD2	3:a:3300[B]:LEU:HD12	2.53	0.43
3:a:3232[A]:VAL:HG21	3:a:3273[A]:LEU:HD11	2.00	0.43
1:b:136:ALA:HB3	1:b:190:PHE:CE2	2.53	0.43
1:b:244:MET:HG3	1:b:261:SER:O	2.18	0.43
1:b:293:LEU:O	1:b:296:ARG:HG2	2.18	0.43
1:b:610:THR:HB	1:b:629:MET:HE1	2.01	0.43
2:c:2505:ILE:HD11	2:c:2779:ASP:HA	2.01	0.43
2:c:2811:HIS:HB3	2:c:2847:HIS:HD2	1.82	0.43
3:d:3001[A]:LYS:H	3:d:3003[A]:LYS:HG3	1.83	0.43
3:d:3200[A]:LEU:CD2	3:d:3204[A]:LEU:HD11	2.48	0.43
3:d:3217[A]:PHE:CD2	3:d:3300[A]:LEU:HD12	2.53	0.43
3:d:3266[A]:ILE:O	3:d:3269[A]:SER:HB2	2.17	0.43
1:A:830:ASN:HB3	1:A:832:LYS:H	1.82	0.43
1:A:831:VAL:HG12	1:A:831:VAL:O	2.18	0.43
1:A:1114:TYR:HE2	1:A:1116:TYR:CE2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:VAL:HA	1:A:1321:HIS:ND1	2.33	0.43
2:B:2302:ASP:HB3	2:B:2368:TYR:OH	2.18	0.43
2:B:2648:ALA:HA	2:B:2654:SER:HB2	2.00	0.43
3:C:3083[A]:ILE:HD11	3:C:3260[A]:ARG:CG	2.49	0.43
3:C:3293[B]:LYS:CB	3:C:3294[B]:SER:CA	2.96	0.43
1:D:448:SER:HA	1:D:449:ASP:HA	1.40	0.43
1:D:449:ASP:HB2	1:D:1280:GLN:HE22	1.82	0.43
1:D:460:GLU:OE2	1:D:1368:ARG:NH2	2.51	0.43
1:D:1286:ARG:NE	1:D:1333:GLU:OE1	2.51	0.43
1:D:1362:ALA:HA	1:D:1378:PHE:CG	2.54	0.43
2:E:2666:GLN:OE1	2:E:2671:ASP:HB3	2.19	0.43
2:E:2840:GLY:O	2:E:2843:GLU:HB2	2.19	0.43
2:E:2848:PHE:HD1	2:E:2848:PHE:HA	1.70	0.43
3:F:2948[B]:ASP:HB3	3:F:2949[B]:LYS:C	2.43	0.43
3:F:2963[A]:MET:SD	3:F:2963[A]:MET:C	3.01	0.43
3:F:2967[B]:CYS:N	3:a:3256[B]:TRP:HD1	1.90	0.43
3:F:3024[A]:LEU:CD1	3:F:3024[A]:LEU:C	2.85	0.43
3:F:3083[A]:ILE:HD11	3:F:3260[A]:ARG:CG	2.49	0.43
3:F:3107[B]:LEU:HD12	3:a:2973[B]:THR:HB	2.01	0.43
3:F:3245[A]:PHE:CD1	3:F:3245[A]:PHE:C	2.97	0.43
3:F:3285[B]:VAL:CG2	3:F:3286[B]:THR:H	2.27	0.43
1:G:37:ILE:O	1:G:40:TYR:HB2	2.19	0.43
1:G:590:ASP:HB3	1:G:653:LYS:NZ	2.33	0.43
1:G:816:PRO:HA	1:G:817:PRO:HD3	1.92	0.43
1:G:926:LEU:HD11	1:G:1043:MET:HB3	2.01	0.43
1:G:946:GLU:HG2	1:G:955:LYS:HD3	2.01	0.43
1:G:988:TYR:HB3	1:G:992:ALA:HB3	2.00	0.43
1:G:1147:MET:HB3	1:G:1230:LEU:HD11	2.01	0.43
1:G:1247:ARG:HA	1:G:1247:ARG:HD3	1.85	0.43
1:G:1315:GLY:HA3	1:G:1601:TRP:CG	2.53	0.43
2:H:2356:ASP:O	2:H:2363:ASN:ND2	2.51	0.43
2:H:2571:ARG:HG3	2:H:2715:ASP:OD1	2.19	0.43
2:H:2782:ASN:O	2:H:2782:ASN:ND2	2.50	0.43
3:I:2940[B]:ASN:O	3:I:2943[B]:ALA:HB3	2.18	0.43
3:I:2948[A]:ASP:HB3	3:I:2949[A]:LYS:C	2.44	0.43
3:I:2948[B]:ASP:HB3	3:I:2949[B]:LYS:C	2.43	0.43
3:I:2951[B]:ASP:OD2	3:I:2952[B]:ALA:CB	2.66	0.43
3:I:3013[B]:ASP:CA	3:I:3122[B]:ASN:ND2	2.74	0.43
3:I:3093[B]:HIS:HD2	3:I:3248[B]:LEU:CD2	2.31	0.43
3:I:3151[B]:LEU:H	3:R:3169[B]:LYS:CG	2.19	0.43
3:I:3217[A]:PHE:CD2	3:I:3300[A]:LEU:HD12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3218[B]:LEU:HD13	3:I:3261[B]:LEU:HD23	2.01	0.43
3:I:3293[B]:LYS:CB	3:I:3294[B]:SER:CA	2.96	0.43
1:J:409:PHE:O	1:J:654:PRO:HG3	2.18	0.43
1:J:982:LYS:N	1:J:983:PRO:CD	2.81	0.43
1:J:1094:ALA:O	1:J:1097:ARG:HB3	2.18	0.43
1:J:1286:ARG:O	1:J:1289:GLU:HB3	2.18	0.43
1:J:1528:ASP:OD1	1:J:1528:ASP:N	2.51	0.43
3:L:2948[B]:ASP:HB3	3:L:2949[B]:LYS:C	2.43	0.43
3:L:2951[B]:ASP:OD2	3:L:2952[B]:ALA:CB	2.66	0.43
3:L:2989[A]:HIS:C	3:L:2991[A]:LEU:N	2.75	0.43
3:L:3182[A]:GLN:H	3:L:3182[A]:GLN:HG2	1.56	0.43
1:M:417:MET:HE2	1:M:417:MET:HA	2.01	0.43
1:M:573:LYS:HB3	1:M:574:GLY:HA2	2.01	0.43
1:M:945:ALA:O	1:M:957:ASN:ND2	2.51	0.43
2:N:2477:PRO:O	2:N:2479:SER:N	2.51	0.43
2:N:2861:LYS:HE3	3:O:2936[A]:GLU:OE1	2.19	0.43
3:O:3083[B]:ILE:HD11	3:O:3260[B]:ARG:CG	2.49	0.43
3:O:3196[A]:THR:N	3:O:3199[A]:GLN:CB	2.65	0.43
1:P:552:PHE:HZ	1:P:623:TYR:HE1	1.65	0.43
1:P:1144:VAL:N	1:P:1194:SER:O	2.49	0.43
1:P:1219:ASP:N	1:P:1223:ALA:O	2.38	0.43
1:P:1321:HIS:HD2	1:P:1465:TRP:HH2	1.64	0.43
1:P:1638:SER:HA	1:P:1639:LYS:HA	1.62	0.43
2:Q:2252:GLU:HG3	2:Q:2385:ILE:HG23	2.00	0.43
3:R:2933[B]:SER:CA	3:R:2936[B]:GLU:HB3	2.48	0.43
3:R:2940[B]:ASN:O	3:R:2943[B]:ALA:HB3	2.18	0.43
3:R:2948[A]:ASP:HB3	3:R:2949[A]:LYS:C	2.43	0.43
3:R:2989[B]:HIS:C	3:R:2991[B]:LEU:N	2.75	0.43
3:R:3148[B]:ILE:HG22	3:R:3152[B]:LYS:HE3	2.01	0.43
3:R:3218[A]:LEU:HD13	3:R:3261[A]:LEU:HD23	2.01	0.43
1:S:135:THR:HG22	1:S:192:HIS:HB3	2.00	0.43
1:S:1299:GLN:O	1:S:1301:PRO:HD3	2.19	0.43
3:U:2969[B]:TYR:O	3:d:3086[B]:GLU:OE1	2.37	0.43
3:U:3135[B]:LYS:HB2	3:U:3141[B]:TYR:CD1	2.51	0.43
3:U:3148[B]:ILE:HG22	3:U:3152[B]:LYS:HE3	2.01	0.43
3:U:3218[A]:LEU:HD12	3:U:3218[A]:LEU:HA	1.78	0.43
3:U:3252[B]:TYR:CZ	3:d:3222[B]:ILE:HD13	2.42	0.43
1:V:228:GLY:H	1:V:229:LEU:HG	1.83	0.43
2:W:2116:SER:HA	2:W:2121:THR:HG21	2.01	0.43
2:W:2246:ASN:HB3	2:W:2266:VAL:HG22	2.01	0.43
2:W:2312:GLN:HB2	2:W:2319:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2988[B]:TRP:CD1	3:X:3158[B]:PHE:CE2	3.06	0.43
3:X:2995[B]:GLN:CG	3:X:3168[B]:THR:HG21	2.48	0.43
3:X:3001[A]:LYS:H	3:X:3003[A]:LYS:HG3	1.83	0.43
3:X:3149[A]:ASN:OD1	3:X:3149[A]:ASN:N	2.51	0.43
3:X:3293[B]:LYS:CB	3:X:3294[B]:SER:CA	2.96	0.43
1:Y:195:SER:HB2	1:Y:386:ILE:HD11	2.00	0.43
1:Y:514:TRP:CZ3	1:Y:606:ILE:HD11	2.53	0.43
1:Y:931:TRP:CB	1:Y:1018:ILE:HD11	2.48	0.43
1:Y:1018:ILE:HD12	1:Y:1045:HIS:HD2	1.84	0.43
1:Y:1025:THR:HG23	1:Y:1221:THR:HA	2.01	0.43
1:Y:1245:GLU:HB3	2:c:2730:LEU:HA	1.99	0.43
1:Y:1401:ARG:HH11	1:Y:1401:ARG:HB3	1.84	0.43
1:Y:1427:HIS:HD2	1:Y:1457:HIS:HE1	1.67	0.43
1:Y:1599:MET:SD	1:Y:1600:PRO:HD2	2.59	0.43
2:Z:2562:GLY:H	2:Z:2846:TRP:CB	2.31	0.43
3:a:2931[B]:THR:O	3:a:2934[B]:GLU:HG3	2.18	0.43
3:a:2951[B]:ASP:OD2	3:a:2952[B]:ALA:CB	2.66	0.43
3:a:3048[B]:ASP:HB3	3:a:3099[B]:PRO:HD2	2.01	0.43
3:a:3093[A]:HIS:HB2	3:a:3248[A]:LEU:CD1	2.48	0.43
3:a:3148[B]:ILE:O	3:a:3148[B]:ILE:HG22	2.17	0.43
3:a:3245[B]:PHE:CD1	3:a:3245[B]:PHE:C	2.97	0.43
1:b:61:GLY:N	1:b:176:GLU:OE2	2.48	0.43
1:b:149:GLU:HG3	1:b:150:GLY:N	2.34	0.43
1:b:896:HIS:HB2	1:b:905:TRP:CG	2.54	0.43
1:b:928:TYR:HB2	1:b:1048:ASN:HB2	2.00	0.43
1:b:1030:MET:HA	1:b:1036:SER:HA	2.00	0.43
2:c:2551:PRO:HA	2:c:2552:GLU:HA	1.73	0.43
3:d:3001[B]:LYS:H	3:d:3003[B]:LYS:HG3	1.83	0.43
3:d:3025[B]:VAL:CG2	3:d:3047[B]:ARG:NH1	2.73	0.43
3:d:3083[A]:ILE:HD11	3:d:3260[A]:ARG:CG	2.49	0.43
3:d:3104[B]:MET:HA	3:d:3110[B]:THR:CG2	2.17	0.43
3:d:3148[A]:ILE:HG22	3:d:3152[A]:LYS:HE3	2.01	0.43
6:3:1:NAG:O3	6:3:2:NAG:N2	2.51	0.43
1:A:150:GLY:HA2	1:A:151:GLN:C	2.42	0.43
1:A:183:HIS:CD2	1:A:344:LEU:HD21	2.54	0.43
1:A:535:PRO:HG3	1:A:985:PHE:CE1	2.53	0.43
1:A:784:ALA:O	1:A:788:LEU:HB2	2.18	0.43
1:A:838:ARG:HD3	1:A:1114:TYR:HB3	2.00	0.43
1:A:854:LEU:HG	1:A:959:PHE:CE2	2.53	0.43
1:A:899:MET:HB3	1:A:1012:GLU:OE1	2.19	0.43
1:A:1638:SER:HA	1:A:1639:LYS:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2346:PRO:O	2:B:2349:THR:OG1	2.33	0.43
2:B:2361:LYS:H	2:B:2361:LYS:HG3	1.53	0.43
3:C:2972[B]:GLY:HA3	3:L:3086[B]:GLU:O	2.19	0.43
3:C:3083[B]:ILE:HD11	3:C:3260[B]:ARG:CG	2.49	0.43
3:C:3093[A]:HIS:HD2	3:C:3248[A]:LEU:CD2	2.31	0.43
3:C:3172[B]:SER:CB	3:L:3152[B]:LYS:CB	2.96	0.43
3:C:3180[A]:TYR:CB	3:C:3183[A]:LEU:CD2	2.89	0.43
3:C:3183[B]:LEU:N	3:C:3184[B]:ASN:CA	2.80	0.43
3:C:3217[B]:PHE:CD2	3:C:3300[B]:LEU:HD12	2.53	0.43
3:C:3284[A]:LYS:CE	3:C:3284[A]:LYS:CA	2.86	0.43
1:D:132:ASN:HA	1:D:133:LYS:HA	1.86	0.43
1:D:361:GLU:HG2	1:D:363:THR:HG22	2.00	0.43
1:D:754:GLU:CD	1:D:799:ARG:HH21	2.26	0.43
2:E:2244:PHE:HA	2:E:2373:MET:HE1	2.01	0.43
2:E:2270:ILE:HB	2:E:2297:HIS:CD2	2.54	0.43
2:E:2830:GLN:N	2:E:2830:GLN:OE1	2.52	0.43
3:F:2933[B]:SER:CA	3:F:2936[B]:GLU:HB3	2.48	0.43
3:F:2965[A]:LEU:CG	3:F:2974[A]:ALA:CB	2.85	0.43
3:F:2988[A]:TRP:CZ3	3:F:2989[A]:HIS:CE1	3.07	0.43
3:F:3147[B]:GLU:HG3	3:a:3160[B]:SER:C	2.43	0.43
3:F:3148[A]:ILE:HG22	3:F:3152[A]:LYS:HE3	2.01	0.43
3:F:3155[B]:MET:SD	3:a:3153[B]:LYS:HG2	2.59	0.43
1:G:1369:THR:HB	1:G:1371:GLN:HG2	2.01	0.43
2:H:2808:PHE:HZ	2:H:2821:LEU:HD13	1.83	0.43
3:I:3001[A]:LYS:H	3:I:3003[A]:LYS:HG3	1.83	0.43
3:I:3001[A]:LYS:N	3:I:3003[A]:LYS:HG3	2.34	0.43
3:I:3149[A]:ASN:OD1	3:I:3149[A]:ASN:N	2.51	0.43
3:I:3173[B]:THR:HA	3:R:3154[B]:PRO:CA	2.48	0.43
3:I:3228[B]:VAL:CG2	3:I:3245[B]:PHE:CD2	3.02	0.43
1:J:1315:GLY:HA3	1:J:1601:TRP:HB2	2.00	0.43
2:K:2403:PHE:CE2	2:K:2476:LEU:HD13	2.54	0.43
3:L:2949[B]:LYS:C	3:L:2949[B]:LYS:HZ3	2.13	0.43
3:L:3023[B]:ILE:HA	3:L:3026[B]:THR:HG1	1.82	0.43
3:L:3180[A]:TYR:CB	3:L:3183[A]:LEU:CD2	2.89	0.43
3:L:3218[A]:LEU:HD13	3:L:3261[A]:LEU:HD23	2.01	0.43
1:M:17:ASN:ND2	1:M:86:THR:H	2.10	0.43
1:M:494:VAL:HG13	1:M:631:TRP:CZ3	2.54	0.43
1:M:1166:THR:HB	1:M:1167:ASP:C	2.44	0.43
2:N:2117:ASP:OD1	2:N:2168:ARG:NH2	2.52	0.43
2:N:2231:LEU:HD12	2:N:2273:TRP:HE3	1.83	0.43
2:N:2286:HIS:NE2	2:N:2433:THR:HG22	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:2311:LEU:O	2:N:2315:ARG:HG3	2.19	0.43
3:O:2976[B]:ALA:O	3:O:2978[B]:CYS:N	2.46	0.43
3:O:2988[B]:TRP:CZ3	3:O:2989[B]:HIS:CE1	3.07	0.43
3:O:3028[A]:PRO:HG2	3:O:3029[A]:LYS:HG3	2.00	0.43
3:O:3185[A]:TYR:HE2	3:O:3187[A]:TYR:CD2	2.35	0.43
3:O:3200[A]:LEU:CD2	3:O:3204[A]:LEU:HD11	2.48	0.43
3:O:3293[A]:LYS:CB	3:O:3294[A]:SER:CA	2.96	0.43
1:P:195:SER:HB2	1:P:386:ILE:HD11	2.00	0.43
1:P:669:LYS:HB2	1:P:670:PRO:HD3	2.01	0.43
1:P:977:GLU:HB3	1:P:979:LEU:HD21	2.00	0.43
1:P:1329:LEU:HB2	1:P:1507:THR:HG21	2.01	0.43
2:Q:2596:THR:HG21	2:Q:2783:PHE:CZ	2.53	0.43
2:Q:2695:MET:HE3	2:Q:2706:ILE:HG23	2.01	0.43
3:R:2951[A]:ASP:OD2	3:R:2952[A]:ALA:CB	2.66	0.43
3:R:3044[B]:LYS:H	3:R:3044[B]:LYS:HG2	1.64	0.43
3:R:3047[B]:ARG:NH2	3:R:3113[B]:ASP:OD1	2.43	0.43
3:R:3217[B]:PHE:CD2	3:R:3300[B]:LEU:HD12	2.53	0.43
3:R:3245[A]:PHE:CD1	3:R:3245[A]:PHE:C	2.97	0.43
1:S:926:LEU:HA	1:S:927:PRO:HD3	1.81	0.43
1:S:1394:GLN:HB2	1:S:1433:TRP:CB	2.48	0.43
3:U:2933[A]:SER:CA	3:U:2936[A]:GLU:HB3	2.48	0.43
3:U:2937[A]:ASN:CG	3:U:3006[A]:LYS:HD3	2.43	0.43
3:U:2963[A]:MET:SD	3:U:2963[A]:MET:C	3.01	0.43
3:U:3001[B]:LYS:N	3:U:3003[B]:LYS:HG3	2.34	0.43
3:U:3047[B]:ARG:NH2	3:U:3113[B]:ASP:OD1	2.43	0.43
3:U:3083[B]:ILE:HD11	3:U:3260[B]:ARG:CG	2.49	0.43
3:U:3146[B]:CYS:HA	3:U:3147[B]:GLU:HA	1.70	0.43
3:U:3170[B]:ALA:CA	3:d:3148[B]:ILE:CB	2.96	0.43
3:U:3228[A]:VAL:CG2	3:U:3245[A]:PHE:CD2	3.02	0.43
3:U:3228[B]:VAL:CG2	3:U:3245[B]:PHE:CD2	3.02	0.43
1:V:226:HIS:O	1:V:227:ARG:HG2	2.19	0.43
1:V:562:GLN:HG2	1:V:614:GLU:HG3	2.00	0.43
1:V:1559:LEU:HD21	1:V:1590:PHE:HE1	1.83	0.43
2:W:2275:GLY:HA3	2:W:2283:ASN:H	1.84	0.43
2:W:2840:GLY:O	2:W:2843:GLU:HB2	2.19	0.43
3:X:3023[A]:ILE:O	3:X:3026[A]:THR:OG1	2.34	0.43
3:X:3228[A]:VAL:CG2	3:X:3245[A]:PHE:CD2	3.02	0.43
3:X:3284[A]:LYS:CE	3:X:3284[A]:LYS:CA	2.85	0.43
1:Y:63:PRO:HA	1:Y:172:GLU:HG3	2.00	0.43
1:Y:1108:TYR:HB2	1:Y:1114:TYR:CE1	2.54	0.43
1:Y:1313:LEU:HD13	1:Y:1322:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:2390:GLN:O	2:Z:2491:PRO:HB3	2.18	0.43
2:Z:2515:ARG:HD2	2:c:2168:ARG:CZ	2.49	0.43
2:Z:2547:MET:O	2:Z:2751:TRP:HH2	2.02	0.43
3:a:2933[A]:SER:CA	3:a:2936[A]:GLU:HB3	2.48	0.43
3:a:2938[B]:LEU:O	3:a:2939[B]:ARG:C	2.58	0.43
3:a:2961[B]:HIS:NE2	3:a:2980[B]:HIS:CE1	2.73	0.43
3:a:2965[B]:LEU:CD1	3:a:2974[B]:ALA:CA	2.89	0.43
3:a:3001[B]:LYS:H	3:a:3003[B]:LYS:HG3	1.83	0.43
3:a:3083[B]:ILE:HD11	3:a:3260[B]:ARG:CG	2.49	0.43
3:a:3281[B]:PHE:HE1	3:a:3305[B]:ILE:HG21	1.81	0.43
1:b:190:PHE:HD1	1:b:191:THR:N	2.17	0.43
1:b:1260:ARG:HD2	1:b:1343:VAL:O	2.18	0.43
1:b:1321:HIS:HD2	1:b:1465:TRP:CH2	2.36	0.43
3:d:2948[B]:ASP:HB3	3:d:2949[B]:LYS:C	2.43	0.43
3:d:2965[A]:LEU:CD1	3:d:2974[A]:ALA:CA	2.89	0.43
3:d:3013[B]:ASP:CG	3:d:3015[B]:THR:HG1	2.26	0.43
3:d:3148[B]:ILE:HG22	3:d:3148[B]:ILE:O	2.17	0.43
3:d:3149[A]:ASN:OD1	3:d:3149[A]:ASN:N	2.50	0.43
3:d:3217[B]:PHE:CD2	3:d:3300[B]:LEU:HD12	2.53	0.43
3:d:3218[A]:LEU:HD13	3:d:3261[A]:LEU:HD23	2.01	0.43
3:d:3230[A]:PHE:CB	3:d:3242[A]:GLY:C	2.91	0.43
6:LA:1:NAG:H62	6:LA:2:NAG:C8	2.48	0.43
1:A:177:VAL:HG11	1:A:358:TYR:CE1	2.54	0.43
1:A:398:ARG:HA	1:A:399:PRO:HD3	1.87	0.43
1:A:641:TRP:HZ2	1:A:693:TYR:HD1	1.65	0.43
1:A:904:HIS:HE1	1:A:1106:PHE:CZ	2.37	0.43
1:A:1022:VAL:O	1:A:1029:SER:OG	2.34	0.43
3:C:2969[B]:TYR:CG	3:L:2989[B]:HIS:NE2	2.87	0.43
3:C:3245[A]:PHE:CD1	3:C:3245[A]:PHE:C	2.97	0.43
1:D:956:PRO:CD	1:D:957:ASN:HA	2.48	0.43
1:D:1427:HIS:HD2	1:D:1457:HIS:HE2	1.66	0.43
2:E:2240:GLN:HG2	2:E:2244:PHE:CD1	2.53	0.43
3:F:2995[A]:GLN:CG	3:F:3168[A]:THR:HG21	2.48	0.43
3:F:3083[B]:ILE:HD11	3:F:3260[B]:ARG:CG	2.49	0.43
3:F:3171[B]:HIS:C	3:F:3173[B]:THR:N	2.73	0.43
3:F:3183[B]:LEU:N	3:F:3184[B]:ASN:CA	2.80	0.43
3:F:3228[B]:VAL:CG2	3:F:3245[B]:PHE:CD2	3.02	0.43
3:F:3294[A]:SER:O	3:F:3294[A]:SER:OG	2.34	0.43
1:G:260:ASN:OD1	1:G:260:ASN:N	2.50	0.43
1:G:425:ARG:NE	1:G:499:GLU:OE2	2.51	0.43
1:G:1028:VAL:HA	1:G:1035:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1078:ARG:NH2	2:K:2875:SER:O	2.33	0.43
1:G:1146:PHE:CE2	1:G:1175:PHE:HE1	2.37	0.43
1:G:1158:GLU:HG2	1:G:1174:GLU:HB3	2.01	0.43
2:H:2156:ARG:HD2	2:H:2357:VAL:HG12	2.01	0.43
3:I:2951[A]:ASP:OD2	3:I:2952[A]:ALA:CB	2.66	0.43
3:I:3169[B]:LYS:NZ	3:R:3149[B]:ASN:ND2	2.66	0.43
3:I:3174[B]:GLY:HA3	3:R:3154[B]:PRO:HB2	1.96	0.43
3:I:3194[B]:GLY:C	3:I:3195[B]:MET:CG	2.90	0.43
3:I:3255[B]:PRO:HB3	3:R:2964[B]:PRO:N	2.33	0.43
3:I:3256[B]:TRP:N	3:R:2965[B]:LEU:C	2.77	0.43
3:I:3299[B]:LEU:HB3	3:I:3300[B]:LEU:H	1.53	0.43
1:J:121:ASN:ND2	1:J:124:TYR:H	2.16	0.43
1:J:922:TRP:CD1	1:J:924:GLY:H	2.37	0.43
1:J:1146:PHE:HZ	1:J:1159:TYR:CG	2.36	0.43
1:J:1303:GLU:HA	1:J:1304:ASP:HA	1.80	0.43
3:L:2951[A]:ASP:OD2	3:L:2952[A]:ALA:CB	2.66	0.43
3:L:3001[A]:LYS:N	3:L:3003[A]:LYS:HG3	2.34	0.43
3:L:3093[B]:HIS:HB2	3:L:3248[B]:LEU:CD1	2.48	0.43
3:L:3148[A]:ILE:HG22	3:L:3152[A]:LYS:HE3	2.01	0.43
3:L:3148[B]:ILE:HG22	3:L:3152[B]:LYS:HE3	2.01	0.43
3:L:3217[A]:PHE:CD2	3:L:3300[A]:LEU:HD12	2.53	0.43
3:L:3228[B]:VAL:CG2	3:L:3245[B]:PHE:CD2	3.02	0.43
3:L:3300[B]:LEU:HD23	3:L:3300[B]:LEU:H	1.83	0.43
3:O:2931[A]:THR:O	3:O:2934[A]:GLU:HG3	2.18	0.43
3:O:2948[A]:ASP:HB3	3:O:2949[A]:LYS:C	2.43	0.43
3:O:2948[B]:ASP:HB3	3:O:2949[B]:LYS:C	2.43	0.43
3:O:2968[B]:GLN:C	3:X:2988[B]:TRP:N	2.77	0.43
3:O:2989[A]:HIS:C	3:O:2991[A]:LEU:N	2.75	0.43
3:O:3031[A]:ASN:HA	3:O:3032[A]:PRO:HD2	1.87	0.43
3:O:3149[B]:ASN:OD1	3:O:3149[B]:ASN:N	2.51	0.43
3:O:3242[A]:GLY:C	3:O:3243[A]:GLY:O	2.58	0.43
3:O:3284[B]:LYS:CE	3:O:3284[B]:LYS:CA	2.85	0.43
1:P:278:ASP:O	1:P:279:LEU:HG	2.19	0.43
2:Q:2603:PRO:HG2	2:Q:2606:LEU:HD12	2.00	0.43
2:Q:2808:PHE:CZ	2:Q:2899:PRO:HG3	2.54	0.43
2:Q:2890:VAL:H	2:Q:2891:LEU:HA	1.81	0.43
3:R:2956[B]:LYS:O	3:R:2959[B]:SER:OG	2.33	0.43
3:R:3013[B]:ASP:CA	3:R:3122[B]:ASN:ND2	2.73	0.43
3:R:3048[B]:ASP:HB3	3:R:3099[B]:PRO:HD2	2.01	0.43
3:R:3104[A]:MET:SD	3:R:3110[A]:THR:CG2	3.06	0.43
2:T:2722:GLN:NE2	2:T:2769:PHE:O	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2951[B]:ASP:OD2	3:U:2952[B]:ALA:CB	2.66	0.43
3:U:2988[A]:TRP:CZ3	3:U:2989[A]:HIS:CE1	3.07	0.43
3:U:2995[A]:GLN:CG	3:U:3168[A]:THR:HG21	2.48	0.43
3:U:3001[A]:LYS:H	3:U:3003[A]:LYS:HG3	1.83	0.43
3:U:3093[B]:HIS:HB2	3:U:3248[B]:LEU:CD1	2.48	0.43
3:U:3245[A]:PHE:C	3:U:3245[A]:PHE:CD1	2.97	0.43
1:V:7:VAL:HG23	1:V:91:TYR:O	2.19	0.43
1:V:943:LEU:HD12	1:V:944:GLU:N	2.33	0.43
1:V:1274:LEU:HD11	1:V:1334:LEU:HD21	2.00	0.43
1:V:1581:GLU:HG3	1:V:1582:ASN:H	1.84	0.43
2:W:2244:PHE:CE1	2:W:2248:ILE:HG13	2.53	0.43
3:X:2932[A]:PRO:CA	3:X:2935[A]:ILE:CD1	2.85	0.43
3:X:2933[B]:SER:CA	3:X:2936[B]:GLU:HB3	2.48	0.43
3:X:2951[B]:ASP:OD2	3:X:2952[B]:ALA:CB	2.66	0.43
3:X:3228[B]:VAL:CG2	3:X:3245[B]:PHE:CD2	3.02	0.43
1:Y:564:ASP:HA	1:Y:609:TRP:O	2.19	0.43
2:Z:2257:CYS:N	2:Z:2324:CYS:SG	2.91	0.43
3:a:2933[B]:SER:CA	3:a:2936[B]:GLU:HB3	2.48	0.43
3:a:3014[B]:TRP:CH2	3:a:3123[B]:THR:HG23	2.53	0.43
3:a:3023[A]:ILE:O	3:a:3026[A]:THR:OG1	2.34	0.43
3:a:3028[A]:PRO:HG2	3:a:3029[A]:LYS:HG3	2.00	0.43
3:a:3133[A]:LEU:HD12	3:a:3133[A]:LEU:HA	1.86	0.43
3:a:3299[B]:LEU:O	3:a:3300[B]:LEU:C	2.60	0.43
1:b:120:LYS:N	1:b:121:ASN:HA	2.34	0.43
1:b:407:GLN:HA	1:b:408:GLY:HA2	1.79	0.43
1:b:516:TRP:NE1	1:b:636:GLN:HG2	2.34	0.43
1:b:946:GLU:HA	1:b:955:LYS:HB3	2.01	0.43
2:c:2131:LEU:HD12	2:c:2335:PRO:HB3	2.01	0.43
2:c:2569:TRP:O	2:c:2572:VAL:HG23	2.19	0.43
3:d:2951[B]:ASP:OD2	3:d:2952[B]:ALA:CB	2.66	0.43
3:d:3014[A]:TRP:CH2	3:d:3123[A]:THR:HG23	2.53	0.43
3:d:3047[A]:ARG:NH2	3:d:3113[A]:ASP:OD1	2.43	0.43
3:d:3228[A]:VAL:CG2	3:d:3245[A]:PHE:CD2	3.02	0.43
3:d:3232[A]:VAL:HG21	3:d:3273[A]:LEU:HD11	2.00	0.43
1:A:1152:LYS:HD2	1:A:1152:LYS:N	2.34	0.43
1:A:1286:ARG:HA	1:A:1286:ARG:HD2	1.58	0.43
1:A:1417:CYS:N	1:A:1484:CYS:SG	2.92	0.43
2:B:2094:ARG:NH2	2:E:2094:ARG:HH21	2.15	0.43
2:B:2114:ARG:HG3	2:E:2526:ARG:HE	1.83	0.43
2:B:2244:PHE:CD1	2:B:2373:MET:HE2	2.54	0.43
2:B:2549:PRO:HA	2:B:2550:THR:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2716:ARG:NH2	2:B:2780:HIS:O	2.44	0.43
3:C:2974[B]:ALA:C	3:L:3253[B]:GLU:OE1	2.62	0.43
3:C:2979[A]:GLN:HA	3:C:2979[A]:GLN:OE1	2.19	0.43
3:C:3001[B]:LYS:H	3:C:3003[B]:LYS:HG3	1.83	0.43
3:C:3048[B]:ASP:HB3	3:C:3099[B]:PRO:HD2	2.01	0.43
3:C:3229[B]:ASN:N	3:C:3286[B]:THR:O	2.52	0.43
1:D:801:ASP:OD1	1:D:801:ASP:N	2.49	0.43
2:E:2435:MET:HA	2:E:2436:PRO:HD3	1.91	0.43
2:E:2807:GLY:O	2:E:2899:PRO:HA	2.18	0.43
3:F:2956[A]:LYS:O	3:F:2959[A]:SER:OG	2.33	0.43
3:F:2961[B]:HIS:CB	3:a:2975[B]:PHE:HZ	2.31	0.43
3:F:2988[B]:TRP:CZ3	3:F:2989[B]:HIS:CE1	3.07	0.43
3:F:2989[B]:HIS:C	3:F:2991[B]:LEU:N	2.75	0.43
1:G:483:GLY:HA3	1:G:771:TRP:CE3	2.54	0.43
1:G:499:GLU:HG3	1:G:511:VAL:H	1.83	0.43
1:G:1161:ILE:HG13	1:G:1196:ILE:HD11	2.01	0.43
2:H:2226:GLU:CD	2:H:2277:LYS:HD2	2.44	0.43
2:H:2266:VAL:O	2:H:2269:SER:OG	2.24	0.43
3:I:3150[B]:LYS:O	3:R:3159[B]:SER:OG	2.36	0.43
3:I:3229[A]:ASN:O	3:I:3286[A]:THR:N	2.50	0.43
3:I:3255[B]:PRO:HD3	3:R:2962[B]:GLY:N	2.34	0.43
3:I:3299[B]:LEU:O	3:I:3300[B]:LEU:C	2.60	0.43
1:J:473:ALA:HB2	1:M:1639:LYS:HG3	2.01	0.43
3:L:3083[A]:ILE:HD11	3:L:3260[A]:ARG:CG	2.49	0.43
3:L:3093[A]:HIS:HD2	3:L:3248[A]:LEU:CD2	2.31	0.43
3:L:3218[B]:LEU:HD13	3:L:3261[B]:LEU:HD23	2.01	0.43
3:L:3293[B]:LYS:CB	3:L:3294[B]:SER:CA	2.96	0.43
1:M:70:ARG:HB2	1:M:214:GLU:CD	2.44	0.43
1:M:633:HIS:C	1:M:633:HIS:ND1	2.75	0.43
1:M:877:HIS:HB3	1:M:1034:GLU:HA	2.01	0.43
2:N:2280:TYR:HD1	2:N:2287:TYR:CD1	2.37	0.43
2:N:2740:ASP:OD1	2:N:2740:ASP:N	2.51	0.43
2:N:2854:MET:HE3	2:N:2854:MET:HB2	1.92	0.43
3:O:2988[B]:TRP:CD1	3:O:3158[B]:PHE:CE2	3.06	0.43
3:O:2989[B]:HIS:O	3:O:2990[B]:ARG:C	2.61	0.43
3:O:3171[A]:HIS:C	3:O:3173[A]:THR:N	2.73	0.43
3:O:3301[A]:PRO:HB2	3:O:3302[A]:SER:H	1.33	0.43
1:P:117:LYS:HG3	2:T:2634:THR:OG1	2.18	0.43
1:P:605:SER:HA	1:P:761:ALA:HB3	2.01	0.43
1:P:622:HIS:HE1	1:P:767:LYS:H	1.63	0.43
1:P:1209:ASP:O	1:P:1211:TYR:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2937[B]:ASN:CG	3:R:3006[B]:LYS:HD3	2.43	0.43
3:R:2976[B]:ALA:O	3:R:2978[B]:CYS:N	2.46	0.43
3:R:3083[B]:ILE:HD11	3:R:3260[B]:ARG:CG	2.49	0.43
3:R:3135[B]:LYS:HB2	3:R:3141[B]:TYR:CD1	2.51	0.43
3:R:3183[B]:LEU:N	3:R:3184[B]:ASN:CA	2.80	0.43
1:S:543:ASN:HA	1:S:544:PRO:HD3	1.86	0.43
1:S:803:LYS:HA	1:S:809:ALA:HA	2.00	0.43
1:S:804:ASP:C	1:S:807:GLY:H	2.26	0.43
1:S:931:TRP:HE3	1:S:991:LEU:HD13	1.83	0.43
2:T:2109:ARG:O	2:T:2113:ASP:N	2.51	0.43
2:T:2130:PRO:CB	2:T:2142:ALA:HB3	2.49	0.43
2:T:2336:PHE:HB3	2:T:2348:THR:HG22	2.00	0.43
2:T:2390:GLN:O	2:T:2491:PRO:HB3	2.19	0.43
2:T:2559:CYS:SG	2:T:2560:LEU:N	2.91	0.43
2:T:2568:HIS:CD2	2:T:2718:TRP:HH2	2.36	0.43
2:T:2684:HIS:CE1	2:T:2711:HIS:HE1	2.37	0.43
3:U:2933[B]:SER:CA	3:U:2936[B]:GLU:HB3	2.48	0.43
3:U:2948[B]:ASP:HB3	3:U:2949[B]:LYS:C	2.43	0.43
3:U:2951[A]:ASP:OD2	3:U:2952[A]:ALA:CB	2.66	0.43
3:U:3023[A]:ILE:HA	3:U:3026[A]:THR:HG1	1.82	0.43
3:U:3220[B]:ARG:HH11	3:d:2974[B]:ALA:HB2	1.83	0.43
1:V:435:GLU:HB3	1:V:509:ILE:HD11	2.01	0.43
2:W:2275:GLY:HA3	2:W:2283:ASN:HB2	2.01	0.43
2:W:2830:GLN:HE21	2:W:2830:GLN:H	1.67	0.43
3:X:2971[A]:ASP:CG	3:X:2973[A]:THR:HG1	2.12	0.43
3:X:2979[A]:GLN:HG2	3:X:3155[A]:MET:HE2	1.85	0.43
3:X:2988[B]:TRP:CZ3	3:X:2989[B]:HIS:CE1	3.07	0.43
3:X:3013[A]:ASP:CA	3:X:3122[A]:ASN:ND2	2.73	0.43
3:X:3047[A]:ARG:NH2	3:X:3113[A]:ASP:OD1	2.43	0.43
3:X:3194[B]:GLY:C	3:X:3195[B]:MET:CG	2.90	0.43
3:X:3230[B]:PHE:CB	3:X:3242[B]:GLY:C	2.91	0.43
1:Y:744:VAL:HG12	1:Y:802:ILE:HG23	2.01	0.43
1:Y:1059:LEU:O	1:Y:1063:ARG:N	2.50	0.43
1:Y:1407:THR:HG22	1:Y:1426:LEU:HD21	2.01	0.43
2:Z:2329:MET:HE2	2:Z:2358:PHE:HE2	1.83	0.43
3:a:2995[B]:GLN:CG	3:a:3168[B]:THR:HG21	2.48	0.43
3:a:3230[B]:PHE:CB	3:a:3242[B]:GLY:C	2.91	0.43
3:a:3293[A]:LYS:CB	3:a:3294[A]:SER:CA	2.96	0.43
1:b:235:CYS:SG	1:b:819:ILE:HD11	2.59	0.43
1:b:732:GLY:HA2	1:b:777:TYR:O	2.19	0.43
2:c:2244:PHE:HZ	2:c:2376:MET:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3034[A]:HIS:HB3	3:d:3035[A]:HIS:CE1	2.50	0.43
3:d:3083[B]:ILE:HD11	3:d:3260[B]:ARG:CG	2.49	0.43
3:d:3131[B]:GLN:HE21	3:d:3131[B]:GLN:HB3	1.66	0.43
2:B:2884:LYS:HG3	2:B:2891:LEU:HG	2.01	0.42
3:C:2933[A]:SER:CA	3:C:2936[A]:GLU:HB3	2.48	0.42
3:C:3090[B]:ASN:HA	3:L:2971[B]:ASP:HB2	2.01	0.42
3:C:3150[B]:LYS:N	3:L:3158[B]:PHE:O	2.42	0.42
3:C:3153[B]:LYS:CD	3:L:2988[B]:TRP:HD1	2.29	0.42
3:C:3218[A]:LEU:HD13	3:C:3261[A]:LEU:HD23	2.01	0.42
3:C:3245[B]:PHE:CD1	3:C:3245[B]:PHE:C	2.97	0.42
1:D:905:TRP:HE1	1:D:1083:PRO:CD	2.32	0.42
1:D:1155:LEU:HD11	1:D:1228:LEU:HD11	2.00	0.42
1:D:1578:ILE:HA	1:D:1579:GLY:HA2	1.63	0.42
1:D:1616:LYS:HA	1:D:1616:LYS:HD3	1.90	0.42
2:E:2446:GLU:HG2	2:E:2448:THR:HG23	2.01	0.42
2:E:2866:PRO:HA	2:E:2867:PRO:HD3	1.65	0.42
3:F:2938[B]:LEU:HD12	3:F:2938[B]:LEU:HA	1.85	0.42
3:F:2948[A]:ASP:HB3	3:F:2949[A]:LYS:C	2.43	0.42
3:F:3174[B]:GLY:N	3:a:3154[B]:PRO:N	2.66	0.42
3:F:3185[A]:TYR:HE2	3:F:3187[A]:TYR:CD2	2.35	0.42
3:F:3293[A]:LYS:CB	3:F:3294[A]:SER:CA	2.96	0.42
1:G:449:ASP:HB2	1:G:1338:GLY:HA3	1.99	0.42
1:G:979:LEU:HD23	1:G:1021:LEU:HD22	2.01	0.42
1:G:1500:THR:HA	1:G:1501:ALA:HA	1.76	0.42
2:H:2252:GLU:HA	2:H:2385:ILE:HD13	2.01	0.42
2:H:2304:LEU:HA	2:H:2304:LEU:HD12	1.76	0.42
3:I:2965[B]:LEU:O	3:R:3221[B]:ALA:HB2	2.19	0.42
3:I:2969[B]:TYR:CE2	3:I:2970[B]:PRO:CG	2.86	0.42
3:I:2979[B]:GLN:CD	3:I:3155[B]:MET:CE	2.92	0.42
3:I:3001[B]:LYS:N	3:I:3003[B]:LYS:HG3	2.34	0.42
3:I:3028[B]:PRO:HG2	3:I:3029[B]:LYS:HG3	2.00	0.42
3:I:3108[B]:HIS:HE1	3:R:3251[B]:ASP:CB	2.32	0.42
3:I:3149[B]:ASN:OD1	3:I:3149[B]:ASN:N	2.50	0.42
3:I:3152[B]:LYS:HB2	3:R:3171[B]:HIS:CA	2.49	0.42
3:I:3155[B]:MET:CG	3:R:3153[B]:LYS:HG2	2.49	0.42
3:I:3165[B]:ASN:O	3:R:3149[B]:ASN:CB	2.42	0.42
1:J:1323:HIS:CD2	1:J:1458:HIS:CE1	3.07	0.42
3:L:2931[A]:THR:O	3:L:2934[A]:GLU:HG3	2.18	0.42
3:L:2979[B]:GLN:CD	3:L:3155[B]:MET:CE	2.92	0.42
3:L:3276[A]:ASP:C	3:L:3278[A]:HIS:N	2.75	0.42
3:L:3299[B]:LEU:HB3	3:L:3300[B]:LEU:H	1.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:868:THR:HG23	1:M:919:ARG:NE	2.34	0.42
3:O:3001[A]:LYS:H	3:O:3003[A]:LYS:HG3	1.83	0.42
3:O:3013[B]:ASP:CG	3:O:3015[B]:THR:HG1	2.26	0.42
3:O:3083[A]:ILE:HD11	3:O:3260[A]:ARG:CG	2.49	0.42
3:O:3148[B]:ILE:HG22	3:O:3152[B]:LYS:HE3	2.01	0.42
3:O:3171[B]:HIS:C	3:O:3173[B]:THR:N	2.73	0.42
3:O:3229[A]:ASN:O	3:O:3286[A]:THR:N	2.50	0.42
3:O:3245[B]:PHE:CD1	3:O:3245[B]:PHE:C	2.97	0.42
1:P:838:ARG:HD2	1:P:914:GLU:CD	2.44	0.42
1:P:929:TRP:CZ3	1:P:935:ILE:HD12	2.54	0.42
1:P:999:LEU:HD21	1:P:1121:LEU:HD22	1.99	0.42
1:P:1243:PHE:HD2	1:P:1474:TYR:HA	1.84	0.42
2:Q:2758:THR:O	2:Q:2762:VAL:HG22	2.19	0.42
3:R:2932[A]:PRO:CA	3:R:2935[A]:ILE:CD1	2.85	0.42
3:R:2948[B]:ASP:HB3	3:R:2949[B]:LYS:C	2.43	0.42
3:R:3028[B]:PRO:HG2	3:R:3029[B]:LYS:HG3	2.00	0.42
3:R:3132[B]:ALA:HB3	3:R:3197[B]:ILE:HD13	1.99	0.42
3:R:3301[B]:PRO:HB2	3:R:3302[B]:SER:H	1.33	0.42
1:S:488:PRO:HB2	1:S:641:TRP:CE3	2.53	0.42
1:S:741:SER:OG	1:S:763:LEU:HA	2.19	0.42
1:S:896:HIS:HB2	1:S:905:TRP:CD1	2.54	0.42
2:T:2497:GLU:HB2	2:T:2498:VAL:HA	2.00	0.42
2:T:2726:LYS:HE3	2:T:2726:LYS:HB2	1.71	0.42
3:U:2988[B]:TRP:CZ3	3:U:2989[B]:HIS:CE1	3.07	0.42
3:U:3038[B]:ILE:HG23	3:U:3040[B]:VAL:HG22	1.90	0.42
3:U:3218[B]:LEU:HD13	3:U:3261[B]:LEU:HD23	2.01	0.42
1:V:7:VAL:HG21	1:V:208:LEU:HD23	2.00	0.42
1:V:424:PHE:CE1	1:V:1125:SER:HB2	2.54	0.42
1:V:754:GLU:CD	1:V:799:ARG:HH21	2.23	0.42
1:V:980:TYR:CD2	1:V:1021:LEU:HD13	2.54	0.42
1:V:1328:SER:HB2	1:V:1523:LEU:HD13	2.00	0.42
1:V:1539:GLN:O	1:V:1542:ARG:HB3	2.19	0.42
1:V:1549:GLY:O	1:V:1655:SER:HB2	2.18	0.42
2:W:2386:ARG:HB3	2:W:2496:LEU:HD21	2.01	0.42
3:X:3048[A]:ASP:HB3	3:X:3099[A]:PRO:HD2	2.01	0.42
3:X:3094[A]:SER:HG	3:X:3227[A]:ASP:CG	2.27	0.42
3:X:3148[A]:ILE:HG22	3:X:3152[A]:LYS:HE3	2.01	0.42
3:X:3217[B]:PHE:CD2	3:X:3300[B]:LEU:HD12	2.53	0.42
1:Y:137:ARG:HA	1:Y:193:SER:OG	2.18	0.42
1:Y:1382:ILE:N	1:Y:1387:ALA:O	2.38	0.42
1:Y:1616:LYS:C	3:d:3187[B]:TYR:CB	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:2795:ILE:O	2:Z:2798:GLN:HG2	2.19	0.42
2:Z:2820:HIS:HB2	2:Z:2882:GLU:HG3	2.01	0.42
3:a:2951[A]:ASP:OD2	3:a:2952[A]:ALA:CB	2.66	0.42
3:a:2951[A]:ASP:C	3:a:2956[A]:LYS:HZ1	2.19	0.42
3:a:2979[A]:GLN:HA	3:a:2979[A]:GLN:OE1	2.19	0.42
3:a:3083[A]:ILE:HD11	3:a:3260[A]:ARG:CG	2.49	0.42
3:a:3182[B]:GLN:H	3:a:3182[B]:GLN:HG2	1.56	0.42
1:b:398:ARG:HA	1:b:399:PRO:HD3	1.86	0.42
1:b:745:ASP:HB2	1:b:801:ASP:OD1	2.18	0.42
1:b:868:THR:HG23	1:b:919:ARG:HH21	1.84	0.42
1:b:1243:PHE:O	1:b:1476:LYS:HD3	2.19	0.42
2:c:2132:CYS:O	2:c:2334:LYS:HD3	2.19	0.42
2:c:2189:GLY:HA2	2:c:2192:THR:HG22	2.01	0.42
3:d:2979[B]:GLN:CD	3:d:3155[B]:MET:CE	2.92	0.42
3:d:2988[A]:TRP:CZ3	3:d:2989[A]:HIS:CE1	3.07	0.42
1:A:995:ILE:HG22	1:A:999:LEU:HD22	2.00	0.42
1:A:1553:ILE:HD11	1:A:1622:GLN:HG3	2.01	0.42
3:C:2938[A]:LEU:HD12	3:C:2938[A]:LEU:HA	1.85	0.42
3:C:2951[B]:ASP:OD2	3:C:2952[B]:ALA:CB	2.66	0.42
3:C:2967[B]:CYS:SG	3:L:2982[B]:MET:N	2.89	0.42
3:C:2988[A]:TRP:CZ3	3:C:2989[A]:HIS:CE1	3.07	0.42
3:C:3023[B]:ILE:HA	3:C:3026[B]:THR:HG1	1.83	0.42
3:C:3086[B]:GLU:HG2	3:L:2968[B]:GLN:NE2	2.34	0.42
3:C:3131[B]:GLN:HE21	3:C:3131[B]:GLN:HB3	1.66	0.42
3:C:3153[B]:LYS:CD	3:L:3155[B]:MET:HE2	2.49	0.42
3:C:3228[B]:VAL:CG2	3:C:3245[B]:PHE:CD2	3.02	0.42
3:C:3299[B]:LEU:O	3:C:3300[B]:LEU:C	2.60	0.42
1:D:447:MET:HE1	1:D:544:PRO:O	2.19	0.42
1:D:468:CYS:SG	1:D:669:LYS:HB3	2.59	0.42
3:F:2969[B]:TYR:HD2	3:a:3093[B]:HIS:NE2	2.15	0.42
3:F:2971[B]:ASP:N	9:F:3401[B]:CUO:CU1	1.40	0.42
3:F:3137[A]:ARG:HD3	3:F:3137[A]:ARG:HA	1.71	0.42
3:F:3154[B]:PRO:CG	3:a:3155[B]:MET:CG	2.84	0.42
3:F:3196[B]:THR:OG1	3:F:3199[B]:GLN:OE1	2.38	0.42
3:F:3218[A]:LEU:HD13	3:F:3261[A]:LEU:HD23	2.01	0.42
3:F:3232[B]:VAL:HG21	3:F:3273[B]:LEU:CD1	2.49	0.42
3:F:3299[B]:LEU:HB3	3:F:3300[B]:LEU:H	1.54	0.42
1:G:40:TYR:CE2	1:G:75:GLN:HG2	2.54	0.42
1:G:323:ILE:HA	1:G:324:PRO:HD3	1.92	0.42
1:G:449:ASP:OD2	1:G:1280:GLN:NE2	2.51	0.42
1:G:767:LYS:HE2	1:G:767:LYS:HB3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:929:TRP:CZ3	1:G:935:ILE:HD12	2.53	0.42
1:G:1582:ASN:HB3	1:G:1583:CYS:CB	2.37	0.42
2:H:2457:LYS:NZ	1:J:1206:HIS:HB3	2.34	0.42
2:H:2470:ALA:HB2	2:H:2476:LEU:HD11	2.00	0.42
2:H:2647:LEU:HD12	2:H:2647:LEU:HA	1.81	0.42
3:I:2961[B]:HIS:HB2	3:I:2992[B]:TYR:HE2	1.81	0.42
3:I:2976[B]:ALA:O	3:I:2978[B]:CYS:N	2.46	0.42
3:I:3281[A]:PHE:HE1	3:I:3305[A]:ILE:HG21	1.81	0.42
1:J:219:LEU:O	1:J:223:LEU:HB2	2.19	0.42
1:J:285:THR:HG22	1:J:287:GLU:H	1.83	0.42
1:J:567:LEU:HD13	1:J:567:LEU:HA	1.79	0.42
1:J:634:HIS:HA	1:J:637:VAL:CG2	2.49	0.42
1:J:689:PRO:HA	1:J:692:VAL:HG23	2.01	0.42
1:J:1263:LEU:HD11	1:J:1358:LEU:HD22	2.01	0.42
1:J:1298:ALA:O	4:v:2:NAG:H62	2.19	0.42
2:K:2128:LEU:HD12	2:K:2128:LEU:HA	1.78	0.42
2:K:2822:LYS:HB3	2:K:2829:CYS:HB3	2.01	0.42
3:L:2938[A]:LEU:O	3:L:2939[A]:ARG:C	2.58	0.42
3:L:2979[B]:GLN:HA	3:L:2979[B]:GLN:OE1	2.19	0.42
3:L:2988[A]:TRP:CZ3	3:L:2989[A]:HIS:CE1	3.07	0.42
3:L:2995[A]:GLN:CG	3:L:3168[A]:THR:HG21	2.48	0.42
3:L:3096[B]:VAL:CG1	3:L:3115[B]:LEU:CD1	2.86	0.42
3:L:3149[A]:ASN:OD1	3:L:3149[A]:ASN:N	2.51	0.42
3:L:3301[B]:PRO:HB2	3:L:3302[B]:SER:H	1.33	0.42
1:M:597:VAL:O	1:M:601:VAL:HG13	2.19	0.42
1:M:893:ALA:HB2	1:M:1182:ASN:HB2	2.01	0.42
1:M:1424:GLU:O	1:M:1427:HIS:HB3	2.19	0.42
2:N:2180:TRP:CH2	2:N:2300:ASN:HB3	2.55	0.42
2:N:2744:PHE:HA	2:N:2745:PRO:HD3	1.87	0.42
2:N:2874:ASP:O	2:N:2876:LYS:HG3	2.19	0.42
3:O:3160[B]:SER:HG	3:X:3150[B]:LYS:HB2	1.81	0.42
3:O:3228[B]:VAL:CG2	3:O:3245[B]:PHE:CD2	3.02	0.42
1:P:145:GLN:OE1	1:P:151:GLN:HG3	2.19	0.42
1:P:607:HIS:NE2	1:P:634:HIS:CE1	2.88	0.42
1:P:1473:ARG:HG3	1:P:1479:TYR:CG	2.55	0.42
2:Q:2128:LEU:HD22	2:Q:2287:TYR:CE1	2.55	0.42
3:R:2988[A]:TRP:CZ3	3:R:2989[A]:HIS:CE1	3.07	0.42
3:R:2995[A]:GLN:CG	3:R:3168[A]:THR:HG21	2.49	0.42
3:R:3182[B]:GLN:H	3:R:3182[B]:GLN:HG2	1.56	0.42
3:R:3185[B]:TYR:HE2	3:R:3187[B]:TYR:CD2	2.35	0.42
3:R:3191[A]:ASN:C	3:R:3192[A]:PHE:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3196[B]:THR:OG1	3:R:3199[B]:GLN:OE1	2.37	0.42
3:R:3281[B]:PHE:HE1	3:R:3305[B]:ILE:HG21	1.81	0.42
1:S:361:GLU:HG2	1:S:363:THR:HG22	2.01	0.42
1:S:516:TRP:HD1	1:S:579:LEU:HB3	1.84	0.42
1:S:1382:ILE:HD13	1:S:1447:TYR:HD2	1.84	0.42
1:S:1398:PHE:HA	1:S:1399:GLY:HA2	1.53	0.42
2:T:2576:HIS:CD2	2:T:2759:THR:HG21	2.54	0.42
3:U:2937[B]:ASN:CG	3:U:3006[B]:LYS:HD3	2.43	0.42
3:U:2979[A]:GLN:CD	3:U:3155[A]:MET:CE	2.92	0.42
3:U:3083[A]:ILE:HD11	3:U:3260[A]:ARG:CG	2.49	0.42
3:U:3232[B]:VAL:HG21	3:U:3273[B]:LEU:CD1	2.49	0.42
3:U:3299[B]:LEU:HB3	3:U:3300[B]:LEU:H	1.54	0.42
3:U:3300[A]:LEU:HD23	3:U:3300[A]:LEU:H	1.83	0.42
1:V:25:MET:HE2	1:V:34:TYR:HA	2.01	0.42
1:V:80:LEU:HD12	1:V:80:LEU:HA	1.81	0.42
1:V:109:LEU:HD13	2:Z:2626:ARG:NH1	2.34	0.42
1:V:163:LEU:HB3	1:V:293:LEU:HD21	2.00	0.42
3:X:2969[A]:TYR:CD2	3:X:2971[A]:ASP:CG	2.97	0.42
3:X:3038[B]:ILE:HG23	3:X:3040[B]:VAL:HG22	1.90	0.42
3:X:3196[A]:THR:OG1	3:X:3199[A]:GLN:OE1	2.38	0.42
3:X:3293[A]:LYS:CD	3:X:3293[A]:LYS:C	2.85	0.42
1:Y:450:LYS:H	1:Y:450:LYS:HG3	1.54	0.42
1:Y:1190:ARG:HA	1:Y:1191:PRO:HD3	1.92	0.42
2:Z:2521:MET:HE3	2:Z:2605:LEU:HD12	2.01	0.42
2:Z:2542:TYR:HB2	2:Z:2573:TYR:CE1	2.51	0.42
2:Z:2561:HIS:ND1	2:Z:2561:HIS:N	2.67	0.42
3:a:2937[B]:ASN:CG	3:a:3006[B]:LYS:HD3	2.44	0.42
3:a:3001[A]:LYS:N	3:a:3003[A]:LYS:HG3	2.34	0.42
3:a:3148[B]:ILE:HG22	3:a:3152[B]:LYS:HE3	2.01	0.42
3:a:3218[B]:LEU:HD13	3:a:3261[B]:LEU:HD23	2.01	0.42
3:a:3245[A]:PHE:CD1	3:a:3245[A]:PHE:C	2.97	0.42
3:a:3267[A]:SER:HG	3:a:3267[A]:SER:H	1.42	0.42
1:b:531:THR:HG22	1:b:542:PRO:HA	2.01	0.42
1:b:1329:LEU:HB2	1:b:1507:THR:HG21	2.01	0.42
3:d:2951[A]:ASP:OD2	3:d:2952[A]:ALA:CB	2.66	0.42
3:d:3001[A]:LYS:N	3:d:3003[A]:LYS:HG3	2.34	0.42
3:d:3048[A]:ASP:HB3	3:d:3099[A]:PRO:HD2	2.01	0.42
1:A:81:VAL:C	1:A:83:HIS:N	2.77	0.42
1:A:496:MET:O	1:A:500:ASN:ND2	2.50	0.42
1:A:843:VAL:HG13	1:A:927:PRO:HB2	1.99	0.42
1:A:905:TRP:CZ3	1:A:909:ILE:HG13	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:GLU:HG2	1:A:1216:ARG:O	2.19	0.42
1:A:1321:HIS:O	1:A:1324:ARG:HB3	2.19	0.42
1:A:1633:THR:HA	1:A:1639:LYS:O	2.19	0.42
2:B:2107:LEU:O	2:B:2111:GLN:HB2	2.19	0.42
2:B:2181:THR:HB	2:B:2373:MET:SD	2.59	0.42
2:B:2505:ILE:HD12	2:B:2507:ARG:HH21	1.84	0.42
2:B:2643:GLU:O	2:B:2647:LEU:N	2.46	0.42
2:B:2884:LYS:HD2	2:B:2889:ALA:HB3	2.02	0.42
3:C:2956[A]:LYS:O	3:C:2959[A]:SER:OG	2.33	0.42
3:C:2959[B]:SER:C	3:L:3255[B]:PRO:HB2	2.33	0.42
3:C:2979[B]:GLN:HA	3:C:2979[B]:GLN:OE1	2.19	0.42
3:C:3149[B]:ASN:HD21	3:L:3163[B]:ASN:HB3	1.82	0.42
3:C:3174[B]:GLY:N	3:L:3154[B]:PRO:HB3	2.30	0.42
3:C:3232[A]:VAL:HG21	3:C:3273[A]:LEU:CD1	2.50	0.42
3:C:3284[A]:LYS:CD	3:C:3284[A]:LYS:C	2.86	0.42
1:D:931:TRP:CZ3	1:D:995:ILE:HD11	2.54	0.42
1:D:1385:GLU:OE1	1:D:1440:HIS:HE1	2.02	0.42
2:E:2549:PRO:HA	2:E:2550:THR:HA	1.56	0.42
2:E:2660:VAL:HG11	2:E:2783:PHE:CE1	2.54	0.42
3:F:2951[B]:ASP:C	3:F:2956[B]:LYS:HZ1	2.13	0.42
3:F:2972[B]:GLY:HA3	3:a:3090[B]:ASN:CG	2.44	0.42
3:F:2979[A]:GLN:CD	3:F:3155[A]:MET:CE	2.92	0.42
3:F:2985[B]:PHE:HD2	3:a:2968[B]:GLN:O	2.02	0.42
3:F:3104[A]:MET:SD	3:F:3110[A]:THR:CG2	3.06	0.42
1:G:497:GLN:CG	1:G:683:THR:HG21	2.50	0.42
1:G:736:MET:HG3	1:G:772:ARG:HD2	2.00	0.42
1:G:945:ALA:C	1:G:957:ASN:HD22	2.27	0.42
1:G:1321:HIS:HE1	1:G:1489:MET:SD	2.42	0.42
3:I:2937[A]:ASN:CG	3:I:3006[A]:LYS:HD3	2.43	0.42
3:I:3038[A]:ILE:HG23	3:I:3040[A]:VAL:HG22	1.89	0.42
3:I:3228[A]:VAL:CG2	3:I:3245[A]:PHE:CD2	3.02	0.42
3:I:3245[A]:PHE:CD1	3:I:3245[A]:PHE:C	2.97	0.42
3:I:3255[B]:PRO:CB	3:R:2959[B]:SER:HA	2.46	0.42
1:J:179:HIS:HD2	1:J:209:HIS:HE2	1.67	0.42
1:J:227:ARG:HH22	1:J:297:ARG:HH22	1.67	0.42
1:J:514:TRP:CZ2	1:J:606:ILE:HD11	2.54	0.42
1:J:545:PHE:O	1:J:561:ARG:NH2	2.52	0.42
1:J:804:ASP:OD2	4:u:1:NAG:O6	2.37	0.42
1:J:902:PHE:N	1:J:903:PRO:HD2	2.34	0.42
1:J:1002:GLU:HG3	1:J:1003:ASP:N	2.34	0.42
1:J:1355:LEU:HB2	1:J:1360:ASN:CG	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2180:TRP:NE1	2:K:2300:ASN:HD22	2.17	0.42
2:K:2536:PHE:HE1	2:K:2708:TYR:HE2	1.67	0.42
2:K:2545:SER:HB3	2:K:2547:MET:HB3	2.01	0.42
3:L:2940[B]:ASN:O	3:L:2943[B]:ALA:HB3	2.18	0.42
3:L:3096[A]:VAL:CG1	3:L:3115[A]:LEU:CD1	2.86	0.42
3:L:3185[A]:TYR:CE2	3:L:3187[A]:TYR:HE2	2.31	0.42
3:L:3228[A]:VAL:CG2	3:L:3245[A]:PHE:CD2	3.02	0.42
1:M:797:THR:HG22	1:M:798:LEU:H	1.84	0.42
1:M:1077:LEU:HB3	1:M:1103:PHE:CE1	2.53	0.42
1:M:1435:GLY:O	1:M:1441:SER:OG	2.29	0.42
2:N:2126:HIS:O	2:N:2143:CYS:HB3	2.20	0.42
2:N:2844:MET:O	2:N:2846:TRP:HD1	2.03	0.42
3:O:2971[B]:ASP:OD2	3:X:3158[B]:PHE:CZ	2.73	0.42
3:O:2979[A]:GLN:CD	3:O:3155[A]:MET:CE	2.92	0.42
3:O:3001[A]:LYS:N	3:O:3003[A]:LYS:HG3	2.34	0.42
3:O:3013[A]:ASP:CA	3:O:3122[A]:ASN:ND2	2.74	0.42
3:O:3276[B]:ASP:C	3:O:3278[B]:HIS:N	2.75	0.42
3:O:3293[A]:LYS:CD	3:O:3293[A]:LYS:C	2.86	0.42
1:P:554:LYS:HA	1:P:554:LYS:HD3	1.76	0.42
1:P:566:ARG:HH22	1:P:803:LYS:CD	2.31	0.42
1:P:816:PRO:HA	1:P:817:PRO:HD3	1.87	0.42
1:P:865:LYS:HA	1:P:865:LYS:HD2	1.80	0.42
1:P:1001:GLN:HG3	1:P:1007:PHE:HA	2.00	0.42
1:P:1438:ASP:HB3	1:P:1441:SER:HB3	2.01	0.42
2:Q:2579:GLU:HG2	2:Q:2756:ASN:HD22	1.84	0.42
3:R:2979[B]:GLN:HA	3:R:2979[B]:GLN:OE1	2.19	0.42
3:R:2988[B]:TRP:CZ3	3:R:2989[B]:HIS:CE1	3.07	0.42
3:R:3148[A]:ILE:HG22	3:R:3152[A]:LYS:HE3	2.01	0.42
1:S:554:LYS:HA	1:S:554:LYS:HD2	1.63	0.42
1:S:585:LEU:O	1:S:588:GLU:HB3	2.19	0.42
1:S:1081:MET:O	1:S:1085:SER:HB3	2.20	0.42
1:S:1491:GLN:HA	1:S:1492:PRO:HD3	1.90	0.42
2:T:2402:GLY:HA3	2:T:2403:PHE:HB2	2.02	0.42
2:T:2551:PRO:HA	2:T:2552:GLU:HA	1.51	0.42
3:U:2969[A]:TYR:CD2	3:U:2971[A]:ASP:CG	2.98	0.42
3:U:2973[B]:THR:CA	3:d:3247[B]:VAL:CG1	2.97	0.42
3:U:2976[A]:ALA:O	3:U:2978[A]:CYS:N	2.46	0.42
3:U:3048[B]:ASP:HB3	3:U:3099[B]:PRO:HD2	2.01	0.42
3:U:3104[A]:MET:SD	3:U:3110[A]:THR:CG2	3.06	0.42
3:U:3196[B]:THR:OG1	3:U:3199[B]:GLN:OE1	2.38	0.42
3:U:3229[B]:ASN:O	3:U:3286[B]:THR:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:302:ALA:H	1:V:363:THR:HB	1.84	0.42
2:W:2825:ILE:HG23	2:W:2826:GLU:H	1.83	0.42
3:X:2931[B]:THR:O	3:X:2934[B]:GLU:HG3	2.18	0.42
3:X:2965[B]:LEU:CG	3:X:2974[B]:ALA:CB	2.85	0.42
3:X:2988[A]:TRP:CZ3	3:X:2989[A]:HIS:CE1	3.07	0.42
3:X:3180[B]:TYR:CB	3:X:3183[B]:LEU:CD2	2.90	0.42
3:X:3196[B]:THR:OG1	3:X:3199[B]:GLN:OE1	2.38	0.42
3:X:3232[B]:VAL:HG21	3:X:3273[B]:LEU:CD1	2.50	0.42
3:X:3232[B]:VAL:HG21	3:X:3273[B]:LEU:HD11	2.00	0.42
1:Y:37:ILE:O	1:Y:72:TYR:OH	2.30	0.42
1:Y:516:TRP:CD1	1:Y:579:LEU:HD13	2.54	0.42
1:Y:568:PHE:CE2	1:Y:609:TRP:HD1	2.37	0.42
1:Y:637:VAL:HA	1:Y:640:LEU:HD12	2.01	0.42
1:Y:801:ASP:N	1:Y:801:ASP:OD1	2.52	0.42
1:Y:1018:ILE:O	1:Y:1022:VAL:HG12	2.19	0.42
3:a:2948[A]:ASP:HB3	3:a:2949[A]:LYS:C	2.43	0.42
3:a:3180[B]:TYR:CA	3:a:3183[B]:LEU:CD2	2.95	0.42
3:a:3232[A]:VAL:HG21	3:a:3273[A]:LEU:CD1	2.49	0.42
1:b:516:TRP:CG	1:b:606:ILE:HD12	2.54	0.42
1:b:980:TYR:HE2	1:b:1021:LEU:HB3	1.84	0.42
1:b:1144:VAL:HG11	1:b:1196:ILE:HD12	2.01	0.42
1:b:1170:MET:SD	1:b:1199:VAL:HG23	2.60	0.42
3:d:2949[A]:LYS:C	3:d:2949[A]:LYS:HZ3	2.17	0.42
3:d:2951[B]:ASP:CG	3:d:2952[B]:ALA:N	2.74	0.42
3:d:2988[B]:TRP:CZ3	3:d:2989[B]:HIS:CE1	3.07	0.42
3:d:3228[B]:VAL:CG2	3:d:3245[B]:PHE:CD2	3.02	0.42
1:A:177:VAL:HG11	1:A:358:TYR:CZ	2.54	0.42
1:A:792:MET:HE3	1:A:822:PHE:HE2	1.83	0.42
1:A:909:ILE:HG12	1:A:1084:PHE:HZ	1.85	0.42
1:A:1518:ASP:OD2	1:A:1521:ASN:HB2	2.19	0.42
2:B:2336:PHE:HA	2:B:2343:ASN:ND2	2.34	0.42
2:B:2904:ALA:HA	2:B:2905:PRO:HD2	1.95	0.42
3:C:2948[B]:ASP:HB3	3:C:2949[B]:LYS:C	2.44	0.42
3:C:2952[B]:ALA:CA	3:C:2956[B]:LYS:CB	2.89	0.42
3:C:2965[B]:LEU:CG	3:C:2974[B]:ALA:CB	2.85	0.42
3:C:3001[A]:LYS:H	3:C:3003[A]:LYS:HG3	1.83	0.42
3:C:3025[A]:VAL:CG2	3:C:3047[A]:ARG:NH1	2.73	0.42
3:C:3148[B]:ILE:O	3:C:3148[B]:ILE:HG22	2.17	0.42
3:C:3172[B]:SER:CA	3:L:3149[B]:ASN:O	2.66	0.42
3:C:3183[A]:LEU:N	3:C:3184[A]:ASN:CA	2.80	0.42
3:C:3196[B]:THR:OG1	3:C:3199[B]:GLN:OE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3299[B]:LEU:HB3	3:C:3300[B]:LEU:H	1.54	0.42
1:D:398:ARG:HA	1:D:399:PRO:HD3	1.90	0.42
2:E:2814:LYS:HD3	2:E:2814:LYS:HA	1.83	0.42
2:E:2879:LEU:HG	2:E:2901:LEU:HD11	2.02	0.42
3:F:2937[B]:ASN:CG	3:F:3006[B]:LYS:HD3	2.44	0.42
3:F:3001[A]:LYS:H	3:F:3003[A]:LYS:HG3	1.83	0.42
3:F:3211[B]:ASP:OD1	3:F:3211[B]:ASP:N	2.28	0.42
3:F:3218[A]:LEU:HD12	3:F:3218[A]:LEU:HA	1.78	0.42
3:F:3255[B]:PRO:CA	3:a:2965[B]:LEU:C	2.92	0.42
1:G:107:HIS:CE1	1:G:109:LEU:HB2	2.54	0.42
1:G:572:SER:HA	1:G:573:LYS:HA	1.54	0.42
1:G:1137:LYS:HA	1:G:1141:ARG:NH1	2.35	0.42
2:H:2317:LEU:HB3	2:H:2318:PRO:HD2	2.00	0.42
2:H:2402:GLY:HA3	2:H:2403:PHE:CD1	2.54	0.42
2:H:2651:GLN:HE21	2:H:2652:LYS:HD3	1.84	0.42
3:I:2952[A]:ALA:N	3:I:2953[A]:GLY:CA	2.71	0.42
3:I:3153[B]:LYS:CB	3:R:3158[B]:PHE:CB	2.76	0.42
3:I:3174[B]:GLY:N	3:R:3154[B]:PRO:CD	2.78	0.42
3:I:3183[A]:LEU:N	3:I:3184[A]:ASN:CA	2.80	0.42
3:I:3276[A]:ASP:C	3:I:3278[A]:HIS:N	2.75	0.42
1:J:95:THR:HB	1:J:156:LEU:HD13	2.01	0.42
1:J:403:TYR:O	1:J:658:TYR:HB3	2.20	0.42
1:J:904:HIS:O	1:J:907:ARG:HB3	2.19	0.42
1:J:1206:HIS:CE1	1:J:1209:ASP:HB2	2.54	0.42
2:K:2156:ARG:HD2	2:K:2357:VAL:HG12	2.01	0.42
3:L:2937[A]:ASN:CG	3:L:3006[A]:LYS:HD3	2.43	0.42
3:L:2969[A]:TYR:CD2	3:L:2971[A]:ASP:CG	2.98	0.42
1:M:133:LYS:HB3	1:M:134:VAL:H	1.48	0.42
1:M:518:LYS:O	1:M:520:PHE:HD1	2.01	0.42
1:M:982:LYS:N	1:M:983:PRO:HD3	2.34	0.42
1:M:1195:ASP:OD1	1:M:1197:THR:OG1	2.24	0.42
1:M:1210:LYS:CA	1:M:1211:TYR:HB2	2.46	0.42
1:M:1486:LEU:HD12	2:Q:2486:ILE:HG22	2.02	0.42
3:O:2969[A]:TYR:CD2	3:O:2971[A]:ASP:CG	2.97	0.42
3:O:2979[B]:GLN:HA	3:O:2979[B]:GLN:OE1	2.20	0.42
3:O:2989[A]:HIS:O	3:O:2990[A]:ARG:C	2.61	0.42
3:O:3135[A]:LYS:HB2	3:O:3141[A]:TYR:CD1	2.51	0.42
1:P:897:HIS:HD2	1:P:899:MET:HE1	1.84	0.42
1:P:1039:ASP:OD1	1:P:1041:ILE:HG12	2.18	0.42
2:Q:2637:VAL:HG11	1:S:111:ILE:HG23	2.02	0.42
3:R:2969[A]:TYR:CD2	3:R:2971[A]:ASP:CG	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:3245[B]:PHE:CD1	3:R:3245[B]:PHE:C	2.97	0.42
2:T:2179:ASP:HB3	2:T:2303:ARG:HH12	1.85	0.42
3:U:2974[B]:ALA:HB2	3:d:3220[B]:ARG:HD2	2.01	0.42
3:U:3133[A]:LEU:HD12	3:U:3133[A]:LEU:HA	1.86	0.42
3:U:3185[A]:TYR:CE2	3:U:3187[A]:TYR:HE2	2.31	0.42
3:U:3232[A]:VAL:HG21	3:U:3273[A]:LEU:CD1	2.50	0.42
1:V:426:LYS:HE3	1:V:435:GLU:OE2	2.19	0.42
1:V:464:LEU:HD22	1:V:622:HIS:HB3	2.02	0.42
1:V:760:ILE:HG21	1:V:777:TYR:CE2	2.52	0.42
1:V:1034:GLU:HB2	1:V:1180:SER:OG	2.20	0.42
1:V:1528:ASP:OD1	1:V:1528:ASP:N	2.53	0.42
2:W:2641:GLN:HA	2:W:2642:PRO:HD3	1.85	0.42
3:X:2979[A]:GLN:HA	3:X:2979[A]:GLN:OE1	2.19	0.42
3:X:3180[A]:TYR:CB	3:X:3183[A]:LEU:CD2	2.90	0.42
3:X:3299[A]:LEU:O	3:X:3300[A]:LEU:C	2.60	0.42
1:Y:142:ARG:O	1:Y:145:GLN:HG2	2.18	0.42
1:Y:170:HIS:O	1:Y:174:GLN:HG3	2.19	0.42
1:Y:282:ASN:OD1	1:Y:282:ASN:N	2.52	0.42
2:Z:2797:LYS:HA	2:Z:2800:LYS:HD3	2.02	0.42
3:a:2979[B]:GLN:CD	3:a:3155[B]:MET:CE	2.92	0.42
3:a:2989[B]:HIS:C	3:a:2991[B]:LEU:N	2.75	0.42
3:a:3013[A]:ASP:CG	3:a:3015[A]:THR:HG1	2.23	0.42
1:b:15:ILE:HG23	1:b:104:LEU:HD21	2.01	0.42
1:b:365:THR:O	1:b:369:LEU:HG	2.19	0.42
1:b:899:MET:HB3	1:b:1012:GLU:OE1	2.19	0.42
1:b:1125:SER:O	1:b:1129:LEU:HB2	2.19	0.42
1:b:1315:GLY:HA3	1:b:1601:TRP:CG	2.55	0.42
2:c:2856:ILE:HG22	2:c:2859:VAL:HB	2.01	0.42
3:d:2948[A]:ASP:HB3	3:d:2949[A]:LYS:C	2.43	0.42
3:d:2989[A]:HIS:O	3:d:2990[A]:ARG:C	2.61	0.42
3:d:3023[B]:ILE:HA	3:d:3026[B]:THR:HG1	1.84	0.42
3:d:3023[B]:ILE:C	3:d:3026[B]:THR:HG1	2.27	0.42
3:d:3104[B]:MET:SD	3:d:3110[B]:THR:CG2	3.06	0.42
3:d:3245[A]:PHE:CD1	3:d:3245[A]:PHE:C	2.97	0.42
4:q:1:NAG:C4	4:q:2:NAG:N2	2.80	0.42
1:A:882:TRP:CD1	1:A:1086:LEU:HD13	2.54	0.42
1:A:977:GLU:OE1	1:A:978:ALA:N	2.49	0.42
2:B:2128:LEU:O	2:B:2130:PRO:HD3	2.20	0.42
2:B:2854:MET:HE3	2:B:2854:MET:HB2	1.80	0.42
3:C:2969[B]:TYR:CD2	3:C:2971[B]:ASP:CG	2.98	0.42
3:C:2969[B]:TYR:HH	3:L:3120[B]:HIS:CD2	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3133[B]:LEU:HD13	3:C:3197[B]:ILE:HG23	2.02	0.42
3:C:3156[B]:MET:C	3:L:3153[B]:LYS:NZ	2.72	0.42
1:D:109:LEU:HG	1:D:119:LYS:HB3	2.01	0.42
1:D:177:VAL:HG11	1:D:358:TYR:CZ	2.55	0.42
1:D:851:MET:HE1	1:D:940:ALA:HB3	2.01	0.42
1:D:956:PRO:HB2	1:D:957:ASN:C	2.44	0.42
1:D:1575:PRO:HA	1:D:1581:GLU:O	2.20	0.42
2:E:2092:VAL:HG23	2:E:2177:TYR:O	2.20	0.42
2:E:2128:LEU:O	2:E:2130:PRO:HD3	2.19	0.42
3:F:2977[B]:CYS:HB3	3:a:2982[B]:MET:HE3	1.97	0.42
3:F:2979[A]:GLN:HA	3:F:2979[A]:GLN:OE1	2.19	0.42
3:F:3024[B]:LEU:CD1	3:F:3024[B]:LEU:C	2.85	0.42
3:F:3028[A]:PRO:HG2	3:F:3029[A]:LYS:HG3	2.00	0.42
3:F:3048[A]:ASP:HB3	3:F:3099[A]:PRO:HD2	2.01	0.42
3:F:3222[A]:ILE:CD1	3:F:3223[A]:GLY:N	2.73	0.42
3:F:3245[B]:PHE:CD1	3:F:3245[B]:PHE:C	2.97	0.42
3:F:3299[A]:LEU:HB3	3:F:3300[A]:LEU:H	1.54	0.42
1:G:516:TRP:CD1	1:G:579:LEU:HD13	2.54	0.42
1:G:603:HIS:O	1:G:606:ILE:HG22	2.19	0.42
1:G:673:PHE:HB3	1:G:677:LEU:HB2	2.01	0.42
1:G:858:MET:HG3	1:G:959:PHE:CZ	2.54	0.42
1:G:1275:ARG:HH22	1:G:1357:ARG:HH11	1.65	0.42
1:G:1323:HIS:CD2	1:G:1458:HIS:CE1	3.07	0.42
2:H:2132:CYS:CB	2:H:2143:CYS:HA	2.47	0.42
2:H:2234:GLN:HG3	2:H:2235:PRO:HD2	2.02	0.42
2:H:2573:TYR:HE2	2:H:2707:PHE:CE2	2.37	0.42
3:I:2969[A]:TYR:CD2	3:I:2971[A]:ASP:CG	2.97	0.42
3:I:2979[A]:GLN:CD	3:I:3155[A]:MET:CE	2.92	0.42
3:I:3141[A]:TYR:CD2	3:I:3141[A]:TYR:C	2.86	0.42
3:I:3300[A]:LEU:HD23	3:I:3300[A]:LEU:H	1.83	0.42
1:J:704:ASP:OD1	1:J:704:ASP:N	2.51	0.42
1:J:714:ARG:HH11	1:J:837:HIS:CE1	2.37	0.42
1:J:740:THR:HG21	4:u:1:NAG:O6	2.20	0.42
1:J:907:ARG:HD3	1:J:1050:ASP:OD1	2.19	0.42
1:J:1156:LEU:HB2	1:J:1176:TYR:CE1	2.55	0.42
1:J:1196:ILE:O	1:J:1199:VAL:HG13	2.20	0.42
2:K:2504:ARG:HD2	2:K:2775:GLY:O	2.20	0.42
2:K:2545:SER:O	2:K:2558:CYS:N	2.48	0.42
3:L:3133[B]:LEU:HD12	3:L:3133[B]:LEU:HA	1.85	0.42
3:L:3151[A]:LEU:CB	3:L:3175[A]:TYR:CE2	2.86	0.42
3:L:3245[A]:PHE:CD1	3:L:3245[A]:PHE:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:447:MET:HE2	1:M:447:MET:HB3	1.86	0.42
1:M:535:PRO:O	1:M:538:LYS:HE3	2.19	0.42
1:M:1308:VAL:HG11	8:O:2:NAG:O6	2.19	0.42
1:M:1473:ARG:HG3	1:M:1479:TYR:CG	2.54	0.42
2:N:2178:TRP:CZ3	2:N:2188:PRO:HD3	2.55	0.42
2:N:2870:LEU:HA	2:N:2877:ILE:HD11	2.00	0.42
3:O:2937[A]:ASN:CG	3:O:3006[A]:LYS:HD3	2.43	0.42
3:O:2937[B]:ASN:CG	3:O:3006[B]:LYS:HD3	2.43	0.42
3:O:2938[B]:LEU:O	3:O:2939[B]:ARG:C	2.58	0.42
3:O:2946[B]:GLN:CD	3:O:2947[B]:ALA:N	2.72	0.42
3:O:2951[A]:ASP:CG	3:O:2952[A]:ALA:N	2.74	0.42
3:O:2961[A]:HIS:HB2	3:O:2992[A]:TYR:HE2	1.80	0.42
3:O:3048[B]:ASP:HB3	3:O:3099[B]:PRO:HD2	2.01	0.42
3:O:3154[B]:PRO:HD2	3:X:3176[B]:LYS:HE2	1.86	0.42
3:O:3232[B]:VAL:HG21	3:O:3273[B]:LEU:CD1	2.50	0.42
1:P:77:GLU:O	1:P:81:VAL:HG23	2.19	0.42
1:P:450:LYS:HZ1	1:P:1273:SER:CB	2.29	0.42
1:P:1319:PHE:CE2	1:P:1424:GLU:HG3	2.55	0.42
2:Q:2562:GLY:H	2:Q:2846:TRP:HB2	1.85	0.42
2:Q:2783:PHE:HB2	2:Q:2791:LEU:HD11	2.02	0.42
2:Q:2808:PHE:CE2	2:Q:2899:PRO:HG3	2.54	0.42
2:Q:2889:ALA:H	2:Q:2890:VAL:HA	1.82	0.42
3:R:2938[A]:LEU:O	3:R:2939[A]:ARG:C	2.58	0.42
3:R:2989[B]:HIS:O	3:R:2990[B]:ARG:C	2.61	0.42
3:R:3083[A]:ILE:HD11	3:R:3260[A]:ARG:CG	2.49	0.42
3:R:3093[B]:HIS:HB2	3:R:3248[B]:LEU:CD1	2.48	0.42
3:R:3217[A]:PHE:CD2	3:R:3300[A]:LEU:HD12	2.53	0.42
1:S:401:VAL:HG23	1:S:661:ASN:HB3	2.00	0.42
1:S:633:HIS:O	1:S:636:GLN:HB3	2.19	0.42
1:S:980:TYR:CZ	1:S:1021:LEU:HD22	2.54	0.42
2:T:2606:LEU:HD22	2:T:2706:ILE:HG12	2.02	0.42
2:T:2731:PRO:HB3	2:T:2734:LYS:HG3	1.99	0.42
2:T:2819:VAL:HG13	2:T:2883:ILE:HG12	2.02	0.42
3:U:3082[B]:GLU:OE2	3:d:2970[B]:PRO:CB	2.67	0.42
3:U:3245[B]:PHE:CD1	3:U:3245[B]:PHE:C	2.97	0.42
1:V:904:HIS:HE1	1:V:1106:PHE:CZ	2.37	0.42
1:V:975:PRO:HG2	1:V:1024:GLY:H	1.84	0.42
2:W:2252:GLU:CD	2:W:2393:ARG:HH12	2.26	0.42
2:W:2670:CYS:N	2:W:2737:CYS:SG	2.93	0.42
2:W:2830:GLN:HG2	2:W:2863:ARG:CZ	2.50	0.42
3:X:2995[A]:GLN:CG	3:X:3168[A]:THR:HG21	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3034[B]:HIS:HB3	3:X:3035[B]:HIS:CE1	2.50	0.42
3:X:3041[B]:ALA:O	3:X:3042[B]:ASP:HB2	2.20	0.42
3:X:3083[B]:ILE:HD11	3:X:3260[B]:ARG:CG	2.49	0.42
3:X:3133[A]:LEU:HD13	3:X:3197[A]:ILE:HG23	2.02	0.42
3:X:3293[A]:LYS:CB	3:X:3294[A]:SER:CA	2.96	0.42
1:Y:48:LYS:HE3	1:Y:54:THR:HG22	2.02	0.42
1:Y:1263:LEU:HD11	1:Y:1358:LEU:HD22	2.01	0.42
2:Z:2431:GLY:O	2:Z:2434:GLU:HG2	2.19	0.42
2:Z:2647:LEU:HD12	2:Z:2647:LEU:HA	1.75	0.42
2:Z:2874:ASP:HA	2:Z:2875:SER:C	2.45	0.42
3:a:2969[B]:TYR:CD2	3:a:2971[B]:ASP:CG	2.97	0.42
3:a:3023[B]:ILE:HA	3:a:3026[B]:THR:HG1	1.82	0.42
1:b:19:GLN:HG3	1:b:122:VAL:HG22	2.02	0.42
1:b:1137:LYS:HA	1:b:1141:ARG:NH1	2.34	0.42
2:c:2400:LEU:HB2	2:c:2439:PHE:HD2	1.84	0.42
3:d:2969[B]:TYR:CD2	3:d:2971[B]:ASP:CG	2.98	0.42
3:d:2976[A]:ALA:O	3:d:2978[A]:CYS:N	2.46	0.42
3:d:2979[A]:GLN:HA	3:d:2979[A]:GLN:OE1	2.19	0.42
3:d:2979[A]:GLN:CD	3:d:3155[A]:MET:CE	2.92	0.42
3:d:2995[A]:GLN:O	3:d:2996[A]:MET:C	2.63	0.42
3:d:3093[B]:HIS:HD2	3:d:3248[B]:LEU:CD2	2.31	0.42
3:d:3218[B]:LEU:HD13	3:d:3261[B]:LEU:HD23	2.01	0.42
3:d:3232[A]:VAL:HG21	3:d:3273[A]:LEU:CD1	2.50	0.42
3:d:3232[B]:VAL:HG21	3:d:3273[B]:LEU:CD1	2.50	0.42
1:A:561:ARG:NH2	1:A:629:MET:HB2	2.35	0.42
1:A:899:MET:HE2	1:A:1186:TRP:CE2	2.55	0.42
1:A:979:LEU:CD2	1:A:1021:LEU:HD22	2.50	0.42
1:A:1140:ASN:OD1	1:A:1239:GLY:N	2.52	0.42
2:B:2581:MET:HE2	2:B:2581:MET:HB3	1.78	0.42
3:C:2937[A]:ASN:CG	3:C:3006[A]:LYS:HD3	2.44	0.42
3:C:2965[B]:LEU:HB2	3:L:3221[B]:ALA:HA	0.84	0.42
3:C:2966[B]:SER:HB2	3:C:2977[B]:CYS:H	1.85	0.42
3:C:2969[B]:TYR:CD2	3:C:2971[B]:ASP:N	2.73	0.42
3:C:3148[A]:ILE:HG22	3:C:3152[A]:LYS:HE3	2.01	0.42
3:C:3152[B]:LYS:CG	3:L:3172[B]:SER:OG	2.66	0.42
3:C:3172[B]:SER:OG	3:L:3152[B]:LYS:HB2	2.11	0.42
3:C:3196[A]:THR:OG1	3:C:3199[A]:GLN:OE1	2.38	0.42
1:D:1438:ASP:OD1	1:D:1439:VAL:N	2.52	0.42
2:E:2403:PHE:N	2:E:2403:PHE:CD1	2.85	0.42
2:E:2544:GLY:HA3	2:E:2699:MET:O	2.18	0.42
2:E:2550:THR:N	2:E:2554:PRO:HD3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2568:HIS:HE1	2:E:2742:MET:SD	2.43	0.42
3:F:2975[B]:PHE:HE1	3:a:3107[B]:LEU:HG	1.81	0.42
3:F:2982[B]:MET:HE2	3:a:2966[B]:SER:CA	2.49	0.42
3:F:3028[A]:PRO:HG2	3:F:3029[A]:LYS:HG2	2.02	0.42
3:F:3146[A]:CYS:O	3:F:3146[A]:CYS:SG	2.78	0.42
3:F:3151[B]:LEU:O	3:a:3154[B]:PRO:CB	2.67	0.42
3:F:3191[A]:ASN:ND2	3:F:3191[A]:ASN:N	2.60	0.42
1:G:127:GLU:HG2	1:G:135:THR:HG23	2.02	0.42
1:G:304:ALA:HB1	1:G:306:PHE:CE1	2.51	0.42
2:H:2746:MET:HG3	2:H:2765:PRO:HD3	2.02	0.42
2:H:2808:PHE:HB3	2:H:2810:LEU:HD21	2.01	0.42
2:H:2888:GLY:HA2	2:H:2889:ALA:HA	1.86	0.42
3:I:2969[B]:TYR:CD2	3:I:2971[B]:ASP:CG	2.98	0.42
3:I:2983[B]:VAL:CG2	3:R:3162[B]:ASP:N	2.65	0.42
3:I:2985[B]:PHE:CE2	3:R:2969[B]:TYR:O	2.73	0.42
3:I:3090[B]:ASN:HB3	3:R:2971[B]:ASP:O	2.20	0.42
3:I:3146[A]:CYS:O	3:I:3146[A]:CYS:SG	2.78	0.42
3:I:3196[B]:THR:OG1	3:I:3199[B]:GLN:OE1	2.37	0.42
3:I:3218[B]:LEU:HD12	3:I:3218[B]:LEU:HA	1.78	0.42
1:J:468:CYS:HB2	1:J:477:VAL:O	2.20	0.42
1:J:1034:GLU:CB	1:J:1182:ASN:HD21	2.33	0.42
2:K:2667:GLU:HB3	2:K:2730:LEU:CD2	2.50	0.42
2:K:2805:PHE:HB2	2:K:2902:ILE:CG1	2.50	0.42
3:L:2979[A]:GLN:HA	3:L:2979[A]:GLN:OE1	2.19	0.42
3:L:3171[A]:HIS:O	3:L:3172[A]:SER:C	2.63	0.42
1:M:17:ASN:O	1:M:21:SER:OG	2.35	0.42
1:M:282:ASN:OD1	1:M:282:ASN:N	2.51	0.42
1:M:843:VAL:HG22	1:M:928:TYR:O	2.20	0.42
1:M:1146:PHE:HZ	1:M:1159:TYR:CG	2.38	0.42
1:M:1427:HIS:HE1	1:M:1458:HIS:CD2	2.38	0.42
2:N:2168:ARG:CZ	2:Q:2515:ARG:HD2	2.49	0.42
2:N:2664:PHE:HB3	2:N:2795:ILE:HD11	2.01	0.42
3:O:2970[B]:PRO:HD2	3:X:2991[B]:LEU:HD22	2.01	0.42
3:O:3023[B]:ILE:O	3:O:3026[B]:THR:OG1	2.34	0.42
3:O:3024[B]:LEU:CD1	3:O:3024[B]:LEU:C	2.85	0.42
3:O:3251[B]:ASP:HB2	3:X:2968[B]:GLN:CG	2.49	0.42
2:Q:2562:GLY:H	2:Q:2846:TRP:CB	2.33	0.42
2:Q:2780:HIS:ND1	2:Q:2782:ASN:OD1	2.53	0.42
3:R:2937[A]:ASN:CG	3:R:3006[A]:LYS:HD3	2.44	0.42
1:S:630:PHE:O	1:S:633:HIS:HB3	2.19	0.42
1:S:647:LEU:HD13	1:S:651:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:2181:THR:HB	2:T:2373:MET:SD	2.60	0.42
2:T:2884:LYS:HG2	2:T:2891:LEU:HB3	2.01	0.42
3:U:2979[B]:GLN:CD	3:U:3155[B]:MET:CE	2.92	0.42
3:U:3025[B]:VAL:CG2	3:U:3047[B]:ARG:NH1	2.73	0.42
3:U:3048[A]:ASP:HB3	3:U:3099[A]:PRO:HD2	2.01	0.42
3:U:3133[A]:LEU:HD13	3:U:3197[A]:ILE:HG23	2.02	0.42
3:U:3171[A]:HIS:O	3:U:3172[A]:SER:C	2.63	0.42
3:U:3183[B]:LEU:N	3:U:3184[B]:ASN:CA	2.80	0.42
3:U:3220[B]:ARG:CB	3:d:2973[B]:THR:CG2	2.80	0.42
1:V:386:ILE:HD13	1:V:386:ILE:O	2.20	0.42
1:V:387:ASN:OD1	1:V:387:ASN:N	2.41	0.42
1:V:563:ILE:HG13	1:V:614:GLU:HG2	2.02	0.42
1:V:630:PHE:CE2	1:V:634:HIS:CE1	3.08	0.42
1:V:938:LEU:H	1:V:938:LEU:HD12	1.85	0.42
1:V:1323:HIS:CD2	9:V:5004:CUO:O1	2.72	0.42
2:W:2275:GLY:HA2	2:W:2281:SER:HB2	2.01	0.42
2:W:2279:LEU:HD12	2:W:2284:HIS:HD2	1.84	0.42
3:X:2937[B]:ASN:CG	3:X:3006[B]:LYS:HD3	2.43	0.42
1:Y:51:ASP:HA	1:Y:52:GLY:HA3	1.70	0.42
1:Y:177:VAL:O	1:Y:181:PRO:HD3	2.20	0.42
1:Y:668:MET:HA	1:Y:668:MET:HE2	2.02	0.42
1:Y:880:THR:O	1:Y:882:TRP:N	2.51	0.42
1:Y:915:ASN:O	1:Y:919:ARG:N	2.31	0.42
1:Y:1327:VAL:O	1:Y:1331:GLU:HB3	2.20	0.42
2:Z:2643:GLU:HA	2:Z:2646:ALA:HB3	2.00	0.42
2:Z:2678:VAL:HG11	2:Z:2852:TYR:CE2	2.55	0.42
3:a:2952[B]:ALA:CA	3:a:2956[B]:LYS:CB	2.89	0.42
3:a:2971[B]:ASP:CG	3:a:2973[B]:THR:HG1	2.10	0.42
3:a:3028[A]:PRO:HG2	3:a:3029[A]:LYS:HG2	2.02	0.42
3:a:3135[A]:LYS:HB2	3:a:3141[A]:TYR:CD1	2.52	0.42
1:b:543:ASN:HA	1:b:544:PRO:HD3	1.81	0.42
2:c:2489:ILE:HA	2:c:2490:PRO:HD3	1.87	0.42
3:d:2937[B]:ASN:CG	3:d:3006[B]:LYS:HD3	2.43	0.42
3:d:3041[B]:ALA:O	3:d:3042[B]:ASP:HB2	2.20	0.42
3:d:3133[B]:LEU:HD13	3:d:3197[B]:ILE:HG23	2.02	0.42
3:d:3293[B]:LYS:CB	3:d:3294[B]:SER:CA	2.96	0.42
1:A:1077:LEU:HB3	1:A:1103:PHE:CE1	2.55	0.42
1:A:1542:ARG:O	1:A:1546:LYS:HG2	2.19	0.42
2:B:2718:TRP:HZ3	2:B:2721:TRP:CE3	2.37	0.42
3:C:2963[B]:MET:C	3:L:3255[B]:PRO:HG3	2.45	0.42
3:C:2989[B]:HIS:NE2	3:L:2969[B]:TYR:CA	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3155[B]:MET:O	3:L:3150[B]:LYS:O	2.37	0.42
3:C:3232[B]:VAL:HG21	3:C:3273[B]:LEU:CD1	2.50	0.42
1:D:21:SER:HB2	1:D:83:HIS:O	2.19	0.42
1:D:276:PHE:HB2	1:D:279:LEU:HD23	2.02	0.42
1:D:682:LYS:O	1:D:685:GLU:HB3	2.19	0.42
2:E:2116:SER:HA	2:E:2121:THR:HG21	2.02	0.42
2:E:2333:LEU:HB3	2:E:2336:PHE:HD2	1.84	0.42
3:F:2932[A]:PRO:CA	3:F:2935[A]:ILE:CD1	2.85	0.42
3:F:2969[A]:TYR:CD2	3:F:2971[A]:ASP:CG	2.97	0.42
3:F:2969[B]:TYR:CD2	3:F:2971[B]:ASP:CG	2.98	0.42
3:F:3034[A]:HIS:HB3	3:F:3035[A]:HIS:CE1	2.50	0.42
3:F:3196[A]:THR:OG1	3:F:3199[A]:GLN:OE1	2.38	0.42
3:F:3252[B]:TYR:O	3:a:2976[B]:ALA:CB	2.68	0.42
3:F:3252[B]:TYR:CD2	3:a:3108[B]:HIS:CE1	3.08	0.42
1:G:428:ILE:HG13	1:G:513:TYR:O	2.20	0.42
1:G:483:GLY:HA2	1:G:773:PHE:CZ	2.54	0.42
1:G:1028:VAL:HA	1:G:1035:TYR:HD2	1.85	0.42
1:G:1245:GLU:HG2	2:K:2729:LYS:O	2.20	0.42
1:G:1638:SER:OG	1:G:1639:LYS:N	2.53	0.42
2:H:2129:PRO:O	2:H:2131:LEU:HD23	2.20	0.42
2:H:2667:GLU:HG2	2:H:2728:ARG:NH2	2.34	0.42
3:I:2933[A]:SER:CA	3:I:2936[A]:GLU:HB3	2.48	0.42
3:I:2979[B]:GLN:HA	3:I:2979[B]:GLN:OE1	2.20	0.42
3:I:2981[B]:GLY:C	3:R:2966[B]:SER:O	2.62	0.42
3:I:2982[B]:MET:HE1	3:R:3157[B]:PRO:HD3	2.00	0.42
3:I:2988[A]:TRP:CZ3	3:I:2989[A]:HIS:CE1	3.07	0.42
3:I:3023[A]:ILE:HA	3:I:3026[A]:THR:HG1	1.83	0.42
3:I:3048[B]:ASP:HB3	3:I:3099[B]:PRO:HD2	2.01	0.42
3:I:3083[A]:ILE:HD11	3:I:3260[A]:ARG:CG	2.49	0.42
3:I:3146[B]:CYS:O	3:I:3146[B]:CYS:SG	2.78	0.42
3:I:3245[B]:PHE:CD1	3:I:3245[B]:PHE:C	2.97	0.42
1:J:499:GLU:HG3	1:J:511:VAL:H	1.85	0.42
1:J:872:GLN:O	1:J:875:ALA:HB3	2.19	0.42
1:J:1019:HIS:ND1	1:J:1030:MET:HE2	2.34	0.42
2:K:2758:THR:O	2:K:2762:VAL:HG22	2.20	0.42
3:L:2939[A]:ARG:CB	3:L:3032[A]:PRO:HG2	2.44	0.42
3:L:2948[A]:ASP:HB3	3:L:2949[A]:LYS:C	2.43	0.42
3:L:3083[B]:ILE:HD11	3:L:3260[B]:ARG:CG	2.49	0.42
3:L:3133[B]:LEU:HD13	3:L:3197[B]:ILE:HG23	2.02	0.42
3:L:3232[B]:VAL:HG21	3:L:3273[B]:LEU:CD1	2.50	0.42
1:M:187:GLY:HA2	1:M:193:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:492:ARG:HG3	1:M:638:ASP:OD1	2.18	0.42
1:M:639:ARG:NH2	1:M:707:PHE:O	2.53	0.42
1:M:870:TYR:HA	1:M:873:VAL:HG12	2.02	0.42
1:M:1171:LYS:HG2	1:M:1173:GLY:H	1.85	0.42
1:M:1243:PHE:O	1:M:1476:LYS:HD3	2.19	0.42
3:O:2969[B]:TYR:CD2	3:O:2971[B]:ASP:CG	2.98	0.42
3:O:2979[B]:GLN:CD	3:O:3155[B]:MET:CE	2.92	0.42
3:O:3001[B]:LYS:H	3:O:3003[B]:LYS:HG3	1.83	0.42
3:O:3048[A]:ASP:HB3	3:O:3099[A]:PRO:HD2	2.01	0.42
3:O:3108[B]:HIS:CG	3:X:2969[B]:TYR:O	2.70	0.42
3:O:3133[B]:LEU:HD13	3:O:3197[B]:ILE:HG23	2.02	0.42
3:O:3157[B]:PRO:O	3:X:3148[B]:ILE:C	2.61	0.42
3:O:3159[B]:SER:CB	3:X:3151[B]:LEU:HB2	2.42	0.42
3:O:3196[A]:THR:OG1	3:O:3199[A]:GLN:OE1	2.38	0.42
3:O:3228[A]:VAL:CG2	3:O:3245[A]:PHE:CD2	3.02	0.42
3:O:3229[A]:ASN:N	3:O:3286[A]:THR:O	2.52	0.42
3:O:3232[A]:VAL:HG21	3:O:3273[A]:LEU:CD1	2.49	0.42
3:O:3299[A]:LEU:O	3:O:3300[A]:LEU:C	2.60	0.42
1:P:131:GLU:OE2	1:P:192:HIS:HE1	2.02	0.42
1:P:929:TRP:CE3	1:P:939:PRO:HD3	2.54	0.42
1:P:1035:TYR:O	1:P:1038:PHE:HD1	2.02	0.42
1:P:1086:LEU:HD13	1:P:1090:ILE:HD11	2.01	0.42
2:Q:2680:HIS:CE1	2:Q:2711:HIS:CE1	3.08	0.42
3:R:2946[B]:GLN:CD	3:R:2947[B]:ALA:N	2.72	0.42
3:R:2965[A]:LEU:CG	3:R:2974[A]:ALA:CB	2.85	0.42
3:R:2966[A]:SER:HB2	3:R:2977[A]:CYS:H	1.85	0.42
3:R:3001[A]:LYS:H	3:R:3003[A]:LYS:HG3	1.83	0.42
3:R:3014[B]:TRP:CH2	3:R:3123[B]:THR:HG23	2.53	0.42
3:R:3028[A]:PRO:HG2	3:R:3029[A]:LYS:HG2	2.02	0.42
3:R:3180[A]:TYR:CB	3:R:3183[A]:LEU:CD2	2.90	0.42
3:R:3185[A]:TYR:HE2	3:R:3187[A]:TYR:CD2	2.36	0.42
1:S:446:PHE:CZ	1:S:455:TYR:HA	2.55	0.42
1:S:904:HIS:HB2	1:S:1081:MET:HE1	2.02	0.42
2:T:2234:GLN:HG3	2:T:2235:PRO:HD2	2.00	0.42
2:T:2442:LEU:HG	1:V:1604:ASP:HB2	2.01	0.42
3:U:2946[B]:GLN:CD	3:U:2947[B]:ALA:N	2.72	0.42
3:U:2973[B]:THR:OG1	3:d:3249[B]:GLY:HA3	2.19	0.42
3:U:2979[A]:GLN:HA	3:U:2979[A]:GLN:OE1	2.19	0.42
3:U:3156[B]:MET:HG2	3:d:3150[B]:LYS:HD3	1.48	0.42
3:U:3299[B]:LEU:O	3:U:3300[B]:LEU:C	2.60	0.42
1:V:452:ILE:HA	1:V:1368:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:995:ILE:O	1:V:999:LEU:HD22	2.20	0.42
1:V:1392:ASP:H	1:V:1435:GLY:HA2	1.85	0.42
2:W:2533:ASP:HB2	2:W:2755:PRO:HG3	2.01	0.42
2:W:2625:LEU:HD23	2:W:2625:LEU:H	1.85	0.42
3:X:2966[B]:SER:HB2	3:X:2977[B]:CYS:H	1.85	0.42
3:X:2979[B]:GLN:OE1	3:X:2979[B]:GLN:HA	2.19	0.42
3:X:2989[B]:HIS:C	3:X:2991[B]:LEU:N	2.75	0.42
3:X:3146[B]:CYS:SG	3:X:3146[B]:CYS:O	2.78	0.42
3:X:3232[A]:VAL:HG21	3:X:3273[A]:LEU:CD1	2.50	0.42
3:X:3245[B]:PHE:CD1	3:X:3245[B]:PHE:C	2.97	0.42
1:Y:217:PHE:O	1:Y:220:TRP:HB3	2.19	0.42
1:Y:486:THR:HA	1:Y:489:HIS:HD1	1.84	0.42
1:Y:1172:ALA:CB	1:Y:1196:ILE:HG13	2.50	0.42
2:Z:2177:TYR:HB2	2:Z:2300:ASN:HB2	2.01	0.42
3:a:2979[A]:GLN:CD	3:a:3155[A]:MET:CE	2.92	0.42
3:a:2988[A]:TRP:CZ3	3:a:2989[A]:HIS:CE1	3.07	0.42
3:a:3148[A]:ILE:HG22	3:a:3152[A]:LYS:HE3	2.01	0.42
3:a:3276[A]:ASP:C	3:a:3278[A]:HIS:N	2.75	0.42
1:b:435:GLU:HB3	1:b:509:ILE:HD11	2.01	0.42
1:b:579:LEU:HD12	1:b:579:LEU:H	1.84	0.42
1:b:639:ARG:HB2	1:b:703:TYR:CE2	2.55	0.42
1:b:949:ASP:H	1:b:953:GLU:H	1.68	0.42
1:b:977:GLU:HB3	1:b:979:LEU:CD2	2.49	0.42
1:b:979:LEU:HD23	1:b:980:TYR:CD2	2.55	0.42
1:b:989:THR:HG22	1:b:991:LEU:H	1.84	0.42
1:b:1550:ARG:HD3	1:b:1550:ARG:HA	1.72	0.42
2:c:2244:PHE:CZ	2:c:2376:MET:HE1	2.55	0.42
2:c:2261:VAL:O	2:c:2265:ILE:HG13	2.19	0.42
2:c:2791:LEU:HA	2:c:2791:LEU:HD23	1.82	0.42
3:d:3041[A]:ALA:O	3:d:3042[A]:ASP:HB2	2.20	0.42
3:d:3120[B]:HIS:HA	3:d:3123[B]:THR:HG1	1.82	0.42
3:d:3146[A]:CYS:O	3:d:3146[A]:CYS:SG	2.78	0.42
3:d:3196[A]:THR:OG1	3:d:3199[A]:GLN:OE1	2.37	0.42
3:d:3232[B]:VAL:HG21	3:d:3273[B]:LEU:HD11	2.00	0.42
1:A:1023:GLY:HA2	1:A:1029:SER:HB3	2.00	0.42
1:A:1030:MET:HE2	1:A:1030:MET:HB3	1.98	0.42
1:A:1067:TYR:CD1	1:A:1067:TYR:N	2.87	0.42
2:B:2089:ARG:HD2	2:B:2175:VAL:O	2.20	0.42
2:B:2726:LYS:HB2	2:B:2726:LYS:HE3	1.84	0.42
2:B:2830:GLN:HB2	2:B:2863:ARG:NH2	2.33	0.42
3:C:2966[A]:SER:HB2	3:C:2977[A]:CYS:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2988[B]:TRP:CZ3	3:C:2989[B]:HIS:CE1	3.07	0.42
3:C:3048[A]:ASP:HB3	3:C:3099[A]:PRO:HD2	2.01	0.42
3:C:3113[A]:ASP:OD2	3:C:3115[A]:LEU:HB2	2.20	0.42
3:C:3152[B]:LYS:CB	3:L:3172[B]:SER:OG	2.67	0.42
3:C:3218[B]:LEU:HD13	3:C:3261[B]:LEU:HD23	2.01	0.42
3:C:3252[B]:TYR:HB2	3:L:3253[B]:GLU:CB	2.43	0.42
1:D:187:GLY:HA3	1:D:195:SER:HB3	2.02	0.42
1:D:205:LEU:HD23	1:D:205:LEU:HA	1.88	0.42
1:D:597:VAL:O	1:D:601:VAL:HG12	2.19	0.42
1:D:639:ARG:HB2	1:D:703:TYR:CE2	2.55	0.42
1:D:1319:PHE:CZ	1:D:1424:GLU:HG3	2.55	0.42
1:D:1636:ASN:OD1	4:m:1:NAG:C7	2.67	0.42
2:E:2447:ILE:O	2:E:2450:ILE:HG22	2.20	0.42
3:F:3154[B]:PRO:HD2	3:a:3155[B]:MET:HG3	1.85	0.42
3:F:3182[A]:GLN:H	3:F:3182[A]:GLN:HG2	1.56	0.42
3:F:3293[B]:LYS:CG	3:F:3294[B]:SER:CB	2.98	0.42
1:G:105:VAL:CG1	1:G:123:PHE:HB3	2.48	0.42
1:G:127:GLU:OE2	1:G:134:VAL:HG13	2.19	0.42
1:G:212:ASN:O	1:G:215:ARG:HB3	2.19	0.42
1:G:227:ARG:HA	1:G:228:GLY:HA2	1.85	0.42
1:G:838:ARG:NH1	1:G:915:ASN:OD1	2.50	0.42
2:H:2302:ASP:OD2	2:H:2366:TYR:OH	2.30	0.42
2:H:2303:ARG:NH2	2:H:2372:GLU:O	2.53	0.42
2:H:2656:LEU:HD23	2:H:2656:LEU:HA	1.81	0.42
3:I:2937[B]:ASN:CB	3:I:3006[B]:LYS:CE	2.86	0.42
3:I:2956[A]:LYS:O	3:I:2959[A]:SER:OG	2.33	0.42
3:I:2961[B]:HIS:ND1	3:R:2969[B]:TYR:CD1	2.72	0.42
3:I:3041[A]:ALA:O	3:I:3042[A]:ASP:HB2	2.20	0.42
3:I:3041[B]:ALA:O	3:I:3042[B]:ASP:HB2	2.20	0.42
3:I:3149[B]:ASN:HD22	3:R:3163[B]:ASN:CA	2.31	0.42
3:I:3171[B]:HIS:O	3:I:3172[B]:SER:C	2.63	0.42
3:I:3196[A]:THR:OG1	3:I:3199[A]:GLN:OE1	2.38	0.42
1:J:1166:THR:N	1:J:1167:ASP:HA	2.34	0.42
1:J:1286:ARG:HA	1:J:1286:ARG:HD3	1.82	0.42
1:J:1427:HIS:HD1	1:J:1461:VAL:HG21	1.85	0.42
2:K:2849:ASP:HB3	2:K:2850:ARG:NH1	2.34	0.42
2:K:2888:GLY:HA2	2:K:2889:ALA:HA	1.83	0.42
2:K:2898:LYS:H	2:K:2898:LYS:HG3	1.47	0.42
3:L:3001[A]:LYS:H	3:L:3003[A]:LYS:HG3	1.83	0.42
3:L:3001[B]:LYS:H	3:L:3003[B]:LYS:HG3	1.83	0.42
3:L:3146[A]:CYS:O	3:L:3146[A]:CYS:SG	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3183[B]:LEU:N	3:L:3184[B]:ASN:CA	2.80	0.42
1:M:415:VAL:CB	1:M:697:ALA:HB2	2.50	0.42
1:M:1392:ASP:H	1:M:1435:GLY:HA2	1.84	0.42
2:N:2235:PRO:HG2	2:Q:2097:LEU:HD12	2.02	0.42
2:N:2764:THR:HA	2:N:2765:PRO:HD3	1.95	0.42
3:O:2961[B]:HIS:HB2	3:O:2992[B]:TYR:HE2	1.81	0.42
3:O:3041[B]:ALA:O	3:O:3042[B]:ASP:HB2	2.20	0.42
3:O:3096[A]:VAL:CG1	3:O:3115[A]:LEU:CD1	2.86	0.42
3:O:3148[A]:ILE:HG22	3:O:3152[A]:LYS:HE3	2.01	0.42
3:O:3154[B]:PRO:HG3	3:X:3175[B]:TYR:CG	2.51	0.42
3:O:3232[A]:VAL:HG21	3:O:3273[A]:LEU:HD11	2.00	0.42
3:O:3232[B]:VAL:HG21	3:O:3273[B]:LEU:HD11	2.00	0.42
3:O:3285[A]:VAL:CG2	3:O:3286[A]:THR:H	2.27	0.42
1:P:353:ASN:HD22	1:P:772:ARG:NH2	2.17	0.42
1:P:416:ASN:ND2	1:P:416:ASN:H	2.17	0.42
1:P:990:HIS:O	1:P:991:LEU:HB2	2.20	0.42
1:P:1562:ILE:HG22	1:P:1563:LYS:N	2.35	0.42
2:Q:2128:LEU:HB2	2:Q:2286:HIS:HB3	2.02	0.42
2:Q:2353:LYS:HB2	2:Q:2356:ASP:OD2	2.19	0.42
2:Q:2545:SER:HA	2:Q:2546:LEU:CB	2.49	0.42
2:Q:2811:HIS:HB3	2:Q:2847:HIS:CD2	2.54	0.42
3:R:3041[B]:ALA:O	3:R:3042[B]:ASP:HB2	2.20	0.42
3:R:3299[B]:LEU:O	3:R:3300[B]:LEU:C	2.60	0.42
1:S:639:ARG:O	1:S:643:ILE:HG13	2.20	0.42
2:T:2089:ARG:HD3	2:T:2163:GLU:OE2	2.20	0.42
2:T:2521:MET:HE3	2:T:2605:LEU:HD12	2.02	0.42
2:T:2556:TYR:HE1	2:T:2845:PRO:HD2	1.84	0.42
3:U:2969[B]:TYR:CD2	3:U:2971[B]:ASP:CG	2.97	0.42
3:U:2975[B]:PHE:HE1	3:d:3253[B]:GLU:OE1	2.03	0.42
3:U:3028[A]:PRO:HG2	3:U:3029[A]:LYS:HG3	2.00	0.42
3:U:3044[A]:LYS:H	3:U:3044[A]:LYS:HG2	1.64	0.42
3:U:3182[B]:GLN:H	3:U:3182[B]:GLN:HG2	1.56	0.42
1:V:400:ILE:HD13	1:V:484:MET:HE1	2.02	0.42
1:V:1059:LEU:HD22	1:V:1063:ARG:HH21	1.85	0.42
1:V:1203:MET:HB2	1:V:1205:LEU:HB2	2.00	0.42
1:V:1562:ILE:HG22	1:V:1563:LYS:N	2.35	0.42
2:W:2092:VAL:HG13	2:W:2190:LEU:HD23	2.01	0.42
3:X:2938[B]:LEU:HD12	3:X:2938[B]:LEU:HA	1.85	0.42
3:X:3013[A]:ASP:CG	3:X:3015[A]:THR:HG1	2.26	0.42
3:X:3133[A]:LEU:HD12	3:X:3133[A]:LEU:HA	1.86	0.42
3:X:3200[A]:LEU:O	3:X:3203[A]:HIS:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3273[B]:LEU:HB2	3:X:3275[B]:LEU:CD1	2.34	0.42
1:Y:486:THR:HA	1:Y:489:HIS:ND1	2.35	0.42
1:Y:1345:TYR:HB2	1:Y:1460:ASN:HB2	2.02	0.42
1:Y:1578:ILE:HA	1:Y:1579:GLY:HA2	1.53	0.42
3:a:3137[B]:ARG:HB3	3:a:3139[B]:LEU:HD21	1.97	0.42
3:a:3232[B]:VAL:HG21	3:a:3273[B]:LEU:CD1	2.50	0.42
1:b:638:ASP:OD2	1:b:703:TYR:OH	2.37	0.42
1:b:879:SER:O	1:b:879:SER:OG	2.26	0.42
2:c:2274:LEU:HD23	2:c:2274:LEU:HA	1.91	0.42
2:c:2823:ILE:CD1	2:c:2856:ILE:HG21	2.50	0.42
3:d:2989[A]:HIS:C	3:d:2991[A]:LEU:N	2.75	0.42
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.92	0.42
1:A:566:ARG:HA	1:A:567:LEU:HB2	2.02	0.42
1:A:956:PRO:HD2	1:A:957:ASN:O	2.20	0.42
1:A:1142:VAL:O	1:A:1195:ASP:HB2	2.19	0.42
2:B:2086:ASN:H	2:B:2086:ASN:HD22	1.67	0.42
2:B:2121:THR:O	2:B:2124:SER:HB3	2.20	0.42
2:B:2779:ASP:HA	2:B:2780:HIS:HA	1.66	0.42
3:C:2933[B]:SER:CA	3:C:2936[B]:GLU:HB3	2.48	0.42
3:C:3154[B]:PRO:C	3:L:3155[B]:MET:HG2	2.41	0.42
3:C:3161[A]:GLU:CD	3:C:3161[A]:GLU:H	2.19	0.42
3:C:3171[B]:HIS:O	3:C:3172[B]:SER:C	2.63	0.42
3:C:3182[A]:GLN:H	3:C:3182[A]:GLN:HG2	1.56	0.42
1:D:319:ILE:O	1:D:338:ALA:N	2.51	0.42
1:D:716:LEU:O	1:D:720:VAL:HG13	2.20	0.42
2:E:2257:CYS:O	2:E:2261:VAL:HG23	2.20	0.42
2:E:2551:PRO:HA	2:E:2552:GLU:HA	1.60	0.42
3:F:3151[B]:LEU:H	3:a:3169[B]:LYS:HG2	1.84	0.42
3:F:3171[B]:HIS:O	3:F:3172[B]:SER:C	2.63	0.42
3:F:3229[B]:ASN:O	3:F:3286[B]:THR:N	2.50	0.42
3:F:3251[B]:ASP:CG	3:a:3251[B]:ASP:HB2	2.41	0.42
3:F:3293[B]:LYS:CB	3:F:3294[B]:SER:CA	2.96	0.42
1:G:43:GLU:HG3	1:G:44:PRO:HA	2.02	0.42
1:G:832:LYS:HE2	1:G:832:LYS:HB3	1.77	0.42
1:G:858:MET:HG3	1:G:959:PHE:CE1	2.55	0.42
1:G:1078:ARG:NH1	2:K:2872:GLU:O	2.43	0.42
1:G:1091:ASN:HA	1:G:1092:PRO:HD3	1.79	0.42
1:G:1438:ASP:OD1	1:G:1439:VAL:N	2.53	0.42
3:I:2985[B]:PHE:HE2	3:R:2969[B]:TYR:C	2.27	0.42
3:I:2988[B]:TRP:CZ3	3:I:2989[B]:HIS:CE1	3.07	0.42
3:I:3183[B]:LEU:N	3:I:3184[B]:ASN:CA	2.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:84:GLY:CA	1:J:85:SER:HB3	2.50	0.42
1:J:187:GLY:HA2	1:J:193:SER:HB2	2.02	0.42
1:J:843:VAL:HG22	1:J:929:TRP:HB3	2.02	0.42
1:J:1145:THR:OG1	1:J:1233:SER:HB3	2.20	0.42
1:J:1166:THR:HB	1:J:1167:ASP:C	2.45	0.42
1:J:1325:LEU:HG	1:J:1516:VAL:HG11	2.02	0.42
2:K:2502:LEU:HD12	2:K:2502:LEU:HA	1.85	0.42
2:K:2568:HIS:CB	2:K:2746:MET:HE1	2.50	0.42
2:K:2805:PHE:HA	2:K:2855:ASP:HA	2.01	0.42
2:K:2808:PHE:HB3	2:K:2810:LEU:HD21	2.02	0.42
3:L:2969[B]:TYR:CD2	3:L:2971[B]:ASP:CG	2.98	0.42
3:L:2988[B]:TRP:CZ3	3:L:2989[B]:HIS:CE1	3.07	0.42
3:L:2995[B]:GLN:CG	3:L:3168[B]:THR:HG21	2.48	0.42
3:L:3028[B]:PRO:HG2	3:L:3029[B]:LYS:HG2	2.02	0.42
3:L:3041[B]:ALA:O	3:L:3042[B]:ASP:HB2	2.20	0.42
3:L:3048[A]:ASP:HB3	3:L:3099[A]:PRO:HD2	2.01	0.42
3:L:3146[B]:CYS:O	3:L:3146[B]:CYS:SG	2.78	0.42
1:M:855:ARG:HD2	1:M:947:TYR:CG	2.55	0.42
2:N:2565:THR:HG21	2:N:2741:GLN:HB3	2.02	0.42
3:O:2967[B]:CYS:CB	3:X:3155[B]:MET:SD	3.08	0.42
3:O:3096[B]:VAL:CG1	3:O:3115[B]:LEU:CD1	2.86	0.42
3:O:3113[B]:ASP:OD2	3:O:3115[B]:LEU:HB2	2.20	0.42
3:O:3133[A]:LEU:HD13	3:O:3197[A]:ILE:HG23	2.02	0.42
3:O:3185[B]:TYR:HE2	3:O:3187[B]:TYR:CD2	2.35	0.42
3:O:3293[B]:LYS:CB	3:O:3294[B]:SER:CA	2.96	0.42
1:P:62:MET:HE3	1:P:62:MET:HB3	1.71	0.42
1:P:73:LEU:HD11	1:P:210:HIS:O	2.19	0.42
1:P:610:THR:HB	1:P:629:MET:HE1	2.02	0.42
1:P:1400:ASN:OD1	1:P:1402:TYR:N	2.52	0.42
2:Q:2244:PHE:HE2	2:Q:2374:ASN:HD22	1.66	0.42
2:Q:2251:LEU:HA	2:Q:2308:TRP:HD1	1.85	0.42
3:R:3133[A]:LEU:HD13	3:R:3197[A]:ILE:HG23	2.02	0.42
3:R:3146[B]:CYS:O	3:R:3146[B]:CYS:SG	2.78	0.42
3:R:3200[A]:LEU:O	3:R:3203[A]:HIS:HB3	2.20	0.42
1:S:116:LYS:O	1:S:117:LYS:HD2	2.20	0.42
1:S:1347:ASP:HA	1:S:1460:ASN:ND2	2.34	0.42
3:U:2975[B]:PHE:CZ	3:d:3256[B]:TRP:CD1	3.06	0.42
3:U:3001[A]:LYS:N	3:U:3003[A]:LYS:HG3	2.34	0.42
3:U:3169[B]:LYS:HE2	3:d:3146[B]:CYS:HB2	1.99	0.42
3:U:3196[A]:THR:N	3:U:3199[A]:GLN:CB	2.64	0.42
1:V:1248:ARG:HD2	1:V:1249:TRP:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1567:ASP:OD1	1:V:1591:SER:OG	2.33	0.42
2:W:2302:ASP:HB3	2:W:2368:TYR:OH	2.20	0.42
2:W:2377:SER:HB3	2:W:2380:GLN:HG3	2.02	0.42
2:W:2500:ILE:HD11	2:W:2776:TYR:HA	2.00	0.42
3:X:3001[A]:LYS:N	3:X:3003[A]:LYS:HG3	2.34	0.42
3:X:3048[B]:ASP:HB3	3:X:3099[B]:PRO:HD2	2.01	0.42
3:X:3083[A]:ILE:HD11	3:X:3260[A]:ARG:CG	2.49	0.42
3:X:3113[A]:ASP:OD2	3:X:3115[A]:LEU:HB2	2.20	0.42
3:X:3113[B]:ASP:OD2	3:X:3115[B]:LEU:HB2	2.20	0.42
3:X:3146[A]:CYS:O	3:X:3146[A]:CYS:SG	2.78	0.42
3:X:3148[A]:ILE:HD12	3:X:3175[A]:TYR:OH	2.20	0.42
3:X:3200[B]:LEU:O	3:X:3203[B]:HIS:HB3	2.20	0.42
3:X:3242[A]:GLY:C	3:X:3243[A]:GLY:O	2.58	0.42
3:X:3245[A]:PHE:CD1	3:X:3245[A]:PHE:C	2.97	0.42
1:Y:73:LEU:HD11	1:Y:210:HIS:O	2.20	0.42
1:Y:98:MET:HB3	1:Y:144:TYR:HD1	1.85	0.42
1:Y:718:ARG:HH21	1:Y:830:ASN:CG	2.28	0.42
1:Y:956:PRO:C	1:Y:958:PRO:HD2	2.45	0.42
2:Z:2142:ALA:N	2:Z:2433:THR:O	2.36	0.42
3:a:3113[B]:ASP:OD2	3:a:3115[B]:LEU:HB2	2.20	0.42
1:b:567:LEU:HB3	1:b:571:PRO:HD2	2.02	0.42
1:b:899:MET:HG3	1:b:1188:PHE:CZ	2.55	0.42
2:c:2390:GLN:O	2:c:2491:PRO:HB3	2.19	0.42
2:c:2628:HIS:CE1	2:c:2630:LYS:HA	2.55	0.42
3:d:2966[A]:SER:HB2	3:d:2977[A]:CYS:H	1.85	0.42
3:d:3222[A]:ILE:CD1	3:d:3223[A]:GLY:N	2.73	0.42
3:d:3245[B]:PHE:C	3:d:3245[B]:PHE:CD1	2.97	0.42
3:d:3301[B]:PRO:HB2	3:d:3302[B]:SER:H	1.33	0.42
1:A:1279:LYS:HE3	1:A:1376:PRO:HG3	2.02	0.42
2:B:2326:ILE:HD11	1:D:1650:ILE:HG12	2.01	0.42
2:B:2606:LEU:HB3	2:B:2706:ILE:HD11	2.02	0.42
3:C:2969[A]:TYR:CD2	3:C:2971[A]:ASP:CG	2.98	0.42
3:C:2995[B]:GLN:CG	3:C:3168[B]:THR:HG21	2.48	0.42
3:C:3041[A]:ALA:O	3:C:3042[A]:ASP:HB2	2.20	0.42
3:C:3161[B]:GLU:HA	3:L:3147[B]:GLU:HG2	0.76	0.42
3:C:3196[A]:THR:HG21	1:D:416:ASN:HB2	2.01	0.42
3:C:3299[A]:LEU:O	3:C:3300[A]:LEU:C	2.60	0.42
1:D:128:ILE:HG22	1:D:134:VAL:HA	2.01	0.42
1:D:593:CYS:O	1:D:597:VAL:HG23	2.20	0.42
2:E:2830:GLN:HB2	2:E:2863:ARG:NH2	2.35	0.42
3:F:2979[B]:GLN:CD	3:F:3155[B]:MET:CE	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3133[B]:LEU:HD13	3:F:3197[B]:ILE:HG23	2.02	0.42
3:F:3255[B]:PRO:HG2	3:a:2959[B]:SER:HA	2.01	0.42
1:G:904:HIS:O	1:G:907:ARG:HB3	2.20	0.42
1:G:907:ARG:HD3	1:G:1050:ASP:OD1	2.20	0.42
1:G:907:ARG:NH1	1:G:1114:TYR:OH	2.50	0.42
1:G:1231:VAL:O	1:G:1233:SER:N	2.53	0.42
1:G:1304:ASP:N	1:G:1305:GLY:HA2	2.35	0.42
1:G:1328:SER:HB2	1:G:1523:LEU:HD13	2.01	0.42
3:I:2982[B]:MET:CB	3:R:3156[B]:MET:HB3	2.50	0.42
3:I:3028[A]:PRO:HG2	3:I:3029[A]:LYS:HG2	2.02	0.42
3:I:3048[A]:ASP:HB3	3:I:3099[A]:PRO:HD2	2.01	0.42
3:I:3137[B]:ARG:HD3	3:I:3137[B]:ARG:HA	1.72	0.42
3:I:3149[B]:ASN:HB2	3:R:3163[B]:ASN:HD21	0.46	0.42
3:I:3155[B]:MET:CG	3:R:3154[B]:PRO:CD	2.96	0.42
3:I:3200[B]:LEU:O	3:I:3203[B]:HIS:HB3	2.20	0.42
3:I:3272[A]:HIS:CD2	1:J:1543:ILE:HD11	2.55	0.42
1:J:601:VAL:HG11	1:J:777:TYR:CG	2.55	0.42
1:J:730:PHE:CD2	1:J:780:GLU:HB3	2.54	0.42
1:J:1150:GLY:HA2	1:J:1186:TRP:CE2	2.55	0.42
3:L:3148[B]:ILE:HD12	3:L:3175[B]:TYR:OH	2.20	0.42
3:L:3180[B]:TYR:CA	3:L:3183[B]:LEU:CD2	2.95	0.42
3:L:3196[A]:THR:OG1	3:L:3199[A]:GLN:OE1	2.37	0.42
3:L:3200[B]:LEU:O	3:L:3203[B]:HIS:HB3	2.20	0.42
3:L:3294[B]:SER:O	3:L:3294[B]:SER:OG	2.34	0.42
1:M:1140:ASN:OD1	1:M:1239:GLY:N	2.43	0.42
1:M:1369:THR:HB	1:M:1371:GLN:HG2	2.00	0.42
1:M:1406:HIS:O	1:M:1410:VAL:HG23	2.20	0.42
1:M:1639:LYS:HG2	1:M:1640:ILE:C	2.45	0.42
2:N:2207:ASN:HA	2:N:2208:PRO:HD2	1.92	0.42
3:O:2966[A]:SER:HB2	3:O:2977[A]:CYS:H	1.85	0.42
3:O:2979[A]:GLN:OE1	3:O:2979[A]:GLN:HA	2.19	0.42
3:O:2989[A]:HIS:NE2	9:O:3401[A]:CUO:O1	2.53	0.42
3:O:3146[A]:CYS:O	3:O:3146[A]:CYS:SG	2.78	0.42
3:O:3200[A]:LEU:O	3:O:3203[A]:HIS:HB3	2.20	0.42
3:O:3218[A]:LEU:HD13	3:O:3261[A]:LEU:HD23	2.01	0.42
3:O:3222[B]:ILE:H	3:X:3161[B]:GLU:HG2	1.85	0.42
3:O:3229[B]:ASN:N	3:O:3286[B]:THR:O	2.52	0.42
1:P:307:ARG:NH1	1:P:400:ILE:HD11	2.35	0.42
1:P:718:ARG:HD2	1:P:718:ARG:HA	1.89	0.42
1:P:1077:LEU:HD12	1:P:1077:LEU:HA	1.92	0.42
1:P:1178:LEU:HD12	1:P:1178:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1346:TRP:CE3	1:P:1356:PRO:HG3	2.54	0.42
2:Q:2622:ASN:HA	2:Q:2623:PRO:HD3	1.94	0.42
3:R:2969[B]:TYR:CD2	3:R:2971[B]:ASP:CG	2.98	0.42
3:R:3171[B]:HIS:O	3:R:3172[B]:SER:C	2.63	0.42
3:R:3222[A]:ILE:CD1	3:R:3223[A]:GLY:N	2.73	0.42
1:S:523:LEU:HA	1:S:524:PRO:HD3	1.94	0.42
1:S:1007:PHE:CE1	1:S:1011:TYR:HB2	2.54	0.42
1:S:1275:ARG:HH12	1:S:1357:ARG:NH1	2.06	0.42
2:T:2201:THR:C	2:T:2203:ILE:H	2.24	0.42
3:U:2973[B]:THR:CG2	3:d:3222[B]:ILE:HG22	2.32	0.42
3:U:2979[B]:GLN:HA	3:U:2979[B]:GLN:OE1	2.20	0.42
3:U:3028[B]:PRO:HG2	3:U:3029[B]:LYS:HG2	2.02	0.42
3:U:3149[A]:ASN:OD1	3:U:3149[A]:ASN:N	2.51	0.42
3:U:3200[B]:LEU:O	3:U:3203[B]:HIS:HB3	2.20	0.42
1:V:173:VAL:HG23	1:V:174:GLN:HG2	2.01	0.42
1:V:1406:HIS:HB3	1:V:1426:LEU:HD13	2.01	0.42
3:X:3025[B]:VAL:CG2	3:X:3047[B]:ARG:NH1	2.73	0.42
3:X:3133[B]:LEU:HD13	3:X:3197[B]:ILE:HG23	2.02	0.42
3:X:3151[A]:LEU:CB	3:X:3175[A]:TYR:CE2	2.86	0.42
1:Y:494:VAL:CG2	1:Y:671:PHE:HZ	2.33	0.42
1:Y:866:GLU:HG3	1:Y:867:VAL:N	2.35	0.42
1:Y:891:LYS:HB2	1:Y:892:TYR:HA	2.02	0.42
1:Y:1171:LYS:NZ	1:Y:1174:GLU:OE2	2.50	0.42
1:Y:1228:LEU:HD22	1:Y:1228:LEU:O	2.20	0.42
1:Y:1415:ASP:OD1	1:Y:1416:PHE:N	2.53	0.42
1:Y:1650:ILE:HB	2:c:2326:ILE:HG23	2.02	0.42
2:Z:2092:VAL:HG23	2:Z:2177:TYR:O	2.20	0.42
2:Z:2145:LEU:HD22	2:Z:2154:TRP:CD1	2.55	0.42
2:Z:2876:LYS:NZ	2:Z:2876:LYS:HB3	2.34	0.42
3:a:3013[B]:ASP:CA	3:a:3122[B]:ASN:ND2	2.74	0.42
3:a:3028[B]:PRO:HG2	3:a:3029[B]:LYS:HG2	2.02	0.42
3:a:3133[A]:LEU:HD13	3:a:3197[A]:ILE:HG23	2.02	0.42
3:a:3133[B]:LEU:HD13	3:a:3197[B]:ILE:HG23	2.02	0.42
3:a:3218[A]:LEU:HD13	3:a:3261[A]:LEU:HD23	2.01	0.42
1:b:109:LEU:HD12	1:b:119:LYS:HB3	2.02	0.42
1:b:564:ASP:HA	1:b:609:TRP:O	2.19	0.42
1:b:897:HIS:C	1:b:899:MET:HA	2.45	0.42
1:b:1500:THR:HA	1:b:1501:ALA:HA	1.80	0.42
2:c:2327:GLU:H	2:c:2327:GLU:HG3	1.50	0.42
2:c:2569:TRP:CZ2	2:c:2748:PRO:HG3	2.55	0.42
3:d:2937[A]:ASN:CB	3:d:3006[A]:LYS:CE	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2966[B]:SER:HB2	3:d:2977[B]:CYS:H	1.85	0.42
3:d:3001[B]:LYS:N	3:d:3003[B]:LYS:HG3	2.34	0.42
3:d:3148[B]:ILE:HD12	3:d:3175[B]:TYR:OH	2.20	0.42
3:d:3276[A]:ASP:C	3:d:3278[A]:HIS:N	2.75	0.42
3:d:3293[B]:LYS:CD	3:d:3293[B]:LYS:C	2.86	0.42
1:A:480:CYS:SG	1:A:621:LEU:HD11	2.59	0.41
1:A:816:PRO:HA	1:A:817:PRO:HD3	1.95	0.41
2:B:2600:ASP:OD1	2:B:2601:ASN:N	2.53	0.41
3:C:2959[B]:SER:O	3:L:3255[B]:PRO:CD	2.68	0.41
3:C:2995[A]:GLN:CG	3:C:3168[A]:THR:HG21	2.48	0.41
3:C:3027[A]:GLU:CD	3:C:3027[A]:GLU:C	2.85	0.41
3:C:3067[B]:ARG:HA	3:C:3067[B]:ARG:HD3	1.87	0.41
3:C:3158[B]:PHE:CG	3:L:3153[B]:LYS:HE2	2.29	0.41
3:C:3182[B]:GLN:H	3:C:3182[B]:GLN:HG2	1.56	0.41
3:C:3185[B]:TYR:CE2	3:C:3187[B]:TYR:HE2	2.31	0.41
3:C:3193[B]:HIS:ND1	3:C:3193[B]:HIS:N	2.68	0.41
1:D:517:THR:HG21	1:D:708:PHE:HE1	1.85	0.41
1:D:671:PHE:O	1:D:684:ARG:HG3	2.20	0.41
1:D:1156:LEU:HD13	1:D:1176:TYR:CE1	2.55	0.41
1:D:1211:TYR:OH	1:D:1234:VAL:HB	2.20	0.41
1:D:1564:ALA:HB1	4:m:1:NAG:C8	2.50	0.41
2:E:2180:TRP:CD1	2:E:2243:LEU:HD22	2.55	0.41
2:E:2400:LEU:HB2	2:E:2439:PHE:HD2	1.84	0.41
2:E:2644:LEU:HD13	2:E:2686:LEU:HB3	2.01	0.41
2:E:2667:GLU:HB3	2:E:2730:LEU:HD13	2.02	0.41
3:F:2965[B]:LEU:C	3:a:3255[B]:PRO:C	2.87	0.41
3:F:2975[B]:PHE:HZ	3:a:2961[B]:HIS:CB	2.33	0.41
3:F:3146[B]:CYS:HA	3:F:3147[B]:GLU:HA	1.70	0.41
1:G:1148:LEU:HD23	1:G:1229:LYS:HE2	2.01	0.41
3:I:2995[B]:GLN:CG	3:I:3168[B]:THR:HG21	2.48	0.41
3:I:3185[B]:TYR:HE2	3:I:3187[B]:TYR:CD2	2.35	0.41
3:I:3232[B]:VAL:HG21	3:I:3273[B]:LEU:CD1	2.50	0.41
1:J:322:CYS:HA	1:J:333:ASN:O	2.20	0.41
1:J:464:LEU:HA	1:J:464:LEU:HD12	1.85	0.41
1:J:566:ARG:HH22	1:J:803:LYS:NZ	2.18	0.41
1:J:905:TRP:HB2	1:J:1081:MET:HE3	2.02	0.41
1:J:913:PHE:CD2	1:J:1043:MET:HG2	2.55	0.41
1:J:1148:LEU:HB2	1:J:1188:PHE:CD2	2.46	0.41
1:J:1494:ARG:HH11	1:J:1494:ARG:CG	2.33	0.41
1:J:1562:ILE:HG13	1:J:1564:ALA:O	2.20	0.41
2:K:2561:HIS:HB3	2:K:2677:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2711:HIS:HA	2:K:2714:VAL:HG22	2.01	0.41
3:L:2979[A]:GLN:CD	3:L:3155[A]:MET:CE	2.92	0.41
3:L:3200[A]:LEU:O	3:L:3203[A]:HIS:HB3	2.20	0.41
3:L:3232[A]:VAL:HG21	3:L:3273[A]:LEU:CD1	2.50	0.41
1:M:84:GLY:HA2	1:M:85:SER:HB3	2.02	0.41
1:M:1484:CYS:O	2:Q:2487:VAL:HG22	2.20	0.41
1:M:1485:ALA:O	1:M:1489:MET:HG2	2.20	0.41
2:N:2778:TYR:HB2	2:N:2781:LEU:CD1	2.50	0.41
3:O:2988[A]:TRP:CZ3	3:O:2989[A]:HIS:CE1	3.07	0.41
3:O:3023[A]:ILE:HA	3:O:3026[A]:THR:HG1	1.83	0.41
3:O:3149[A]:ASN:OD1	3:O:3149[A]:ASN:N	2.51	0.41
3:O:3185[A]:TYR:CE2	3:O:3187[A]:TYR:HE2	2.31	0.41
1:P:40:TYR:HE2	1:P:75:GLN:HG2	1.85	0.41
1:P:71:LEU:HD13	1:P:266:LEU:HD21	2.01	0.41
1:P:107:HIS:HA	1:P:108:PRO:HD3	1.89	0.41
1:P:468:CYS:HA	1:P:469:PRO:C	2.45	0.41
1:P:524:PRO:HD2	1:P:527:LEU:HD11	2.01	0.41
1:P:930:ASP:OD1	1:P:1051:ARG:NH2	2.53	0.41
2:Q:2261:VAL:HG21	2:Q:2441:ARG:HG3	2.01	0.41
2:Q:2398:PHE:HE1	2:Q:2466:THR:HG21	1.85	0.41
2:Q:2568:HIS:CD2	2:Q:2718:TRP:CH2	3.08	0.41
3:R:2952[B]:ALA:CA	3:R:2956[B]:LYS:CB	2.89	0.41
3:R:3048[A]:ASP:HB3	3:R:3099[A]:PRO:HD2	2.01	0.41
3:R:3133[B]:LEU:HD13	3:R:3197[B]:ILE:HG23	2.02	0.41
3:R:3171[A]:HIS:O	3:R:3172[A]:SER:C	2.63	0.41
3:R:3228[B]:VAL:CG2	3:R:3245[B]:PHE:CD2	3.02	0.41
3:R:3232[B]:VAL:HG21	3:R:3273[B]:LEU:CD1	2.49	0.41
3:R:3281[A]:PHE:CZ	3:R:3305[A]:ILE:HG21	2.55	0.41
1:S:285:THR:HB	1:S:288:GLU:H	1.85	0.41
1:S:932:THR:O	1:S:989:THR:OG1	2.37	0.41
1:S:1019:HIS:CE1	1:S:1046:HIS:CE1	3.08	0.41
1:S:1055:THR:HG21	1:S:1121:LEU:HD13	2.01	0.41
1:S:1263:LEU:HD11	1:S:1358:LEU:HD22	2.02	0.41
2:T:2104:ILE:O	2:T:2108:LYS:HB2	2.20	0.41
3:U:2949[A]:LYS:C	3:U:2949[A]:LYS:HZ3	2.18	0.41
3:U:2987[B]:HIS:CD2	3:U:3178[B]:PHE:CE1	3.08	0.41
3:U:2989[B]:HIS:NE2	9:U:3401[B]:CUO:O1	2.53	0.41
3:U:3041[B]:ALA:O	3:U:3042[B]:ASP:HB2	2.20	0.41
3:U:3096[A]:VAL:CG1	3:U:3115[A]:LEU:CD1	2.86	0.41
3:U:3193[B]:HIS:ND1	3:U:3193[B]:HIS:N	2.68	0.41
1:V:109:LEU:HD21	2:Z:2635:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:128:ILE:HG12	1:V:130:PHE:O	2.20	0.41
1:V:664:VAL:HG12	1:V:690:THR:HG22	2.00	0.41
2:W:2191:LEU:HD13	2:W:2296:LEU:HD22	2.01	0.41
2:W:2381:LEU:HD23	2:W:2381:LEU:HA	1.92	0.41
3:X:2969[B]:TYR:CD2	3:X:2971[B]:ASP:CG	2.98	0.41
1:Y:843:VAL:CG1	1:Y:927:PRO:HB2	2.50	0.41
1:Y:1019:HIS:CE1	1:Y:1046:HIS:HE1	2.37	0.41
2:Z:2235:PRO:HG2	2:c:2097:LEU:HD12	2.02	0.41
3:a:3047[A]:ARG:NH2	3:a:3113[A]:ASP:OD1	2.43	0.41
3:a:3148[B]:ILE:HD12	3:a:3175[B]:TYR:OH	2.20	0.41
3:a:3200[A]:LEU:O	3:a:3203[A]:HIS:HB3	2.20	0.41
1:b:891:LYS:HB2	1:b:892:TYR:HB3	2.00	0.41
1:b:1180:SER:OG	1:b:1181:GLU:N	2.53	0.41
2:c:2336:PHE:HB3	2:c:2348:THR:HG22	2.02	0.41
3:d:2965[A]:LEU:CG	3:d:2974[A]:ALA:CB	2.85	0.41
3:d:2979[B]:GLN:HA	3:d:2979[B]:GLN:OE1	2.19	0.41
3:d:2989[B]:HIS:NE2	9:d:3401[B]:CUO:O1	2.53	0.41
3:d:2995[B]:GLN:CG	3:d:3168[B]:THR:HG21	2.48	0.41
3:d:3149[B]:ASN:OD1	3:d:3149[B]:ASN:N	2.51	0.41
3:d:3183[B]:LEU:N	3:d:3184[B]:ASN:CA	2.80	0.41
3:d:3185[A]:TYR:HE2	3:d:3187[A]:TYR:CD2	2.35	0.41
1:A:119:LYS:CB	1:A:120:LYS:HA	2.34	0.41
1:A:139:VAL:HG11	1:A:144:TYR:CZ	2.55	0.41
1:A:418:ASP:C	1:A:420:SER:HA	2.44	0.41
1:A:473:ALA:HB1	1:b:1639:LYS:HD2	2.02	0.41
1:A:718:ARG:HD3	1:A:834:ASP:OD2	2.19	0.41
1:A:1091:ASN:HA	1:A:1092:PRO:HD3	1.76	0.41
1:A:1361:GLU:HG3	1:A:1363:THR:H	1.85	0.41
3:C:2979[A]:GLN:CD	3:C:3155[A]:MET:CE	2.92	0.41
3:C:3146[B]:CYS:SG	3:C:3146[B]:CYS:O	2.78	0.41
3:C:3163[B]:ASN:O	3:L:3147[B]:GLU:OE2	2.38	0.41
3:C:3171[B]:HIS:C	3:L:3152[B]:LYS:CB	2.82	0.41
3:C:3180[A]:TYR:CA	3:C:3183[A]:LEU:CD2	2.95	0.41
3:C:3185[A]:TYR:CE2	3:C:3187[A]:TYR:HE2	2.31	0.41
3:C:3200[B]:LEU:O	3:C:3203[B]:HIS:HB3	2.20	0.41
3:C:3222[A]:ILE:CD1	3:C:3223[A]:GLY:N	2.73	0.41
9:C:3401[A]:CUO:O1	3:L:2989[A]:HIS:NE2	2.53	0.41
1:D:23:ARG:HD3	1:D:120:LYS:HD3	2.02	0.41
1:D:472:ASP:HA	1:D:473:ALA:HA	1.74	0.41
1:D:1634:ALA:HB1	4:m:1:NAG:O7	2.19	0.41
2:E:2107:LEU:HA	2:E:2110:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2597:MET:HE2	2:E:2598:PRO:HD2	2.02	0.41
2:E:2711:HIS:O	2:E:2712:SER:C	2.63	0.41
3:F:3041[A]:ALA:O	3:F:3042[A]:ASP:HB2	2.20	0.41
3:F:3150[B]:LYS:NZ	3:a:3162[B]:ASP:C	2.77	0.41
3:F:3150[B]:LYS:HB2	3:a:3169[B]:LYS:HE3	2.02	0.41
3:F:3193[B]:HIS:ND1	3:F:3193[B]:HIS:N	2.68	0.41
1:G:149:GLU:O	1:G:151:GLN:N	2.53	0.41
1:G:806:ASN:OD1	1:G:808:THR:HG22	2.20	0.41
1:G:1144:VAL:HG12	1:G:1194:SER:O	2.19	0.41
1:G:1339:SER:HB3	1:G:1340:GLY:CA	2.40	0.41
2:H:2406:SER:OG	2:H:2430:GLY:N	2.33	0.41
2:H:2521:MET:HE3	2:H:2605:LEU:HD12	2.01	0.41
2:H:2744:PHE:CZ	1:J:1212:HIS:HB3	2.55	0.41
2:H:2800:LYS:HB3	3:I:3023[A]:ILE:HD13	2.02	0.41
3:I:3153[B]:LYS:HG2	3:R:3155[B]:MET:CG	2.50	0.41
3:I:3259[B]:ASP:N	3:R:3162[B]:ASP:CB	2.77	0.41
3:I:3259[B]:ASP:H	3:R:3162[B]:ASP:CG	2.27	0.41
1:J:19:GLN:HG2	1:J:110:PHE:CD2	2.55	0.41
1:J:494:VAL:HG23	1:J:671:PHE:CZ	2.56	0.41
1:J:946:GLU:HG2	1:J:955:LYS:HD3	2.01	0.41
2:K:2481:LEU:HA	2:K:2482:PRO:HD3	1.94	0.41
2:K:2568:HIS:CD2	2:K:2718:TRP:CH2	3.08	0.41
3:L:3041[A]:ALA:O	3:L:3042[A]:ASP:HB2	2.20	0.41
3:L:3048[B]:ASP:HB3	3:L:3099[B]:PRO:HD2	2.01	0.41
3:L:3161[B]:GLU:H	3:L:3161[B]:GLU:CD	2.19	0.41
3:L:3299[A]:LEU:HB3	3:L:3300[A]:LEU:H	1.54	0.41
1:M:603:HIS:HD2	1:M:633:HIS:CE1	2.38	0.41
1:M:1636:ASN:HB2	1:M:1638:SER:O	2.19	0.41
2:N:2155:HIS:O	2:N:2159:VAL:HG23	2.21	0.41
3:O:2966[B]:SER:HB2	3:O:2977[B]:CYS:H	1.85	0.41
3:O:3148[B]:ILE:HD12	3:O:3175[B]:TYR:OH	2.20	0.41
3:O:3171[A]:HIS:O	3:O:3172[A]:SER:C	2.63	0.41
3:O:3200[B]:LEU:O	3:O:3203[B]:HIS:HB3	2.20	0.41
1:P:64:THR:HG22	1:P:240:PHE:CE1	2.55	0.41
1:P:92:TRP:CE3	1:P:102:PRO:HD3	2.55	0.41
1:P:489:HIS:CD2	1:P:689:PRO:HB2	2.56	0.41
1:P:492:ARG:HD2	1:P:692:VAL:HG13	2.01	0.41
1:P:1324:ARG:NH1	1:P:1519:TYR:HB3	2.34	0.41
2:Q:2660:VAL:HG13	2:Q:2663:MET:HE2	2.02	0.41
3:R:2979[B]:GLN:CD	3:R:3155[B]:MET:CE	2.93	0.41
1:S:72:TYR:HD1	1:S:247:PHE:HZ	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:305:ASN:HB3	1:S:400:ILE:HB	2.02	0.41
1:S:714:ARG:NH1	1:S:1115:GLU:OE1	2.52	0.41
1:S:1166:THR:N	1:S:1167:ASP:HA	2.35	0.41
1:S:1312:CYS:HA	1:S:1322:TRP:CE2	2.54	0.41
1:S:1438:ASP:HB3	1:S:1441:SER:HB3	2.01	0.41
2:T:2132:CYS:O	2:T:2334:LYS:HD3	2.21	0.41
3:U:2970[B]:PRO:N	3:d:2981[B]:GLY:N	2.68	0.41
3:U:2975[B]:PHE:HD1	3:d:3221[B]:ALA:CB	2.33	0.41
3:U:2980[B]:HIS:O	3:d:2969[B]:TYR:HD1	1.92	0.41
3:U:3011[A]:TYR:CB	3:U:3121[A]:SER:HB2	2.49	0.41
3:U:3133[B]:LEU:HD13	3:U:3197[B]:ILE:HG23	2.02	0.41
3:U:3148[A]:ILE:HD12	3:U:3175[A]:TYR:OH	2.20	0.41
1:V:482:HIS:CE1	1:V:621:LEU:HD11	2.55	0.41
1:V:949:ASP:O	1:V:952:GLY:N	2.52	0.41
2:W:2553:ALA:N	2:W:2554:PRO:CD	2.84	0.41
3:X:2952[B]:ALA:CA	3:X:2956[B]:LYS:CB	2.89	0.41
3:X:2987[B]:HIS:CD2	3:X:3178[B]:PHE:CE1	3.08	0.41
3:X:2988[A]:TRP:HE3	3:X:2989[A]:HIS:CE1	2.25	0.41
3:X:3028[A]:PRO:HG2	3:X:3029[A]:LYS:HG2	2.02	0.41
3:X:3171[A]:HIS:O	3:X:3172[A]:SER:C	2.63	0.41
3:X:3194[A]:GLY:C	3:X:3195[A]:MET:CG	2.90	0.41
3:X:3281[A]:PHE:CZ	3:X:3305[A]:ILE:HG21	2.55	0.41
3:X:3284[A]:LYS:CD	3:X:3284[A]:LYS:C	2.86	0.41
3:X:3299[A]:LEU:HB3	3:X:3300[A]:LEU:H	1.54	0.41
3:X:3301[A]:PRO:HB2	3:X:3302[A]:SER:H	1.33	0.41
1:Y:1319:PHE:CE2	1:Y:1424:GLU:HG3	2.55	0.41
1:Y:1489:MET:HB3	1:Y:1514:ASN:ND2	2.36	0.41
2:Z:2327:GLU:HG2	1:b:1649:THR:HA	2.02	0.41
2:Z:2469:VAL:HG12	2:Z:2475:GLU:HG2	2.02	0.41
3:a:3048[A]:ASP:HB3	3:a:3099[A]:PRO:HD2	2.01	0.41
3:a:3084[B]:GLN:HE21	3:a:3084[B]:GLN:HB3	1.71	0.41
1:b:51:ASP:HA	1:b:52:GLY:HA2	1.62	0.41
1:b:882:TRP:CD1	1:b:1086:LEU:HD13	2.55	0.41
1:b:1070:ALA:HB3	1:b:1077:LEU:HD21	2.01	0.41
2:c:2858:ASP:O	2:c:2862:LYS:HG2	2.20	0.41
3:d:2969[A]:TYR:CD2	3:d:2971[A]:ASP:CG	2.98	0.41
3:d:3133[A]:LEU:HD13	3:d:3197[A]:ILE:HG23	2.02	0.41
3:d:3230[A]:PHE:HB2	3:d:3242[A]:GLY:C	2.45	0.41
3:d:3281[A]:PHE:HE1	3:d:3305[A]:ILE:HG21	1.81	0.41
1:A:1010:GLN:H	1:A:1010:GLN:HG2	1.67	0.41
2:B:2191:LEU:HD12	2:B:2191:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2406:SER:O	2:B:2471:HIS:HB2	2.20	0.41
3:C:2949[A]:LYS:NZ	3:C:2949[A]:LYS:C	2.73	0.41
3:C:3028[A]:PRO:HG2	3:C:3029[A]:LYS:HG2	2.02	0.41
3:C:3146[A]:CYS:HA	3:C:3147[A]:GLU:HA	1.70	0.41
1:D:40:TYR:CD1	1:D:246:PRO:HG2	2.54	0.41
1:D:282:ASN:OD1	1:D:282:ASN:N	2.53	0.41
1:D:601:VAL:HG11	1:D:777:TYR:CG	2.56	0.41
1:D:1023:GLY:HA2	1:D:1029:SER:OG	2.21	0.41
1:D:1248:ARG:HG3	1:D:1249:TRP:H	1.85	0.41
1:D:1260:ARG:HD2	1:D:1343:VAL:O	2.21	0.41
2:E:2089:ARG:HD3	2:E:2163:GLU:OE2	2.20	0.41
2:E:2304:LEU:HD12	2:E:2304:LEU:HA	1.89	0.41
2:E:2554:PRO:CB	2:E:2556:TYR:HB2	2.51	0.41
3:F:2931[A]:THR:HG1	3:F:2934[A]:GLU:CD	2.04	0.41
3:F:3120[B]:HIS:HA	3:F:3123[B]:THR:HG1	1.82	0.41
3:F:3148[B]:ILE:O	3:a:3170[B]:ALA:N	2.53	0.41
1:G:104:LEU:HD23	1:G:123:PHE:CE2	2.51	0.41
1:G:590:ASP:OD1	1:G:590:ASP:N	2.54	0.41
1:G:938:LEU:HD11	1:G:976:THR:HG21	2.02	0.41
2:H:2089:ARG:HB2	2:H:2368:TYR:CD1	2.56	0.41
2:H:2157:LEU:O	2:H:2160:VAL:HG22	2.20	0.41
2:H:2680:HIS:CD2	2:H:2684:HIS:CD2	3.08	0.41
3:I:2963[A]:MET:SD	3:I:2963[A]:MET:O	2.79	0.41
3:I:2968[B]:GLN:O	3:R:2985[B]:PHE:CE2	2.74	0.41
3:I:2971[B]:ASP:O	3:R:3093[B]:HIS:CB	2.67	0.41
3:I:2979[A]:GLN:HA	3:I:2979[A]:GLN:OE1	2.19	0.41
3:I:2989[A]:HIS:NE2	9:R:3401[A]:CUO:O1	2.53	0.41
3:I:2989[B]:HIS:C	3:I:2991[B]:LEU:N	2.75	0.41
3:I:2995[A]:GLN:O	3:I:2996[A]:MET:C	2.63	0.41
3:I:3148[A]:ILE:HD12	3:I:3175[A]:TYR:OH	2.20	0.41
3:I:3200[A]:LEU:O	3:I:3203[A]:HIS:HB3	2.20	0.41
3:I:3218[A]:LEU:HD13	3:I:3261[A]:LEU:HD23	2.01	0.41
1:J:464:LEU:HD22	1:J:622:HIS:CD2	2.54	0.41
1:J:728:ARG:HE	1:J:730:PHE:HZ	1.68	0.41
2:K:2361:LYS:HE2	2:K:2362:GLN:HG3	2.01	0.41
2:K:2575:LEU:HD23	2:K:2575:LEU:HA	1.87	0.41
3:L:2931[A]:THR:HG1	3:L:2934[A]:GLU:CD	2.04	0.41
3:L:2963[A]:MET:SD	3:L:2963[A]:MET:O	2.78	0.41
3:L:2963[B]:MET:SD	3:L:2963[B]:MET:O	2.79	0.41
3:L:3196[A]:THR:N	3:L:3199[A]:GLN:CB	2.65	0.41
3:L:3196[B]:THR:OG1	3:L:3199[B]:GLN:OE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3281[B]:PHE:CZ	3:L:3305[B]:ILE:HG21	2.55	0.41
1:M:164:GLU:OE2	1:M:301:ARG:NH2	2.53	0.41
1:M:705:THR:HG22	1:M:1118:THR:HG22	2.02	0.41
1:M:862:ALA:HA	1:M:870:TYR:HD2	1.85	0.41
1:M:1458:HIS:CE1	9:M:2105:CUO:O1	2.74	0.41
2:N:2641:GLN:HA	2:N:2642:PRO:HD3	1.87	0.41
3:O:3047[B]:ARG:NH2	3:O:3113[B]:ASP:OD1	2.43	0.41
3:O:3131[A]:GLN:HE21	3:O:3131[A]:GLN:HB3	1.66	0.41
3:O:3180[B]:TYR:HA	3:O:3183[B]:LEU:CD2	2.51	0.41
1:P:150:GLY:HA2	1:P:151:GLN:HA	1.77	0.41
1:P:177:VAL:HA	1:P:180:ASN:ND2	2.35	0.41
1:P:450:LYS:HZ2	1:P:505:ARG:HH21	1.67	0.41
3:R:2979[A]:GLN:HA	3:R:2979[A]:GLN:OE1	2.19	0.41
3:R:2987[A]:HIS:CD2	3:R:3178[A]:PHE:CE1	3.08	0.41
3:R:3041[A]:ALA:O	3:R:3042[A]:ASP:HB2	2.20	0.41
3:R:3083[B]:ILE:HD11	3:R:3260[B]:ARG:HG3	2.03	0.41
3:R:3173[B]:THR:HG22	3:R:3174[B]:GLY:H	1.67	0.41
3:R:3180[B]:TYR:CB	3:R:3183[B]:LEU:CD2	2.90	0.41
3:R:3294[B]:SER:O	3:R:3294[B]:SER:OG	2.34	0.41
1:S:858:MET:HE1	1:S:870:TYR:CZ	2.55	0.41
1:S:980:TYR:CE1	1:S:1021:LEU:HB3	2.55	0.41
1:S:1166:THR:OG1	1:S:1168:GLN:N	2.52	0.41
2:T:2549:PRO:HA	2:T:2550:THR:HA	1.56	0.41
2:T:2575:LEU:HD11	2:T:2774:LEU:HB3	2.01	0.41
3:U:2963[A]:MET:SD	3:U:2963[A]:MET:O	2.79	0.41
3:U:3034[A]:HIS:HB3	3:U:3035[A]:HIS:CE1	2.50	0.41
3:U:3094[B]:SER:HG	3:U:3227[B]:ASP:CG	2.28	0.41
3:U:3169[B]:LYS:HG2	3:d:3148[B]:ILE:H	0.62	0.41
3:U:3182[A]:GLN:H	3:U:3182[A]:GLN:HG2	1.56	0.41
3:U:3200[A]:LEU:O	3:U:3203[A]:HIS:HB3	2.20	0.41
3:U:3218[A]:LEU:HD13	3:U:3261[A]:LEU:HD23	2.01	0.41
3:U:3222[B]:ILE:CD1	3:U:3223[B]:GLY:N	2.73	0.41
1:V:225:LYS:HE2	1:V:225:LYS:HB2	1.93	0.41
1:V:518:LYS:HE2	1:V:520:PHE:HB3	2.00	0.41
1:V:567:LEU:HB2	1:V:571:PRO:HD2	2.01	0.41
1:V:1249:TRP:HZ2	1:V:1537:ILE:HD12	1.85	0.41
1:V:1304:ASP:OD1	1:V:1306:THR:N	2.53	0.41
1:V:1573:CYS:HB2	1:V:1627:ARG:CG	2.49	0.41
2:W:2180:TRP:HH2	2:W:2297:HIS:O	2.02	0.41
3:X:3185[B]:TYR:HE2	3:X:3187[B]:TYR:CD2	2.35	0.41
1:Y:859:ALA:HB2	1:Y:957:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:898:GLY:HA2	1:Y:1186:TRP:CB	2.44	0.41
2:Z:2638:ARG:HG2	2:Z:2687:ILE:O	2.20	0.41
3:a:2969[A]:TYR:CD2	3:a:2971[A]:ASP:CG	2.97	0.41
3:a:2995[A]:GLN:CG	3:a:3168[A]:THR:HG21	2.48	0.41
3:a:3041[A]:ALA:O	3:a:3042[A]:ASP:HB2	2.20	0.41
3:a:3196[B]:THR:OG1	3:a:3199[B]:GLN:OE1	2.37	0.41
3:a:3285[A]:VAL:CG2	3:a:3286[A]:THR:H	2.27	0.41
1:b:59:LEU:HD23	1:b:64:THR:OG1	2.20	0.41
1:b:350:MET:O	1:b:352:TRP:HD1	2.04	0.41
1:b:619:SER:HB2	1:b:805:VAL:HG11	2.02	0.41
1:b:843:VAL:HG21	1:b:1044:LEU:HD13	2.02	0.41
1:b:882:TRP:N	1:b:894:CYS:SG	2.94	0.41
1:b:907:ARG:HD3	1:b:1050:ASP:OD1	2.19	0.41
1:b:949:ASP:OD1	1:b:950:ALA:N	2.51	0.41
1:b:1081:MET:HG2	1:b:1100:SER:O	2.20	0.41
1:b:1166:THR:N	1:b:1167:ASP:HA	2.34	0.41
1:b:1361:GLU:HG3	1:b:1363:THR:H	1.84	0.41
1:b:1492:PRO:HA	1:b:1512:ARG:HA	2.02	0.41
1:b:1614:GLU:OE1	1:b:1614:GLU:N	2.53	0.41
2:c:2393:ARG:O	2:c:2489:ILE:N	2.42	0.41
2:c:2562:GLY:H	2:c:2846:TRP:CB	2.33	0.41
2:c:2571:ARG:NH1	2:c:2771:TYR:HB3	2.35	0.41
2:c:2656:LEU:HD23	2:c:2656:LEU:HA	1.91	0.41
2:c:2762:VAL:O	2:c:2768:LEU:HD23	2.20	0.41
3:d:3193[A]:HIS:ND1	3:d:3193[A]:HIS:N	2.69	0.41
1:A:100:GLN:HA	1:A:100:GLN:HE21	1.85	0.41
1:A:103:GLU:OE2	1:A:106:GLN:NE2	2.54	0.41
1:A:119:LYS:HA	1:A:119:LYS:HD2	1.86	0.41
1:A:232:ARG:NE	1:A:267:PHE:HE2	2.19	0.41
1:A:307:ARG:HH12	1:A:484:MET:HE1	1.86	0.41
1:A:328:LYS:NZ	1:b:1631:GLU:OE1	2.42	0.41
1:A:331:SER:HB3	1:b:1582:ASN:O	2.20	0.41
1:A:1180:SER:N	1:A:1183:GLU:OE1	2.53	0.41
1:A:1322:TRP:HZ2	1:A:1495:PRO:HG3	1.85	0.41
1:A:1498:ASN:ND2	1:A:1500:THR:O	2.54	0.41
3:C:2987[B]:HIS:CD2	3:C:3178[B]:PHE:CE1	3.08	0.41
3:C:3158[B]:PHE:HE2	3:L:3153[B]:LYS:HZ1	1.49	0.41
3:C:3232[B]:VAL:HG21	3:C:3273[B]:LEU:HD11	2.00	0.41
3:C:3252[B]:TYR:HB3	3:L:3253[B]:GLU:CD	2.45	0.41
3:C:3276[A]:ASP:C	3:C:3278[A]:HIS:N	2.75	0.41
3:C:3281[A]:PHE:HE1	3:C:3305[A]:ILE:HG21	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3300[A]:LEU:HD23	3:C:3300[A]:LEU:H	1.83	0.41
1:D:81:VAL:C	1:D:83:HIS:N	2.76	0.41
1:D:442:ALA:HB2	1:D:507:SER:HB3	2.01	0.41
1:D:1099:TYR:CD2	1:D:1112:PHE:HE1	2.39	0.41
1:D:1170:MET:SD	1:D:1199:VAL:HG23	2.60	0.41
1:D:1275:ARG:HH21	1:D:1375:ASN:ND2	2.17	0.41
1:D:1319:PHE:CE2	1:D:1424:GLU:HG3	2.54	0.41
1:D:1562:ILE:CG2	1:D:1644:ILE:HG21	2.50	0.41
2:E:2240:GLN:HG3	2:E:2241:THR:N	2.35	0.41
3:F:2969[B]:TYR:HE2	3:a:3120[B]:HIS:CD2	2.36	0.41
3:F:2979[A]:GLN:NE2	3:F:3155[A]:MET:HE3	2.19	0.41
3:F:3083[A]:ILE:HD11	3:F:3260[A]:ARG:HG3	2.03	0.41
3:F:3232[A]:VAL:HG21	3:F:3273[A]:LEU:CD1	2.50	0.41
3:F:3232[B]:VAL:CG2	3:F:3273[B]:LEU:CD1	2.98	0.41
9:F:3401[A]:CUO:O1	3:a:2989[A]:HIS:NE2	2.53	0.41
1:G:69:HIS:CD2	1:G:210:HIS:CE1	3.08	0.41
1:G:104:LEU:HB3	1:G:123:PHE:CD2	2.50	0.41
1:G:686:HIS:NE2	1:G:698:GLU:HB3	2.35	0.41
1:G:1018:ILE:HD12	1:G:1045:HIS:CD2	2.55	0.41
1:G:1280:GLN:HE21	1:G:1280:GLN:HB3	1.66	0.41
2:H:2502:LEU:HD12	2:H:2502:LEU:HA	1.89	0.41
3:I:3232[A]:VAL:HG21	3:I:3273[A]:LEU:CD1	2.50	0.41
1:J:385:ALA:HB2	1:J:391:MET:SD	2.60	0.41
2:K:2263:PHE:HE1	2:K:2304:LEU:HB3	1.85	0.41
2:K:2304:LEU:O	2:K:2307:VAL:HB	2.20	0.41
2:K:2536:PHE:HE1	2:K:2708:TYR:CE2	2.38	0.41
2:K:2549:PRO:HA	2:K:2550:THR:HA	1.48	0.41
3:L:2952[B]:ALA:CA	3:L:2956[B]:LYS:CB	2.89	0.41
3:L:2965[A]:LEU:CG	3:L:2974[A]:ALA:CB	2.85	0.41
3:L:3229[A]:ASN:N	3:L:3286[A]:THR:O	2.52	0.41
1:M:84:GLY:CA	1:M:85:SER:HB3	2.50	0.41
1:M:132:ASN:HB2	1:M:133:LYS:HG2	2.02	0.41
1:M:200:THR:O	1:M:206:PHE:HB2	2.20	0.41
1:M:419:THR:HA	1:M:420:SER:HA	1.60	0.41
1:M:979:LEU:CB	1:M:980:TYR:HD1	2.33	0.41
1:M:1207:TYR:O	1:M:1207:TYR:HD1	2.03	0.41
1:M:1256:ALA:HB1	1:M:1526:LYS:HB2	2.02	0.41
2:N:2107:LEU:O	2:N:2111:GLN:HB2	2.20	0.41
2:N:2181:THR:HB	2:N:2374:ASN:H	1.86	0.41
2:N:2187:VAL:HG12	2:N:2188:PRO:HD2	2.02	0.41
2:N:2638:ARG:NH2	2:N:2706:ILE:HD11	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2952[B]:ALA:CA	3:O:2956[B]:LYS:CB	2.89	0.41
3:O:2963[B]:MET:SD	3:O:2963[B]:MET:O	2.79	0.41
3:O:2980[B]:HIS:HA	3:O:2985[B]:PHE:HD2	1.86	0.41
3:O:3028[B]:PRO:HG2	3:O:3029[B]:LYS:HG2	2.02	0.41
3:O:3146[B]:CYS:O	3:O:3146[B]:CYS:SG	2.78	0.41
3:O:3148[A]:ILE:HD12	3:O:3175[A]:TYR:OH	2.20	0.41
3:O:3161[B]:GLU:OE1	3:X:3144[B]:ALA:CB	2.68	0.41
3:O:3196[B]:THR:OG1	3:O:3199[B]:GLN:OE1	2.37	0.41
3:O:3276[A]:ASP:C	3:O:3278[A]:HIS:N	2.75	0.41
1:P:1118:THR:HB	1:P:1120:GLU:HG2	2.02	0.41
2:Q:2764:THR:HG22	2:Q:2766:SER:H	1.84	0.41
2:Q:2823:ILE:HD12	2:Q:2860:LEU:HD21	2.03	0.41
2:Q:2829:CYS:C	2:Q:2830:GLN:HG2	2.46	0.41
3:R:2963[B]:MET:SD	3:R:2963[B]:MET:O	2.79	0.41
3:R:3229[A]:ASN:N	3:R:3286[A]:THR:O	2.52	0.41
3:R:3232[A]:VAL:HG21	3:R:3273[A]:LEU:CD1	2.50	0.41
3:R:3300[B]:LEU:HD23	3:R:3300[B]:LEU:H	1.83	0.41
1:S:407:GLN:HA	1:S:408:GLY:HA2	1.68	0.41
1:S:834:ASP:HB2	1:S:837:HIS:HB3	2.02	0.41
1:S:977:GLU:HG3	1:S:978:ALA:H	1.84	0.41
1:S:995:ILE:HG22	1:S:999:LEU:HD22	2.02	0.41
1:S:1248:ARG:HG3	1:S:1249:TRP:H	1.86	0.41
1:S:1634:ALA:HB3	1:S:1639:LYS:HD3	2.02	0.41
2:T:2339:GLY:HA2	2:T:2349:THR:HG21	2.03	0.41
2:T:2866:PRO:HA	2:T:2867:PRO:HD3	1.96	0.41
3:U:2963[B]:MET:SD	3:U:2963[B]:MET:O	2.79	0.41
3:U:2995[B]:GLN:CG	3:U:3168[B]:THR:HG21	2.48	0.41
3:U:3013[B]:ASP:CA	3:U:3122[B]:ASN:ND2	2.73	0.41
3:U:3137[A]:ARG:HD3	3:U:3137[A]:ARG:HA	1.71	0.41
3:U:3146[A]:CYS:O	3:U:3146[A]:CYS:SG	2.78	0.41
3:U:3148[B]:ILE:HD12	3:U:3175[B]:TYR:OH	2.20	0.41
3:U:3158[B]:PHE:O	3:d:3149[B]:ASN:HB3	2.14	0.41
3:U:3196[A]:THR:OG1	3:U:3199[A]:GLN:OE1	2.38	0.41
1:V:407:GLN:HA	1:V:408:GLY:HA2	1.73	0.41
1:V:480:CYS:HA	1:V:490:TRP:CE2	2.54	0.41
1:V:547:LYS:HG2	1:V:558:HIS:HB3	2.02	0.41
1:V:587:PHE:HA	1:V:644:TRP:HD1	1.86	0.41
1:V:879:SER:O	1:V:879:SER:OG	2.34	0.41
1:V:897:HIS:HB3	1:V:899:MET:CE	2.48	0.41
1:V:1147:MET:HE2	1:V:1147:MET:HB2	1.79	0.41
1:V:1161:ILE:O	1:V:1203:MET:HE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:2092:VAL:HG23	2:W:2177:TYR:O	2.19	0.41
2:W:2191:LEU:O	2:W:2225:ARG:NH2	2.53	0.41
3:X:2946[A]:GLN:CD	3:X:2947[A]:ALA:N	2.72	0.41
3:X:3137[B]:ARG:HD3	3:X:3137[B]:ARG:HA	1.71	0.41
3:X:3192[A]:PHE:HD2	3:X:3192[A]:PHE:HA	1.77	0.41
3:X:3218[A]:LEU:HD12	3:X:3218[A]:LEU:HA	1.78	0.41
1:Y:266:LEU:HD12	1:Y:266:LEU:HA	1.90	0.41
2:Z:2398:PHE:CE1	2:Z:2484:ALA:HB2	2.55	0.41
2:Z:2575:LEU:HD23	2:Z:2575:LEU:HA	1.94	0.41
2:Z:2745:PRO:HA	2:Z:2764:THR:HA	2.02	0.41
3:a:3113[A]:ASP:OD2	3:a:3115[A]:LEU:HB2	2.20	0.41
3:a:3200[B]:LEU:O	3:a:3203[B]:HIS:HB3	2.20	0.41
1:b:77:GLU:O	1:b:81:VAL:HG23	2.21	0.41
1:b:361:GLU:HG2	1:b:363:THR:HG22	2.02	0.41
1:b:494:VAL:HG13	1:b:631:TRP:HZ3	1.85	0.41
3:d:2995[A]:GLN:CG	3:d:3168[A]:THR:HG21	2.48	0.41
3:d:3048[B]:ASP:HB3	3:d:3099[B]:PRO:HD2	2.01	0.41
3:d:3176[A]:LYS:C	3:d:3177[A]:SER:HG	2.13	0.41
1:A:70:ARG:HA	1:A:214:GLU:CD	2.43	0.41
1:A:1470:GLU:HG3	1:A:1530:LEU:HD12	2.02	0.41
1:A:1649:THR:HG22	2:E:2325:ALA:HA	2.02	0.41
3:C:3146[A]:CYS:O	3:C:3146[A]:CYS:SG	2.78	0.41
3:C:3146[B]:CYS:C	3:L:3161[B]:GLU:HG3	2.45	0.41
3:C:3148[B]:ILE:HD12	3:C:3175[B]:TYR:OH	2.21	0.41
3:C:3151[B]:LEU:O	3:L:3154[B]:PRO:CB	2.61	0.41
3:C:3281[B]:PHE:CZ	3:C:3305[B]:ILE:HG21	2.55	0.41
1:D:11:THR:HG22	1:D:13:ASP:H	1.86	0.41
1:D:407:GLN:HA	1:D:408:GLY:HA2	1.69	0.41
2:E:2725:GLN:OE1	2:E:2728:ARG:NH2	2.31	0.41
2:E:2858:ASP:O	2:E:2862:LYS:HG2	2.20	0.41
3:F:2961[A]:HIS:HB2	3:F:2992[A]:TYR:HE2	1.80	0.41
3:F:2973[B]:THR:C	3:a:3107[B]:LEU:HD12	2.45	0.41
3:F:2976[B]:ALA:O	3:F:2978[B]:CYS:N	2.46	0.41
3:F:3067[A]:ARG:HA	3:F:3067[A]:ARG:HD3	1.87	0.41
3:F:3173[B]:THR:OG1	3:a:3152[B]:LYS:HA	2.21	0.41
3:F:3298[A]:ASN:CA	3:F:3299[A]:LEU:HB2	2.44	0.41
1:G:897:HIS:HB3	1:G:899:MET:SD	2.61	0.41
1:G:1108:TYR:HB2	1:G:1114:TYR:CE1	2.55	0.41
1:G:1275:ARG:HH21	1:G:1375:ASN:ND2	2.18	0.41
1:G:1415:ASP:OD1	1:G:1484:CYS:HB2	2.19	0.41
2:H:2554:PRO:HB3	2:H:2556:TYR:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2938[B]:LEU:HD12	3:I:2938[B]:LEU:HA	1.85	0.41
3:I:2966[A]:SER:HB2	3:I:2977[A]:CYS:H	1.85	0.41
3:I:2975[B]:PHE:CE2	3:R:2988[B]:TRP:CH2	3.04	0.41
3:I:2995[B]:GLN:O	3:I:2996[B]:MET:C	2.62	0.41
3:I:3180[A]:TYR:HA	3:I:3183[A]:LEU:CD2	2.51	0.41
3:I:3276[B]:ASP:C	3:I:3278[B]:HIS:N	2.75	0.41
1:J:4:ARG:HD2	1:J:89:ILE:O	2.20	0.41
1:J:212:ASN:O	1:J:215:ARG:HB3	2.21	0.41
1:J:474:LEU:HD22	1:J:475:ASN:H	1.85	0.41
1:J:543:ASN:HA	1:J:544:PRO:HD3	1.87	0.41
1:J:604:ASN:O	1:J:607:HIS:HB2	2.20	0.41
1:J:1289:GLU:O	1:J:1292:SER:OG	2.24	0.41
1:J:1482:ALA:HB3	1:J:1489:MET:HE3	2.03	0.41
2:K:2650:GLY:N	2:K:2651:GLN:HA	2.35	0.41
3:L:3010[B]:PRO:HG2	3:L:3118[B]:VAL:HG13	2.03	0.41
3:L:3133[A]:LEU:HD12	3:L:3133[A]:LEU:HA	1.86	0.41
3:L:3133[A]:LEU:HD13	3:L:3197[A]:ILE:HG23	2.02	0.41
3:L:3185[A]:TYR:HD2	3:L:3186[A]:GLU:N	2.19	0.41
3:L:3185[B]:TYR:HD2	3:L:3186[B]:GLU:N	2.19	0.41
3:L:3230[B]:PHE:HB2	3:L:3242[B]:GLY:C	2.45	0.41
1:M:294:LYS:O	1:M:297:ARG:HB2	2.20	0.41
1:M:319:ILE:HG23	1:M:379:VAL:HG13	2.01	0.41
1:M:323:ILE:HA	1:M:324:PRO:HD3	1.84	0.41
1:M:627:ASP:HA	1:M:628:PRO:HD3	1.88	0.41
1:M:1301:PRO:HB3	1:M:1308:VAL:HG12	2.03	0.41
2:N:2089:ARG:HH11	2:N:2163:GLU:CD	2.28	0.41
2:N:2454:MET:HB3	2:N:2456:LEU:HG	2.03	0.41
3:O:2965[A]:LEU:CG	3:O:2974[A]:ALA:CB	2.85	0.41
3:O:3281[A]:PHE:CZ	3:O:3305[A]:ILE:HG21	2.55	0.41
1:P:35:GLN:HE22	1:P:127:GLU:HG3	1.86	0.41
1:P:604:ASN:ND2	1:P:763:LEU:H	2.19	0.41
1:P:1081:MET:HG2	1:P:1100:SER:O	2.20	0.41
2:Q:2695:MET:HE1	2:Q:2707:PHE:HB2	2.03	0.41
2:Q:2858:ASP:O	2:Q:2862:LYS:HG2	2.20	0.41
3:R:2933[A]:SER:CA	3:R:2936[A]:GLU:HB3	2.48	0.41
3:R:2939[B]:ARG:CB	3:R:3032[B]:PRO:HG2	2.44	0.41
3:R:3148[B]:ILE:HD12	3:R:3175[B]:TYR:OH	2.20	0.41
3:R:3196[A]:THR:OG1	3:R:3199[A]:GLN:OE1	2.38	0.41
1:S:320:LYS:HB2	1:S:380:THR:HG23	2.01	0.41
1:S:486:THR:HA	1:S:489:HIS:ND1	2.35	0.41
1:S:490:TRP:HE1	1:S:670:PRO:CD	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2995[A]:GLN:O	3:U:2996[A]:MET:C	2.63	0.41
3:U:3023[A]:ILE:O	3:U:3026[A]:THR:OG1	2.34	0.41
3:U:3113[A]:ASP:OD2	3:U:3115[A]:LEU:HB2	2.20	0.41
3:U:3113[B]:ASP:OD2	3:U:3115[B]:LEU:HB2	2.20	0.41
3:U:3229[B]:ASN:N	3:U:3286[B]:THR:O	2.52	0.41
3:U:3258[B]:PHE:CZ	3:d:2969[B]:TYR:CD2	3.09	0.41
1:V:151:GLN:H	1:V:151:GLN:HG3	1.54	0.41
1:V:1013:ILE:HG21	1:V:1192:TYR:CE1	2.54	0.41
1:V:1311:CYS:HB3	1:V:1495:PRO:HD3	2.01	0.41
2:W:2534:PHE:CE2	2:W:2755:PRO:HB3	2.55	0.41
3:X:2963[B]:MET:SD	3:X:2963[B]:MET:O	2.79	0.41
3:X:2989[A]:HIS:NE2	9:X:3401[A]:CUO:O1	2.54	0.41
3:X:3185[B]:TYR:CZ	3:X:3187[B]:TYR:CE2	3.09	0.41
1:Y:94:TRP:NE1	1:Y:212:ASN:HD22	2.18	0.41
1:Y:893:ALA:HB2	1:Y:1182:ASN:HD22	1.85	0.41
1:Y:1458:HIS:HA	1:Y:1461:VAL:HB	2.01	0.41
1:Y:1568:VAL:HB	1:Y:1632:LEU:HG	2.02	0.41
2:Z:2360:TYR:HB2	2:Z:2366:TYR:CE1	2.55	0.41
2:Z:2392:ASP:OD2	2:Z:2488:ARG:NH2	2.49	0.41
3:a:2963[A]:MET:SD	3:a:2963[A]:MET:O	2.79	0.41
3:a:3013[B]:ASP:CG	3:a:3015[B]:THR:HG1	2.25	0.41
3:a:3192[B]:PHE:HD2	3:a:3192[B]:PHE:HA	1.77	0.41
1:b:118:ALA:HB1	1:b:119:LYS:CA	2.46	0.41
1:b:387:ASN:OD1	1:b:387:ASN:N	2.41	0.41
1:b:464:LEU:HD22	1:b:622:HIS:CG	2.54	0.41
1:b:1321:HIS:CD2	1:b:1465:TRP:CH2	3.09	0.41
2:c:2720:ILE:HG12	2:c:2781:LEU:HG	2.02	0.41
3:d:2963[A]:MET:SD	3:d:2963[A]:MET:O	2.79	0.41
3:d:2963[B]:MET:SD	3:d:2963[B]:MET:O	2.79	0.41
3:d:3028[A]:PRO:HG2	3:d:3029[A]:LYS:HG2	2.02	0.41
3:d:3113[A]:ASP:OD2	3:d:3115[A]:LEU:HB2	2.20	0.41
3:d:3180[B]:TYR:HA	3:d:3183[B]:LEU:CD2	2.51	0.41
1:A:71:LEU:HA	1:A:71:LEU:HD12	1.83	0.41
1:A:120:LYS:HB3	1:A:121:ASN:CA	2.50	0.41
1:A:443:MET:HE1	1:A:455:TYR:CE1	2.56	0.41
1:A:451:SER:CB	1:A:1273:SER:HA	2.51	0.41
1:A:1033:LEU:H	1:A:1180:SER:HB2	1.85	0.41
1:A:1090:ILE:H	1:A:1090:ILE:HG12	1.60	0.41
2:B:2867:PRO:CG	3:C:2932[A]:PRO:HG2	2.42	0.41
3:C:3028[B]:PRO:HG2	3:C:3029[B]:LYS:HG2	2.02	0.41
3:C:3113[B]:ASP:OD2	3:C:3115[B]:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3200[A]:LEU:O	3:C:3203[A]:HIS:HB3	2.20	0.41
1:D:1148:LEU:HD23	1:D:1229:LYS:HD2	2.02	0.41
1:D:1406:HIS:O	1:D:1410:VAL:HG23	2.20	0.41
3:F:3146[B]:CYS:O	3:F:3146[B]:CYS:SG	2.78	0.41
3:F:3148[A]:ILE:HD12	3:F:3175[A]:TYR:OH	2.20	0.41
3:F:3150[B]:LYS:NZ	3:a:3162[B]:ASP:O	2.42	0.41
3:F:3230[A]:PHE:HB2	3:F:3242[A]:GLY:C	2.44	0.41
3:F:3248[B]:LEU:HB2	3:a:2972[B]:GLY:C	2.37	0.41
3:F:3259[B]:ASP:HB3	3:a:3162[B]:ASP:HA	2.03	0.41
3:F:3281[B]:PHE:CZ	3:F:3305[B]:ILE:HG21	2.55	0.41
1:G:456:GLN:HG2	1:G:551:GLU:CB	2.47	0.41
1:G:618:MET:SD	1:G:629:MET:HE3	2.60	0.41
1:G:733:PHE:HZ	1:G:746:LEU:HD13	1.86	0.41
1:G:891:LYS:HB2	1:G:892:TYR:HB3	2.01	0.41
1:G:1074:ILE:HG21	2:K:2870:LEU:HD22	2.02	0.41
1:G:1082:SER:OG	1:G:1083:PRO:HD3	2.20	0.41
2:H:2110:MET:O	2:H:2119:PHE:N	2.52	0.41
3:I:2963[B]:MET:SD	3:I:2963[B]:MET:O	2.79	0.41
3:I:3094[A]:SER:HG	3:I:3227[A]:ASP:CG	2.28	0.41
3:I:3096[A]:VAL:CG1	3:I:3115[A]:LEU:CD1	2.86	0.41
3:I:3113[A]:ASP:OD2	3:I:3115[A]:LEU:HB2	2.20	0.41
3:I:3133[A]:LEU:HD13	3:I:3197[A]:ILE:HG23	2.02	0.41
3:I:3155[B]:MET:CA	3:R:3153[B]:LYS:HD2	2.40	0.41
3:I:3196[A]:THR:N	3:I:3199[A]:GLN:CB	2.64	0.41
1:J:260:ASN:OD1	1:J:271:HIS:NE2	2.51	0.41
1:J:319:ILE:HG22	1:J:338:ALA:HB3	2.03	0.41
1:J:415:VAL:HG11	1:J:697:ALA:HB2	2.03	0.41
1:J:767:LYS:HE2	1:J:767:LYS:HB3	1.83	0.41
1:J:1018:ILE:HB	1:J:1045:HIS:NE2	2.35	0.41
1:J:1182:ASN:HD22	1:J:1182:ASN:N	2.09	0.41
2:K:2179:ASP:HB3	2:K:2303:ARG:NH1	2.35	0.41
2:K:2296:LEU:O	2:K:2299:SER:HB3	2.20	0.41
3:L:3028[B]:PRO:HG2	3:L:3029[B]:LYS:N	2.36	0.41
3:L:3299[A]:LEU:O	3:L:3300[A]:LEU:C	2.60	0.41
1:M:804:ASP:HB2	1:M:810:LEU:HD11	2.02	0.41
1:M:1207:TYR:O	1:M:1207:TYR:CD1	2.74	0.41
1:M:1215:LEU:HD11	1:M:1228:LEU:HD21	2.03	0.41
1:M:1300:CYS:HB3	1:M:1494:ARG:NH1	2.34	0.41
2:N:2097:LEU:HD12	2:Q:2235:PRO:HG2	2.03	0.41
2:N:2421:TYR:HB2	2:N:2454:MET:HE3	2.03	0.41
2:N:2742:MET:HA	2:N:2765:PRO:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:2963[B]:MET:HE2	3:X:2968[B]:GLN:C	2.46	0.41
3:O:2995[B]:GLN:O	3:O:2996[B]:MET:C	2.63	0.41
3:O:3041[A]:ALA:O	3:O:3042[A]:ASP:HB2	2.20	0.41
3:O:3185[B]:TYR:HD2	3:O:3186[B]:GLU:N	2.19	0.41
1:P:1225:VAL:HG12	1:P:1226:THR:H	1.85	0.41
1:P:1299:GLN:HB2	1:P:1311:CYS:SG	2.60	0.41
2:Q:2451:LEU:HD23	2:Q:2451:LEU:HA	1.87	0.41
2:Q:2561:HIS:HA	2:Q:2562:GLY:HA2	1.80	0.41
3:R:2995[B]:GLN:O	3:R:2996[B]:MET:C	2.63	0.41
3:R:3024[B]:LEU:CD1	3:R:3024[B]:LEU:C	2.85	0.41
3:R:3028[B]:PRO:HG2	3:R:3029[B]:LYS:HG2	2.02	0.41
3:R:3148[A]:ILE:HD12	3:R:3175[A]:TYR:OH	2.20	0.41
1:S:41:HIS:O	1:S:201:SER:OG	2.27	0.41
1:S:241:HIS:CD2	1:S:795:GLU:HA	2.56	0.41
2:T:2740:ASP:OD2	1:V:1232:THR:HA	2.20	0.41
3:U:2931[B]:THR:HG1	3:U:2934[B]:GLU:CD	2.04	0.41
3:U:2952[B]:ALA:CA	3:U:2956[B]:LYS:CB	2.89	0.41
3:U:3028[B]:PRO:HG2	3:U:3029[B]:LYS:N	2.36	0.41
3:U:3041[A]:ALA:O	3:U:3042[A]:ASP:HB2	2.20	0.41
3:U:3161[A]:GLU:H	3:U:3161[A]:GLU:CD	2.19	0.41
1:V:4:ARG:HD2	1:V:89:ILE:O	2.20	0.41
1:V:319:ILE:HG22	1:V:338:ALA:HB3	2.02	0.41
1:V:669:LYS:HB2	1:V:670:PRO:HD3	2.03	0.41
1:V:1018:ILE:HB	1:V:1045:HIS:NE2	2.36	0.41
2:W:2525:LYS:NZ	2:W:2526:ARG:HH12	2.18	0.41
2:W:2656:LEU:HA	2:W:2656:LEU:HD23	1.84	0.41
3:X:3010[B]:PRO:HG2	3:X:3118[B]:VAL:HG13	2.03	0.41
3:X:3182[B]:GLN:H	3:X:3182[B]:GLN:HG2	1.56	0.41
3:X:3298[A]:ASN:CB	3:X:3300[A]:LEU:CD2	2.61	0.41
1:Y:260:ASN:OD1	1:Y:271:HIS:NE2	2.49	0.41
1:Y:385:ALA:HB2	1:Y:391:MET:SD	2.61	0.41
1:Y:474:LEU:HD12	1:Y:474:LEU:HA	1.78	0.41
2:Z:2394:VAL:H	2:Z:2448:THR:HB	1.85	0.41
3:a:3171[B]:HIS:O	3:a:3172[B]:SER:C	2.63	0.41
3:a:3274[A]:ARG:NE	3:a:3274[A]:ARG:CA	2.84	0.41
1:b:112:ASP:N	1:b:112:ASP:OD1	2.51	0.41
1:b:306:PHE:CE2	1:b:399:PRO:HG3	2.55	0.41
1:b:855:ARG:HD3	1:b:957:ASN:O	2.20	0.41
1:b:1237:GLU:HA	1:b:1238:PRO:HD2	1.88	0.41
1:b:1423:TYR:OH	1:b:1461:VAL:O	2.38	0.41
2:c:2404:GLY:HA2	2:c:2405:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:2500:ILE:HD11	2:c:2504:ARG:HB3	2.02	0.41
2:c:2625:LEU:HA	2:c:2638:ARG:NH1	2.26	0.41
3:d:3028[B]:PRO:HG2	3:d:3029[B]:LYS:N	2.36	0.41
3:d:3096[B]:VAL:CG1	3:d:3115[B]:LEU:CD1	2.86	0.41
3:d:3148[B]:ILE:HG22	3:d:3152[B]:LYS:HE3	2.01	0.41
3:d:3281[A]:PHE:CZ	3:d:3305[A]:ILE:HG21	2.55	0.41
3:d:3299[A]:LEU:O	3:d:3300[A]:LEU:C	2.60	0.41
1:A:293:LEU:O	1:A:296:ARG:HG2	2.20	0.41
1:A:1319:PHE:HB3	1:A:1420:GLU:OE2	2.21	0.41
1:A:1647:ASN:HA	1:A:1648:PRO:HD3	1.93	0.41
2:B:2469:VAL:HG12	2:B:2475:GLU:HG2	2.03	0.41
3:C:2969[B]:TYR:CE2	3:L:3093[B]:HIS:NE2	2.78	0.41
3:C:2989[A]:HIS:NE2	9:L:3401[A]:CUO:O1	2.54	0.41
3:C:3041[B]:ALA:O	3:C:3042[B]:ASP:HB2	2.20	0.41
3:C:3171[A]:HIS:O	3:C:3172[A]:SER:C	2.63	0.41
3:C:3276[B]:ASP:C	3:C:3278[B]:HIS:N	2.75	0.41
1:D:425:ARG:HB2	1:D:703:TYR:CD2	2.55	0.41
1:D:622:HIS:HE1	1:D:766:SER:HB3	1.85	0.41
3:F:3180[B]:TYR:CA	3:F:3183[B]:LEU:CD2	2.95	0.41
3:F:3200[A]:LEU:O	3:F:3203[A]:HIS:HB3	2.20	0.41
1:G:614:GLU:O	1:G:617:SER:OG	2.28	0.41
1:G:905:TRP:HE1	1:G:1083:PRO:HD2	1.85	0.41
1:G:1576:THR:H	1:G:1581:GLU:CG	2.32	0.41
2:H:2765:PRO:HA	2:H:2768:LEU:HD11	2.01	0.41
3:I:3013[A]:ASP:CG	3:I:3015[A]:THR:HG1	2.24	0.41
3:I:3028[A]:PRO:HG2	3:I:3029[A]:LYS:N	2.36	0.41
3:I:3155[A]:MET:HE2	3:I:3155[A]:MET:HB3	1.99	0.41
3:I:3185[B]:TYR:CE2	3:I:3187[B]:TYR:HE2	2.31	0.41
1:J:1312:CYS:HA	1:J:1322:TRP:CE2	2.56	0.41
1:J:1599:MET:HA	1:J:1600:PRO:HD2	1.93	0.41
2:K:2398:PHE:HE2	2:K:2466:THR:HG21	1.86	0.41
3:L:2966[B]:SER:HB2	3:L:2977[B]:CYS:H	1.85	0.41
3:L:3028[A]:PRO:HG2	3:L:3029[A]:LYS:N	2.36	0.41
3:L:3067[B]:ARG:HA	3:L:3067[B]:ARG:HD3	1.87	0.41
3:L:3171[B]:HIS:C	3:L:3173[B]:THR:N	2.73	0.41
3:L:3180[A]:TYR:HA	3:L:3183[A]:LEU:CD2	2.51	0.41
3:L:3185[A]:TYR:HE2	3:L:3187[A]:TYR:CD2	2.35	0.41
1:M:89:ILE:H	1:M:89:ILE:HG12	1.69	0.41
1:M:436:GLU:O	1:M:440:ARG:HB2	2.20	0.41
1:M:450:LYS:NZ	1:M:505:ARG:HH21	2.18	0.41
1:M:548:ALA:HA	1:M:549:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:597:VAL:HG23	1:M:598:GLN:H	1.85	0.41
1:M:1146:PHE:CD2	1:M:1231:VAL:HG12	2.55	0.41
1:M:1156:LEU:HB2	1:M:1176:TYR:CE1	2.56	0.41
2:N:2515:ARG:HD2	2:Q:2168:ARG:NH2	2.36	0.41
3:O:2933[A]:SER:CA	3:O:2936[A]:GLU:HB3	2.48	0.41
3:O:2989[B]:HIS:NE2	9:O:3401[B]:CUO:O1	2.53	0.41
3:O:3028[A]:PRO:HG2	3:O:3029[A]:LYS:HG2	2.02	0.41
3:O:3083[A]:ILE:HD11	3:O:3260[A]:ARG:HG3	2.03	0.41
3:O:3113[A]:ASP:OD2	3:O:3115[A]:LEU:HB2	2.20	0.41
3:O:3194[B]:GLY:C	3:O:3195[B]:MET:CG	2.90	0.41
3:O:3293[B]:LYS:CG	3:O:3294[B]:SER:CB	2.98	0.41
3:O:3299[B]:LEU:O	3:O:3300[B]:LEU:C	2.60	0.41
1:P:639:ARG:HB2	1:P:703:TYR:CE1	2.55	0.41
1:P:745:ASP:OD1	1:P:759:SER:OG	2.31	0.41
1:P:975:PRO:HG3	1:P:1026:GLU:HG2	2.03	0.41
1:P:1560:HIS:HB3	1:P:1602:GLN:HG3	2.03	0.41
2:Q:2156:ARG:HD2	2:Q:2357:VAL:HG12	2.02	0.41
2:Q:2800:LYS:HB3	3:R:3023[A]:ILE:CD1	2.51	0.41
2:Q:2898:LYS:H	2:Q:2898:LYS:HG3	1.43	0.41
3:R:3034[B]:HIS:HB3	3:R:3035[B]:HIS:CE1	2.50	0.41
3:R:3113[A]:ASP:OD2	3:R:3115[A]:LEU:HB2	2.20	0.41
3:R:3133[B]:LEU:HD12	3:R:3133[B]:LEU:HA	1.86	0.41
3:R:3193[A]:HIS:ND1	3:R:3193[A]:HIS:N	2.68	0.41
3:R:3232[B]:VAL:HG21	3:R:3273[B]:LEU:HD11	2.00	0.41
1:S:25:MET:HE2	1:S:34:TYR:HA	2.02	0.41
1:S:285:THR:HG22	1:S:287:GLU:H	1.85	0.41
1:S:817:PRO:HA	1:S:818:PRO:HD3	1.87	0.41
1:S:1234:VAL:O	2:W:2739:LEU:HG	2.21	0.41
1:S:1339:SER:CB	1:S:1340:GLY:HA2	2.51	0.41
2:T:2323:ASN:HB3	1:V:1652:PHE:O	2.21	0.41
2:T:2345:ASN:HA	2:T:2346:PRO:HD2	1.96	0.41
2:T:2648:ALA:HB2	2:T:2656:LEU:HD12	2.03	0.41
3:U:2966[A]:SER:HB2	3:U:2977[A]:CYS:H	1.85	0.41
3:U:2989[A]:HIS:NE2	9:U:3401[A]:CUO:O1	2.53	0.41
3:U:3146[B]:CYS:O	3:U:3146[B]:CYS:SG	2.78	0.41
3:U:3185[B]:TYR:HD2	3:U:3186[B]:GLU:N	2.19	0.41
3:U:3256[B]:TRP:CE3	3:d:2969[B]:TYR:CG	3.05	0.41
1:V:40:TYR:HE2	1:V:75:GLN:HG2	1.85	0.41
1:V:95:THR:HG21	1:V:159:VAL:HG21	2.02	0.41
1:V:816:PRO:HA	1:V:817:PRO:HD3	1.95	0.41
1:V:877:HIS:HE1	1:V:1042:PHE:CE2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:2622:ASN:HA	2:W:2623:PRO:HD3	1.94	0.41
3:X:2989[B]:HIS:O	3:X:2991[B]:LEU:N	2.54	0.41
3:X:2995[B]:GLN:O	3:X:2996[B]:MET:C	2.63	0.41
3:X:3031[B]:ASN:HA	3:X:3032[B]:PRO:HD2	1.87	0.41
3:X:3183[B]:LEU:N	3:X:3184[B]:ASN:CA	2.80	0.41
3:X:3193[A]:HIS:ND1	3:X:3193[A]:HIS:N	2.68	0.41
1:Y:183:HIS:HE1	1:Y:206:PHE:HD1	1.69	0.41
1:Y:407:GLN:HA	1:Y:408:GLY:HA2	1.78	0.41
1:Y:1229:LYS:HD3	1:Y:1230:LEU:N	2.34	0.41
1:Y:1417:CYS:O	1:Y:1421:VAL:HG22	2.20	0.41
2:Z:2133:PRO:HG2	2:Z:2140:ARG:HA	2.03	0.41
2:Z:2779:ASP:HA	2:Z:2780:HIS:HA	1.73	0.41
3:a:2957[B]:ILE:HD11	3:a:2995[B]:GLN:C	2.46	0.41
3:a:3028[B]:PRO:HG2	3:a:3029[B]:LYS:N	2.36	0.41
3:a:3041[B]:ALA:O	3:a:3042[B]:ASP:HB2	2.20	0.41
3:a:3146[B]:CYS:O	3:a:3146[B]:CYS:SG	2.78	0.41
3:a:3193[B]:HIS:ND1	3:a:3193[B]:HIS:N	2.68	0.41
1:b:975:PRO:HG2	1:b:1024:GLY:CA	2.51	0.41
2:c:2277:LYS:H	2:c:2277:LYS:HE2	1.86	0.41
2:c:2552:GLU:HA	2:c:2553:ALA:HA	1.78	0.41
2:c:2610:ASP:OD1	2:c:2610:ASP:N	2.54	0.41
3:d:2957[B]:ILE:HD11	3:d:2995[B]:GLN:C	2.46	0.41
3:d:3010[B]:PRO:HG2	3:d:3118[B]:VAL:HG13	2.03	0.41
3:d:3096[A]:VAL:CG1	3:d:3115[A]:LEU:CD1	2.86	0.41
3:d:3148[A]:ILE:HD12	3:d:3175[A]:TYR:OH	2.20	0.41
3:d:3171[A]:HIS:C	3:d:3173[A]:THR:N	2.73	0.41
3:d:3254[B]:MET:H	3:d:3254[B]:MET:HG2	1.71	0.41
1:A:450:LYS:HG3	1:A:551:GLU:OE1	2.20	0.41
1:A:456:GLN:O	1:A:460:GLU:HG3	2.21	0.41
1:A:747:PHE:CE1	1:A:756:PHE:HD2	2.38	0.41
1:A:901:THR:HG22	1:A:904:HIS:HB2	2.01	0.41
1:A:1560:HIS:HB3	1:A:1602:GLN:HG3	2.03	0.41
2:B:2824:CYS:HB3	2:B:2826:GLU:O	2.20	0.41
2:B:2885:SER:OG	2:B:2886:VAL:N	2.54	0.41
3:C:3077[B]:ASP:HB3	3:C:3080[B]:ASP:OD2	2.21	0.41
3:C:3137[B]:ARG:HB3	3:C:3139[B]:LEU:HD21	1.97	0.41
3:C:3180[A]:TYR:HA	3:C:3183[A]:LEU:CD2	2.51	0.41
3:C:3281[B]:PHE:HE1	3:C:3305[B]:ILE:HG21	1.81	0.41
1:D:514:TRP:HZ2	1:D:606:ILE:HD11	1.86	0.41
1:D:736:MET:HE2	1:D:816:PRO:HD3	2.03	0.41
1:D:829:ALA:HA	1:D:830:ASN:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2097:LEU:HD23	2:E:2097:LEU:HA	1.92	0.41
2:E:2104:ILE:HG21	2:E:2196:TYR:CD2	2.56	0.41
2:E:2145:LEU:HD22	2:E:2154:TRP:CD1	2.56	0.41
3:F:2963[B]:MET:SD	3:F:2963[B]:MET:O	2.79	0.41
3:F:3152[B]:LYS:HB3	3:a:3172[B]:SER:N	2.23	0.41
3:F:3180[A]:TYR:HA	3:F:3183[A]:LEU:CD2	2.51	0.41
3:F:3274[B]:ARG:NE	3:F:3274[B]:ARG:CA	2.84	0.41
3:F:3300[A]:LEU:HD23	3:F:3300[A]:LEU:H	1.83	0.41
1:G:41:HIS:HD2	1:G:68:TRP:CZ3	2.38	0.41
1:G:674:LYS:HE3	1:G:674:LYS:HB2	1.89	0.41
1:G:737:GLY:HA2	1:G:771:TRP:CZ2	2.55	0.41
2:H:2625:LEU:HD13	2:H:2626:ARG:HG2	2.01	0.41
2:H:2811:HIS:NE2	2:H:2896:LEU:HD22	2.36	0.41
3:I:2980[B]:HIS:HA	3:I:2985[B]:PHE:HD2	1.86	0.41
3:I:3139[A]:LEU:CD2	3:I:3139[A]:LEU:H	2.34	0.41
3:I:3180[B]:TYR:CA	3:I:3183[B]:LEU:CD2	2.95	0.41
9:I:3401[A]:CUO:O1	3:R:2989[A]:HIS:NE2	2.54	0.41
1:J:306:PHE:CE2	1:J:399:PRO:HG3	2.56	0.41
1:J:705:THR:HG22	1:J:1118:THR:HG23	2.02	0.41
1:J:1252:PRO:HD3	1:J:1473:ARG:NH2	2.36	0.41
1:J:1647:ASN:HA	1:J:1648:PRO:HD3	1.93	0.41
2:K:2562:GLY:H	2:K:2846:TRP:CB	2.34	0.41
2:K:2569:TRP:HZ2	2:K:2748:PRO:HG3	1.86	0.41
2:K:2677:GLU:O	2:K:2680:HIS:HB3	2.20	0.41
3:L:3011[A]:TYR:CB	3:L:3121[A]:SER:HB2	2.49	0.41
3:L:3024[B]:LEU:CD1	3:L:3024[B]:LEU:C	2.85	0.41
3:L:3137[B]:ARG:HA	3:L:3137[B]:ARG:HD3	1.71	0.41
3:L:3192[A]:PHE:HD2	3:L:3192[A]:PHE:HA	1.77	0.41
3:L:3274[A]:ARG:NE	3:L:3274[A]:ARG:CA	2.84	0.41
3:L:3281[A]:PHE:CZ	3:L:3305[A]:ILE:HG21	2.55	0.41
1:M:447:MET:HA	1:M:455:TYR:CB	2.50	0.41
2:N:2695:MET:HE2	2:N:2695:MET:HB2	1.87	0.41
3:O:2951[B]:ASP:CG	3:O:2952[B]:ALA:H	2.28	0.41
3:O:2968[B]:GLN:HB3	3:X:2979[B]:GLN:HG2	2.03	0.41
3:O:2989[B]:HIS:O	3:O:2991[B]:LEU:N	2.54	0.41
3:O:3028[A]:PRO:HG2	3:O:3029[A]:LYS:N	2.36	0.41
3:O:3034[A]:HIS:HB3	3:O:3035[A]:HIS:CE1	2.50	0.41
3:O:3083[B]:ILE:HD11	3:O:3260[B]:ARG:HG3	2.03	0.41
3:O:3180[A]:TYR:HA	3:O:3183[A]:LEU:CD2	2.51	0.41
3:O:3221[B]:ALA:HA	3:X:3161[B]:GLU:HG2	1.21	0.41
3:O:3281[A]:PHE:HE1	3:O:3305[A]:ILE:HG21	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3281[B]:PHE:CZ	3:O:3305[B]:ILE:HG21	2.56	0.41
1:P:187:GLY:HA2	1:P:193:SER:HB2	2.03	0.41
1:P:327:ASP:OD1	1:P:328:LYS:N	2.54	0.41
1:P:732:GLY:HA2	1:P:777:TYR:O	2.20	0.41
1:P:891:LYS:HB3	1:P:892:TYR:HD2	1.81	0.41
1:P:1077:LEU:O	1:P:1102:PRO:HG2	2.21	0.41
1:P:1380:GLY:HA3	1:P:1450:TYR:O	2.21	0.41
1:P:1562:ILE:HG22	1:P:1563:LYS:H	1.85	0.41
2:Q:2377:SER:HB3	2:Q:2380:GLN:HG3	2.02	0.41
3:R:2957[B]:ILE:HD11	3:R:2995[B]:GLN:C	2.46	0.41
3:R:2963[A]:MET:SD	3:R:2963[A]:MET:O	2.79	0.41
3:R:3139[B]:LEU:CD2	3:R:3139[B]:LEU:H	2.34	0.41
1:S:120:LYS:H	1:S:121:ASN:HA	1.86	0.41
2:T:2527:LEU:HD22	2:T:2581:MET:HG2	2.02	0.41
3:U:2965[A]:LEU:CG	3:U:2974[A]:ALA:CB	2.85	0.41
3:U:2969[B]:TYR:CA	3:d:2981[B]:GLY:CA	2.97	0.41
3:U:3180[B]:TYR:HA	3:U:3183[B]:LEU:CD2	2.51	0.41
3:U:3255[B]:PRO:CG	3:d:3252[B]:TYR:HB3	2.51	0.41
3:U:3281[B]:PHE:CZ	3:U:3305[B]:ILE:HG21	2.55	0.41
1:V:548:ALA:N	1:V:559:THR:HG22	2.35	0.41
1:V:904:HIS:CD2	1:V:904:HIS:H	2.38	0.41
3:X:2948[B]:ASP:HB2	3:X:2953[B]:GLY:HA3	1.99	0.41
3:X:2980[B]:HIS:HA	3:X:2985[B]:PHE:HD2	1.86	0.41
3:X:2989[B]:HIS:NE2	9:X:3401[B]:CUO:O1	2.53	0.41
3:X:3028[B]:PRO:HG2	3:X:3029[B]:LYS:N	2.36	0.41
3:X:3083[A]:ILE:HD11	3:X:3260[A]:ARG:HG3	2.03	0.41
1:Y:148:GLN:C	1:Y:150:GLY:N	2.78	0.41
1:Y:554:LYS:HD3	1:Y:554:LYS:HA	1.79	0.41
1:Y:1401:ARG:NE	3:d:3182[B]:GLN:OE1	2.53	0.41
1:Y:1621:ASN:HA	3:d:3188[B]:ASP:CB	2.51	0.41
2:Z:2602:LEU:HG	2:Z:2603:PRO:HD2	2.02	0.41
2:Z:2716:ARG:O	2:Z:2720:ILE:HG13	2.21	0.41
3:a:3089[A]:HIS:CE1	3:a:3119[A]:HIS:CE1	2.81	0.41
3:a:3146[A]:CYS:O	3:a:3146[A]:CYS:SG	2.78	0.41
3:a:3171[A]:HIS:O	3:a:3172[A]:SER:C	2.63	0.41
3:a:3180[B]:TYR:HA	3:a:3183[B]:LEU:CD2	2.51	0.41
3:a:3193[A]:HIS:ND1	3:a:3193[A]:HIS:N	2.69	0.41
1:b:1430:ILE:HD13	1:b:1457:HIS:CD2	2.56	0.41
1:b:1647:ASN:HA	1:b:1648:PRO:HD3	1.96	0.41
2:c:2446:GLU:CG	2:c:2448:THR:HG23	2.50	0.41
2:c:2670:CYS:HB3	2:c:2850:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:2970[B]:PRO:C	3:d:2972[B]:GLY:H	2.23	0.41
3:d:3200[B]:LEU:O	3:d:3203[B]:HIS:HB3	2.20	0.41
3:d:3281[B]:PHE:CZ	3:d:3305[B]:ILE:HG21	2.56	0.41
1:A:236:GLY:HA2	1:A:819:ILE:HB	2.03	0.41
1:A:468:CYS:SG	1:A:669:LYS:HB3	2.61	0.41
1:A:749:VAL:HB	1:A:754:GLU:HB3	2.03	0.41
1:A:837:HIS:HA	1:A:1113:HIS:O	2.21	0.41
1:A:1059:LEU:HB3	1:A:1063:ARG:NH2	2.36	0.41
1:A:1075:GLU:H	1:A:1075:GLU:HG3	1.61	0.41
2:B:2235:PRO:HB3	2:B:2240:GLN:CD	2.46	0.41
2:B:2582:ARG:HG2	2:E:2109:ARG:HD3	2.02	0.41
3:C:2969[B]:TYR:CE2	3:L:3089[B]:HIS:NE2	2.86	0.41
3:C:2975[B]:PHE:CZ	3:L:2961[B]:HIS:CD2	3.09	0.41
3:C:2976[A]:ALA:O	3:C:2978[A]:CYS:N	2.46	0.41
3:C:2979[A]:GLN:NE2	3:C:3155[A]:MET:HE3	2.19	0.41
3:C:2980[A]:HIS:HA	3:C:2985[A]:PHE:HD2	1.86	0.41
3:C:2980[B]:HIS:HA	3:C:2985[B]:PHE:HD2	1.86	0.41
3:C:2995[A]:GLN:O	3:C:2996[A]:MET:C	2.63	0.41
3:C:3028[A]:PRO:HG2	3:C:3029[A]:LYS:N	2.36	0.41
3:C:3148[A]:ILE:HD12	3:C:3175[A]:TYR:OH	2.20	0.41
3:C:3180[B]:TYR:HA	3:C:3183[B]:LEU:CD2	2.51	0.41
3:C:3185[B]:TYR:HD2	3:C:3186[B]:GLU:N	2.19	0.41
3:C:3192[B]:PHE:HD2	3:C:3192[B]:PHE:HA	1.77	0.41
3:C:3232[B]:VAL:CG2	3:C:3273[B]:LEU:CD1	2.99	0.41
3:C:3298[B]:ASN:HA	3:C:3300[B]:LEU:N	2.36	0.41
1:D:588:GLU:OE2	1:D:728:ARG:NH1	2.53	0.41
1:D:946:GLU:CG	1:D:955:LYS:HB3	2.51	0.41
1:D:1200:MET:HE1	1:D:1205:LEU:HD23	2.03	0.41
1:D:1278:PHE:HD2	1:D:1376:PRO:HB2	1.85	0.41
1:D:1528:ASP:OD1	1:D:1528:ASP:N	2.53	0.41
1:D:1564:ALA:HB1	4:m:1:NAG:H81	2.03	0.41
2:E:2100:ILE:O	2:E:2104:ILE:HG12	2.21	0.41
2:E:2132:CYS:HA	2:E:2133:PRO:C	2.46	0.41
2:E:2361:LYS:HD3	2:E:2367:GLU:HG2	2.03	0.41
2:E:2568:HIS:CD2	2:E:2718:TRP:CH2	3.08	0.41
2:E:2647:LEU:HD12	2:E:2647:LEU:HA	1.64	0.41
3:F:3028[A]:PRO:HG2	3:F:3029[A]:LYS:N	2.36	0.41
3:F:3113[B]:ASP:OD2	3:F:3115[B]:LEU:HB2	2.20	0.41
3:F:3133[A]:LEU:HD13	3:F:3197[A]:ILE:HG23	2.02	0.41
3:F:3139[A]:LEU:CD2	3:F:3139[A]:LEU:H	2.34	0.41
3:F:3149[B]:ASN:HA	3:a:3169[B]:LYS:H	1.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3153[B]:LYS:HE3	3:a:3155[B]:MET:O	2.21	0.41
3:F:3158[B]:PHE:HB2	3:a:3153[B]:LYS:CG	2.51	0.41
3:F:3172[B]:SER:HB3	3:a:3150[B]:LYS:C	2.46	0.41
1:G:294:LYS:HA	1:G:297:ARG:HD2	2.03	0.41
1:G:745:ASP:OD1	1:G:759:SER:OG	2.37	0.41
1:G:792:MET:HB2	1:G:793:PHE:HD1	1.86	0.41
1:G:943:LEU:HD12	1:G:944:GLU:H	1.86	0.41
1:G:977:GLU:OE1	1:G:978:ALA:N	2.54	0.41
1:G:1002:GLU:HG3	1:G:1065:LYS:HD3	2.01	0.41
1:G:1037:ALA:HA	1:G:1042:PHE:CG	2.56	0.41
1:G:1081:MET:HG2	1:G:1100:SER:O	2.21	0.41
1:G:1302:SER:CB	1:G:1494:ARG:HH22	2.34	0.41
1:G:1319:PHE:CZ	1:G:1424:GLU:HG3	2.55	0.41
2:H:2218:SER:HG	2:H:2221:THR:HG1	1.60	0.41
2:H:2309:GLN:HG2	2:H:2319:ALA:HB1	2.02	0.41
2:H:2442:LEU:HG	1:J:1604:ASP:HB2	2.02	0.41
2:H:2527:LEU:HG	2:H:2536:PHE:HB2	2.03	0.41
2:H:2561:HIS:HA	2:H:2562:GLY:HA2	1.83	0.41
2:H:2742:MET:HA	2:H:2765:PRO:HB2	2.02	0.41
2:H:2816:SER:HB2	2:H:2886:VAL:HG21	2.03	0.41
3:I:2946[B]:GLN:CD	3:I:2947[B]:ALA:N	2.72	0.41
3:I:2954[B]:TYR:HA	3:I:2957[B]:ILE:CG2	2.50	0.41
3:I:2965[A]:LEU:CG	3:I:2974[A]:ALA:CB	2.85	0.41
3:I:2982[B]:MET:SD	3:R:3156[B]:MET:HB2	2.60	0.41
3:I:2987[B]:HIS:CD2	3:I:3178[B]:PHE:CE1	3.08	0.41
3:I:3096[B]:VAL:CG1	3:I:3115[B]:LEU:CD1	2.86	0.41
3:I:3148[B]:ILE:HD12	3:I:3175[B]:TYR:OH	2.20	0.41
3:I:3153[B]:LYS:NZ	3:R:3156[B]:MET:C	2.79	0.41
3:I:3163[B]:ASN:ND2	3:R:3150[B]:LYS:CG	2.37	0.41
3:I:3173[B]:THR:HG21	3:R:3173[B]:THR:HG1	1.77	0.41
3:I:3180[B]:TYR:HA	3:I:3183[B]:LEU:CD2	2.51	0.41
3:I:3185[B]:TYR:HD2	3:I:3186[B]:GLU:N	2.19	0.41
3:I:3281[A]:PHE:CZ	3:I:3305[A]:ILE:HG21	2.55	0.41
1:J:51:ASP:HA	1:J:52:GLY:HA2	1.66	0.41
1:J:418:ASP:OD1	1:J:418:ASP:N	2.53	0.41
1:J:572:SER:OG	1:J:574:GLY:HA3	2.21	0.41
1:J:876:PHE:CD2	1:J:1083:PRO:HB2	2.56	0.41
1:J:877:HIS:CE1	1:J:905:TRP:HZ3	2.39	0.41
1:J:1258:ARG:HG2	1:J:1335:LEU:HD11	2.01	0.41
1:J:1480:ASN:ND2	1:J:1518:ASP:HB3	2.34	0.41
1:J:1550:ARG:HD2	1:J:1551:ASP:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2130:PRO:CB	2:K:2142:ALA:HB3	2.51	0.41
2:K:2305:TRP:HZ2	2:K:2358:PHE:CE1	2.39	0.41
2:K:2746:MET:HG2	2:K:2763:SER:O	2.20	0.41
3:L:2951[A]:ASP:C	3:L:2956[A]:LYS:HZ1	2.17	0.41
3:L:2957[B]:ILE:HD11	3:L:2995[B]:GLN:C	2.46	0.41
3:L:2980[A]:HIS:HA	3:L:2985[A]:PHE:HD2	1.86	0.41
3:L:2980[B]:HIS:HA	3:L:2985[B]:PHE:HD2	1.86	0.41
3:L:3028[A]:PRO:HG2	3:L:3029[A]:LYS:HG2	2.02	0.41
3:L:3067[A]:ARG:HA	3:L:3067[A]:ARG:HD3	1.87	0.41
3:L:3083[A]:ILE:HD11	3:L:3260[A]:ARG:HG3	2.03	0.41
3:L:3089[A]:HIS:HD1	3:L:3119[A]:HIS:HE1	1.65	0.41
3:L:3139[B]:LEU:CD2	3:L:3139[B]:LEU:H	2.34	0.41
3:L:3194[B]:GLY:C	3:L:3195[B]:MET:CG	2.90	0.41
3:L:3196[B]:THR:N	3:L:3199[B]:GLN:CB	2.64	0.41
3:L:3218[A]:LEU:HD12	3:L:3218[A]:LEU:HA	1.78	0.41
3:L:3218[B]:LEU:HD12	3:L:3218[B]:LEU:HA	1.78	0.41
3:L:3230[A]:PHE:HB2	3:L:3242[A]:GLY:C	2.44	0.41
1:M:67:MET:H	1:M:67:MET:HG2	1.57	0.41
1:M:92:TRP:CE3	1:M:102:PRO:HD3	2.55	0.41
1:M:416:ASN:N	1:M:416:ASN:HD22	2.17	0.41
1:M:629:MET:HE2	1:M:629:MET:HB3	1.96	0.41
1:M:988:TYR:HB3	1:M:992:ALA:HB3	2.02	0.41
1:M:1007:PHE:CE1	1:M:1011:TYR:HB2	2.55	0.41
1:M:1080:PRO:HB2	1:M:1085:SER:CB	2.50	0.41
1:M:1156:LEU:HD13	1:M:1176:TYR:CE1	2.56	0.41
1:M:1528:ASP:OD1	1:M:1528:ASP:N	2.54	0.41
2:N:2184:MET:HB2	2:N:2231:LEU:O	2.20	0.41
2:N:2398:PHE:CE2	2:N:2484:ALA:HB2	2.56	0.41
2:N:2570:HIS:CD2	2:N:2711:HIS:CE1	3.09	0.41
2:N:2595:TRP:CD2	2:N:2683:ILE:HG13	2.56	0.41
2:N:2606:LEU:HD21	2:N:2709:VAL:HG21	2.03	0.41
3:O:2957[A]:ILE:HD11	3:O:2995[A]:GLN:C	2.46	0.41
3:O:2970[B]:PRO:CG	3:X:2991[B]:LEU:HD12	2.50	0.41
3:O:2989[A]:HIS:O	3:O:2991[A]:LEU:N	2.54	0.41
3:O:3031[B]:ASN:HA	3:O:3032[B]:PRO:HD2	1.87	0.41
3:O:3084[A]:GLN:HE21	3:O:3084[A]:GLN:HB3	1.71	0.41
3:O:3106[B]:THR:CG2	3:X:2970[B]:PRO:O	2.46	0.41
3:O:3139[B]:LEU:CD2	3:O:3139[B]:LEU:H	2.34	0.41
3:O:3151[A]:LEU:HB2	3:O:3175[A]:TYR:HE2	1.68	0.41
3:O:3194[A]:GLY:C	3:O:3195[A]:MET:CG	2.91	0.41
3:O:3218[B]:LEU:HD12	3:O:3218[B]:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3223[B]:GLY:N	3:X:3162[B]:ASP:OD1	2.53	0.41
3:O:3253[B]:GLU:OE1	3:X:3161[B]:GLU:CD	2.44	0.41
1:P:16:LEU:HD12	1:P:113:PRO:HG2	2.02	0.41
1:P:119:LYS:H	1:P:119:LYS:HG2	1.71	0.41
1:P:567:LEU:HB2	1:P:571:PRO:HB3	2.01	0.41
1:P:1573:CYS:HA	1:P:1583:CYS:O	2.21	0.41
2:Q:2134:ASN:OD1	2:Q:2137:ALA:HB2	2.20	0.41
2:Q:2471:HIS:O	2:Q:2471:HIS:ND1	2.47	0.41
3:R:2980[B]:HIS:HA	3:R:2985[B]:PHE:HD2	1.86	0.41
3:R:3010[A]:PRO:HG2	3:R:3118[A]:VAL:HG13	2.03	0.41
3:R:3023[A]:ILE:O	3:R:3026[A]:THR:OG1	2.34	0.41
3:R:3028[A]:PRO:HG2	3:R:3029[A]:LYS:N	2.36	0.41
3:R:3028[B]:PRO:HG2	3:R:3029[B]:LYS:N	2.36	0.41
3:R:3113[B]:ASP:OD2	3:R:3115[B]:LEU:HB2	2.20	0.41
3:R:3146[A]:CYS:O	3:R:3146[A]:CYS:SG	2.78	0.41
3:R:3151[B]:LEU:CB	3:R:3175[B]:TYR:CE2	2.85	0.41
3:R:3180[A]:TYR:HA	3:R:3183[A]:LEU:CD2	2.51	0.41
3:R:3200[B]:LEU:O	3:R:3203[B]:HIS:HB3	2.20	0.41
3:R:3218[B]:LEU:HD13	3:R:3261[B]:LEU:HD23	2.01	0.41
3:R:3265[A]:ASP:OD1	3:R:3266[A]:ILE:N	2.54	0.41
1:S:664:VAL:HG12	1:S:690:THR:HG22	2.02	0.41
1:S:718:ARG:HD2	1:S:718:ARG:HA	1.81	0.41
1:S:902:PHE:N	1:S:903:PRO:HD2	2.36	0.41
1:S:913:PHE:O	1:S:917:LEU:HB2	2.21	0.41
1:S:1057:GLN:NE2	1:S:1067:TYR:O	2.43	0.41
1:S:1078:ARG:NH1	2:W:2872:GLU:O	2.45	0.41
1:S:1086:LEU:HB3	1:S:1090:ILE:HD12	2.03	0.41
1:S:1348:TRP:CZ3	1:S:1460:ASN:HB3	2.56	0.41
1:S:1359:ILE:O	1:S:1391:ARG:NH2	2.54	0.41
1:S:1426:LEU:O	1:S:1429:THR:HB	2.20	0.41
1:S:1487:PRO:O	1:S:1491:GLN:NE2	2.52	0.41
2:T:2361:LYS:HD2	2:T:2362:GLN:H	1.85	0.41
2:T:2381:LEU:HD23	2:T:2381:LEU:HA	1.90	0.41
2:T:2481:LEU:HD23	2:T:2481:LEU:HA	1.96	0.41
2:T:2679:ILE:O	2:T:2682:SER:HB3	2.21	0.41
2:T:2749:PHE:HA	2:T:2754:ASN:ND2	2.36	0.41
3:U:2969[B]:TYR:CZ	3:d:2980[B]:HIS:CG	3.08	0.41
3:U:2974[B]:ALA:N	3:d:3222[B]:ILE:N	2.58	0.41
3:U:3010[A]:PRO:HG2	3:U:3118[A]:VAL:HG13	2.03	0.41
3:U:3034[B]:HIS:HB3	3:U:3035[B]:HIS:CE1	2.50	0.41
3:U:3077[B]:ASP:HB3	3:U:3080[B]:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:3134[A]:GLN:C	3:U:3136[A]:TYR:N	2.77	0.41
3:U:3193[A]:HIS:ND1	3:U:3193[A]:HIS:N	2.69	0.41
3:U:3281[A]:PHE:CZ	3:U:3305[A]:ILE:HG21	2.55	0.41
1:V:227:ARG:HA	1:V:228:GLY:HA2	1.84	0.41
1:V:237:LEU:HA	1:V:240:PHE:CD2	2.56	0.41
1:V:425:ARG:HD2	1:V:703:TYR:CE1	2.56	0.41
1:V:450:LYS:HZ2	1:V:451:SER:H	1.66	0.41
1:V:468:CYS:HA	1:V:469:PRO:C	2.45	0.41
1:V:912:ASN:OD1	1:V:1096:THR:HG21	2.21	0.41
1:V:1008:GLU:HA	1:V:1011:TYR:HB3	2.03	0.41
1:V:1145:THR:HB	1:V:1191:PRO:HB2	2.03	0.41
1:V:1149:GLU:HG3	1:V:1187:LYS:HB3	2.02	0.41
1:V:1267:GLU:H	1:V:1267:GLU:HG2	1.74	0.41
1:V:1492:PRO:HB2	1:V:1497:SER:HB3	2.03	0.41
2:W:2506:ARG:NH1	2:W:2778:TYR:OH	2.51	0.41
2:W:2612:TYR:HB2	1:Y:138:ALA:HB1	2.02	0.41
2:W:2667:GLU:HB3	2:W:2730:LEU:HD13	2.03	0.41
2:W:2744:PHE:HA	2:W:2745:PRO:HD3	1.84	0.41
2:W:2745:PRO:HB2	2:W:2750:ILE:HD12	2.03	0.41
3:X:2942[A]:LEU:CD1	3:X:3033[A]:PHE:CZ	3.04	0.41
3:X:2963[A]:MET:SD	3:X:2963[A]:MET:O	2.79	0.41
3:X:2966[A]:SER:HB2	3:X:2977[A]:CYS:H	1.85	0.41
3:X:2995[A]:GLN:O	3:X:2996[A]:MET:C	2.63	0.41
3:X:3010[A]:PRO:HG2	3:X:3118[A]:VAL:HG13	2.03	0.41
3:X:3023[A]:ILE:HA	3:X:3026[A]:THR:HG1	1.82	0.41
3:X:3023[B]:ILE:HA	3:X:3026[B]:THR:HG1	1.84	0.41
3:X:3067[B]:ARG:HA	3:X:3067[B]:ARG:HD3	1.87	0.41
3:X:3180[A]:TYR:HA	3:X:3183[A]:LEU:CD2	2.51	0.41
3:X:3265[A]:ASP:OD1	3:X:3266[A]:ILE:N	2.54	0.41
1:Y:398:ARG:HA	1:Y:399:PRO:HD3	1.91	0.41
1:Y:548:ALA:HA	1:Y:549:PRO:HD3	1.97	0.41
1:Y:566:ARG:HH11	1:Y:803:LYS:HZ2	1.69	0.41
1:Y:806:ASN:ND2	1:Y:806:ASN:C	2.72	0.41
1:Y:834:ASP:OD1	1:Y:834:ASP:N	2.54	0.41
1:Y:899:MET:HB3	1:Y:1012:GLU:OE1	2.21	0.41
1:Y:913:PHE:O	1:Y:917:LEU:HB2	2.20	0.41
1:Y:1300:CYS:SG	1:Y:1494:ARG:HB3	2.61	0.41
1:Y:1301:PRO:HD2	5:KA:1:NAG:H83	2.02	0.41
1:Y:1403:LEU:HD21	1:Y:1429:THR:HG21	2.03	0.41
1:Y:1493:MET:HG2	1:Y:1511:SER:O	2.21	0.41
1:Y:1573:CYS:HB2	1:Y:1627:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:2122:ILE:O	2:Z:2125:PHE:HB2	2.21	0.41
2:Z:2168:ARG:O	2:c:2503:ASN:HB3	2.21	0.41
2:Z:2180:TRP:HB3	2:Z:2184:MET:HE2	2.02	0.41
2:Z:2724:LEU:O	2:Z:2728:ARG:HG3	2.21	0.41
3:a:2957[A]:ILE:HD11	3:a:2995[A]:GLN:C	2.46	0.41
3:a:2980[B]:HIS:HA	3:a:2985[B]:PHE:HD2	1.86	0.41
3:a:3010[A]:PRO:HG2	3:a:3118[A]:VAL:HG13	2.03	0.41
3:a:3010[B]:PRO:HG2	3:a:3118[B]:VAL:HG13	2.03	0.41
3:a:3023[A]:ILE:HA	3:a:3026[A]:THR:HG1	1.84	0.41
3:a:3025[A]:VAL:CG2	3:a:3047[A]:ARG:NH1	2.73	0.41
3:a:3155[A]:MET:HE2	3:a:3155[A]:MET:HB3	1.99	0.41
3:a:3185[B]:TYR:CZ	3:a:3187[B]:TYR:CE2	3.09	0.41
3:a:3196[A]:THR:OG1	3:a:3199[A]:GLN:OE1	2.38	0.41
1:b:35:GLN:OE1	1:b:127:GLU:HG2	2.21	0.41
1:b:93:ASP:HA	1:b:212:ASN:HD21	1.85	0.41
1:b:468:CYS:HA	1:b:469:PRO:C	2.46	0.41
1:b:740:THR:OG1	1:b:741:SER:N	2.54	0.41
1:b:1002:GLU:HG3	1:b:1065:LYS:HD3	2.03	0.41
1:b:1017:HIS:ND1	1:b:1021:LEU:HD11	2.36	0.41
1:b:1109:LYS:H	1:b:1109:LYS:HG3	1.57	0.41
1:b:1161:ILE:HG21	1:b:1200:MET:HE3	2.02	0.41
1:b:1228:LEU:HA	1:b:1228:LEU:HD23	1.77	0.41
1:b:1481:GLU:HG2	1:b:1482:ALA:H	1.86	0.41
2:c:2153:GLN:OE1	2:c:2153:GLN:N	2.48	0.41
2:c:2490:PRO:HA	2:c:2491:PRO:HD3	1.97	0.41
2:c:2521:MET:HE3	2:c:2605:LEU:HD12	2.03	0.41
2:c:2640:ILE:HD13	2:c:2687:ILE:O	2.20	0.41
3:d:2942[B]:LEU:CD1	3:d:3033[B]:PHE:CZ	3.04	0.41
3:d:3028[A]:PRO:HG2	3:d:3029[A]:LYS:N	2.36	0.41
3:d:3028[B]:PRO:HG2	3:d:3029[B]:LYS:HG2	2.02	0.41
3:d:3113[B]:ASP:OD2	3:d:3115[B]:LEU:HB2	2.20	0.41
3:d:3134[B]:GLN:C	3:d:3136[B]:TYR:N	2.77	0.41
3:d:3196[B]:THR:OG1	3:d:3199[B]:GLN:OE1	2.38	0.41
3:d:3229[A]:ASN:N	3:d:3286[A]:THR:O	2.52	0.41
3:d:3229[B]:ASN:O	3:d:3286[B]:THR:N	2.50	0.41
3:d:3265[A]:ASP:OD1	3:d:3266[A]:ILE:N	2.54	0.41
3:d:3276[B]:ASP:C	3:d:3278[B]:HIS:N	2.75	0.41
3:d:3284[A]:LYS:CD	3:d:3284[A]:LYS:C	2.86	0.41
6:k:1:NAG:O4	6:k:2:NAG:O7	2.39	0.41
1:A:40:TYR:CD1	1:A:246:PRO:HG2	2.56	0.41
1:A:203:ASP:HA	1:A:204:PRO:HD2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1492:PRO:HB2	1:A:1497:SER:CB	2.48	0.41
1:A:1508:PHE:CD1	1:A:1508:PHE:C	2.99	0.41
3:C:2954[A]:TYR:HA	3:C:2957[A]:ILE:CG2	2.50	0.41
3:C:2963[A]:MET:SD	3:C:2963[A]:MET:O	2.79	0.41
3:C:2995[B]:GLN:O	3:C:2996[B]:MET:C	2.63	0.41
3:C:3242[A]:GLY:O	3:C:3243[A]:GLY:O	2.39	0.41
3:C:3274[A]:ARG:NE	3:C:3274[A]:ARG:CA	2.84	0.41
1:D:59:LEU:HD13	1:D:68:TRP:CD1	2.56	0.41
1:D:225:LYS:HD2	1:D:231:THR:HG21	2.03	0.41
1:D:568:PHE:O	1:D:569:LYS:HD2	2.20	0.41
1:D:587:PHE:O	1:D:651:ARG:NH2	2.43	0.41
1:D:717:GLN:NE2	1:D:832:LYS:HE3	2.35	0.41
2:E:2582:ARG:HG2	2:E:2586:ALA:O	2.20	0.41
2:E:2651:GLN:C	2:E:2653:GLU:H	2.27	0.41
2:E:2764:THR:HA	2:E:2765:PRO:HD3	1.96	0.41
3:F:2952[B]:ALA:N	3:F:2953[B]:GLY:CA	2.71	0.41
3:F:2957[B]:ILE:HD11	3:F:2995[B]:GLN:C	2.46	0.41
3:F:2966[A]:SER:HB2	3:F:2977[A]:CYS:H	1.85	0.41
3:F:2966[B]:SER:HB3	3:a:2982[B]:MET:HE1	2.00	0.41
3:F:2972[B]:GLY:N	3:a:3248[B]:LEU:HD22	2.35	0.41
3:F:3048[B]:ASP:HB3	3:F:3099[B]:PRO:HD2	2.01	0.41
3:F:3137[B]:ARG:HB3	3:F:3139[B]:LEU:HD21	1.97	0.41
3:F:3152[B]:LYS:HB3	3:a:3170[B]:ALA:O	2.21	0.41
3:F:3229[A]:ASN:N	3:F:3286[A]:THR:O	2.52	0.41
3:F:3265[B]:ASP:OD1	3:F:3266[B]:ILE:N	2.54	0.41
1:G:35:GLN:NE2	1:G:129:LYS:HB2	2.36	0.41
1:G:164:GLU:OE2	1:G:297:ARG:HG2	2.21	0.41
1:G:1033:LEU:HA	1:G:1036:SER:OG	2.21	0.41
1:G:1149:GLU:HG3	1:G:1187:LYS:HE2	2.03	0.41
1:G:1380:GLY:O	1:G:1389:THR:HG23	2.21	0.41
3:I:2980[A]:HIS:HA	3:I:2985[A]:PHE:HD2	1.86	0.41
3:I:2989[B]:HIS:O	3:I:2991[B]:LEU:N	2.54	0.41
3:I:2991[B]:LEU:CD2	3:R:3153[B]:LYS:HG3	2.51	0.41
3:I:3028[B]:PRO:HG2	3:I:3029[B]:LYS:HG2	2.02	0.41
3:I:3169[B]:LYS:C	3:R:3152[B]:LYS:HB2	2.46	0.41
3:I:3193[A]:HIS:ND1	3:I:3193[A]:HIS:N	2.69	0.41
3:I:3281[B]:PHE:CZ	3:I:3305[B]:ILE:HG21	2.55	0.41
1:J:750:ALA:HA	1:J:796:TYR:HB3	2.02	0.41
1:J:842:ASN:OD1	1:J:843:VAL:N	2.54	0.41
1:J:891:LYS:HA	1:J:892:TYR:HA	1.92	0.41
1:J:1302:SER:HA	1:J:1303:GLU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2399:LEU:HA	2:K:2399:LEU:HD12	1.87	0.41
2:K:2818:ASP:OD2	2:K:2820:HIS:NE2	2.54	0.41
3:L:2989[A]:HIS:O	3:L:2991[A]:LEU:N	2.54	0.41
3:L:3010[A]:PRO:HG2	3:L:3118[A]:VAL:HG13	2.03	0.41
3:L:3083[B]:ILE:HD11	3:L:3260[B]:ARG:HG3	2.03	0.41
3:L:3134[A]:GLN:C	3:L:3136[A]:TYR:N	2.77	0.41
3:L:3139[A]:LEU:CD2	3:L:3139[A]:LEU:H	2.34	0.41
3:L:3242[A]:GLY:O	3:L:3243[A]:GLY:O	2.39	0.41
1:M:131:GLU:OE2	1:M:192:HIS:HE1	2.04	0.41
1:M:876:PHE:CE2	1:M:1083:PRO:HB2	2.56	0.41
2:N:2534:PHE:CD2	2:N:2755:PRO:HB3	2.56	0.41
3:O:2975[B]:PHE:CD2	3:X:3172[B]:SER:O	2.74	0.41
3:O:3028[B]:PRO:HG2	3:O:3029[B]:LYS:N	2.36	0.41
3:O:3160[B]:SER:OG	3:X:3150[B]:LYS:HB3	2.15	0.41
3:O:3180[A]:TYR:CA	3:O:3183[A]:LEU:CD2	2.95	0.41
3:O:3182[A]:GLN:H	3:O:3182[A]:GLN:HG2	1.56	0.41
3:O:3284[B]:LYS:CD	3:O:3284[B]:LYS:C	2.86	0.41
1:P:197:LEU:HG	1:P:345:GLY:C	2.46	0.41
1:P:305:ASN:HB3	1:P:400:ILE:HB	2.03	0.41
1:P:450:LYS:HD3	1:P:1338:GLY:O	2.20	0.41
1:P:1086:LEU:HD12	1:P:1086:LEU:N	2.36	0.41
3:R:2942[A]:LEU:CD1	3:R:3033[A]:PHE:CZ	3.04	0.41
3:R:3193[B]:HIS:ND1	3:R:3193[B]:HIS:N	2.68	0.41
1:S:188:GLY:O	1:S:386:ILE:HD11	2.20	0.41
1:S:1258:ARG:HG2	1:S:1335:LEU:CD1	2.51	0.41
1:S:1319:PHE:CE2	1:S:1424:GLU:HG3	2.56	0.41
2:T:2132:CYS:HB2	2:T:2142:ALA:CB	2.51	0.41
2:T:2568:HIS:HB2	2:T:2746:MET:HE1	2.02	0.41
2:T:2764:THR:HG22	2:T:2766:SER:H	1.84	0.41
2:T:2889:ALA:H	2:T:2890:VAL:HA	1.84	0.41
3:U:2957[A]:ILE:HD11	3:U:2995[A]:GLN:C	2.46	0.41
3:U:3134[B]:GLN:C	3:U:3136[B]:TYR:N	2.77	0.41
3:U:3232[B]:VAL:HG21	3:U:3273[B]:LEU:HD11	2.00	0.41
3:U:3298[B]:ASN:HA	3:U:3300[B]:LEU:N	2.36	0.41
1:V:570:GLN:HE21	1:V:570:GLN:HB2	1.54	0.41
1:V:1258:ARG:HD2	1:V:1524:HIS:O	2.20	0.41
1:V:1350:GLU:HA	1:V:1351:PRO:HD2	1.93	0.41
1:V:1410:VAL:HG22	1:V:1422:HIS:HB3	2.03	0.41
1:V:1571:TYR:HA	1:V:1585:ASN:O	2.21	0.41
2:W:2156:ARG:O	2:W:2160:VAL:HG13	2.21	0.41
2:W:2373:MET:HE3	2:W:2374:ASN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2976[B]:ALA:O	3:X:2978[B]:CYS:N	2.46	0.41
3:X:2980[A]:HIS:HA	3:X:2985[A]:PHE:HD2	1.86	0.41
3:X:2980[A]:HIS:ND1	3:X:2980[A]:HIS:N	2.59	0.41
3:X:3025[A]:VAL:CG2	3:X:3047[A]:ARG:NH1	2.73	0.41
3:X:3041[A]:ALA:O	3:X:3042[A]:ASP:HB2	2.20	0.41
3:X:3276[A]:ASP:C	3:X:3278[A]:HIS:N	2.75	0.41
3:X:3281[B]:PHE:CZ	3:X:3305[B]:ILE:HG21	2.55	0.41
1:Y:69:HIS:NE2	9:Y:2102:CUO:O2	2.53	0.41
1:Y:589:GLN:HG2	1:Y:594:ASP:CB	2.49	0.41
1:Y:704:ASP:OD1	1:Y:705:THR:N	2.49	0.41
1:Y:907:ARG:NH1	1:Y:1114:TYR:OH	2.54	0.41
1:Y:1195:ASP:O	1:Y:1197:THR:N	2.54	0.41
1:Y:1334:LEU:HD12	1:Y:1334:LEU:HA	1.90	0.41
1:Y:1613:ASP:CG	3:d:3185[B]:TYR:C	2.89	0.41
1:Y:1622:GLN:H	1:Y:1622:GLN:HG3	1.43	0.41
2:Z:2866:PRO:HB3	3:a:2933[A]:SER:N	2.36	0.41
2:Z:2903:TYR:OH	3:a:2932[A]:PRO:HD2	2.21	0.41
3:a:2930[B]:LEU:N	3:a:2930[B]:LEU:HD13	2.36	0.41
3:a:2932[A]:PRO:CA	3:a:2935[A]:ILE:CD1	2.85	0.41
3:a:2948[A]:ASP:HB2	3:a:2953[A]:GLY:HA3	1.99	0.41
3:a:2966[A]:SER:HB2	3:a:2977[A]:CYS:H	1.85	0.41
3:a:3084[A]:GLN:HE21	3:a:3084[A]:GLN:HB3	1.71	0.41
3:a:3133[B]:LEU:HD12	3:a:3133[B]:LEU:HA	1.86	0.41
3:a:3148[A]:ILE:HD12	3:a:3175[A]:TYR:OH	2.20	0.41
1:b:447:MET:HA	1:b:455:TYR:HB3	2.01	0.41
1:b:491:HIS:CD2	1:b:634:HIS:CE1	3.09	0.41
1:b:514:TRP:CZ2	1:b:606:ILE:HD11	2.56	0.41
1:b:535:PRO:O	1:b:538:LYS:HE3	2.21	0.41
1:b:1401:ARG:H	1:b:1401:ARG:HG3	1.55	0.41
1:b:1470:GLU:HB3	1:b:1537:ILE:HD13	2.03	0.41
2:c:2089:ARG:HB2	2:c:2368:TYR:CD1	2.56	0.41
2:c:2606:LEU:HD13	2:c:2706:ILE:HG23	2.03	0.41
3:d:2938[A]:LEU:HD12	3:d:2938[A]:LEU:HA	1.85	0.41
3:d:2952[A]:ALA:CA	3:d:2956[A]:LYS:CB	2.89	0.41
3:d:2989[A]:HIS:O	3:d:2991[A]:LEU:N	2.54	0.41
3:d:3133[B]:LEU:HD12	3:d:3133[B]:LEU:HA	1.86	0.41
3:d:3185[B]:TYR:HD2	3:d:3186[B]:GLU:N	2.19	0.41
1:A:128:ILE:N	1:A:133:LYS:O	2.49	0.40
1:A:462:HIS:HA	1:A:490:TRP:CH2	2.56	0.40
1:A:492:ARG:HH22	1:A:641:TRP:CD1	2.40	0.40
1:A:1400:ASN:HD22	1:A:1400:ASN:HA	1.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1519:TYR:CE2	1:A:1520:GLN:HG3	2.56	0.40
1:A:1528:ASP:N	1:A:1528:ASP:OD1	2.55	0.40
1:A:1565:SER:HB3	1:A:1594:GLY:H	1.86	0.40
2:B:2647:LEU:O	2:B:2654:SER:HB2	2.20	0.40
2:B:2687:ILE:HD11	2:B:2695:MET:HG2	2.04	0.40
3:C:2963[B]:MET:SD	3:C:2963[B]:MET:O	2.79	0.40
3:C:3010[B]:PRO:HG2	3:C:3118[B]:VAL:HG13	2.03	0.40
3:C:3023[B]:ILE:O	3:C:3026[B]:THR:OG1	2.34	0.40
3:C:3133[A]:LEU:HD13	3:C:3197[A]:ILE:HG23	2.02	0.40
3:C:3183[B]:LEU:H	3:C:3184[B]:ASN:CA	2.22	0.40
1:D:7:VAL:HG21	1:D:208:LEU:HD23	2.03	0.40
1:D:753:ASN:HD22	1:D:753:ASN:C	2.29	0.40
3:F:2931[A]:THR:O	3:F:2934[A]:GLU:HB2	2.22	0.40
3:F:2975[B]:PHE:O	3:a:3253[B]:GLU:CG	2.65	0.40
3:F:2983[B]:VAL:CG2	3:a:3161[B]:GLU:HB2	2.49	0.40
3:F:3028[B]:PRO:HG2	3:F:3029[B]:LYS:HG2	2.02	0.40
3:F:3084[A]:GLN:HE21	3:F:3084[A]:GLN:HB3	1.71	0.40
3:F:3150[B]:LYS:C	3:a:3172[B]:SER:HB3	2.46	0.40
3:F:3306[A]:LEU:C	3:F:3306[A]:LEU:CD1	2.85	0.40
1:G:695:TYR:N	1:G:695:TYR:HD1	2.19	0.40
1:G:1025:THR:HG23	1:G:1221:THR:HA	2.02	0.40
1:G:1156:LEU:HB2	1:G:1176:TYR:CE1	2.55	0.40
1:G:1248:ARG:HG3	1:G:1249:TRP:N	2.36	0.40
2:H:2107:LEU:HD22	2:H:2209:PHE:CE1	2.55	0.40
2:H:2145:LEU:HD12	2:H:2145:LEU:HA	1.93	0.40
2:H:2311:LEU:HD23	2:H:2311:LEU:HA	1.98	0.40
2:H:2568:HIS:HD2	2:H:2718:TRP:CH2	2.40	0.40
2:H:2590:VAL:HA	2:H:2591:PRO:HD3	1.90	0.40
2:H:2901:LEU:H	1:J:1075:GLU:HG3	1.86	0.40
3:I:2952[A]:ALA:CA	3:I:2956[A]:LYS:CB	2.89	0.40
3:I:2970[B]:PRO:CA	3:R:2989[B]:HIS:HD2	2.29	0.40
3:I:3010[B]:PRO:HG2	3:I:3118[B]:VAL:HG13	2.03	0.40
3:I:3023[A]:ILE:C	3:I:3025[A]:VAL:N	2.79	0.40
3:I:3093[B]:HIS:NE2	3:R:2969[B]:TYR:CD2	2.90	0.40
3:I:3113[B]:ASP:OD2	3:I:3115[B]:LEU:HB2	2.20	0.40
3:I:3139[B]:LEU:CD2	3:I:3139[B]:LEU:H	2.34	0.40
3:I:3153[B]:LYS:O	3:R:3154[B]:PRO:CA	2.68	0.40
3:I:3229[B]:ASN:N	3:I:3286[B]:THR:O	2.52	0.40
3:I:3265[B]:ASP:OD1	3:I:3266[B]:ILE:N	2.54	0.40
3:I:3299[A]:LEU:HB3	3:I:3300[A]:LEU:H	1.54	0.40
1:J:1051:ARG:HD2	1:J:1118:THR:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2303:ARG:NH2	2:K:2372:GLU:O	2.53	0.40
3:L:3031[B]:ASN:HA	3:L:3032[B]:PRO:HD2	1.87	0.40
3:L:3113[A]:ASP:OD2	3:L:3115[A]:LEU:HB2	2.20	0.40
3:L:3113[B]:ASP:OD2	3:L:3115[B]:LEU:HB2	2.20	0.40
1:M:1339:SER:OG	1:M:1340:GLY:HA2	2.21	0.40
2:N:2403:PHE:CZ	2:N:2428:VAL:HG21	2.56	0.40
2:N:2622:ASN:HA	2:N:2623:PRO:HD3	1.96	0.40
2:N:2651:GLN:C	2:N:2653:GLU:H	2.29	0.40
3:O:2963[A]:MET:SD	3:O:2963[A]:MET:O	2.79	0.40
3:O:2987[A]:HIS:CD2	3:O:3178[A]:PHE:CE1	3.08	0.40
3:O:2987[B]:HIS:CD2	3:O:3178[B]:PHE:CE1	3.08	0.40
3:O:2995[A]:GLN:O	3:O:2996[A]:MET:C	2.63	0.40
3:O:3010[B]:PRO:HG2	3:O:3118[B]:VAL:HG13	2.03	0.40
3:O:3139[A]:LEU:CD2	3:O:3139[A]:LEU:H	2.34	0.40
1:P:424:PHE:HB2	1:P:1128:GLN:NE2	2.36	0.40
1:P:953:GLU:HG3	1:P:954:ALA:O	2.21	0.40
1:P:1137:LYS:HA	1:P:1141:ARG:NH1	2.36	0.40
1:P:1293:PHE:O	1:P:1311:CYS:HB2	2.20	0.40
2:Q:2361:LYS:HD2	2:Q:2362:GLN:H	1.85	0.40
2:Q:2470:ALA:HB2	2:Q:2476:LEU:HD21	2.02	0.40
3:R:2957[A]:ILE:HD11	3:R:2995[A]:GLN:C	2.46	0.40
3:R:3180[B]:TYR:HA	3:R:3183[B]:LEU:CD2	2.51	0.40
3:R:3230[A]:PHE:HB2	3:R:3242[A]:GLY:C	2.45	0.40
3:R:3232[A]:VAL:HG21	3:R:3273[A]:LEU:HD11	2.00	0.40
3:R:3276[A]:ASP:C	3:R:3278[A]:HIS:N	2.75	0.40
3:R:3298[A]:ASN:HA	3:R:3300[A]:LEU:N	2.36	0.40
1:S:474:LEU:HD12	1:S:475:ASN:N	2.36	0.40
1:S:909:ILE:HG12	1:S:1084:PHE:CZ	2.50	0.40
1:S:1034:GLU:HG3	1:S:1182:ASN:HD21	1.86	0.40
2:T:2344:LEU:HA	2:T:2344:LEU:HD13	1.89	0.40
2:T:2446:GLU:HG2	2:T:2448:THR:HG22	2.04	0.40
3:U:2957[B]:ILE:HD11	3:U:2995[B]:GLN:C	2.46	0.40
3:U:2966[B]:SER:HB2	3:U:2977[B]:CYS:H	1.85	0.40
3:U:2989[A]:HIS:O	3:U:2991[A]:LEU:N	2.54	0.40
3:U:2989[B]:HIS:O	3:U:2991[B]:LEU:N	2.54	0.40
3:U:3028[A]:PRO:HG2	3:U:3029[A]:LYS:HG2	2.02	0.40
3:U:3083[B]:ILE:CD1	3:U:3260[B]:ARG:HB2	2.52	0.40
3:U:3274[A]:ARG:NE	3:U:3274[A]:ARG:CA	2.84	0.40
1:V:78:GLN:HE21	1:V:256:ILE:HG21	1.85	0.40
1:V:1572:ILE:HD13	1:V:1615:LEU:HD23	2.02	0.40
3:X:2989[A]:HIS:O	3:X:2991[A]:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3028[B]:PRO:HG2	3:X:3029[B]:LYS:HG2	2.02	0.40
3:X:3180[B]:TYR:HA	3:X:3183[B]:LEU:CD2	2.51	0.40
1:Y:194:MET:HA	1:Y:200:THR:CA	2.48	0.40
1:Y:710:GLY:O	1:Y:841:LYS:HE2	2.21	0.40
1:Y:1347:ASP:HA	1:Y:1460:ASN:ND2	2.36	0.40
1:Y:1356:PRO:HD2	1:Y:1359:ILE:HD11	2.04	0.40
2:Z:2353:LYS:O	2:Z:2357:VAL:HG23	2.21	0.40
3:a:2963[B]:MET:SD	3:a:2963[B]:MET:O	2.79	0.40
3:a:3013[A]:ASP:CA	3:a:3122[A]:ASN:ND2	2.74	0.40
3:a:3028[A]:PRO:HG2	3:a:3029[A]:LYS:N	2.36	0.40
3:a:3185[B]:TYR:HD2	3:a:3186[B]:GLU:N	2.19	0.40
3:a:3281[B]:PHE:CZ	3:a:3305[B]:ILE:HG21	2.56	0.40
3:a:3298[B]:ASN:HA	3:a:3300[B]:LEU:N	2.36	0.40
1:b:168:PHE:O	1:b:172:GLU:N	2.54	0.40
1:b:760:ILE:HG21	1:b:777:TYR:HE2	1.86	0.40
1:b:991:LEU:HD23	1:b:991:LEU:HA	1.86	0.40
1:b:1480:ASN:CG	1:b:1518:ASP:HB3	2.46	0.40
2:c:2179:ASP:HB3	2:c:2303:ARG:NH1	2.36	0.40
2:c:2849:ASP:OD2	2:c:2850:ARG:NH2	2.54	0.40
3:d:2931[B]:THR:O	3:d:2934[B]:GLU:HB2	2.22	0.40
3:d:2987[A]:HIS:CD2	3:d:3178[A]:PHE:CE1	3.08	0.40
3:d:3044[B]:LYS:H	3:d:3044[B]:LYS:HG2	1.65	0.40
3:d:3083[B]:ILE:HD11	3:d:3260[B]:ARG:HG3	2.03	0.40
3:d:3139[A]:LEU:CD2	3:d:3139[A]:LEU:H	2.34	0.40
3:d:3139[B]:LEU:CD2	3:d:3139[B]:LEU:H	2.34	0.40
3:d:3146[B]:CYS:O	3:d:3146[B]:CYS:SG	2.78	0.40
3:d:3232[B]:VAL:CG2	3:d:3273[B]:LEU:CD1	2.99	0.40
1:A:1030:MET:HE3	1:A:1036:SER:O	2.21	0.40
1:A:1260:ARG:HD2	1:A:1343:VAL:O	2.21	0.40
2:B:2528:LYS:NZ	2:B:2626:ARG:O	2.54	0.40
2:B:2547:MET:O	2:B:2554:PRO:HG2	2.21	0.40
2:B:2556:TYR:CE1	2:B:2844:MET:HG3	2.57	0.40
2:B:2840:GLY:O	2:B:2843:GLU:HB2	2.21	0.40
3:C:2957[A]:ILE:HD11	3:C:2995[A]:GLN:C	2.46	0.40
3:C:2957[B]:ILE:HD11	3:C:2995[B]:GLN:C	2.46	0.40
3:C:3013[A]:ASP:CA	3:C:3122[A]:ASN:ND2	2.74	0.40
3:C:3185[B]:TYR:CZ	3:C:3187[B]:TYR:CE2	3.09	0.40
3:C:3194[B]:GLY:C	3:C:3195[B]:MET:CG	2.90	0.40
3:C:3281[A]:PHE:CZ	3:C:3305[A]:ILE:HG21	2.55	0.40
3:C:3298[A]:ASN:HA	3:C:3300[A]:LEU:N	2.36	0.40
1:D:177:VAL:O	1:D:181:PRO:HD3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ASP:O	1:D:279:LEU:HG	2.21	0.40
1:D:417:MET:HB3	1:D:418:ASP:H	1.59	0.40
1:D:512:PRO:HG2	1:D:632:LEU:HD23	2.02	0.40
1:D:564:ASP:HA	1:D:609:TRP:O	2.21	0.40
1:D:639:ARG:O	1:D:642:ALA:HB3	2.21	0.40
1:D:979:LEU:CB	1:D:980:TYR:HA	2.51	0.40
1:D:1016:ASN:HD22	1:D:1177:VAL:HA	1.85	0.40
1:D:1037:ALA:HA	1:D:1042:PHE:CD2	2.57	0.40
2:E:2403:PHE:HD2	2:E:2480:LEU:HG	1.87	0.40
3:F:2942[A]:LEU:CD1	3:F:3033[A]:PHE:CZ	3.04	0.40
3:F:2957[A]:ILE:HD11	3:F:2995[A]:GLN:C	2.46	0.40
3:F:2961[B]:HIS:CG	3:a:2975[B]:PHE:CE1	3.09	0.40
3:F:2963[A]:MET:SD	3:F:2963[A]:MET:O	2.79	0.40
3:F:2965[B]:LEU:CG	3:F:2974[B]:ALA:CB	2.85	0.40
3:F:2966[B]:SER:CB	3:a:2982[B]:MET:HE2	2.49	0.40
3:F:2989[B]:HIS:O	3:F:2991[B]:LEU:N	2.54	0.40
3:F:3067[B]:ARG:HA	3:F:3067[B]:ARG:HD3	1.87	0.40
3:F:3108[B]:HIS:CE1	3:a:3251[B]:ASP:CG	2.87	0.40
3:F:3160[B]:SER:C	3:a:3150[B]:LYS:NZ	2.63	0.40
3:F:3306[B]:LEU:C	3:F:3306[B]:LEU:CD1	2.86	0.40
1:G:930:ASP:HB3	1:G:933:ARG:HD2	2.03	0.40
1:G:1290:ILE:HD11	1:G:1333:GLU:HG3	2.03	0.40
1:G:1454:PHE:O	1:G:1457:HIS:HB3	2.21	0.40
1:G:1512:ARG:O	1:G:1516:VAL:HG23	2.21	0.40
2:H:2275:GLY:HA2	2:H:2281:SER:HB2	2.03	0.40
2:H:2398:PHE:HE2	2:H:2466:THR:HG21	1.86	0.40
2:H:2400:LEU:HD23	2:H:2400:LEU:HA	1.85	0.40
2:H:2547:MET:C	2:H:2554:PRO:HG3	2.46	0.40
2:H:2825:ILE:HG23	2:H:2826:GLU:N	2.36	0.40
3:I:2965[B]:LEU:HD12	3:R:3256[B]:TRP:HE1	1.81	0.40
3:I:3083[A]:ILE:HD11	3:I:3260[A]:ARG:HG3	2.03	0.40
3:I:3083[B]:ILE:CD1	3:I:3260[B]:ARG:HB2	2.52	0.40
3:I:3185[A]:TYR:HD2	3:I:3186[A]:GLU:N	2.19	0.40
3:I:3185[B]:TYR:CZ	3:I:3187[B]:TYR:CE2	3.09	0.40
3:I:3193[B]:HIS:ND1	3:I:3193[B]:HIS:N	2.69	0.40
3:I:3301[A]:PRO:HB2	3:I:3302[A]:SER:H	1.33	0.40
1:J:148:GLN:O	1:J:149:GLU:HB2	2.22	0.40
1:J:320:LYS:HZ3	1:J:337:ASP:HB3	1.85	0.40
1:J:639:ARG:O	1:J:643:ILE:HG13	2.21	0.40
1:J:810:LEU:HD12	1:J:810:LEU:HA	1.93	0.40
1:J:876:PHE:N	1:J:876:PHE:CD1	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1081:MET:SD	1:J:1102:PRO:HG3	2.62	0.40
2:K:2135:PRO:HG2	2:K:2342:TYR:CZ	2.56	0.40
2:K:2224:THR:HG23	2:K:2278:GLU:HG3	2.04	0.40
2:K:2271:HIS:O	2:K:2283:ASN:HB3	2.21	0.40
3:L:2938[B]:LEU:HD12	3:L:2938[B]:LEU:HA	1.85	0.40
3:L:2951[A]:ASP:CG	3:L:2952[A]:ALA:H	2.28	0.40
3:L:2966[A]:SER:HB2	3:L:2977[A]:CYS:H	1.85	0.40
3:L:3180[B]:TYR:HA	3:L:3183[B]:LEU:CD2	2.51	0.40
3:L:3300[A]:LEU:HD23	3:L:3300[A]:LEU:H	1.83	0.40
1:M:95:THR:O	1:M:153:ASN:ND2	2.54	0.40
1:M:318:ARG:HB2	1:M:382:GLU:HB2	2.02	0.40
1:M:320:LYS:HB2	1:M:380:THR:HG23	2.02	0.40
1:M:324:PRO:HA	1:M:332:ASP:OD2	2.21	0.40
1:M:747:PHE:HD1	1:M:756:PHE:HA	1.87	0.40
1:M:876:PHE:CD2	1:M:1083:PRO:HB2	2.56	0.40
1:M:884:PRO:O	1:M:888:ALA:HB2	2.22	0.40
1:M:1005:CYS:O	1:M:1009:VAL:HG23	2.21	0.40
1:M:1019:HIS:CE1	1:M:1046:HIS:HE1	2.38	0.40
1:M:1091:ASN:HA	1:M:1092:PRO:HD3	1.83	0.40
1:M:1390:ASP:HB2	1:M:1438:ASP:OD2	2.22	0.40
2:N:2235:PRO:HG3	2:N:2240:GLN:HE22	1.85	0.40
2:N:2668:ASP:HB3	2:N:2671:ASP:HB2	2.04	0.40
3:O:2980[A]:HIS:HA	3:O:2985[A]:PHE:HD2	1.86	0.40
3:O:3112[B]:TYR:CZ	3:X:2969[B]:TYR:CE1	3.09	0.40
3:O:3157[B]:PRO:CD	3:X:3153[B]:LYS:CA	2.99	0.40
3:O:3242[B]:GLY:O	3:O:3243[B]:GLY:O	2.39	0.40
1:P:450:LYS:HA	1:P:450:LYS:HD2	1.71	0.40
1:P:1380:GLY:O	1:P:1389:THR:HG23	2.22	0.40
1:P:1616:LYS:HA	1:P:1616:LYS:HD3	1.89	0.40
2:Q:2891:LEU:HD12	2:Q:2891:LEU:H	1.86	0.40
3:R:2989[A]:HIS:O	3:R:2991[A]:LEU:N	2.54	0.40
3:R:3242[B]:GLY:O	3:R:3243[B]:GLY:O	2.40	0.40
1:S:982:LYS:N	1:S:983:PRO:CD	2.84	0.40
2:T:2092:VAL:HG23	2:T:2177:TYR:O	2.22	0.40
3:U:2931[B]:THR:O	3:U:2934[B]:GLU:HB2	2.22	0.40
3:U:3185[A]:TYR:HD2	3:U:3186[A]:GLU:N	2.19	0.40
3:U:3256[B]:TRP:CA	3:d:2969[B]:TYR:N	2.84	0.40
3:U:3276[B]:ASP:C	3:U:3278[B]:HIS:N	2.75	0.40
1:V:71:LEU:HB2	1:V:266:LEU:HD21	2.03	0.40
1:V:524:PRO:HD2	1:V:527:LEU:HD11	2.03	0.40
1:V:566:ARG:HH12	1:V:745:ASP:CG	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:729:VAL:HG11	1:V:785:LEU:HD12	2.03	0.40
2:W:2184:MET:HB2	2:W:2231:LEU:O	2.21	0.40
2:W:2684:HIS:HA	2:W:2695:MET:HG3	2.03	0.40
3:X:2957[A]:ILE:HD11	3:X:2995[A]:GLN:C	2.46	0.40
3:X:3023[B]:ILE:C	3:X:3025[B]:VAL:N	2.79	0.40
3:X:3044[B]:LYS:H	3:X:3044[B]:LYS:HG2	1.65	0.40
3:X:3171[B]:HIS:O	3:X:3172[B]:SER:C	2.63	0.40
3:X:3176[B]:LYS:O	3:X:3177[B]:SER:CB	2.70	0.40
3:X:3180[B]:TYR:CA	3:X:3183[B]:LEU:CD2	2.95	0.40
3:X:3191[B]:ASN:ND2	3:X:3191[B]:ASN:N	2.60	0.40
1:Y:810:LEU:HD11	4:JA:1:NAG:O6	2.21	0.40
2:Z:2098:GLN:HE22	2:c:2374:ASN:ND2	2.19	0.40
2:Z:2771:TYR:HB2	2:Z:2776:TYR:CE1	2.56	0.40
2:Z:2819:VAL:HB	2:Z:2835:ILE:HG23	2.03	0.40
3:a:2931[B]:THR:O	3:a:2934[B]:GLU:HB2	2.22	0.40
3:a:2989[A]:HIS:O	3:a:2991[A]:LEU:N	2.54	0.40
3:a:2989[B]:HIS:O	3:a:2991[B]:LEU:N	2.54	0.40
3:a:3134[A]:GLN:C	3:a:3136[A]:TYR:N	2.77	0.40
3:a:3180[A]:TYR:HA	3:a:3183[A]:LEU:CD2	2.51	0.40
3:a:3242[B]:GLY:O	3:a:3243[B]:GLY:O	2.40	0.40
3:a:3265[A]:ASP:OD1	3:a:3266[A]:ILE:N	2.54	0.40
1:b:93:ASP:HA	1:b:212:ASN:ND2	2.37	0.40
1:b:907:ARG:NH2	1:b:1106:PHE:O	2.53	0.40
1:b:1304:ASP:OD2	1:b:1306:THR:HG23	2.22	0.40
2:c:2179:ASP:HA	2:c:2300:ASN:ND2	2.35	0.40
2:c:2569:TRP:HE3	2:c:2570:HIS:ND1	2.18	0.40
2:c:2590:VAL:HA	2:c:2591:PRO:HD3	1.90	0.40
3:d:2957[A]:ILE:HD11	3:d:2995[A]:GLN:C	2.46	0.40
3:d:2980[B]:HIS:HA	3:d:2985[B]:PHE:HD2	1.86	0.40
3:d:3083[A]:ILE:CD1	3:d:3260[A]:ARG:HB2	2.52	0.40
3:d:3094[A]:SER:HG	3:d:3227[A]:ASP:CG	2.28	0.40
3:d:3185[A]:TYR:CE2	3:d:3187[A]:TYR:HE2	2.31	0.40
3:d:3274[A]:ARG:NE	3:d:3274[A]:ARG:CA	2.84	0.40
3:d:3298[B]:ASN:HA	3:d:3300[B]:LEU:N	2.36	0.40
1:A:243:PRO:HB2	1:A:248:GLY:HA3	2.02	0.40
1:A:597:VAL:O	1:A:601:VAL:HG12	2.21	0.40
1:A:745:ASP:OD1	1:A:759:SER:OG	2.35	0.40
1:A:896:HIS:HB2	1:A:905:TRP:CD1	2.56	0.40
1:A:1001:GLN:HE21	1:A:1001:GLN:HB3	1.77	0.40
1:A:1390:ASP:HB3	1:b:1372:ILE:HD11	2.03	0.40
2:B:2145:LEU:HD12	2:B:2145:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2848:PHE:HD1	2:B:2848:PHE:HA	1.76	0.40
3:C:2965[B]:LEU:HB3	3:L:3256[B]:TRP:CD2	2.11	0.40
3:C:2989[A]:HIS:O	3:C:2991[A]:LEU:N	2.54	0.40
3:C:3023[A]:ILE:HA	3:C:3026[A]:THR:HG1	1.83	0.40
3:C:3139[A]:LEU:CD2	3:C:3139[A]:LEU:H	2.34	0.40
3:C:3168[A]:THR:O	3:C:3172[A]:SER:N	2.55	0.40
3:C:3185[B]:TYR:C	3:C:3185[B]:TYR:HD2	2.30	0.40
3:C:3265[A]:ASP:OD1	3:C:3266[A]:ILE:N	2.54	0.40
1:D:3:ILE:O	1:D:88:GLY:N	2.48	0.40
1:D:450:LYS:O	1:D:450:LYS:HD3	2.22	0.40
1:D:513:TYR:HB2	1:D:636:GLN:HB2	2.02	0.40
1:D:843:VAL:HG13	1:D:927:PRO:HB2	2.03	0.40
1:D:899:MET:HE2	1:D:1012:GLU:OE1	2.21	0.40
1:D:907:ARG:HD3	1:D:1050:ASP:OD1	2.22	0.40
1:D:1249:TRP:CZ2	1:D:1537:ILE:HD12	2.55	0.40
1:D:1470:GLU:HB3	1:D:1537:ILE:HD11	2.03	0.40
2:E:2122:ILE:HD11	2:E:2165:SER:OG	2.21	0.40
3:F:2931[B]:THR:O	3:F:2934[B]:GLU:HB2	2.22	0.40
3:F:2961[B]:HIS:O	3:a:2975[B]:PHE:CE1	2.75	0.40
3:F:2980[B]:HIS:HB3	3:a:2968[B]:GLN:CG	1.76	0.40
3:F:2987[B]:HIS:CD2	3:F:3178[B]:PHE:CE1	3.08	0.40
3:F:3010[B]:PRO:HG2	3:F:3118[B]:VAL:HG13	2.03	0.40
3:F:3041[B]:ALA:O	3:F:3042[B]:ASP:HB2	2.20	0.40
3:F:3221[B]:ALA:HB2	3:a:2965[B]:LEU:O	2.21	0.40
3:F:3298[A]:ASN:HA	3:F:3300[A]:LEU:N	2.37	0.40
3:F:3301[B]:PRO:HB2	3:F:3302[B]:SER:H	1.33	0.40
1:G:1303:GLU:C	1:G:1306:THR:H	2.29	0.40
1:G:1408:LEU:HD23	1:G:1547:ASN:HD21	1.86	0.40
1:G:1473:ARG:HG3	1:G:1479:TYR:CG	2.56	0.40
2:H:2089:ARG:HD3	2:H:2163:GLU:OE2	2.21	0.40
3:I:3011[B]:TYR:CB	3:I:3121[B]:SER:HB2	2.49	0.40
3:I:3133[B]:LEU:HD13	3:I:3197[B]:ILE:HG23	2.02	0.40
3:I:3150[B]:LYS:CD	3:R:3160[B]:SER:CA	2.73	0.40
3:I:3163[B]:ASN:HD22	3:R:3149[B]:ASN:CG	2.23	0.40
1:J:177:VAL:HG11	1:J:358:TYR:CZ	2.56	0.40
1:J:321:LEU:HD11	1:J:377:TYR:CD1	2.55	0.40
1:J:902:PHE:CE2	1:J:1012:GLU:HG3	2.56	0.40
2:K:2117:ASP:OD2	2:K:2168:ARG:NH2	2.54	0.40
2:K:2244:PHE:CD1	2:K:2244:PHE:C	2.99	0.40
2:K:2448:THR:OG1	2:K:2449:ASP:N	2.55	0.40
3:L:2951[B]:ASP:CG	3:L:2952[B]:ALA:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3176[A]:LYS:O	3:L:3177[A]:SER:CB	2.70	0.40
3:L:3222[A]:ILE:CD1	3:L:3223[A]:GLY:N	2.73	0.40
1:M:398:ARG:HA	1:M:399:PRO:HD3	1.85	0.40
1:M:651:ARG:HG3	1:M:717:GLN:HE22	1.87	0.40
1:M:979:LEU:HB3	1:M:980:TYR:CB	2.52	0.40
1:M:1289:GLU:O	1:M:1292:SER:OG	2.34	0.40
1:M:1492:PRO:HA	1:M:1512:ARG:HA	2.02	0.40
2:N:2224:THR:HG23	2:N:2278:GLU:HB3	2.03	0.40
2:N:2527:LEU:HD11	2:N:2580:SER:HB3	2.03	0.40
3:O:3160[B]:SER:HB3	3:X:3149[B]:ASN:CG	2.27	0.40
3:O:3265[B]:ASP:OD1	3:O:3266[B]:ILE:N	2.54	0.40
1:P:754:GLU:OE2	1:P:799:ARG:NH2	2.53	0.40
3:R:2991[A]:LEU:O	3:R:2994[A]:LYS:CB	2.70	0.40
3:R:3083[B]:ILE:CD1	3:R:3260[B]:ARG:HB2	2.52	0.40
3:R:3211[A]:ASP:CB	3:R:3309[A]:PRO:HA	2.46	0.40
3:R:3274[B]:ARG:NE	3:R:3274[B]:ARG:CA	2.84	0.40
3:R:3299[A]:LEU:HB3	3:R:3300[A]:LEU:H	1.54	0.40
1:S:307:ARG:HG2	1:S:774:ASP:HA	2.04	0.40
1:S:403:TYR:HD2	1:S:658:TYR:CD1	2.39	0.40
1:S:843:VAL:HG22	1:S:928:TYR:O	2.21	0.40
1:S:1384:PHE:CZ	1:S:1385:GLU:HG3	2.56	0.40
1:S:1632:LEU:HD22	1:S:1644:ILE:HD11	2.02	0.40
2:T:2526:ARG:HB3	2:T:2584:HIS:CD2	2.57	0.40
2:T:2890:VAL:H	2:T:2891:LEU:HA	1.83	0.40
3:U:2951[A]:ASP:CG	3:U:2952[A]:ALA:H	2.28	0.40
3:U:2991[A]:LEU:O	3:U:2994[A]:LYS:CB	2.70	0.40
3:U:3083[B]:ILE:HD11	3:U:3260[B]:ARG:HG3	2.03	0.40
3:U:3137[B]:ARG:HD3	3:U:3137[B]:ARG:HA	1.71	0.40
3:U:3171[B]:HIS:O	3:U:3172[B]:SER:C	2.63	0.40
1:V:215:ARG:NE	1:V:279:LEU:HA	2.35	0.40
1:V:1565:SER:HB3	1:V:1594:GLY:H	1.86	0.40
2:W:2338:PHE:O	2:W:2343:ASN:HB3	2.20	0.40
3:X:2954[B]:TYR:HA	3:X:2957[B]:ILE:CG2	2.50	0.40
3:X:2957[B]:ILE:HD11	3:X:2995[B]:GLN:C	2.46	0.40
3:X:2979[A]:GLN:CD	3:X:3155[A]:MET:CE	2.92	0.40
3:X:3131[B]:GLN:HE21	3:X:3131[B]:GLN:HB3	1.66	0.40
3:X:3185[B]:TYR:HD2	3:X:3186[B]:GLU:N	2.19	0.40
1:Y:150:GLY:HA2	1:Y:151:GLN:C	2.46	0.40
1:Y:1293:PHE:O	1:Y:1311:CYS:HB2	2.22	0.40
2:Z:2553:ALA:N	2:Z:2554:PRO:CD	2.84	0.40
3:a:3083[B]:ILE:HD11	3:a:3260[B]:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:3139[A]:LEU:CD2	3:a:3139[A]:LEU:H	2.34	0.40
3:a:3176[A]:LYS:O	3:a:3177[A]:SER:CB	2.70	0.40
1:b:566:ARG:N	1:b:567:LEU:HA	2.36	0.40
1:b:904:HIS:HB3	1:b:1105:VAL:HG21	2.02	0.40
1:b:1321:HIS:ND1	1:b:1513:PRO:HB3	2.36	0.40
2:c:2426:PHE:HB3	2:c:2445:MET:HE1	2.04	0.40
2:c:2568:HIS:HD2	2:c:2718:TRP:CH2	2.38	0.40
2:c:2578:GLU:O	2:c:2581:MET:HB2	2.22	0.40
2:c:2685:TYR:OH	2:c:2818:ASP:OD1	2.30	0.40
3:d:3194[B]:GLY:C	3:d:3195[B]:MET:CG	2.91	0.40
3:d:3242[B]:GLY:O	3:d:3243[B]:GLY:O	2.40	0.40
1:A:83:HIS:O	1:A:85:SER:HB3	2.21	0.40
1:A:489:HIS:CD2	1:A:689:PRO:HB3	2.57	0.40
1:A:695:TYR:N	1:A:695:TYR:HD1	2.19	0.40
2:B:2214:ILE:HD13	2:B:2287:TYR:HD1	1.86	0.40
2:B:2502:LEU:HA	2:B:2502:LEU:HD12	1.84	0.40
3:C:2946[B]:GLN:CD	3:C:2947[B]:ALA:N	2.72	0.40
3:C:3083[B]:ILE:HD11	3:C:3260[B]:ARG:HG3	2.03	0.40
3:C:3163[B]:ASN:N	3:L:3147[B]:GLU:OE2	2.32	0.40
1:D:572:SER:HB2	1:D:578:PHE:HB2	2.03	0.40
1:D:627:ASP:HA	1:D:628:PRO:HD3	1.95	0.40
1:D:1017:HIS:CD2	1:D:1176:TYR:HD2	2.39	0.40
2:E:2181:THR:HB	2:E:2374:ASN:N	2.36	0.40
2:E:2262:GLN:O	2:E:2266:VAL:HG23	2.20	0.40
3:F:2963[B]:MET:C	3:a:3255[B]:PRO:HG3	2.46	0.40
3:F:2980[A]:HIS:HA	3:F:2985[A]:PHE:HD2	1.86	0.40
3:F:2989[A]:HIS:NE2	9:a:3401[A]:CUO:O1	2.54	0.40
3:F:3031[B]:ASN:HA	3:F:3032[B]:PRO:HD2	1.87	0.40
3:F:3083[B]:ILE:HD11	3:F:3260[B]:ARG:HG3	2.03	0.40
3:F:3113[A]:ASP:OD2	3:F:3115[A]:LEU:HB2	2.20	0.40
3:F:3148[B]:ILE:HD12	3:F:3175[B]:TYR:OH	2.20	0.40
3:F:3172[B]:SER:CB	3:a:3150[B]:LYS:O	2.68	0.40
3:F:3185[A]:TYR:HD2	3:F:3186[A]:GLU:N	2.19	0.40
3:F:3193[A]:HIS:ND1	3:F:3193[A]:HIS:N	2.68	0.40
3:F:3242[B]:GLY:O	3:F:3243[B]:GLY:O	2.40	0.40
3:F:3254[B]:MET:CA	3:a:2966[B]:SER:OG	2.67	0.40
3:F:3255[B]:PRO:HD3	3:a:2962[B]:GLY:C	2.23	0.40
3:F:3281[A]:PHE:CZ	3:F:3305[A]:ILE:HG21	2.55	0.40
1:G:398:ARG:HA	1:G:399:PRO:HD3	1.93	0.40
1:G:597:VAL:HG12	1:G:773:PHE:CD1	2.57	0.40
2:H:2168:ARG:O	2:K:2503:ASN:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2931[A]:THR:O	3:I:2934[A]:GLU:HB2	2.22	0.40
3:I:2951[B]:ASP:CG	3:I:2952[B]:ALA:H	2.28	0.40
3:I:2951[B]:ASP:C	3:I:2956[B]:LYS:HZ1	2.15	0.40
3:I:2961[A]:HIS:HB2	3:I:2992[A]:TYR:HE2	1.80	0.40
3:I:3010[A]:PRO:HG2	3:I:3118[A]:VAL:HG13	2.03	0.40
3:I:3083[B]:ILE:HD11	3:I:3260[B]:ARG:HG3	2.03	0.40
3:I:3150[B]:LYS:CG	3:R:3163[B]:ASN:ND2	2.52	0.40
3:I:3229[A]:ASN:N	3:I:3286[A]:THR:O	2.52	0.40
3:I:3265[A]:ASP:OD1	3:I:3266[A]:ILE:N	2.54	0.40
3:I:3298[B]:ASN:HA	3:I:3300[B]:LEU:N	2.37	0.40
1:J:472:ASP:HA	1:J:473:ALA:HA	1.82	0.40
1:J:633:HIS:O	1:J:636:GLN:HB3	2.21	0.40
1:J:872:GLN:NE2	1:J:1090:ILE:O	2.47	0.40
2:K:2134:ASN:OD1	2:K:2137:ALA:HB2	2.21	0.40
2:K:2156:ARG:NH1	2:K:2360:TYR:HB3	2.36	0.40
2:K:2241:THR:HG23	2:K:2244:PHE:HB2	2.02	0.40
2:K:2381:LEU:O	2:K:2385:ILE:HG13	2.21	0.40
3:L:2930[A]:LEU:N	3:L:2930[A]:LEU:HD13	2.36	0.40
3:L:2938[A]:LEU:HD12	3:L:2938[A]:LEU:HA	1.85	0.40
3:L:2989[B]:HIS:O	3:L:2991[B]:LEU:N	2.54	0.40
3:L:2991[B]:LEU:O	3:L:2994[B]:LYS:CB	2.70	0.40
3:L:3023[B]:ILE:O	3:L:3026[B]:THR:OG1	2.34	0.40
3:L:3023[B]:ILE:C	3:L:3025[B]:VAL:N	2.79	0.40
3:L:3265[B]:ASP:OD1	3:L:3266[B]:ILE:N	2.54	0.40
3:L:3301[A]:PRO:HB2	3:L:3302[A]:SER:H	1.33	0.40
1:M:73:LEU:HD22	1:M:89:ILE:HD12	2.03	0.40
1:M:837:HIS:HA	1:M:1113:HIS:O	2.21	0.40
1:M:881:GLN:NE2	1:M:888:ALA:HB3	2.34	0.40
1:M:897:HIS:HB3	1:M:899:MET:CE	2.51	0.40
1:M:1022:VAL:HG13	1:M:1030:MET:HB2	2.03	0.40
1:M:1296:VAL:N	1:M:1446:ASP:O	2.54	0.40
3:O:2931[B]:THR:O	3:O:2934[B]:GLU:HB2	2.22	0.40
3:O:2967[B]:CYS:SG	3:X:3150[B]:LYS:O	2.79	0.40
3:O:3120[A]:HIS:HA	3:O:3123[A]:THR:HG1	1.83	0.40
3:O:3185[A]:TYR:C	3:O:3185[A]:TYR:HD2	2.30	0.40
3:O:3185[A]:TYR:HD2	3:O:3186[A]:GLU:N	2.19	0.40
3:O:3193[A]:HIS:ND1	3:O:3193[A]:HIS:N	2.68	0.40
3:O:3228[A]:VAL:CG2	3:O:3245[A]:PHE:CZ	2.86	0.40
1:P:92:TRP:CZ3	1:P:102:PRO:HD3	2.56	0.40
1:P:514:TRP:CZ2	1:P:606:ILE:HD11	2.56	0.40
1:P:550:ILE:HG22	1:P:552:PHE:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:618:MET:HB3	1:P:618:MET:HE3	1.69	0.40
1:P:633:HIS:O	1:P:636:GLN:HB3	2.21	0.40
1:P:991:LEU:HD21	1:P:1017:HIS:CG	2.56	0.40
2:Q:2235:PRO:HG3	2:Q:2240:GLN:OE1	2.21	0.40
2:Q:2861:LYS:NZ	3:R:2936[A]:GLU:OE1	2.52	0.40
3:R:2931[A]:THR:O	3:R:2934[A]:GLU:HB2	2.22	0.40
3:R:3010[B]:PRO:HG2	3:R:3118[B]:VAL:HG13	2.03	0.40
3:R:3131[B]:GLN:HE21	3:R:3131[B]:GLN:HB3	1.66	0.40
3:R:3133[A]:LEU:HD12	3:R:3133[A]:LEU:HA	1.86	0.40
3:R:3155[B]:MET:HB3	3:R:3155[B]:MET:HE2	1.99	0.40
3:R:3168[B]:THR:O	3:R:3172[B]:SER:N	2.55	0.40
3:R:3176[B]:LYS:O	3:R:3177[B]:SER:CB	2.70	0.40
1:S:717:GLN:O	1:S:720:VAL:HG22	2.21	0.40
1:S:816:PRO:HA	1:S:817:PRO:HD3	1.88	0.40
1:S:1348:TRP:CD2	1:S:1430:ILE:HD11	2.56	0.40
3:U:3180[A]:TYR:HA	3:U:3183[A]:LEU:CD2	2.51	0.40
3:U:3298[A]:ASN:HA	3:U:3300[A]:LEU:N	2.36	0.40
1:V:279:LEU:HD12	1:V:279:LEU:O	2.20	0.40
1:V:361:GLU:HG2	1:V:363:THR:HG22	2.03	0.40
1:V:573:LYS:HD2	1:V:573:LYS:HA	1.93	0.40
1:V:1015:HIS:NE2	1:V:1019:HIS:CD2	2.89	0.40
1:V:1143:ALA:O	1:V:1235:ILE:N	2.52	0.40
1:V:1153:LYS:H	1:V:1153:LYS:HG2	1.48	0.40
1:V:1300:CYS:SG	1:V:1494:ARG:HD2	2.62	0.40
1:V:1622:GLN:H	1:V:1622:GLN:HG3	1.45	0.40
2:W:2695:MET:SD	2:W:2701:SER:HB2	2.61	0.40
3:X:2931[A]:THR:O	3:X:2934[A]:GLU:HB2	2.22	0.40
3:X:3028[A]:PRO:HG2	3:X:3029[A]:LYS:N	2.36	0.40
3:X:3148[B]:ILE:HD12	3:X:3175[B]:TYR:OH	2.20	0.40
3:X:3265[B]:ASP:OD1	3:X:3266[B]:ILE:N	2.54	0.40
1:Y:555:ALA:C	1:Y:557:VAL:H	2.28	0.40
1:Y:563:ILE:O	1:Y:612:GLY:N	2.54	0.40
1:Y:975:PRO:HG2	1:Y:1024:GLY:HA3	2.03	0.40
1:Y:1359:ILE:O	1:Y:1391:ARG:NH2	2.53	0.40
2:Z:2465:LYS:HE2	2:Z:2467:LYS:HE3	2.04	0.40
3:a:3122[A]:ASN:O	3:a:3126[A]:ILE:HG13	2.22	0.40
3:a:3146[B]:CYS:HA	3:a:3147[B]:GLU:HA	1.70	0.40
3:a:3176[B]:LYS:O	3:a:3177[B]:SER:CB	2.70	0.40
3:a:3265[B]:ASP:OD1	3:a:3266[B]:ILE:N	2.54	0.40
3:a:3299[B]:LEU:HB3	3:a:3300[B]:LEU:H	1.54	0.40
3:d:3034[B]:HIS:HB3	3:d:3035[B]:HIS:CE1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:3122[B]:ASN:O	3:d:3126[B]:ILE:HG13	2.22	0.40
3:d:3171[A]:HIS:O	3:d:3172[A]:SER:C	2.63	0.40
3:d:3176[B]:LYS:O	3:d:3177[B]:SER:CB	2.70	0.40
3:d:3180[A]:TYR:HA	3:d:3183[A]:LEU:CD2	2.51	0.40
1:A:76:PHE:CE2	1:A:89:ILE:HG21	2.56	0.40
1:A:210:HIS:ND1	1:A:213:VAL:HG21	2.37	0.40
1:A:636:GLN:O	1:A:640:LEU:HG	2.21	0.40
2:B:2500:ILE:HG13	2:B:2501:PRO:CD	2.50	0.40
2:B:2561:HIS:HA	2:B:2562:GLY:HA2	1.85	0.40
3:C:2991[B]:LEU:O	3:C:2994[B]:LYS:CB	2.70	0.40
3:C:3139[B]:LEU:CD2	3:C:3139[B]:LEU:H	2.34	0.40
3:C:3185[A]:TYR:HD2	3:C:3186[A]:GLU:N	2.19	0.40
3:C:3185[A]:TYR:CZ	3:C:3187[A]:TYR:CE2	3.09	0.40
3:C:3185[B]:TYR:HE2	3:C:3187[B]:TYR:CD2	2.35	0.40
3:C:3231[A]:ASP:CA	3:C:3284[A]:LYS:O	2.70	0.40
3:C:3298[A]:ASN:CA	3:C:3299[A]:LEU:HB2	2.44	0.40
1:D:35:GLN:NE2	1:D:127:GLU:O	2.52	0.40
1:D:434:GLU:H	1:D:434:GLU:HG3	1.64	0.40
1:D:882:TRP:HB3	1:D:1086:LEU:HD11	2.03	0.40
2:E:2450:ILE:O	2:E:2454:MET:HG3	2.21	0.40
3:F:3028[B]:PRO:HG2	3:F:3029[B]:LYS:N	2.36	0.40
3:F:3083[B]:ILE:CD1	3:F:3260[B]:ARG:HB2	2.51	0.40
3:F:3139[B]:LEU:CD2	3:F:3139[B]:LEU:H	2.34	0.40
3:F:3148[B]:ILE:HA	3:a:3169[B]:LYS:HD3	1.70	0.40
3:F:3200[B]:LEU:O	3:F:3203[B]:HIS:HB3	2.20	0.40
1:G:512:PRO:HG2	1:G:632:LEU:HD22	2.03	0.40
1:G:892:TYR:HB2	1:G:893:ALA:H	1.70	0.40
1:G:1380:GLY:HA3	1:G:1450:TYR:O	2.21	0.40
3:I:2930[B]:LEU:N	3:I:2930[B]:LEU:HD13	2.36	0.40
3:I:2942[A]:LEU:CD1	3:I:3033[A]:PHE:CZ	3.04	0.40
3:I:2968[B]:GLN:O	3:R:2985[B]:PHE:HE2	2.04	0.40
3:I:2979[B]:GLN:O	3:R:2967[B]:CYS:HB3	2.16	0.40
3:I:3028[B]:PRO:HG2	3:I:3029[B]:LYS:N	2.36	0.40
3:I:3093[B]:HIS:CD2	3:R:2971[B]:ASP:O	2.62	0.40
3:I:3133[B]:LEU:HD12	3:I:3133[B]:LEU:HA	1.86	0.40
3:I:3171[A]:HIS:O	3:I:3172[A]:SER:C	2.63	0.40
3:I:3242[B]:GLY:O	3:I:3243[B]:GLY:O	2.40	0.40
3:I:3268[A]:LYS:HG2	1:J:1539:GLN:HE22	1.86	0.40
1:J:236:GLY:HA2	1:J:819:ILE:HB	2.04	0.40
1:J:492:ARG:HG3	1:J:638:ASP:OD1	2.21	0.40
1:J:1091:ASN:HA	1:J:1092:PRO:HD3	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1618:LEU:O	1:J:1620:LEU:HD13	2.20	0.40
2:K:2800:LYS:O	3:L:3023[A]:ILE:HD11	2.21	0.40
2:K:2814:LYS:HD3	2:K:2814:LYS:HA	1.91	0.40
3:L:2931[A]:THR:O	3:L:2934[A]:GLU:HB2	2.22	0.40
3:L:3122[B]:ASN:O	3:L:3126[B]:ILE:HG13	2.22	0.40
3:L:3148[A]:ILE:HD12	3:L:3175[A]:TYR:OH	2.20	0.40
3:L:3176[B]:LYS:O	3:L:3177[B]:SER:CB	2.70	0.40
3:L:3185[A]:TYR:C	3:L:3185[A]:TYR:HD2	2.30	0.40
3:L:3185[B]:TYR:CZ	3:L:3187[B]:TYR:CE2	3.09	0.40
3:L:3299[B]:LEU:O	3:L:3300[B]:LEU:C	2.60	0.40
1:M:425:ARG:HD2	1:M:703:TYR:CZ	2.57	0.40
2:N:2500:ILE:HD11	2:N:2504:ARG:O	2.21	0.40
3:O:3010[A]:PRO:HG2	3:O:3118[A]:VAL:HG13	2.03	0.40
3:O:3155[A]:MET:HE2	3:O:3155[A]:MET:HB3	1.99	0.40
3:O:3158[B]:PHE:HB2	3:X:3152[B]:LYS:HD2	0.94	0.40
3:O:3168[B]:THR:O	3:O:3172[B]:SER:N	2.55	0.40
3:O:3193[B]:HIS:ND1	3:O:3193[B]:HIS:N	2.69	0.40
3:O:3298[B]:ASN:HA	3:O:3300[B]:LEU:N	2.37	0.40
1:P:449:ASP:HB3	1:P:1280:GLN:CD	2.46	0.40
1:P:599:PHE:HZ	1:P:637:VAL:O	2.04	0.40
1:P:1002:GLU:HB2	1:P:1065:LYS:CD	2.51	0.40
1:P:1055:THR:HA	1:P:1119:LEU:HD13	2.02	0.40
1:P:1312:CYS:HA	1:P:1322:TRP:CE2	2.56	0.40
1:P:1325:LEU:HG	1:P:1516:VAL:HG11	2.03	0.40
2:Q:2457:LYS:HB2	2:Q:2457:LYS:HE2	1.92	0.40
3:R:2995[A]:GLN:O	3:R:2996[A]:MET:C	2.63	0.40
3:R:3265[B]:ASP:OD1	3:R:3266[B]:ILE:N	2.54	0.40
1:S:73:LEU:HD11	1:S:210:HIS:O	2.21	0.40
1:S:246:PRO:HB3	1:S:249:ARG:NE	2.35	0.40
1:S:1557:PHE:HB3	1:S:1559:LEU:HD13	2.04	0.40
2:T:2816:SER:HB2	2:T:2886:VAL:CG2	2.51	0.40
2:T:2823:ILE:HD11	2:T:2863:ARG:HD3	2.04	0.40
3:U:2991[B]:LEU:O	3:U:2994[B]:LYS:CB	2.69	0.40
3:U:3013[A]:ASP:CG	3:U:3015[A]:THR:HG1	2.28	0.40
3:U:3028[A]:PRO:HG2	3:U:3029[A]:LYS:N	2.36	0.40
3:U:3139[A]:LEU:CD2	3:U:3139[A]:LEU:H	2.34	0.40
3:U:3185[B]:TYR:HE2	3:U:3187[B]:TYR:CD2	2.35	0.40
3:U:3231[A]:ASP:CA	3:U:3284[A]:LYS:O	2.70	0.40
3:U:3293[B]:LYS:CG	3:U:3294[B]:SER:CB	2.98	0.40
1:V:109:LEU:HD12	1:V:109:LEU:HA	1.92	0.40
1:V:999:LEU:HA	1:V:1056:TRP:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:3139[A]:LEU:CD2	3:X:3139[A]:LEU:H	2.34	0.40
3:X:3242[B]:GLY:O	3:X:3243[B]:GLY:O	2.40	0.40
3:X:3298[A]:ASN:HA	3:X:3300[A]:LEU:N	2.37	0.40
1:Y:43:GLU:HG3	1:Y:44:PRO:HA	2.04	0.40
1:Y:978:ALA:HB1	1:Y:979:LEU:HD13	2.04	0.40
1:Y:1429:THR:HG23	1:Y:1433:TRP:CE2	2.56	0.40
1:Y:1647:ASN:HA	1:Y:1648:PRO:HD3	1.98	0.40
2:Z:2116:SER:CA	2:Z:2121:THR:HG21	2.52	0.40
2:Z:2304:LEU:HD12	2:Z:2304:LEU:HA	1.95	0.40
2:Z:2502:LEU:HD12	2:Z:2502:LEU:HA	1.85	0.40
2:Z:2764:THR:HG22	2:Z:2766:SER:H	1.87	0.40
3:a:2980[A]:HIS:HA	3:a:2985[A]:PHE:HD2	1.86	0.40
3:a:3139[B]:LEU:CD2	3:a:3139[B]:LEU:H	2.34	0.40
3:a:3185[B]:TYR:HE2	3:a:3187[B]:TYR:CD2	2.35	0.40
3:a:3232[A]:VAL:CG2	3:a:3273[A]:LEU:CD1	2.98	0.40
1:b:525:SER:HA	1:b:528:ALA:HB3	2.03	0.40
1:b:1294:HIS:HB2	1:b:1322:TRP:HH2	1.86	0.40
1:b:1311:CYS:HB3	1:b:1495:PRO:HD3	2.03	0.40
1:b:1316:MET:HE1	1:b:1599:MET:HE2	2.04	0.40
2:c:2303:ARG:NH2	2:c:2372:GLU:O	2.55	0.40
2:c:2854:MET:HB2	2:c:2854:MET:HE3	1.81	0.40
2:c:2888:GLY:HA2	2:c:2889:ALA:HA	1.75	0.40
3:d:2989[A]:HIS:NE2	9:d:3401[A]:CUO:O1	2.53	0.40
3:d:3168[B]:THR:O	3:d:3172[B]:SER:N	2.55	0.40
3:d:3185[A]:TYR:C	3:d:3185[A]:TYR:HD2	2.30	0.40
3:d:3185[A]:TYR:HD2	3:d:3186[A]:GLU:N	2.19	0.40
3:d:3222[B]:ILE:CD1	3:d:3223[B]:GLY:N	2.73	0.40
3:d:3242[A]:GLY:O	3:d:3243[A]:GLY:O	2.40	0.40
3:d:3265[B]:ASP:OD1	3:d:3266[B]:ILE:N	2.54	0.40
3:d:3298[A]:ASN:HA	3:d:3300[A]:LEU:N	2.36	0.40
6:DA:1:NAG:O4	6:DA:2:NAG:O7	2.39	0.40

All (1) 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)
1:A:1:ASN:N	1:b:887:ASP:OD1[1_455]	2.19	0.01

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	1654/2000 (83%)	1552 (94%)	89 (5%)	13 (1%)	16	50
1	D	1654/2000 (83%)	1541 (93%)	100 (6%)	13 (1%)	16	50
1	G	1654/2000 (83%)	1560 (94%)	78 (5%)	16 (1%)	12	45
1	J	1654/2000 (83%)	1537 (93%)	103 (6%)	14 (1%)	16	50
1	M	1654/2000 (83%)	1569 (95%)	73 (4%)	12 (1%)	18	53
1	P	1654/2000 (83%)	1562 (94%)	78 (5%)	14 (1%)	16	50
1	S	1654/2000 (83%)	1581 (96%)	64 (4%)	9 (0%)	24	60
1	V	1654/2000 (83%)	1570 (95%)	68 (4%)	16 (1%)	12	45
1	Y	1654/2000 (83%)	1580 (96%)	66 (4%)	8 (0%)	24	60
1	b	1654/2000 (83%)	1564 (95%)	80 (5%)	10 (1%)	21	56
2	B	823/920 (90%)	778 (94%)	40 (5%)	5 (1%)	21	56
2	E	823/920 (90%)	781 (95%)	34 (4%)	8 (1%)	12	45
2	H	823/920 (90%)	787 (96%)	33 (4%)	3 (0%)	30	65
2	K	823/920 (90%)	778 (94%)	37 (4%)	8 (1%)	12	45
2	N	823/920 (90%)	789 (96%)	32 (4%)	2 (0%)	43	76
2	Q	823/920 (90%)	787 (96%)	32 (4%)	4 (0%)	24	60
2	T	823/920 (90%)	794 (96%)	22 (3%)	7 (1%)	14	48
2	W	823/920 (90%)	791 (96%)	28 (3%)	4 (0%)	24	60
2	Z	823/920 (90%)	797 (97%)	23 (3%)	3 (0%)	30	65
2	c	823/920 (90%)	791 (96%)	29 (4%)	3 (0%)	30	65
3	C	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	F	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	I	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	L	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	O	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	U	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	X	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	a	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	d	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
All	All	31970/33140 (96%)	30149 (94%)	1589 (5%)	232 (1%)	18	53

All (232) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1196	ILE
1	D	695	TYR
1	D	1196	ILE
1	G	331	SER
1	G	1086	LEU
1	J	883	CYS
1	M	127	GLU
1	M	695	TYR
2	N	2340	ALA
1	P	781	ILE
1	P	1436	GLY
1	S	51	ASP
1	S	1196	ILE
2	T	2424	SER
2	T	2631	TYR
1	V	867	VAL
1	Y	148	GLN
2	Z	2340	ALA
1	b	134	VAL
1	b	331	SER
1	b	675	SER
1	b	1301	PRO
1	A	149	GLU
1	A	831	VAL
1	A	1436	GLY
2	B	2343	ASN
2	B	2404	GLY
3	C	3111[A]	SER
3	C	3111[B]	SER
3	C	3301[A]	PRO

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Mol	Chain	Res	Type
3	C	3301[B]	PRO
2	E	2340	ALA
2	E	2419	ASP
3	F	3111[A]	SER
3	F	3111[B]	SER
3	F	3301[A]	PRO
3	F	3301[B]	PRO
1	G	116	LYS
1	G	150	GLY
1	G	563	ILE
1	G	674	LYS
2	H	2340	ALA
3	I	3111[A]	SER
3	I	3111[B]	SER
3	I	3301[A]	PRO
3	I	3301[B]	PRO
1	J	84	GLY
1	J	952	GLY
1	J	1436	GLY
2	K	2738	ALA
2	K	2831	GLU
2	K	2877	ILE
2	K	2894	ASN
3	L	3111[A]	SER
3	L	3111[B]	SER
3	L	3301[A]	PRO
3	L	3301[B]	PRO
1	M	84	GLY
1	M	149	GLU
1	M	447	MET
1	M	1436	GLY
3	O	3111[A]	SER
3	O	3111[B]	SER
3	O	3301[A]	PRO
3	O	3301[B]	PRO
1	P	962	GLY
1	P	1484	CYS
1	P	1485	ALA
2	Q	2340	ALA
3	R	3111[A]	SER
3	R	3111[B]	SER
3	R	3301[A]	PRO

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Mol	Chain	Res	Type
3	R	3301[B]	PRO
1	S	153	ASN
1	S	781	ILE
1	S	1232	THR
1	S	1436	GLY
2	T	2202	GLY
3	U	3111[A]	SER
3	U	3111[B]	SER
3	U	3301[A]	PRO
3	U	3301[B]	PRO
1	V	753	ASN
1	V	1436	GLY
1	V	1485	ALA
3	X	3111[A]	SER
3	X	3111[B]	SER
3	X	3301[A]	PRO
3	X	3301[B]	PRO
1	Y	611	GLY
1	Y	807	GLY
3	a	3111[A]	SER
3	a	3111[B]	SER
3	a	3301[A]	PRO
3	a	3301[B]	PRO
1	b	867	VAL
1	b	1485	ALA
2	c	2404	GLY
2	c	2461	HIS
3	d	3111[A]	SER
3	d	3111[B]	SER
3	d	3301[A]	PRO
3	d	3301[B]	PRO
1	A	333	ASN
2	B	2547	MET
1	D	134	VAL
1	D	417	MET
1	D	867	VAL
1	D	1484	CYS
1	D	1485	ALA
2	E	2779	ASP
1	G	867	VAL
1	G	1211	TYR
1	G	1436	GLY

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Mol	Chain	Res	Type
2	H	2738	ALA
1	M	227	ARG
1	M	867	VAL
1	P	227	ARG
1	P	881	GLN
1	S	149	GLU
2	T	2461	HIS
1	V	781	ILE
1	V	834	ASP
1	V	1037	ALA
1	V	1232	THR
2	W	2344	LEU
2	W	2418	GLY
1	Y	153	ASN
1	Y	881	GLN
1	Y	1228	LEU
1	A	867	VAL
1	A	875	ALA
1	A	1232	THR
2	B	2738	ALA
3	C	3099[A]	PRO
3	C	3099[B]	PRO
1	D	884	PRO
1	D	956	PRO
1	D	1436	GLY
2	E	2344	LEU
2	E	2461	HIS
2	E	2548	CYS
3	F	3099[A]	PRO
3	F	3099[B]	PRO
1	G	153	ASN
3	I	3099[A]	PRO
3	I	3099[B]	PRO
1	J	555	ALA
1	J	867	VAL
1	J	1301	PRO
1	J	1582	ASN
2	K	2830	GLN
3	L	3099[A]	PRO
3	L	3099[B]	PRO
1	M	464	LEU
1	M	1211	TYR

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Mol	Chain	Res	Type
3	O	3099[A]	PRO
3	O	3099[B]	PRO
1	P	571	PRO
1	P	1036	SER
3	R	3099[A]	PRO
3	R	3099[B]	PRO
1	S	1301	PRO
3	U	3099[A]	PRO
3	U	3099[B]	PRO
1	V	116	LYS
1	V	330	GLN
1	V	1583	CYS
2	W	2461	HIS
3	X	3099[A]	PRO
3	X	3099[B]	PRO
3	a	3099[A]	PRO
3	a	3099[B]	PRO
1	b	962	GLY
3	d	3099[A]	PRO
3	d	3099[B]	PRO
1	A	464	LEU
2	B	2548	CYS
1	G	53	SER
1	G	983	PRO
2	H	2894	ASN
1	J	884	PRO
1	J	956	PRO
2	Q	2831	GLU
1	S	1432	SER
2	T	2738	ALA
1	V	570	GLN
2	W	2340	ALA
1	Y	884	PRO
1	A	956	PRO
2	E	2738	ALA
1	G	883	CYS
1	G	956	PRO
1	J	116	LYS
2	K	2340	ALA
1	P	884	PRO
2	Q	2738	ALA
2	T	2237	LEU

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Mol	Chain	Res	Type
2	T	2650	GLY
1	V	153	ASN
2	Z	2499	ALA
1	D	831	VAL
1	G	676	PRO
1	P	956	PRO
2	Q	2217	ILE
1	V	982	LYS
1	b	956	PRO
1	b	1196	ILE
1	G	1196	ILE
1	J	1196	ILE
1	M	982	LYS
1	Y	1196	ILE
1	b	52	GLY
1	M	126	GLY
1	P	867	VAL
1	P	982	LYS
1	V	1083	PRO
2	Z	2650	GLY
2	c	2549	PRO
1	A	921	GLY
1	A	1083	PRO
1	A	1301	PRO
1	D	464	LEU
2	E	2418	GLY
1	J	52	GLY
2	K	2415	PRO
1	P	1196	ILE
1	J	556	GLY
2	K	2339	GLY
1	V	1196	ILE
2	N	2477	PRO
1	D	571	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	1429/1738 (82%)	1263 (88%)	166 (12%)	5	23
1	D	1429/1738 (82%)	1249 (87%)	180 (13%)	4	20
1	G	1429/1738 (82%)	1242 (87%)	187 (13%)	4	19
1	J	1429/1738 (82%)	1246 (87%)	183 (13%)	4	19
1	M	1429/1738 (82%)	1269 (89%)	160 (11%)	6	24
1	P	1429/1738 (82%)	1245 (87%)	184 (13%)	4	19
1	S	1429/1738 (82%)	1241 (87%)	188 (13%)	4	18
1	V	1429/1738 (82%)	1249 (87%)	180 (13%)	4	20
1	Y	1429/1738 (82%)	1243 (87%)	186 (13%)	4	19
1	b	1429/1738 (82%)	1265 (88%)	164 (12%)	5	24
2	B	731/814 (90%)	654 (90%)	77 (10%)	6	27
2	E	731/814 (90%)	651 (89%)	80 (11%)	6	26
2	H	731/814 (90%)	631 (86%)	100 (14%)	3	17
2	K	731/814 (90%)	649 (89%)	82 (11%)	6	24
2	N	731/814 (90%)	646 (88%)	85 (12%)	5	23
2	Q	731/814 (90%)	650 (89%)	81 (11%)	6	25
2	T	731/814 (90%)	653 (89%)	78 (11%)	6	26
2	W	731/814 (90%)	655 (90%)	76 (10%)	7	28
2	Z	731/814 (90%)	639 (87%)	92 (13%)	4	20
2	c	731/814 (90%)	641 (88%)	90 (12%)	4	21
3	C	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	F	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	I	636/343 (185%)	410 (64%)	226 (36%)	0	1
3	L	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	O	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	R	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	U	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	X	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	a	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	d	636/343 (185%)	412 (65%)	224 (35%)	0	1
All	All	27960/28950 (97%)	23099 (83%)	4861 (17%)	3	10

All (4861) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	16	LEU
1	A	26	GLN
1	A	62	MET
1	A	67	MET
1	A	73	LEU
1	A	83	HIS
1	A	109	LEU
1	A	114	THR
1	A	117	LYS
1	A	127	GLU
1	A	133	LYS
1	A	134	VAL
1	A	140	ASP
1	A	149	GLU
1	A	151	GLN
1	A	163	LEU
1	A	174	GLN
1	A	179	HIS
1	A	185	LEU
1	A	205	LEU
1	A	210	HIS
1	A	219	LEU
1	A	235	CYS
1	A	238	ASN
1	A	239	LEU
1	A	245	GLU
1	A	249	ARG
1	A	266	LEU
1	A	277	ASP
1	A	279	LEU
1	A	285	THR
1	A	326	GLU
1	A	336	ASN
1	A	344	LEU
1	A	365	THR
1	A	367	LEU
1	A	368	SER
1	A	373	LEU
1	A	376	ASN
1	A	384	THR
1	A	386	ILE
1	A	417	MET

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Mol	Chain	Res	Type
1	A	430	SER
1	A	432	THR
1	A	434	GLU
1	A	452	ILE
1	A	456	GLN
1	A	494	VAL
1	A	497	GLN
1	A	509	ILE
1	A	511	VAL
1	A	515	ASP
1	A	516	TRP
1	A	527	LEU
1	A	554	LYS
1	A	557	VAL
1	A	568	PHE
1	A	570	GLN
1	A	572	SER
1	A	573	LYS
1	A	579	LEU
1	A	589	GLN
1	A	603	HIS
1	A	610	THR
1	A	624	THR
1	A	650	GLN
1	A	688	VAL
1	A	692	VAL
1	A	695	TYR
1	A	713	ILE
1	A	720	VAL
1	A	729	VAL
1	A	744	VAL
1	A	749	VAL
1	A	754	GLU
1	A	783	ASP
1	A	801	ASP
1	A	810	LEU
1	A	821	ILE
1	A	833	PHE
1	A	836	GLN
1	A	865	LYS
1	A	867	VAL
1	A	881	GLN

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Mol	Chain	Res	Type
1	A	917	LEU
1	A	920	ASN
1	A	935	ILE
1	A	943	LEU
1	A	965	ASP
1	A	979	LEU
1	A	981	GLU
1	A	982	LYS
1	A	999	LEU
1	A	1001	GLN
1	A	1003	ASP
1	A	1013	ILE
1	A	1015	HIS
1	A	1017	HIS
1	A	1033	LEU
1	A	1067	TYR
1	A	1075	GLU
1	A	1077	LEU
1	A	1089	ASP
1	A	1090	ILE
1	A	1098	GLU
1	A	1126	ILE
1	A	1139	LYS
1	A	1144	VAL
1	A	1153	LYS
1	A	1155	LEU
1	A	1157	VAL
1	A	1160	PHE
1	A	1166	THR
1	A	1170	MET
1	A	1196	ILE
1	A	1200	MET
1	A	1210	LYS
1	A	1211	TYR
1	A	1213	VAL
1	A	1219	ASP
1	A	1221	THR
1	A	1225	VAL
1	A	1227	ASP
1	A	1229	LYS
1	A	1230	LEU
1	A	1245	GLU

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Mol	Chain	Res	Type
1	A	1248	ARG
1	A	1249	TRP
1	A	1258	ARG
1	A	1266	PHE
1	A	1280	GLN
1	A	1286	ARG
1	A	1302	SER
1	A	1303	GLU
1	A	1307	MET
1	A	1308	VAL
1	A	1325	LEU
1	A	1331	GLU
1	A	1354	GLU
1	A	1367	SER
1	A	1369	THR
1	A	1372	ILE
1	A	1396	GLU
1	A	1400	ASN
1	A	1407	THR
1	A	1408	LEU
1	A	1427	HIS
1	A	1430	ILE
1	A	1439	VAL
1	A	1441	SER
1	A	1461	VAL
1	A	1494	ARG
1	A	1509	THR
1	A	1516	VAL
1	A	1543	ILE
1	A	1563	LYS
1	A	1568	VAL
1	A	1581	GLU
1	A	1597	THR
1	A	1622	GLN
1	A	1632	LEU
1	A	1642	GLN
1	A	1643	LYS
1	A	1649	THR
1	A	1653	VAL
2	B	2084	ARG
2	B	2089	ARG
2	B	2104	ILE

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Mol	Chain	Res	Type
2	B	2121	THR
2	B	2131	LEU
2	B	2132	CYS
2	B	2145	LEU
2	B	2160	VAL
2	B	2180	TRP
2	B	2184	MET
2	B	2185	THR
2	B	2187	VAL
2	B	2191	LEU
2	B	2205	THR
2	B	2216	PHE
2	B	2237	LEU
2	B	2240	GLN
2	B	2241	THR
2	B	2260	GLU
2	B	2267	HIS
2	B	2274	LEU
2	B	2285	LEU
2	B	2296	LEU
2	B	2326	ILE
2	B	2327	GLU
2	B	2328	LEU
2	B	2329	MET
2	B	2333	LEU
2	B	2334	LYS
2	B	2361	LYS
2	B	2394	VAL
2	B	2406	SER
2	B	2445	MET
2	B	2456	LEU
2	B	2478	GLU
2	B	2500	ILE
2	B	2507	ARG
2	B	2531	GLU
2	B	2546	LEU
2	B	2547	MET
2	B	2550	THR
2	B	2555	GLU
2	B	2556	TYR
2	B	2561	HIS
2	B	2572	VAL

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Mol	Chain	Res	Type
2	B	2581	MET
2	B	2595	TRP
2	B	2597	MET
2	B	2616	THR
2	B	2617	ASP
2	B	2625	LEU
2	B	2644	LEU
2	B	2658	LYS
2	B	2662	LEU
2	B	2680	HIS
2	B	2718	TRP
2	B	2728	ARG
2	B	2750	ILE
2	B	2752	GLU
2	B	2758	THR
2	B	2769	PHE
2	B	2772	LYS
2	B	2798	GLN
2	B	2809	LEU
2	B	2814	LYS
2	B	2822	LYS
2	B	2825	ILE
2	B	2828	ASP
2	B	2838	LEU
2	B	2851	ASN
2	B	2876	LYS
2	B	2879	LEU
2	B	2883	ILE
2	B	2894	ASN
2	B	2898	LYS
2	B	2900	SER
2	B	2907	LYS
3	C	2929[A]	SER
3	C	2929[B]	SER
3	C	2930[A]	LEU
3	C	2930[B]	LEU
3	C	2931[A]	THR
3	C	2931[B]	THR
3	C	2933[A]	SER
3	C	2933[B]	SER
3	C	2935[A]	ILE
3	C	2935[B]	ILE

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Mol	Chain	Res	Type
3	C	2938[A]	LEU
3	C	2938[B]	LEU
3	C	2942[A]	LEU
3	C	2942[B]	LEU
3	C	2946[A]	GLN
3	C	2946[B]	GLN
3	C	2949[A]	LYS
3	C	2949[B]	LYS
3	C	2954[A]	TYR
3	C	2954[B]	TYR
3	C	2956[A]	LYS
3	C	2956[B]	LYS
3	C	2959[A]	SER
3	C	2959[B]	SER
3	C	2960[A]	PHE
3	C	2960[B]	PHE
3	C	2963[A]	MET
3	C	2963[B]	MET
3	C	2965[A]	LEU
3	C	2965[B]	LEU
3	C	2968[A]	GLN
3	C	2968[B]	GLN
3	C	2973[A]	THR
3	C	2973[B]	THR
3	C	2980[A]	HIS
3	C	2980[B]	HIS
3	C	2982[A]	MET
3	C	2982[B]	MET
3	C	2990[A]	ARG
3	C	2990[B]	ARG
3	C	2995[A]	GLN
3	C	2995[B]	GLN
3	C	2996[A]	MET
3	C	2996[B]	MET
3	C	2997[A]	GLU
3	C	2997[B]	GLU
3	C	3000[A]	LEU
3	C	3000[B]	LEU
3	C	3001[A]	LYS
3	C	3001[B]	LYS
3	C	3019[A]	HIS
3	C	3019[B]	HIS

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Mol	Chain	Res	Type
3	C	3021[A]	LEU
3	C	3021[B]	LEU
3	C	3023[A]	ILE
3	C	3023[B]	ILE
3	C	3024[A]	LEU
3	C	3024[B]	LEU
3	C	3026[A]	THR
3	C	3026[B]	THR
3	C	3029[A]	LYS
3	C	3029[B]	LYS
3	C	3040[A]	VAL
3	C	3040[B]	VAL
3	C	3042[A]	ASP
3	C	3042[B]	ASP
3	C	3044[A]	LYS
3	C	3044[B]	LYS
3	C	3048[A]	ASP
3	C	3048[B]	ASP
3	C	3050[A]	ARG
3	C	3050[B]	ARG
3	C	3063[A]	SER
3	C	3063[B]	SER
3	C	3067[A]	ARG
3	C	3067[B]	ARG
3	C	3077[A]	ASP
3	C	3077[B]	ASP
3	C	3081[A]	PHE
3	C	3081[B]	PHE
3	C	3096[A]	VAL
3	C	3096[B]	VAL
3	C	3105[A]	SER
3	C	3105[B]	SER
3	C	3107[A]	LEU
3	C	3107[B]	LEU
3	C	3110[A]	THR
3	C	3110[B]	THR
3	C	3111[A]	SER
3	C	3111[B]	SER
3	C	3115[A]	LEU
3	C	3115[B]	LEU
3	C	3123[A]	THR
3	C	3123[B]	THR

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Mol	Chain	Res	Type
3	C	3131[A]	GLN
3	C	3131[B]	GLN
3	C	3133[A]	LEU
3	C	3133[B]	LEU
3	C	3134[A]	GLN
3	C	3134[B]	GLN
3	C	3135[A]	LYS
3	C	3135[B]	LYS
3	C	3139[A]	LEU
3	C	3139[B]	LEU
3	C	3141[A]	TYR
3	C	3141[B]	TYR
3	C	3147[A]	GLU
3	C	3147[B]	GLU
3	C	3151[A]	LEU
3	C	3151[B]	LEU
3	C	3156[A]	MET
3	C	3156[B]	MET
3	C	3159[A]	SER
3	C	3159[B]	SER
3	C	3160[A]	SER
3	C	3160[B]	SER
3	C	3161[A]	GLU
3	C	3161[B]	GLU
3	C	3162[A]	ASP
3	C	3162[B]	ASP
3	C	3163[A]	ASN
3	C	3163[B]	ASN
3	C	3169[A]	LYS
3	C	3169[B]	LYS
3	C	3172[A]	SER
3	C	3172[B]	SER
3	C	3176[A]	LYS
3	C	3176[B]	LYS
3	C	3181[A]	GLN
3	C	3181[B]	GLN
3	C	3182[A]	GLN
3	C	3182[B]	GLN
3	C	3183[A]	LEU
3	C	3183[B]	LEU
3	C	3185[A]	TYR
3	C	3185[B]	TYR

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Mol	Chain	Res	Type
3	C	3186[A]	GLU
3	C	3186[B]	GLU
3	C	3188[A]	ASP
3	C	3188[B]	ASP
3	C	3191[A]	ASN
3	C	3191[B]	ASN
3	C	3192[A]	PHE
3	C	3192[B]	PHE
3	C	3193[A]	HIS
3	C	3193[B]	HIS
3	C	3195[A]	MET
3	C	3195[B]	MET
3	C	3196[A]	THR
3	C	3196[B]	THR
3	C	3200[A]	LEU
3	C	3200[B]	LEU
3	C	3201[A]	GLU
3	C	3201[B]	GLU
3	C	3204[A]	LEU
3	C	3204[B]	LEU
3	C	3205[A]	LYS
3	C	3205[B]	LYS
3	C	3210[A]	LYS
3	C	3210[B]	LYS
3	C	3211[A]	ASP
3	C	3211[B]	ASP
3	C	3212[A]	ARG
3	C	3212[B]	ARG
3	C	3218[A]	LEU
3	C	3218[B]	LEU
3	C	3220[A]	ARG
3	C	3220[B]	ARG
3	C	3222[A]	ILE
3	C	3222[B]	ILE
3	C	3224[A]	GLN
3	C	3224[B]	GLN
3	C	3225[A]	SER
3	C	3225[B]	SER
3	C	3230[A]	PHE
3	C	3230[B]	PHE
3	C	3244[A]	THR
3	C	3244[B]	THR

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Mol	Chain	Res	Type
3	C	3251[A]	ASP
3	C	3251[B]	ASP
3	C	3254[A]	MET
3	C	3254[B]	MET
3	C	3260[A]	ARG
3	C	3260[B]	ARG
3	C	3267[A]	SER
3	C	3267[B]	SER
3	C	3268[A]	LYS
3	C	3268[B]	LYS
3	C	3271[A]	VAL
3	C	3271[B]	VAL
3	C	3272[A]	HIS
3	C	3272[B]	HIS
3	C	3274[A]	ARG
3	C	3274[B]	ARG
3	C	3276[A]	ASP
3	C	3276[B]	ASP
3	C	3278[A]	HIS
3	C	3278[B]	HIS
3	C	3279[A]	ASP
3	C	3279[B]	ASP
3	C	3283[A]	ILE
3	C	3283[B]	ILE
3	C	3286[A]	THR
3	C	3286[B]	THR
3	C	3287[A]	ILE
3	C	3287[B]	ILE
3	C	3288[A]	MET
3	C	3288[B]	MET
3	C	3290[A]	ILE
3	C	3290[B]	ILE
3	C	3293[A]	LYS
3	C	3293[B]	LYS
3	C	3297[A]	PRO
3	C	3297[B]	PRO
3	C	3299[A]	LEU
3	C	3299[B]	LEU
3	C	3302[A]	SER
3	C	3302[B]	SER
3	C	3304[A]	THR
3	C	3304[B]	THR

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Mol	Chain	Res	Type
3	C	3306[A]	LEU
3	C	3306[B]	LEU
3	C	3308[A]	LYS
3	C	3308[B]	LYS
1	D	2	LEU
1	D	3	ILE
1	D	26	GLN
1	D	28	ASP
1	D	32	SER
1	D	55	ILE
1	D	62	MET
1	D	67	MET
1	D	70	ARG
1	D	83	HIS
1	D	96	LYS
1	D	110	PHE
1	D	119	LYS
1	D	128	ILE
1	D	132	ASN
1	D	133	LYS
1	D	134	VAL
1	D	135	THR
1	D	137	ARG
1	D	140	ASP
1	D	163	LEU
1	D	174	GLN
1	D	179	HIS
1	D	185	LEU
1	D	205	LEU
1	D	214	GLU
1	D	226	HIS
1	D	235	CYS
1	D	238	ASN
1	D	249	ARG
1	D	251	THR
1	D	261	SER
1	D	266	LEU
1	D	281	LEU
1	D	285	THR
1	D	289	LEU
1	D	296	ARG
1	D	297	ARG

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Mol	Chain	Res	Type
1	D	325	THR
1	D	336	ASN
1	D	365	THR
1	D	371	LEU
1	D	384	THR
1	D	386	ILE
1	D	394	GLN
1	D	416	ASN
1	D	419	THR
1	D	423	ARG
1	D	449	ASP
1	D	450	LYS
1	D	456	GLN
1	D	499	GLU
1	D	509	ILE
1	D	511	VAL
1	D	515	ASP
1	D	527	LEU
1	D	557	VAL
1	D	560	SER
1	D	565	GLU
1	D	567	LEU
1	D	568	PHE
1	D	570	GLN
1	D	572	SER
1	D	573	LYS
1	D	579	LEU
1	D	589	GLN
1	D	603	HIS
1	D	606	ILE
1	D	609	TRP
1	D	633	HIS
1	D	674	LYS
1	D	677	LEU
1	D	692	VAL
1	D	695	TYR
1	D	729	VAL
1	D	736	MET
1	D	739	GLN
1	D	744	VAL
1	D	749	VAL
1	D	753	ASN

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Mol	Chain	Res	Type
1	D	781	ILE
1	D	797	THR
1	D	808	THR
1	D	810	LEU
1	D	813	THR
1	D	830	ASN
1	D	835	GLU
1	D	836	GLN
1	D	842	ASN
1	D	851	MET
1	D	865	LYS
1	D	870	TYR
1	D	877	HIS
1	D	880	THR
1	D	891	LYS
1	D	896	HIS
1	D	901	THR
1	D	917	LEU
1	D	935	ILE
1	D	936	ASP
1	D	964	ILE
1	D	979	LEU
1	D	984	ASP
1	D	990	HIS
1	D	999	LEU
1	D	1001	GLN
1	D	1008	GLU
1	D	1013	ILE
1	D	1015	HIS
1	D	1017	HIS
1	D	1067	TYR
1	D	1075	GLU
1	D	1077	LEU
1	D	1078	ARG
1	D	1096	THR
1	D	1105	VAL
1	D	1118	THR
1	D	1122	ASN
1	D	1126	ILE
1	D	1133	ILE
1	D	1140	ASN
1	D	1153	LYS

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Mol	Chain	Res	Type
1	D	1155	LEU
1	D	1156	LEU
1	D	1157	VAL
1	D	1160	PHE
1	D	1167	ASP
1	D	1174	GLU
1	D	1196	ILE
1	D	1200	MET
1	D	1206	HIS
1	D	1210	LYS
1	D	1221	THR
1	D	1225	VAL
1	D	1228	LEU
1	D	1230	LEU
1	D	1232	THR
1	D	1234	VAL
1	D	1242	ASN
1	D	1245	GLU
1	D	1249	TRP
1	D	1258	ARG
1	D	1260	ARG
1	D	1266	PHE
1	D	1283	ASP
1	D	1286	ARG
1	D	1302	SER
1	D	1304	ASP
1	D	1306	THR
1	D	1307	MET
1	D	1328	SER
1	D	1355	LEU
1	D	1369	THR
1	D	1394	GLN
1	D	1408	LEU
1	D	1427	HIS
1	D	1433	TRP
1	D	1439	VAL
1	D	1456	LEU
1	D	1478	SER
1	D	1480	ASN
1	D	1494	ARG
1	D	1505	ARG
1	D	1516	VAL

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Mol	Chain	Res	Type
1	D	1542	ARG
1	D	1550	ARG
1	D	1563	LYS
1	D	1568	VAL
1	D	1598	GLU
1	D	1621	ASN
1	D	1622	GLN
1	D	1629	GLU
1	D	1632	LEU
1	D	1635	VAL
1	D	1636	ASN
1	D	1639	LYS
1	D	1641	THR
1	D	1643	LYS
1	D	1647	ASN
1	D	1650	ILE
2	E	2086	ASN
2	E	2089	ARG
2	E	2117	ASP
2	E	2145	LEU
2	E	2184	MET
2	E	2187	VAL
2	E	2191	LEU
2	E	2205	THR
2	E	2211	HIS
2	E	2220	GLU
2	E	2233	GLU
2	E	2237	LEU
2	E	2239	LYS
2	E	2254	THR
2	E	2260	GLU
2	E	2265	ILE
2	E	2267	HIS
2	E	2274	LEU
2	E	2277	LYS
2	E	2326	ILE
2	E	2328	LEU
2	E	2333	LEU
2	E	2344	LEU
2	E	2378	ILE
2	E	2394	VAL
2	E	2403	PHE

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Mol	Chain	Res	Type
2	E	2435	MET
2	E	2445	MET
2	E	2457	LYS
2	E	2459	ASP
2	E	2474	THR
2	E	2480	LEU
2	E	2489	ILE
2	E	2496	LEU
2	E	2500	ILE
2	E	2533	ASP
2	E	2548	CYS
2	E	2555	GLU
2	E	2556	TYR
2	E	2561	HIS
2	E	2572	VAL
2	E	2579	GLU
2	E	2581	MET
2	E	2595	TRP
2	E	2597	MET
2	E	2600	ASP
2	E	2616	THR
2	E	2617	ASP
2	E	2630	LYS
2	E	2631	TYR
2	E	2647	LEU
2	E	2652	LYS
2	E	2653	GLU
2	E	2662	LEU
2	E	2680	HIS
2	E	2684	HIS
2	E	2686	LEU
2	E	2739	LEU
2	E	2742	MET
2	E	2758	THR
2	E	2769	PHE
2	E	2772	LYS
2	E	2780	HIS
2	E	2814	LYS
2	E	2816	SER
2	E	2824	CYS
2	E	2825	ILE
2	E	2826	GLU

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Mol	Chain	Res	Type
2	E	2828	ASP
2	E	2838	LEU
2	E	2847	HIS
2	E	2848	PHE
2	E	2851	ASN
2	E	2858	ASP
2	E	2868	GLU
2	E	2876	LYS
2	E	2879	LEU
2	E	2883	ILE
2	E	2898	LYS
2	E	2901	LEU
3	F	2929[A]	SER
3	F	2929[B]	SER
3	F	2930[A]	LEU
3	F	2930[B]	LEU
3	F	2931[A]	THR
3	F	2931[B]	THR
3	F	2933[A]	SER
3	F	2933[B]	SER
3	F	2935[A]	ILE
3	F	2935[B]	ILE
3	F	2938[A]	LEU
3	F	2938[B]	LEU
3	F	2942[A]	LEU
3	F	2942[B]	LEU
3	F	2946[A]	GLN
3	F	2946[B]	GLN
3	F	2949[A]	LYS
3	F	2949[B]	LYS
3	F	2954[A]	TYR
3	F	2954[B]	TYR
3	F	2956[A]	LYS
3	F	2956[B]	LYS
3	F	2959[A]	SER
3	F	2959[B]	SER
3	F	2960[A]	PHE
3	F	2960[B]	PHE
3	F	2963[A]	MET
3	F	2963[B]	MET
3	F	2965[A]	LEU
3	F	2965[B]	LEU

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Mol	Chain	Res	Type
3	F	2968[A]	GLN
3	F	2968[B]	GLN
3	F	2973[A]	THR
3	F	2973[B]	THR
3	F	2980[A]	HIS
3	F	2980[B]	HIS
3	F	2982[A]	MET
3	F	2982[B]	MET
3	F	2990[A]	ARG
3	F	2990[B]	ARG
3	F	2995[A]	GLN
3	F	2995[B]	GLN
3	F	2996[A]	MET
3	F	2996[B]	MET
3	F	2997[A]	GLU
3	F	2997[B]	GLU
3	F	3000[A]	LEU
3	F	3000[B]	LEU
3	F	3001[A]	LYS
3	F	3001[B]	LYS
3	F	3019[A]	HIS
3	F	3019[B]	HIS
3	F	3021[A]	LEU
3	F	3021[B]	LEU
3	F	3023[A]	ILE
3	F	3023[B]	ILE
3	F	3024[A]	LEU
3	F	3024[B]	LEU
3	F	3026[A]	THR
3	F	3026[B]	THR
3	F	3029[A]	LYS
3	F	3029[B]	LYS
3	F	3040[A]	VAL
3	F	3040[B]	VAL
3	F	3042[A]	ASP
3	F	3042[B]	ASP
3	F	3044[A]	LYS
3	F	3044[B]	LYS
3	F	3048[A]	ASP
3	F	3048[B]	ASP
3	F	3050[A]	ARG
3	F	3050[B]	ARG

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Mol	Chain	Res	Type
3	F	3063[A]	SER
3	F	3063[B]	SER
3	F	3067[A]	ARG
3	F	3067[B]	ARG
3	F	3077[A]	ASP
3	F	3077[B]	ASP
3	F	3081[A]	PHE
3	F	3081[B]	PHE
3	F	3096[A]	VAL
3	F	3096[B]	VAL
3	F	3105[A]	SER
3	F	3105[B]	SER
3	F	3107[A]	LEU
3	F	3107[B]	LEU
3	F	3110[A]	THR
3	F	3110[B]	THR
3	F	3111[A]	SER
3	F	3111[B]	SER
3	F	3115[A]	LEU
3	F	3115[B]	LEU
3	F	3123[A]	THR
3	F	3123[B]	THR
3	F	3131[A]	GLN
3	F	3131[B]	GLN
3	F	3133[A]	LEU
3	F	3133[B]	LEU
3	F	3134[A]	GLN
3	F	3134[B]	GLN
3	F	3135[A]	LYS
3	F	3135[B]	LYS
3	F	3139[A]	LEU
3	F	3139[B]	LEU
3	F	3141[A]	TYR
3	F	3141[B]	TYR
3	F	3147[A]	GLU
3	F	3147[B]	GLU
3	F	3151[A]	LEU
3	F	3151[B]	LEU
3	F	3156[A]	MET
3	F	3156[B]	MET
3	F	3159[A]	SER
3	F	3159[B]	SER

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Mol	Chain	Res	Type
3	F	3160[A]	SER
3	F	3160[B]	SER
3	F	3161[A]	GLU
3	F	3161[B]	GLU
3	F	3162[A]	ASP
3	F	3162[B]	ASP
3	F	3163[A]	ASN
3	F	3163[B]	ASN
3	F	3169[A]	LYS
3	F	3169[B]	LYS
3	F	3172[A]	SER
3	F	3172[B]	SER
3	F	3176[A]	LYS
3	F	3176[B]	LYS
3	F	3181[A]	GLN
3	F	3181[B]	GLN
3	F	3182[A]	GLN
3	F	3182[B]	GLN
3	F	3183[A]	LEU
3	F	3183[B]	LEU
3	F	3185[A]	TYR
3	F	3185[B]	TYR
3	F	3186[A]	GLU
3	F	3186[B]	GLU
3	F	3188[A]	ASP
3	F	3188[B]	ASP
3	F	3191[A]	ASN
3	F	3191[B]	ASN
3	F	3192[A]	PHE
3	F	3192[B]	PHE
3	F	3193[A]	HIS
3	F	3193[B]	HIS
3	F	3195[A]	MET
3	F	3195[B]	MET
3	F	3196[A]	THR
3	F	3196[B]	THR
3	F	3200[A]	LEU
3	F	3200[B]	LEU
3	F	3201[A]	GLU
3	F	3201[B]	GLU
3	F	3204[A]	LEU
3	F	3204[B]	LEU

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Mol	Chain	Res	Type
3	F	3205[A]	LYS
3	F	3205[B]	LYS
3	F	3210[A]	LYS
3	F	3210[B]	LYS
3	F	3211[A]	ASP
3	F	3211[B]	ASP
3	F	3212[A]	ARG
3	F	3212[B]	ARG
3	F	3218[A]	LEU
3	F	3218[B]	LEU
3	F	3220[A]	ARG
3	F	3220[B]	ARG
3	F	3222[A]	ILE
3	F	3222[B]	ILE
3	F	3224[A]	GLN
3	F	3224[B]	GLN
3	F	3225[A]	SER
3	F	3225[B]	SER
3	F	3230[A]	PHE
3	F	3230[B]	PHE
3	F	3244[A]	THR
3	F	3244[B]	THR
3	F	3251[A]	ASP
3	F	3251[B]	ASP
3	F	3254[A]	MET
3	F	3254[B]	MET
3	F	3260[A]	ARG
3	F	3260[B]	ARG
3	F	3267[A]	SER
3	F	3267[B]	SER
3	F	3268[A]	LYS
3	F	3268[B]	LYS
3	F	3271[A]	VAL
3	F	3271[B]	VAL
3	F	3272[A]	HIS
3	F	3272[B]	HIS
3	F	3274[A]	ARG
3	F	3274[B]	ARG
3	F	3276[A]	ASP
3	F	3276[B]	ASP
3	F	3278[A]	HIS
3	F	3278[B]	HIS

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Mol	Chain	Res	Type
3	F	3279[A]	ASP
3	F	3279[B]	ASP
3	F	3283[A]	ILE
3	F	3283[B]	ILE
3	F	3286[A]	THR
3	F	3286[B]	THR
3	F	3287[A]	ILE
3	F	3287[B]	ILE
3	F	3288[A]	MET
3	F	3288[B]	MET
3	F	3290[A]	ILE
3	F	3290[B]	ILE
3	F	3293[A]	LYS
3	F	3293[B]	LYS
3	F	3297[A]	PRO
3	F	3297[B]	PRO
3	F	3299[A]	LEU
3	F	3299[B]	LEU
3	F	3302[A]	SER
3	F	3302[B]	SER
3	F	3304[A]	THR
3	F	3304[B]	THR
3	F	3306[A]	LEU
3	F	3306[B]	LEU
3	F	3308[A]	LYS
3	F	3308[B]	LYS
1	G	4	ARG
1	G	17	ASN
1	G	19	GLN
1	G	26	GLN
1	G	37	ILE
1	G	53	SER
1	G	62	MET
1	G	67	MET
1	G	70	ARG
1	G	83	HIS
1	G	89	ILE
1	G	116	LYS
1	G	119	LYS
1	G	128	ILE
1	G	131	GLU
1	G	132	ASN

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Mol	Chain	Res	Type
1	G	134	VAL
1	G	148	GLN
1	G	163	LEU
1	G	166	GLU
1	G	182	ILE
1	G	185	LEU
1	G	191	THR
1	G	205	LEU
1	G	214	GLU
1	G	223	LEU
1	G	226	HIS
1	G	238	ASN
1	G	249	ARG
1	G	260	ASN
1	G	266	LEU
1	G	280	SER
1	G	281	LEU
1	G	285	THR
1	G	290	GLU
1	G	308	LEU
1	G	325	THR
1	G	330	GLN
1	G	331	SER
1	G	336	ASN
1	G	337	ASP
1	G	344	LEU
1	G	349	GLU
1	G	353	ASN
1	G	354	PHE
1	G	384	THR
1	G	386	ILE
1	G	387	ASN
1	G	395	THR
1	G	400	ILE
1	G	411	ASP
1	G	415	VAL
1	G	450	LYS
1	G	451	SER
1	G	456	GLN
1	G	472	ASP
1	G	474	LEU
1	G	476	ARG

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Mol	Chain	Res	Type
1	G	494	VAL
1	G	497	GLN
1	G	509	ILE
1	G	515	ASP
1	G	540	THR
1	G	553	LEU
1	G	565	GLU
1	G	566	ARG
1	G	567	LEU
1	G	568	PHE
1	G	570	GLN
1	G	572	SER
1	G	579	LEU
1	G	584	SER
1	G	588	GLU
1	G	597	VAL
1	G	600	GLU
1	G	603	HIS
1	G	610	THR
1	G	618	MET
1	G	624	THR
1	G	674	LYS
1	G	675	SER
1	G	684	ARG
1	G	687	SER
1	G	692	VAL
1	G	695	TYR
1	G	722	GLU
1	G	727	ASP
1	G	744	VAL
1	G	749	VAL
1	G	753	ASN
1	G	762	VAL
1	G	783	ASP
1	G	788	LEU
1	G	797	THR
1	G	808	THR
1	G	821	ILE
1	G	832	LYS
1	G	834	ASP
1	G	838	ARG
1	G	842	ASN

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Mol	Chain	Res	Type
1	G	856	THR
1	G	866	GLU
1	G	885	SER
1	G	894	CYS
1	G	896	HIS
1	G	901	THR
1	G	912	ASN
1	G	930	ASP
1	G	935	ILE
1	G	943	LEU
1	G	953	GLU
1	G	961	SER
1	G	965	ASP
1	G	973	ARG
1	G	977	GLU
1	G	979	LEU
1	G	987	LYS
1	G	999	LEU
1	G	1001	GLN
1	G	1012	GLU
1	G	1013	ILE
1	G	1015	HIS
1	G	1017	HIS
1	G	1026	GLU
1	G	1028	VAL
1	G	1075	GLU
1	G	1077	LEU
1	G	1078	ARG
1	G	1081	MET
1	G	1097	ARG
1	G	1105	VAL
1	G	1118	THR
1	G	1121	LEU
1	G	1126	ILE
1	G	1154	SER
1	G	1156	LEU
1	G	1157	VAL
1	G	1160	PHE
1	G	1166	THR
1	G	1174	GLU
1	G	1182	ASN
1	G	1183	GLU

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Mol	Chain	Res	Type
1	G	1195	ASP
1	G	1199	VAL
1	G	1200	MET
1	G	1210	LYS
1	G	1213	VAL
1	G	1226	THR
1	G	1228	LEU
1	G	1230	LEU
1	G	1240	ILE
1	G	1245	GLU
1	G	1254	THR
1	G	1255	SER
1	G	1258	ARG
1	G	1260	ARG
1	G	1280	GLN
1	G	1303	GLU
1	G	1304	ASP
1	G	1339	SER
1	G	1354	GLU
1	G	1369	THR
1	G	1372	ILE
1	G	1381	LYS
1	G	1401	ARG
1	G	1427	HIS
1	G	1439	VAL
1	G	1441	SER
1	G	1456	LEU
1	G	1470	GLU
1	G	1471	LEU
1	G	1476	LYS
1	G	1478	SER
1	G	1494	ARG
1	G	1509	THR
1	G	1530	LEU
1	G	1543	ILE
1	G	1559	LEU
1	G	1563	LYS
1	G	1568	VAL
1	G	1578	ILE
1	G	1599	MET
1	G	1622	GLN
1	G	1632	LEU

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Mol	Chain	Res	Type
1	G	1642	GLN
1	G	1643	LYS
1	G	1655	SER
2	H	2083	VAL
2	H	2086	ASN
2	H	2089	ARG
2	H	2131	LEU
2	H	2143	CYS
2	H	2145	LEU
2	H	2160	VAL
2	H	2168	ARG
2	H	2186	GLU
2	H	2187	VAL
2	H	2191	LEU
2	H	2203	ILE
2	H	2204	GLU
2	H	2205	THR
2	H	2224	THR
2	H	2226	GLU
2	H	2231	LEU
2	H	2237	LEU
2	H	2241	THR
2	H	2260	GLU
2	H	2267	HIS
2	H	2274	LEU
2	H	2277	LYS
2	H	2296	LEU
2	H	2327	GLU
2	H	2328	LEU
2	H	2333	LEU
2	H	2344	LEU
2	H	2345	ASN
2	H	2359	ASN
2	H	2361	LYS
2	H	2373	MET
2	H	2394	VAL
2	H	2445	MET
2	H	2456	LEU
2	H	2457	LYS
2	H	2469	VAL
2	H	2480	LEU
2	H	2497	GLU

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Mol	Chain	Res	Type
2	H	2500	ILE
2	H	2505	ILE
2	H	2545	SER
2	H	2548	CYS
2	H	2556	TYR
2	H	2561	HIS
2	H	2571	ARG
2	H	2572	VAL
2	H	2575	LEU
2	H	2581	MET
2	H	2595	TRP
2	H	2597	MET
2	H	2600	ASP
2	H	2615	TRP
2	H	2616	THR
2	H	2625	LEU
2	H	2630	LYS
2	H	2631	TYR
2	H	2637	VAL
2	H	2644	LEU
2	H	2652	LYS
2	H	2653	GLU
2	H	2662	LEU
2	H	2680	HIS
2	H	2687	ILE
2	H	2739	LEU
2	H	2742	MET
2	H	2750	ILE
2	H	2758	THR
2	H	2768	LEU
2	H	2769	PHE
2	H	2774	LEU
2	H	2780	HIS
2	H	2781	LEU
2	H	2782	ASN
2	H	2788	ILE
2	H	2791	LEU
2	H	2794	LEU
2	H	2809	LEU
2	H	2822	LYS
2	H	2826	GLU
2	H	2831	GLU

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Mol	Chain	Res	Type
2	H	2838	LEU
2	H	2842	THR
2	H	2844	MET
2	H	2848	PHE
2	H	2849	ASP
2	H	2851	ASN
2	H	2858	ASP
2	H	2864	ASN
2	H	2868	GLU
2	H	2876	LYS
2	H	2878	ARG
2	H	2881	VAL
2	H	2883	ILE
2	H	2884	LYS
2	H	2887	ASP
2	H	2890	VAL
2	H	2891	LEU
2	H	2898	LYS
2	H	2900	SER
3	I	2929[A]	SER
3	I	2929[B]	SER
3	I	2930[A]	LEU
3	I	2930[B]	LEU
3	I	2931[A]	THR
3	I	2931[B]	THR
3	I	2933[A]	SER
3	I	2933[B]	SER
3	I	2935[A]	ILE
3	I	2935[B]	ILE
3	I	2938[A]	LEU
3	I	2938[B]	LEU
3	I	2942[A]	LEU
3	I	2942[B]	LEU
3	I	2946[A]	GLN
3	I	2946[B]	GLN
3	I	2949[A]	LYS
3	I	2949[B]	LYS
3	I	2954[A]	TYR
3	I	2954[B]	TYR
3	I	2956[A]	LYS
3	I	2956[B]	LYS
3	I	2959[A]	SER

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Mol	Chain	Res	Type
3	I	2959[B]	SER
3	I	2960[A]	PHE
3	I	2960[B]	PHE
3	I	2963[A]	MET
3	I	2963[B]	MET
3	I	2965[A]	LEU
3	I	2965[B]	LEU
3	I	2968[A]	GLN
3	I	2968[B]	GLN
3	I	2973[A]	THR
3	I	2973[B]	THR
3	I	2980[A]	HIS
3	I	2980[B]	HIS
3	I	2982[A]	MET
3	I	2982[B]	MET
3	I	2990[A]	ARG
3	I	2990[B]	ARG
3	I	2995[A]	GLN
3	I	2995[B]	GLN
3	I	2996[A]	MET
3	I	2996[B]	MET
3	I	2997[A]	GLU
3	I	2997[B]	GLU
3	I	3000[A]	LEU
3	I	3000[B]	LEU
3	I	3001[A]	LYS
3	I	3001[B]	LYS
3	I	3019[A]	HIS
3	I	3019[B]	HIS
3	I	3021[A]	LEU
3	I	3021[B]	LEU
3	I	3023[A]	ILE
3	I	3023[B]	ILE
3	I	3024[A]	LEU
3	I	3024[B]	LEU
3	I	3026[A]	THR
3	I	3026[B]	THR
3	I	3029[A]	LYS
3	I	3029[B]	LYS
3	I	3040[A]	VAL
3	I	3040[B]	VAL
3	I	3042[A]	ASP

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Mol	Chain	Res	Type
3	I	3042[B]	ASP
3	I	3044[A]	LYS
3	I	3044[B]	LYS
3	I	3048[A]	ASP
3	I	3048[B]	ASP
3	I	3050[A]	ARG
3	I	3050[B]	ARG
3	I	3063[A]	SER
3	I	3063[B]	SER
3	I	3067[A]	ARG
3	I	3067[B]	ARG
3	I	3077[A]	ASP
3	I	3077[B]	ASP
3	I	3081[A]	PHE
3	I	3081[B]	PHE
3	I	3096[A]	VAL
3	I	3096[B]	VAL
3	I	3105[A]	SER
3	I	3105[B]	SER
3	I	3107[A]	LEU
3	I	3107[B]	LEU
3	I	3110[A]	THR
3	I	3110[B]	THR
3	I	3111[A]	SER
3	I	3111[B]	SER
3	I	3115[A]	LEU
3	I	3115[B]	LEU
3	I	3123[A]	THR
3	I	3123[B]	THR
3	I	3131[A]	GLN
3	I	3131[B]	GLN
3	I	3133[A]	LEU
3	I	3133[B]	LEU
3	I	3134[A]	GLN
3	I	3134[B]	GLN
3	I	3135[A]	LYS
3	I	3135[B]	LYS
3	I	3139[A]	LEU
3	I	3139[B]	LEU
3	I	3141[A]	TYR
3	I	3141[B]	TYR
3	I	3147[A]	GLU

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Mol	Chain	Res	Type
3	I	3147[B]	GLU
3	I	3151[A]	LEU
3	I	3151[B]	LEU
3	I	3152[A]	LYS
3	I	3152[B]	LYS
3	I	3156[A]	MET
3	I	3156[B]	MET
3	I	3159[A]	SER
3	I	3159[B]	SER
3	I	3160[A]	SER
3	I	3160[B]	SER
3	I	3161[A]	GLU
3	I	3161[B]	GLU
3	I	3162[A]	ASP
3	I	3162[B]	ASP
3	I	3163[A]	ASN
3	I	3163[B]	ASN
3	I	3169[A]	LYS
3	I	3169[B]	LYS
3	I	3172[A]	SER
3	I	3172[B]	SER
3	I	3176[A]	LYS
3	I	3176[B]	LYS
3	I	3181[A]	GLN
3	I	3181[B]	GLN
3	I	3182[A]	GLN
3	I	3182[B]	GLN
3	I	3183[A]	LEU
3	I	3183[B]	LEU
3	I	3185[A]	TYR
3	I	3185[B]	TYR
3	I	3186[A]	GLU
3	I	3186[B]	GLU
3	I	3188[A]	ASP
3	I	3188[B]	ASP
3	I	3191[A]	ASN
3	I	3191[B]	ASN
3	I	3192[A]	PHE
3	I	3192[B]	PHE
3	I	3193[A]	HIS
3	I	3193[B]	HIS
3	I	3195[A]	MET

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Mol	Chain	Res	Type
3	I	3195[B]	MET
3	I	3196[A]	THR
3	I	3196[B]	THR
3	I	3200[A]	LEU
3	I	3200[B]	LEU
3	I	3201[A]	GLU
3	I	3201[B]	GLU
3	I	3204[A]	LEU
3	I	3204[B]	LEU
3	I	3205[A]	LYS
3	I	3205[B]	LYS
3	I	3210[A]	LYS
3	I	3210[B]	LYS
3	I	3211[A]	ASP
3	I	3211[B]	ASP
3	I	3212[A]	ARG
3	I	3212[B]	ARG
3	I	3218[A]	LEU
3	I	3218[B]	LEU
3	I	3220[A]	ARG
3	I	3220[B]	ARG
3	I	3222[A]	ILE
3	I	3222[B]	ILE
3	I	3224[A]	GLN
3	I	3224[B]	GLN
3	I	3225[A]	SER
3	I	3225[B]	SER
3	I	3230[A]	PHE
3	I	3230[B]	PHE
3	I	3244[A]	THR
3	I	3244[B]	THR
3	I	3251[A]	ASP
3	I	3251[B]	ASP
3	I	3254[A]	MET
3	I	3254[B]	MET
3	I	3260[A]	ARG
3	I	3260[B]	ARG
3	I	3267[A]	SER
3	I	3267[B]	SER
3	I	3268[A]	LYS
3	I	3268[B]	LYS
3	I	3271[A]	VAL

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Mol	Chain	Res	Type
3	I	3271[B]	VAL
3	I	3272[A]	HIS
3	I	3272[B]	HIS
3	I	3274[A]	ARG
3	I	3274[B]	ARG
3	I	3276[A]	ASP
3	I	3276[B]	ASP
3	I	3278[A]	HIS
3	I	3278[B]	HIS
3	I	3279[A]	ASP
3	I	3279[B]	ASP
3	I	3283[A]	ILE
3	I	3283[B]	ILE
3	I	3286[A]	THR
3	I	3286[B]	THR
3	I	3287[A]	ILE
3	I	3287[B]	ILE
3	I	3288[A]	MET
3	I	3288[B]	MET
3	I	3290[A]	ILE
3	I	3290[B]	ILE
3	I	3293[A]	LYS
3	I	3293[B]	LYS
3	I	3297[A]	PRO
3	I	3297[B]	PRO
3	I	3299[A]	LEU
3	I	3299[B]	LEU
3	I	3302[A]	SER
3	I	3302[B]	SER
3	I	3304[A]	THR
3	I	3304[B]	THR
3	I	3306[A]	LEU
3	I	3306[B]	LEU
3	I	3308[A]	LYS
3	I	3308[B]	LYS
1	J	2	LEU
1	J	4	ARG
1	J	17	ASN
1	J	19	GLN
1	J	22	LEU
1	J	25	MET
1	J	26	GLN

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Mol	Chain	Res	Type
1	J	55	ILE
1	J	59	LEU
1	J	62	MET
1	J	67	MET
1	J	70	ARG
1	J	100	GLN
1	J	121	ASN
1	J	133	LYS
1	J	137	ARG
1	J	144	TYR
1	J	151	GLN
1	J	160	LEU
1	J	163	LEU
1	J	179	HIS
1	J	185	LEU
1	J	205	LEU
1	J	211	SER
1	J	214	GLU
1	J	219	LEU
1	J	223	LEU
1	J	225	LYS
1	J	227	ARG
1	J	235	CYS
1	J	237	LEU
1	J	238	ASN
1	J	239	LEU
1	J	249	ARG
1	J	266	LEU
1	J	279	LEU
1	J	281	LEU
1	J	289	LEU
1	J	290	GLU
1	J	308	LEU
1	J	329	ARG
1	J	330	GLN
1	J	332	ASP
1	J	336	ASN
1	J	376	ASN
1	J	384	THR
1	J	386	ILE
1	J	390	LEU
1	J	391	MET

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Mol	Chain	Res	Type
1	J	407	GLN
1	J	419	THR
1	J	420	SER
1	J	432	THR
1	J	433	THR
1	J	434	GLU
1	J	444	GLU
1	J	450	LYS
1	J	452	ILE
1	J	456	GLN
1	J	467	LYS
1	J	472	ASP
1	J	474	LEU
1	J	477	VAL
1	J	494	VAL
1	J	509	ILE
1	J	518	LYS
1	J	527	LEU
1	J	557	VAL
1	J	559	THR
1	J	560	SER
1	J	567	LEU
1	J	568	PHE
1	J	569	LYS
1	J	570	GLN
1	J	573	LYS
1	J	597	VAL
1	J	600	GLU
1	J	603	HIS
1	J	617	SER
1	J	633	HIS
1	J	669	LYS
1	J	675	SER
1	J	695	TYR
1	J	705	THR
1	J	712	SER
1	J	739	GLN
1	J	744	VAL
1	J	749	VAL
1	J	753	ASN
1	J	782	THR
1	J	797	THR

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Mol	Chain	Res	Type
1	J	806	ASN
1	J	810	LEU
1	J	832	LYS
1	J	844	ASP
1	J	871	GLN
1	J	881	GLN
1	J	894	CYS
1	J	901	THR
1	J	912	ASN
1	J	917	LEU
1	J	930	ASP
1	J	935	ILE
1	J	936	ASP
1	J	941	LEU
1	J	953	GLU
1	J	965	ASP
1	J	999	LEU
1	J	1001	GLN
1	J	1015	HIS
1	J	1017	HIS
1	J	1025	THR
1	J	1075	GLU
1	J	1077	LEU
1	J	1078	ARG
1	J	1090	ILE
1	J	1093	ASP
1	J	1105	VAL
1	J	1131	ARG
1	J	1142	VAL
1	J	1145	THR
1	J	1152	LYS
1	J	1157	VAL
1	J	1160	PHE
1	J	1167	ASP
1	J	1168	GLN
1	J	1182	ASN
1	J	1183	GLU
1	J	1199	VAL
1	J	1200	MET
1	J	1206	HIS
1	J	1210	LYS
1	J	1215	LEU

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Mol	Chain	Res	Type
1	J	1221	THR
1	J	1228	LEU
1	J	1231	VAL
1	J	1233	SER
1	J	1249	TRP
1	J	1258	ARG
1	J	1260	ARG
1	J	1266	PHE
1	J	1280	GLN
1	J	1284	GLU
1	J	1286	ARG
1	J	1307	MET
1	J	1331	GLU
1	J	1339	SER
1	J	1341	VAL
1	J	1369	THR
1	J	1372	ILE
1	J	1393	THR
1	J	1396	GLU
1	J	1408	LEU
1	J	1430	ILE
1	J	1439	VAL
1	J	1441	SER
1	J	1458	HIS
1	J	1473	ARG
1	J	1478	SER
1	J	1494	ARG
1	J	1516	VAL
1	J	1541	GLU
1	J	1550	ARG
1	J	1553	ILE
1	J	1559	LEU
1	J	1562	ILE
1	J	1563	LYS
1	J	1567	ASP
1	J	1568	VAL
1	J	1580	GLU
1	J	1581	GLU
1	J	1583	CYS
1	J	1597	THR
1	J	1599	MET
1	J	1602	GLN

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Mol	Chain	Res	Type
1	J	1620	LEU
1	J	1622	GLN
1	J	1629	GLU
1	J	1632	LEU
1	J	1633	THR
1	J	1639	LYS
1	J	1642	GLN
1	J	1644	ILE
2	K	2089	ARG
2	K	2092	VAL
2	K	2108	LYS
2	K	2117	ASP
2	K	2131	LEU
2	K	2145	LEU
2	K	2160	VAL
2	K	2180	TRP
2	K	2184	MET
2	K	2185	THR
2	K	2190	LEU
2	K	2205	THR
2	K	2211	HIS
2	K	2220	GLU
2	K	2222	MET
2	K	2237	LEU
2	K	2239	LYS
2	K	2248	ILE
2	K	2260	GLU
2	K	2267	HIS
2	K	2270	ILE
2	K	2274	LEU
2	K	2282	LEU
2	K	2283	ASN
2	K	2326	ILE
2	K	2327	GLU
2	K	2333	LEU
2	K	2344	LEU
2	K	2355	SER
2	K	2370	MET
2	K	2373	MET
2	K	2460	SER
2	K	2468	ILE
2	K	2480	LEU

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Mol	Chain	Res	Type
2	K	2489	ILE
2	K	2500	ILE
2	K	2502	LEU
2	K	2506	ARG
2	K	2507	ARG
2	K	2533	ASP
2	K	2546	LEU
2	K	2547	MET
2	K	2548	CYS
2	K	2561	HIS
2	K	2572	VAL
2	K	2579	GLU
2	K	2581	MET
2	K	2595	TRP
2	K	2597	MET
2	K	2600	ASP
2	K	2601	ASN
2	K	2616	THR
2	K	2620	ILE
2	K	2625	LEU
2	K	2653	GLU
2	K	2662	LEU
2	K	2714	VAL
2	K	2750	ILE
2	K	2758	THR
2	K	2769	PHE
2	K	2772	LYS
2	K	2780	HIS
2	K	2809	LEU
2	K	2826	GLU
2	K	2835	ILE
2	K	2848	PHE
2	K	2849	ASP
2	K	2860	LEU
2	K	2862	LYS
2	K	2868	GLU
2	K	2870	LEU
2	K	2875	SER
2	K	2879	LEU
2	K	2880	GLU
2	K	2881	VAL
2	K	2883	ILE

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Mol	Chain	Res	Type
2	K	2884	LYS
2	K	2891	LEU
2	K	2895	SER
2	K	2898	LYS
2	K	2900	SER
2	K	2902	ILE
3	L	2929[A]	SER
3	L	2929[B]	SER
3	L	2930[A]	LEU
3	L	2930[B]	LEU
3	L	2931[A]	THR
3	L	2931[B]	THR
3	L	2933[A]	SER
3	L	2933[B]	SER
3	L	2935[A]	ILE
3	L	2935[B]	ILE
3	L	2938[A]	LEU
3	L	2938[B]	LEU
3	L	2942[A]	LEU
3	L	2942[B]	LEU
3	L	2946[A]	GLN
3	L	2946[B]	GLN
3	L	2949[A]	LYS
3	L	2949[B]	LYS
3	L	2954[A]	TYR
3	L	2954[B]	TYR
3	L	2956[A]	LYS
3	L	2956[B]	LYS
3	L	2959[A]	SER
3	L	2959[B]	SER
3	L	2960[A]	PHE
3	L	2960[B]	PHE
3	L	2963[A]	MET
3	L	2963[B]	MET
3	L	2965[A]	LEU
3	L	2965[B]	LEU
3	L	2968[A]	GLN
3	L	2968[B]	GLN
3	L	2973[A]	THR
3	L	2973[B]	THR
3	L	2980[A]	HIS
3	L	2980[B]	HIS

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Mol	Chain	Res	Type
3	L	2982[A]	MET
3	L	2982[B]	MET
3	L	2990[A]	ARG
3	L	2990[B]	ARG
3	L	2995[A]	GLN
3	L	2995[B]	GLN
3	L	2996[A]	MET
3	L	2996[B]	MET
3	L	2997[A]	GLU
3	L	2997[B]	GLU
3	L	3000[A]	LEU
3	L	3000[B]	LEU
3	L	3001[A]	LYS
3	L	3001[B]	LYS
3	L	3019[A]	HIS
3	L	3019[B]	HIS
3	L	3021[A]	LEU
3	L	3021[B]	LEU
3	L	3023[A]	ILE
3	L	3023[B]	ILE
3	L	3024[A]	LEU
3	L	3024[B]	LEU
3	L	3026[A]	THR
3	L	3026[B]	THR
3	L	3029[A]	LYS
3	L	3029[B]	LYS
3	L	3040[A]	VAL
3	L	3040[B]	VAL
3	L	3042[A]	ASP
3	L	3042[B]	ASP
3	L	3044[A]	LYS
3	L	3044[B]	LYS
3	L	3048[A]	ASP
3	L	3048[B]	ASP
3	L	3050[A]	ARG
3	L	3050[B]	ARG
3	L	3063[A]	SER
3	L	3063[B]	SER
3	L	3067[A]	ARG
3	L	3067[B]	ARG
3	L	3077[A]	ASP
3	L	3077[B]	ASP

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Mol	Chain	Res	Type
3	L	3081[A]	PHE
3	L	3081[B]	PHE
3	L	3096[A]	VAL
3	L	3096[B]	VAL
3	L	3105[A]	SER
3	L	3105[B]	SER
3	L	3107[A]	LEU
3	L	3107[B]	LEU
3	L	3110[A]	THR
3	L	3110[B]	THR
3	L	3111[A]	SER
3	L	3111[B]	SER
3	L	3115[A]	LEU
3	L	3115[B]	LEU
3	L	3123[A]	THR
3	L	3123[B]	THR
3	L	3131[A]	GLN
3	L	3131[B]	GLN
3	L	3133[A]	LEU
3	L	3133[B]	LEU
3	L	3134[A]	GLN
3	L	3134[B]	GLN
3	L	3135[A]	LYS
3	L	3135[B]	LYS
3	L	3139[A]	LEU
3	L	3139[B]	LEU
3	L	3141[A]	TYR
3	L	3141[B]	TYR
3	L	3147[A]	GLU
3	L	3147[B]	GLU
3	L	3151[A]	LEU
3	L	3151[B]	LEU
3	L	3156[A]	MET
3	L	3156[B]	MET
3	L	3159[A]	SER
3	L	3159[B]	SER
3	L	3160[A]	SER
3	L	3160[B]	SER
3	L	3161[A]	GLU
3	L	3161[B]	GLU
3	L	3162[A]	ASP
3	L	3162[B]	ASP

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Mol	Chain	Res	Type
3	L	3163[A]	ASN
3	L	3163[B]	ASN
3	L	3169[A]	LYS
3	L	3169[B]	LYS
3	L	3172[A]	SER
3	L	3172[B]	SER
3	L	3176[A]	LYS
3	L	3176[B]	LYS
3	L	3181[A]	GLN
3	L	3181[B]	GLN
3	L	3182[A]	GLN
3	L	3182[B]	GLN
3	L	3183[A]	LEU
3	L	3183[B]	LEU
3	L	3185[A]	TYR
3	L	3185[B]	TYR
3	L	3186[A]	GLU
3	L	3186[B]	GLU
3	L	3188[A]	ASP
3	L	3188[B]	ASP
3	L	3191[A]	ASN
3	L	3191[B]	ASN
3	L	3192[A]	PHE
3	L	3192[B]	PHE
3	L	3193[A]	HIS
3	L	3193[B]	HIS
3	L	3195[A]	MET
3	L	3195[B]	MET
3	L	3196[A]	THR
3	L	3196[B]	THR
3	L	3200[A]	LEU
3	L	3200[B]	LEU
3	L	3201[A]	GLU
3	L	3201[B]	GLU
3	L	3204[A]	LEU
3	L	3204[B]	LEU
3	L	3205[A]	LYS
3	L	3205[B]	LYS
3	L	3210[A]	LYS
3	L	3210[B]	LYS
3	L	3211[A]	ASP
3	L	3211[B]	ASP

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Mol	Chain	Res	Type
3	L	3212[A]	ARG
3	L	3212[B]	ARG
3	L	3218[A]	LEU
3	L	3218[B]	LEU
3	L	3220[A]	ARG
3	L	3220[B]	ARG
3	L	3222[A]	ILE
3	L	3222[B]	ILE
3	L	3224[A]	GLN
3	L	3224[B]	GLN
3	L	3225[A]	SER
3	L	3225[B]	SER
3	L	3230[A]	PHE
3	L	3230[B]	PHE
3	L	3244[A]	THR
3	L	3244[B]	THR
3	L	3251[A]	ASP
3	L	3251[B]	ASP
3	L	3254[A]	MET
3	L	3254[B]	MET
3	L	3260[A]	ARG
3	L	3260[B]	ARG
3	L	3267[A]	SER
3	L	3267[B]	SER
3	L	3268[A]	LYS
3	L	3268[B]	LYS
3	L	3271[A]	VAL
3	L	3271[B]	VAL
3	L	3272[A]	HIS
3	L	3272[B]	HIS
3	L	3274[A]	ARG
3	L	3274[B]	ARG
3	L	3276[A]	ASP
3	L	3276[B]	ASP
3	L	3278[A]	HIS
3	L	3278[B]	HIS
3	L	3279[A]	ASP
3	L	3279[B]	ASP
3	L	3283[A]	ILE
3	L	3283[B]	ILE
3	L	3286[A]	THR
3	L	3286[B]	THR

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Mol	Chain	Res	Type
3	L	3287[A]	ILE
3	L	3287[B]	ILE
3	L	3288[A]	MET
3	L	3288[B]	MET
3	L	3290[A]	ILE
3	L	3290[B]	ILE
3	L	3293[A]	LYS
3	L	3293[B]	LYS
3	L	3297[A]	PRO
3	L	3297[B]	PRO
3	L	3299[A]	LEU
3	L	3299[B]	LEU
3	L	3302[A]	SER
3	L	3302[B]	SER
3	L	3304[A]	THR
3	L	3304[B]	THR
3	L	3306[A]	LEU
3	L	3306[B]	LEU
3	L	3308[A]	LYS
3	L	3308[B]	LYS
1	M	4	ARG
1	M	19	GLN
1	M	26	GLN
1	M	51	ASP
1	M	67	MET
1	M	70	ARG
1	M	89	ILE
1	M	100	GLN
1	M	104	LEU
1	M	109	LEU
1	M	114	THR
1	M	116	LYS
1	M	128	ILE
1	M	130	PHE
1	M	133	LYS
1	M	139	VAL
1	M	160	LEU
1	M	163	LEU
1	M	167	ASP
1	M	174	GLN
1	M	179	HIS
1	M	185	LEU

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Mol	Chain	Res	Type
1	M	205	LEU
1	M	227	ARG
1	M	235	CYS
1	M	238	ASN
1	M	245	GLU
1	M	249	ARG
1	M	266	LEU
1	M	281	LEU
1	M	289	LEU
1	M	290	GLU
1	M	308	LEU
1	M	313	THR
1	M	329	ARG
1	M	330	GLN
1	M	336	ASN
1	M	365	THR
1	M	371	LEU
1	M	376	ASN
1	M	386	ILE
1	M	387	ASN
1	M	394	GLN
1	M	395	THR
1	M	407	GLN
1	M	424	PHE
1	M	448	SER
1	M	456	GLN
1	M	474	LEU
1	M	494	VAL
1	M	509	ILE
1	M	511	VAL
1	M	515	ASP
1	M	527	LEU
1	M	539	GLU
1	M	557	VAL
1	M	562	GLN
1	M	563	ILE
1	M	565	GLU
1	M	568	PHE
1	M	570	GLN
1	M	572	SER
1	M	589	GLN
1	M	597	VAL

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Mol	Chain	Res	Type
1	M	601	VAL
1	M	603	HIS
1	M	606	ILE
1	M	618	MET
1	M	633	HIS
1	M	650	GLN
1	M	687	SER
1	M	688	VAL
1	M	695	TYR
1	M	705	THR
1	M	711	LEU
1	M	729	VAL
1	M	744	VAL
1	M	776	VAL
1	M	797	THR
1	M	808	THR
1	M	831	VAL
1	M	834	ASP
1	M	836	GLN
1	M	841	LYS
1	M	867	VAL
1	M	870	TYR
1	M	887	ASP
1	M	891	LYS
1	M	896	HIS
1	M	901	THR
1	M	909	ILE
1	M	913	PHE
1	M	930	ASP
1	M	935	ILE
1	M	938	LEU
1	M	943	LEU
1	M	964	ILE
1	M	965	ASP
1	M	980	TYR
1	M	999	LEU
1	M	1002	GLU
1	M	1013	ILE
1	M	1015	HIS
1	M	1017	HIS
1	M	1075	GLU
1	M	1077	LEU

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Mol	Chain	Res	Type
1	M	1086	LEU
1	M	1098	GLU
1	M	1110	LYS
1	M	1126	ILE
1	M	1139	LYS
1	M	1157	VAL
1	M	1160	PHE
1	M	1164	ASP
1	M	1168	GLN
1	M	1169	LYS
1	M	1174	GLU
1	M	1182	ASN
1	M	1203	MET
1	M	1205	LEU
1	M	1207	TYR
1	M	1210	LYS
1	M	1211	TYR
1	M	1212	HIS
1	M	1213	VAL
1	M	1221	THR
1	M	1229	LYS
1	M	1230	LEU
1	M	1258	ARG
1	M	1260	ARG
1	M	1280	GLN
1	M	1286	ARG
1	M	1307	MET
1	M	1343	VAL
1	M	1357	ARG
1	M	1369	THR
1	M	1430	ILE
1	M	1439	VAL
1	M	1471	LEU
1	M	1473	ARG
1	M	1494	ARG
1	M	1509	THR
1	M	1516	VAL
1	M	1520	GLN
1	M	1537	ILE
1	M	1541	GLU
1	M	1550	ARG
1	M	1559	LEU

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Mol	Chain	Res	Type
1	M	1567	ASP
1	M	1568	VAL
1	M	1580	GLU
1	M	1581	GLU
1	M	1597	THR
1	M	1632	LEU
1	M	1640	ILE
1	M	1642	GLN
1	M	1643	LYS
1	M	1649	THR
1	M	1653	VAL
1	M	1656	ASP
2	N	2089	ARG
2	N	2098	GLN
2	N	2104	ILE
2	N	2131	LEU
2	N	2132	CYS
2	N	2141	HIS
2	N	2145	LEU
2	N	2160	VAL
2	N	2185	THR
2	N	2187	VAL
2	N	2190	LEU
2	N	2191	LEU
2	N	2205	THR
2	N	2211	HIS
2	N	2221	THR
2	N	2222	MET
2	N	2231	LEU
2	N	2241	THR
2	N	2248	ILE
2	N	2260	GLU
2	N	2267	HIS
2	N	2327	GLU
2	N	2333	LEU
2	N	2344	LEU
2	N	2361	LYS
2	N	2432	SER
2	N	2445	MET
2	N	2456	LEU
2	N	2476	LEU
2	N	2479	SER

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Mol	Chain	Res	Type
2	N	2500	ILE
2	N	2505	ILE
2	N	2507	ARG
2	N	2531	GLU
2	N	2552	GLU
2	N	2556	TYR
2	N	2561	HIS
2	N	2571	ARG
2	N	2572	VAL
2	N	2575	LEU
2	N	2579	GLU
2	N	2581	MET
2	N	2595	TRP
2	N	2597	MET
2	N	2616	THR
2	N	2621	GLU
2	N	2625	LEU
2	N	2631	TYR
2	N	2647	LEU
2	N	2649	GLU
2	N	2653	GLU
2	N	2654	SER
2	N	2662	LEU
2	N	2680	HIS
2	N	2723	GLU
2	N	2730	LEU
2	N	2750	ILE
2	N	2752	GLU
2	N	2758	THR
2	N	2760	ARG
2	N	2769	PHE
2	N	2772	LYS
2	N	2780	HIS
2	N	2809	LEU
2	N	2818	ASP
2	N	2826	GLU
2	N	2828	ASP
2	N	2830	GLN
2	N	2848	PHE
2	N	2851	ASN
2	N	2856	ILE
2	N	2868	GLU

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Mol	Chain	Res	Type
2	N	2870	LEU
2	N	2872	GLU
2	N	2873	HIS
2	N	2876	LYS
2	N	2877	ILE
2	N	2882	GLU
2	N	2886	VAL
2	N	2887	ASP
2	N	2890	VAL
2	N	2891	LEU
2	N	2898	LYS
2	N	2900	SER
2	N	2901	LEU
3	O	2929[A]	SER
3	O	2929[B]	SER
3	O	2930[A]	LEU
3	O	2930[B]	LEU
3	O	2931[A]	THR
3	O	2931[B]	THR
3	O	2933[A]	SER
3	O	2933[B]	SER
3	O	2935[A]	ILE
3	O	2935[B]	ILE
3	O	2938[A]	LEU
3	O	2938[B]	LEU
3	O	2942[A]	LEU
3	O	2942[B]	LEU
3	O	2946[A]	GLN
3	O	2946[B]	GLN
3	O	2949[A]	LYS
3	O	2949[B]	LYS
3	O	2954[A]	TYR
3	O	2954[B]	TYR
3	O	2956[A]	LYS
3	O	2956[B]	LYS
3	O	2959[A]	SER
3	O	2959[B]	SER
3	O	2960[A]	PHE
3	O	2960[B]	PHE
3	O	2963[A]	MET
3	O	2963[B]	MET
3	O	2965[A]	LEU

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Mol	Chain	Res	Type
3	O	2965[B]	LEU
3	O	2968[A]	GLN
3	O	2968[B]	GLN
3	O	2973[A]	THR
3	O	2973[B]	THR
3	O	2980[A]	HIS
3	O	2980[B]	HIS
3	O	2982[A]	MET
3	O	2982[B]	MET
3	O	2990[A]	ARG
3	O	2990[B]	ARG
3	O	2995[A]	GLN
3	O	2995[B]	GLN
3	O	2996[A]	MET
3	O	2996[B]	MET
3	O	2997[A]	GLU
3	O	2997[B]	GLU
3	O	3000[A]	LEU
3	O	3000[B]	LEU
3	O	3001[A]	LYS
3	O	3001[B]	LYS
3	O	3019[A]	HIS
3	O	3019[B]	HIS
3	O	3021[A]	LEU
3	O	3021[B]	LEU
3	O	3023[A]	ILE
3	O	3023[B]	ILE
3	O	3024[A]	LEU
3	O	3024[B]	LEU
3	O	3026[A]	THR
3	O	3026[B]	THR
3	O	3029[A]	LYS
3	O	3029[B]	LYS
3	O	3040[A]	VAL
3	O	3040[B]	VAL
3	O	3042[A]	ASP
3	O	3042[B]	ASP
3	O	3044[A]	LYS
3	O	3044[B]	LYS
3	O	3048[A]	ASP
3	O	3048[B]	ASP
3	O	3050[A]	ARG

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Mol	Chain	Res	Type
3	O	3050[B]	ARG
3	O	3063[A]	SER
3	O	3063[B]	SER
3	O	3067[A]	ARG
3	O	3067[B]	ARG
3	O	3077[A]	ASP
3	O	3077[B]	ASP
3	O	3081[A]	PHE
3	O	3081[B]	PHE
3	O	3096[A]	VAL
3	O	3096[B]	VAL
3	O	3105[A]	SER
3	O	3105[B]	SER
3	O	3107[A]	LEU
3	O	3107[B]	LEU
3	O	3110[A]	THR
3	O	3110[B]	THR
3	O	3111[A]	SER
3	O	3111[B]	SER
3	O	3115[A]	LEU
3	O	3115[B]	LEU
3	O	3123[A]	THR
3	O	3123[B]	THR
3	O	3131[A]	GLN
3	O	3131[B]	GLN
3	O	3133[A]	LEU
3	O	3133[B]	LEU
3	O	3134[A]	GLN
3	O	3134[B]	GLN
3	O	3135[A]	LYS
3	O	3135[B]	LYS
3	O	3139[A]	LEU
3	O	3139[B]	LEU
3	O	3141[A]	TYR
3	O	3141[B]	TYR
3	O	3147[A]	GLU
3	O	3147[B]	GLU
3	O	3151[A]	LEU
3	O	3151[B]	LEU
3	O	3156[A]	MET
3	O	3156[B]	MET
3	O	3159[A]	SER

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Mol	Chain	Res	Type
3	O	3159[B]	SER
3	O	3160[A]	SER
3	O	3160[B]	SER
3	O	3161[A]	GLU
3	O	3161[B]	GLU
3	O	3162[A]	ASP
3	O	3162[B]	ASP
3	O	3163[A]	ASN
3	O	3163[B]	ASN
3	O	3169[A]	LYS
3	O	3169[B]	LYS
3	O	3172[A]	SER
3	O	3172[B]	SER
3	O	3176[A]	LYS
3	O	3176[B]	LYS
3	O	3181[A]	GLN
3	O	3181[B]	GLN
3	O	3182[A]	GLN
3	O	3182[B]	GLN
3	O	3183[A]	LEU
3	O	3183[B]	LEU
3	O	3185[A]	TYR
3	O	3185[B]	TYR
3	O	3186[A]	GLU
3	O	3186[B]	GLU
3	O	3188[A]	ASP
3	O	3188[B]	ASP
3	O	3191[A]	ASN
3	O	3191[B]	ASN
3	O	3192[A]	PHE
3	O	3192[B]	PHE
3	O	3193[A]	HIS
3	O	3193[B]	HIS
3	O	3195[A]	MET
3	O	3195[B]	MET
3	O	3196[A]	THR
3	O	3196[B]	THR
3	O	3200[A]	LEU
3	O	3200[B]	LEU
3	O	3201[A]	GLU
3	O	3201[B]	GLU
3	O	3204[A]	LEU

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Mol	Chain	Res	Type
3	O	3204[B]	LEU
3	O	3205[A]	LYS
3	O	3205[B]	LYS
3	O	3210[A]	LYS
3	O	3210[B]	LYS
3	O	3211[A]	ASP
3	O	3211[B]	ASP
3	O	3212[A]	ARG
3	O	3212[B]	ARG
3	O	3218[A]	LEU
3	O	3218[B]	LEU
3	O	3220[A]	ARG
3	O	3220[B]	ARG
3	O	3222[A]	ILE
3	O	3222[B]	ILE
3	O	3224[A]	GLN
3	O	3224[B]	GLN
3	O	3225[A]	SER
3	O	3225[B]	SER
3	O	3230[A]	PHE
3	O	3230[B]	PHE
3	O	3244[A]	THR
3	O	3244[B]	THR
3	O	3251[A]	ASP
3	O	3251[B]	ASP
3	O	3254[A]	MET
3	O	3254[B]	MET
3	O	3260[A]	ARG
3	O	3260[B]	ARG
3	O	3267[A]	SER
3	O	3267[B]	SER
3	O	3268[A]	LYS
3	O	3268[B]	LYS
3	O	3271[A]	VAL
3	O	3271[B]	VAL
3	O	3272[A]	HIS
3	O	3272[B]	HIS
3	O	3274[A]	ARG
3	O	3274[B]	ARG
3	O	3276[A]	ASP
3	O	3276[B]	ASP
3	O	3278[A]	HIS

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Mol	Chain	Res	Type
3	O	3278[B]	HIS
3	O	3279[A]	ASP
3	O	3279[B]	ASP
3	O	3283[A]	ILE
3	O	3283[B]	ILE
3	O	3286[A]	THR
3	O	3286[B]	THR
3	O	3287[A]	ILE
3	O	3287[B]	ILE
3	O	3288[A]	MET
3	O	3288[B]	MET
3	O	3290[A]	ILE
3	O	3290[B]	ILE
3	O	3293[A]	LYS
3	O	3293[B]	LYS
3	O	3297[A]	PRO
3	O	3297[B]	PRO
3	O	3299[A]	LEU
3	O	3299[B]	LEU
3	O	3302[A]	SER
3	O	3302[B]	SER
3	O	3304[A]	THR
3	O	3304[B]	THR
3	O	3306[A]	LEU
3	O	3306[B]	LEU
3	O	3308[A]	LYS
3	O	3308[B]	LYS
1	P	2	LEU
1	P	4	ARG
1	P	17	ASN
1	P	19	GLN
1	P	23	ARG
1	P	28	ASP
1	P	37	ILE
1	P	51	ASP
1	P	62	MET
1	P	67	MET
1	P	70	ARG
1	P	83	HIS
1	P	104	LEU
1	P	109	LEU
1	P	114	THR

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Mol	Chain	Res	Type
1	P	116	LYS
1	P	119	LYS
1	P	120	LYS
1	P	133	LYS
1	P	151	GLN
1	P	152	LYS
1	P	160	LEU
1	P	179	HIS
1	P	185	LEU
1	P	205	LEU
1	P	214	GLU
1	P	223	LEU
1	P	239	LEU
1	P	249	ARG
1	P	266	LEU
1	P	281	LEU
1	P	289	LEU
1	P	308	LEU
1	P	325	THR
1	P	329	ARG
1	P	336	ASN
1	P	365	THR
1	P	371	LEU
1	P	376	ASN
1	P	386	ILE
1	P	407	GLN
1	P	411	ASP
1	P	418	ASP
1	P	420	SER
1	P	423	ARG
1	P	424	PHE
1	P	448	SER
1	P	449	ASP
1	P	450	LYS
1	P	452	ILE
1	P	464	LEU
1	P	474	LEU
1	P	494	VAL
1	P	499	GLU
1	P	504	THR
1	P	515	ASP
1	P	516	TRP

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Mol	Chain	Res	Type
1	P	527	LEU
1	P	547	LYS
1	P	551	GLU
1	P	557	VAL
1	P	558	HIS
1	P	560	SER
1	P	562	GLN
1	P	565	GLU
1	P	568	PHE
1	P	575	ASP
1	P	576	HIS
1	P	579	LEU
1	P	583	LEU
1	P	584	SER
1	P	589	GLN
1	P	603	HIS
1	P	609	TRP
1	P	624	THR
1	P	633	HIS
1	P	674	LYS
1	P	692	VAL
1	P	729	VAL
1	P	734	LEU
1	P	736	MET
1	P	744	VAL
1	P	749	VAL
1	P	762	VAL
1	P	775	ARG
1	P	776	VAL
1	P	781	ILE
1	P	788	LEU
1	P	797	THR
1	P	810	LEU
1	P	832	LYS
1	P	834	ASP
1	P	841	LYS
1	P	847	THR
1	P	870	TYR
1	P	873	VAL
1	P	877	HIS
1	P	881	GLN
1	P	885	SER

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Mol	Chain	Res	Type
1	P	901	THR
1	P	909	ILE
1	P	917	LEU
1	P	930	ASP
1	P	935	ILE
1	P	955	LYS
1	P	961	SER
1	P	965	ASP
1	P	979	LEU
1	P	980	TYR
1	P	984	ASP
1	P	987	LYS
1	P	999	LEU
1	P	1001	GLN
1	P	1003	ASP
1	P	1015	HIS
1	P	1017	HIS
1	P	1018	ILE
1	P	1034	GLU
1	P	1067	TYR
1	P	1068	ASN
1	P	1075	GLU
1	P	1078	ARG
1	P	1086	LEU
1	P	1089	ASP
1	P	1093	ASP
1	P	1105	VAL
1	P	1109	LYS
1	P	1118	THR
1	P	1122	ASN
1	P	1125	SER
1	P	1126	ILE
1	P	1131	ARG
1	P	1137	LYS
1	P	1140	ASN
1	P	1153	LYS
1	P	1156	LEU
1	P	1157	VAL
1	P	1160	PHE
1	P	1161	ILE
1	P	1168	GLN
1	P	1174	GLU

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Mol	Chain	Res	Type
1	P	1182	ASN
1	P	1196	ILE
1	P	1200	MET
1	P	1210	LYS
1	P	1213	VAL
1	P	1221	THR
1	P	1225	VAL
1	P	1226	THR
1	P	1230	LEU
1	P	1247	ARG
1	P	1249	TRP
1	P	1250	ILE
1	P	1255	SER
1	P	1258	ARG
1	P	1260	ARG
1	P	1266	PHE
1	P	1286	ARG
1	P	1302	SER
1	P	1304	ASP
1	P	1310	THR
1	P	1313	LEU
1	P	1330	VAL
1	P	1331	GLU
1	P	1357	ARG
1	P	1394	GLN
1	P	1421	VAL
1	P	1427	HIS
1	P	1430	ILE
1	P	1439	VAL
1	P	1441	SER
1	P	1461	VAL
1	P	1484	CYS
1	P	1494	ARG
1	P	1516	VAL
1	P	1541	GLU
1	P	1543	ILE
1	P	1551	ASP
1	P	1559	LEU
1	P	1568	VAL
1	P	1581	GLU
1	P	1622	GLN
1	P	1643	LYS

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Mol	Chain	Res	Type
1	P	1644	ILE
2	Q	2089	ARG
2	Q	2104	ILE
2	Q	2131	LEU
2	Q	2132	CYS
2	Q	2145	LEU
2	Q	2160	VAL
2	Q	2185	THR
2	Q	2187	VAL
2	Q	2191	LEU
2	Q	2205	THR
2	Q	2211	HIS
2	Q	2220	GLU
2	Q	2222	MET
2	Q	2227	VAL
2	Q	2234	GLN
2	Q	2241	THR
2	Q	2260	GLU
2	Q	2267	HIS
2	Q	2270	ILE
2	Q	2274	LEU
2	Q	2326	ILE
2	Q	2327	GLU
2	Q	2333	LEU
2	Q	2361	LYS
2	Q	2441	ARG
2	Q	2445	MET
2	Q	2448	THR
2	Q	2450	ILE
2	Q	2466	THR
2	Q	2474	THR
2	Q	2497	GLU
2	Q	2500	ILE
2	Q	2502	LEU
2	Q	2547	MET
2	Q	2548	CYS
2	Q	2555	GLU
2	Q	2556	TYR
2	Q	2561	HIS
2	Q	2571	ARG
2	Q	2572	VAL
2	Q	2575	LEU

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Mol	Chain	Res	Type
2	Q	2579	GLU
2	Q	2581	MET
2	Q	2593	TRP
2	Q	2595	TRP
2	Q	2597	MET
2	Q	2600	ASP
2	Q	2630	LYS
2	Q	2631	TYR
2	Q	2643	GLU
2	Q	2651	GLN
2	Q	2662	LEU
2	Q	2699	MET
2	Q	2750	ILE
2	Q	2758	THR
2	Q	2768	LEU
2	Q	2769	PHE
2	Q	2772	LYS
2	Q	2781	LEU
2	Q	2788	ILE
2	Q	2802	ASP
2	Q	2814	LYS
2	Q	2816	SER
2	Q	2823	ILE
2	Q	2829	CYS
2	Q	2847	HIS
2	Q	2848	PHE
2	Q	2851	ASN
2	Q	2863	ARG
2	Q	2868	GLU
2	Q	2877	ILE
2	Q	2878	ARG
2	Q	2879	LEU
2	Q	2880	GLU
2	Q	2882	GLU
2	Q	2883	ILE
2	Q	2891	LEU
2	Q	2895	SER
2	Q	2898	LYS
2	Q	2900	SER
2	Q	2907	LYS
3	R	2929[A]	SER
3	R	2929[B]	SER

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Mol	Chain	Res	Type
3	R	2930[A]	LEU
3	R	2930[B]	LEU
3	R	2931[A]	THR
3	R	2931[B]	THR
3	R	2933[A]	SER
3	R	2933[B]	SER
3	R	2935[A]	ILE
3	R	2935[B]	ILE
3	R	2938[A]	LEU
3	R	2938[B]	LEU
3	R	2942[A]	LEU
3	R	2942[B]	LEU
3	R	2946[A]	GLN
3	R	2946[B]	GLN
3	R	2949[A]	LYS
3	R	2949[B]	LYS
3	R	2954[A]	TYR
3	R	2954[B]	TYR
3	R	2956[A]	LYS
3	R	2956[B]	LYS
3	R	2959[A]	SER
3	R	2959[B]	SER
3	R	2960[A]	PHE
3	R	2960[B]	PHE
3	R	2963[A]	MET
3	R	2963[B]	MET
3	R	2965[A]	LEU
3	R	2965[B]	LEU
3	R	2968[A]	GLN
3	R	2968[B]	GLN
3	R	2973[A]	THR
3	R	2973[B]	THR
3	R	2980[A]	HIS
3	R	2980[B]	HIS
3	R	2982[A]	MET
3	R	2982[B]	MET
3	R	2990[A]	ARG
3	R	2990[B]	ARG
3	R	2995[A]	GLN
3	R	2995[B]	GLN
3	R	2996[A]	MET
3	R	2996[B]	MET

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Mol	Chain	Res	Type
3	R	2997[A]	GLU
3	R	2997[B]	GLU
3	R	3000[A]	LEU
3	R	3000[B]	LEU
3	R	3001[A]	LYS
3	R	3001[B]	LYS
3	R	3019[A]	HIS
3	R	3019[B]	HIS
3	R	3021[A]	LEU
3	R	3021[B]	LEU
3	R	3023[A]	ILE
3	R	3023[B]	ILE
3	R	3024[A]	LEU
3	R	3024[B]	LEU
3	R	3026[A]	THR
3	R	3026[B]	THR
3	R	3029[A]	LYS
3	R	3029[B]	LYS
3	R	3040[A]	VAL
3	R	3040[B]	VAL
3	R	3042[A]	ASP
3	R	3042[B]	ASP
3	R	3044[A]	LYS
3	R	3044[B]	LYS
3	R	3048[A]	ASP
3	R	3048[B]	ASP
3	R	3050[A]	ARG
3	R	3050[B]	ARG
3	R	3063[A]	SER
3	R	3063[B]	SER
3	R	3067[A]	ARG
3	R	3067[B]	ARG
3	R	3077[A]	ASP
3	R	3077[B]	ASP
3	R	3081[A]	PHE
3	R	3081[B]	PHE
3	R	3096[A]	VAL
3	R	3096[B]	VAL
3	R	3105[A]	SER
3	R	3105[B]	SER
3	R	3107[A]	LEU
3	R	3107[B]	LEU

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Mol	Chain	Res	Type
3	R	3110[A]	THR
3	R	3110[B]	THR
3	R	3111[A]	SER
3	R	3111[B]	SER
3	R	3115[A]	LEU
3	R	3115[B]	LEU
3	R	3123[A]	THR
3	R	3123[B]	THR
3	R	3131[A]	GLN
3	R	3131[B]	GLN
3	R	3133[A]	LEU
3	R	3133[B]	LEU
3	R	3134[A]	GLN
3	R	3134[B]	GLN
3	R	3135[A]	LYS
3	R	3135[B]	LYS
3	R	3139[A]	LEU
3	R	3139[B]	LEU
3	R	3141[A]	TYR
3	R	3141[B]	TYR
3	R	3147[A]	GLU
3	R	3147[B]	GLU
3	R	3151[A]	LEU
3	R	3151[B]	LEU
3	R	3156[A]	MET
3	R	3156[B]	MET
3	R	3159[A]	SER
3	R	3159[B]	SER
3	R	3160[A]	SER
3	R	3160[B]	SER
3	R	3161[A]	GLU
3	R	3161[B]	GLU
3	R	3162[A]	ASP
3	R	3162[B]	ASP
3	R	3163[A]	ASN
3	R	3163[B]	ASN
3	R	3169[A]	LYS
3	R	3169[B]	LYS
3	R	3172[A]	SER
3	R	3172[B]	SER
3	R	3176[A]	LYS
3	R	3176[B]	LYS

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Mol	Chain	Res	Type
3	R	3181[A]	GLN
3	R	3181[B]	GLN
3	R	3182[A]	GLN
3	R	3182[B]	GLN
3	R	3183[A]	LEU
3	R	3183[B]	LEU
3	R	3185[A]	TYR
3	R	3185[B]	TYR
3	R	3186[A]	GLU
3	R	3186[B]	GLU
3	R	3188[A]	ASP
3	R	3188[B]	ASP
3	R	3191[A]	ASN
3	R	3191[B]	ASN
3	R	3192[A]	PHE
3	R	3192[B]	PHE
3	R	3193[A]	HIS
3	R	3193[B]	HIS
3	R	3195[A]	MET
3	R	3195[B]	MET
3	R	3196[A]	THR
3	R	3196[B]	THR
3	R	3200[A]	LEU
3	R	3200[B]	LEU
3	R	3201[A]	GLU
3	R	3201[B]	GLU
3	R	3204[A]	LEU
3	R	3204[B]	LEU
3	R	3205[A]	LYS
3	R	3205[B]	LYS
3	R	3210[A]	LYS
3	R	3210[B]	LYS
3	R	3211[A]	ASP
3	R	3211[B]	ASP
3	R	3212[A]	ARG
3	R	3212[B]	ARG
3	R	3218[A]	LEU
3	R	3218[B]	LEU
3	R	3220[A]	ARG
3	R	3220[B]	ARG
3	R	3222[A]	ILE
3	R	3222[B]	ILE

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Mol	Chain	Res	Type
3	R	3224[A]	GLN
3	R	3224[B]	GLN
3	R	3225[A]	SER
3	R	3225[B]	SER
3	R	3230[A]	PHE
3	R	3230[B]	PHE
3	R	3244[A]	THR
3	R	3244[B]	THR
3	R	3251[A]	ASP
3	R	3251[B]	ASP
3	R	3254[A]	MET
3	R	3254[B]	MET
3	R	3260[A]	ARG
3	R	3260[B]	ARG
3	R	3267[A]	SER
3	R	3267[B]	SER
3	R	3268[A]	LYS
3	R	3268[B]	LYS
3	R	3271[A]	VAL
3	R	3271[B]	VAL
3	R	3272[A]	HIS
3	R	3272[B]	HIS
3	R	3274[A]	ARG
3	R	3274[B]	ARG
3	R	3276[A]	ASP
3	R	3276[B]	ASP
3	R	3278[A]	HIS
3	R	3278[B]	HIS
3	R	3279[A]	ASP
3	R	3279[B]	ASP
3	R	3283[A]	ILE
3	R	3283[B]	ILE
3	R	3286[A]	THR
3	R	3286[B]	THR
3	R	3287[A]	ILE
3	R	3287[B]	ILE
3	R	3288[A]	MET
3	R	3288[B]	MET
3	R	3290[A]	ILE
3	R	3290[B]	ILE
3	R	3293[A]	LYS
3	R	3293[B]	LYS

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Mol	Chain	Res	Type
3	R	3297[A]	PRO
3	R	3297[B]	PRO
3	R	3299[A]	LEU
3	R	3299[B]	LEU
3	R	3302[A]	SER
3	R	3302[B]	SER
3	R	3304[A]	THR
3	R	3304[B]	THR
3	R	3306[A]	LEU
3	R	3306[B]	LEU
3	R	3308[A]	LYS
3	R	3308[B]	LYS
1	S	2	LEU
1	S	37	ILE
1	S	62	MET
1	S	67	MET
1	S	70	ARG
1	S	83	HIS
1	S	89	ILE
1	S	111	ILE
1	S	116	LYS
1	S	117	LYS
1	S	119	LYS
1	S	148	GLN
1	S	149	GLU
1	S	152	LYS
1	S	179	HIS
1	S	185	LEU
1	S	205	LEU
1	S	214	GLU
1	S	226	HIS
1	S	227	ARG
1	S	238	ASN
1	S	239	LEU
1	S	249	ARG
1	S	266	LEU
1	S	281	LEU
1	S	289	LEU
1	S	296	ARG
1	S	308	LEU
1	S	326	GLU
1	S	327	ASP

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Mol	Chain	Res	Type
1	S	329	ARG
1	S	331	SER
1	S	332	ASP
1	S	336	ASN
1	S	386	ILE
1	S	391	MET
1	S	393	THR
1	S	394	GLN
1	S	407	GLN
1	S	415	VAL
1	S	420	SER
1	S	424	PHE
1	S	450	LYS
1	S	456	GLN
1	S	472	ASP
1	S	474	LEU
1	S	486	THR
1	S	494	VAL
1	S	509	ILE
1	S	511	VAL
1	S	525	SER
1	S	527	LEU
1	S	547	LYS
1	S	559	THR
1	S	562	GLN
1	S	564	ASP
1	S	568	PHE
1	S	569	LYS
1	S	570	GLN
1	S	572	SER
1	S	573	LYS
1	S	576	HIS
1	S	579	LEU
1	S	589	GLN
1	S	597	VAL
1	S	603	HIS
1	S	609	TRP
1	S	613	SER
1	S	618	MET
1	S	624	THR
1	S	633	HIS
1	S	688	VAL

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Mol	Chain	Res	Type
1	S	705	THR
1	S	720	VAL
1	S	729	VAL
1	S	738	ILE
1	S	741	SER
1	S	744	VAL
1	S	749	VAL
1	S	754	GLU
1	S	757	VAL
1	S	797	THR
1	S	803	LYS
1	S	806	ASN
1	S	810	LEU
1	S	813	THR
1	S	828	ASP
1	S	831	VAL
1	S	832	LYS
1	S	836	GLN
1	S	838	ARG
1	S	841	LYS
1	S	842	ASN
1	S	865	LYS
1	S	868	THR
1	S	873	VAL
1	S	877	HIS
1	S	880	THR
1	S	881	GLN
1	S	890	GLN
1	S	891	LYS
1	S	896	HIS
1	S	917	LEU
1	S	920	ASN
1	S	930	ASP
1	S	935	ILE
1	S	941	LEU
1	S	943	LEU
1	S	944	GLU
1	S	953	GLU
1	S	955	LYS
1	S	977	GLU
1	S	989	THR
1	S	999	LEU

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Mol	Chain	Res	Type
1	S	1012	GLU
1	S	1015	HIS
1	S	1017	HIS
1	S	1025	THR
1	S	1059	LEU
1	S	1061	LYS
1	S	1075	GLU
1	S	1076	ILE
1	S	1077	LEU
1	S	1078	ARG
1	S	1088	SER
1	S	1089	ASP
1	S	1090	ILE
1	S	1097	ARG
1	S	1120	GLU
1	S	1121	LEU
1	S	1122	ASN
1	S	1126	ILE
1	S	1131	ARG
1	S	1137	LYS
1	S	1145	THR
1	S	1153	LYS
1	S	1155	LEU
1	S	1157	VAL
1	S	1160	PHE
1	S	1161	ILE
1	S	1164	ASP
1	S	1166	THR
1	S	1167	ASP
1	S	1174	GLU
1	S	1181	GLU
1	S	1190	ARG
1	S	1196	ILE
1	S	1200	MET
1	S	1213	VAL
1	S	1217	ILE
1	S	1219	ASP
1	S	1224	GLU
1	S	1225	VAL
1	S	1228	LEU
1	S	1230	LEU
1	S	1242	ASN

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Mol	Chain	Res	Type
1	S	1258	ARG
1	S	1260	ARG
1	S	1284	GLU
1	S	1286	ARG
1	S	1313	LEU
1	S	1325	LEU
1	S	1341	VAL
1	S	1354	GLU
1	S	1370	LEU
1	S	1396	GLU
1	S	1398	PHE
1	S	1408	LEU
1	S	1427	HIS
1	S	1429	THR
1	S	1439	VAL
1	S	1441	SER
1	S	1465	TRP
1	S	1473	ARG
1	S	1484	CYS
1	S	1494	ARG
1	S	1500	THR
1	S	1541	GLU
1	S	1559	LEU
1	S	1568	VAL
1	S	1597	THR
1	S	1620	LEU
1	S	1622	GLN
1	S	1632	LEU
1	S	1641	THR
1	S	1643	LYS
1	S	1644	ILE
1	S	1651	ILE
2	T	2089	ARG
2	T	2117	ASP
2	T	2131	LEU
2	T	2132	CYS
2	T	2145	LEU
2	T	2160	VAL
2	T	2166	LEU
2	T	2168	ARG
2	T	2180	TRP
2	T	2185	THR

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Mol	Chain	Res	Type
2	T	2186	GLU
2	T	2191	LEU
2	T	2215	SER
2	T	2222	MET
2	T	2237	LEU
2	T	2241	THR
2	T	2248	ILE
2	T	2260	GLU
2	T	2267	HIS
2	T	2309	GLN
2	T	2327	GLU
2	T	2333	LEU
2	T	2344	LEU
2	T	2349	THR
2	T	2359	ASN
2	T	2361	LYS
2	T	2370	MET
2	T	2424	SER
2	T	2425	HIS
2	T	2445	MET
2	T	2478	GLU
2	T	2505	ILE
2	T	2507	ARG
2	T	2548	CYS
2	T	2556	TYR
2	T	2558	CYS
2	T	2561	HIS
2	T	2572	VAL
2	T	2575	LEU
2	T	2579	GLU
2	T	2580	SER
2	T	2581	MET
2	T	2595	TRP
2	T	2601	ASN
2	T	2617	ASP
2	T	2625	LEU
2	T	2630	LYS
2	T	2643	GLU
2	T	2652	LYS
2	T	2662	LEU
2	T	2680	HIS
2	T	2739	LEU

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Mol	Chain	Res	Type
2	T	2750	ILE
2	T	2758	THR
2	T	2768	LEU
2	T	2769	PHE
2	T	2772	LYS
2	T	2809	LEU
2	T	2823	ILE
2	T	2825	ILE
2	T	2828	ASP
2	T	2830	GLN
2	T	2831	GLU
2	T	2838	LEU
2	T	2848	PHE
2	T	2851	ASN
2	T	2856	ILE
2	T	2865	ILE
2	T	2872	GLU
2	T	2873	HIS
2	T	2876	LYS
2	T	2878	ARG
2	T	2879	LEU
2	T	2882	GLU
2	T	2890	VAL
2	T	2891	LEU
2	T	2892	ASP
2	T	2901	LEU
3	U	2929[A]	SER
3	U	2929[B]	SER
3	U	2930[A]	LEU
3	U	2930[B]	LEU
3	U	2931[A]	THR
3	U	2931[B]	THR
3	U	2933[A]	SER
3	U	2933[B]	SER
3	U	2935[A]	ILE
3	U	2935[B]	ILE
3	U	2938[A]	LEU
3	U	2938[B]	LEU
3	U	2942[A]	LEU
3	U	2942[B]	LEU
3	U	2946[A]	GLN
3	U	2946[B]	GLN

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Mol	Chain	Res	Type
3	U	2949[A]	LYS
3	U	2949[B]	LYS
3	U	2954[A]	TYR
3	U	2954[B]	TYR
3	U	2956[A]	LYS
3	U	2956[B]	LYS
3	U	2959[A]	SER
3	U	2959[B]	SER
3	U	2960[A]	PHE
3	U	2960[B]	PHE
3	U	2963[A]	MET
3	U	2963[B]	MET
3	U	2965[A]	LEU
3	U	2965[B]	LEU
3	U	2968[A]	GLN
3	U	2968[B]	GLN
3	U	2973[A]	THR
3	U	2973[B]	THR
3	U	2980[A]	HIS
3	U	2980[B]	HIS
3	U	2982[A]	MET
3	U	2982[B]	MET
3	U	2990[A]	ARG
3	U	2990[B]	ARG
3	U	2995[A]	GLN
3	U	2995[B]	GLN
3	U	2996[A]	MET
3	U	2996[B]	MET
3	U	2997[A]	GLU
3	U	2997[B]	GLU
3	U	3000[A]	LEU
3	U	3000[B]	LEU
3	U	3001[A]	LYS
3	U	3001[B]	LYS
3	U	3019[A]	HIS
3	U	3019[B]	HIS
3	U	3021[A]	LEU
3	U	3021[B]	LEU
3	U	3023[A]	ILE
3	U	3023[B]	ILE
3	U	3024[A]	LEU
3	U	3024[B]	LEU

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Mol	Chain	Res	Type
3	U	3026[A]	THR
3	U	3026[B]	THR
3	U	3029[A]	LYS
3	U	3029[B]	LYS
3	U	3040[A]	VAL
3	U	3040[B]	VAL
3	U	3042[A]	ASP
3	U	3042[B]	ASP
3	U	3044[A]	LYS
3	U	3044[B]	LYS
3	U	3048[A]	ASP
3	U	3048[B]	ASP
3	U	3050[A]	ARG
3	U	3050[B]	ARG
3	U	3063[A]	SER
3	U	3063[B]	SER
3	U	3067[A]	ARG
3	U	3067[B]	ARG
3	U	3077[A]	ASP
3	U	3077[B]	ASP
3	U	3081[A]	PHE
3	U	3081[B]	PHE
3	U	3096[A]	VAL
3	U	3096[B]	VAL
3	U	3105[A]	SER
3	U	3105[B]	SER
3	U	3107[A]	LEU
3	U	3107[B]	LEU
3	U	3110[A]	THR
3	U	3110[B]	THR
3	U	3111[A]	SER
3	U	3111[B]	SER
3	U	3115[A]	LEU
3	U	3115[B]	LEU
3	U	3123[A]	THR
3	U	3123[B]	THR
3	U	3131[A]	GLN
3	U	3131[B]	GLN
3	U	3133[A]	LEU
3	U	3133[B]	LEU
3	U	3134[A]	GLN
3	U	3134[B]	GLN

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Mol	Chain	Res	Type
3	U	3135[A]	LYS
3	U	3135[B]	LYS
3	U	3139[A]	LEU
3	U	3139[B]	LEU
3	U	3141[A]	TYR
3	U	3141[B]	TYR
3	U	3147[A]	GLU
3	U	3147[B]	GLU
3	U	3151[A]	LEU
3	U	3151[B]	LEU
3	U	3156[A]	MET
3	U	3156[B]	MET
3	U	3159[A]	SER
3	U	3159[B]	SER
3	U	3160[A]	SER
3	U	3160[B]	SER
3	U	3161[A]	GLU
3	U	3161[B]	GLU
3	U	3162[A]	ASP
3	U	3162[B]	ASP
3	U	3163[A]	ASN
3	U	3163[B]	ASN
3	U	3169[A]	LYS
3	U	3169[B]	LYS
3	U	3172[A]	SER
3	U	3172[B]	SER
3	U	3176[A]	LYS
3	U	3176[B]	LYS
3	U	3181[A]	GLN
3	U	3181[B]	GLN
3	U	3182[A]	GLN
3	U	3182[B]	GLN
3	U	3183[A]	LEU
3	U	3183[B]	LEU
3	U	3185[A]	TYR
3	U	3185[B]	TYR
3	U	3186[A]	GLU
3	U	3186[B]	GLU
3	U	3188[A]	ASP
3	U	3188[B]	ASP
3	U	3191[A]	ASN
3	U	3191[B]	ASN

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Mol	Chain	Res	Type
3	U	3192[A]	PHE
3	U	3192[B]	PHE
3	U	3193[A]	HIS
3	U	3193[B]	HIS
3	U	3195[A]	MET
3	U	3195[B]	MET
3	U	3196[A]	THR
3	U	3196[B]	THR
3	U	3200[A]	LEU
3	U	3200[B]	LEU
3	U	3201[A]	GLU
3	U	3201[B]	GLU
3	U	3204[A]	LEU
3	U	3204[B]	LEU
3	U	3205[A]	LYS
3	U	3205[B]	LYS
3	U	3210[A]	LYS
3	U	3210[B]	LYS
3	U	3211[A]	ASP
3	U	3211[B]	ASP
3	U	3212[A]	ARG
3	U	3212[B]	ARG
3	U	3218[A]	LEU
3	U	3218[B]	LEU
3	U	3220[A]	ARG
3	U	3220[B]	ARG
3	U	3222[A]	ILE
3	U	3222[B]	ILE
3	U	3224[A]	GLN
3	U	3224[B]	GLN
3	U	3225[A]	SER
3	U	3225[B]	SER
3	U	3230[A]	PHE
3	U	3230[B]	PHE
3	U	3244[A]	THR
3	U	3244[B]	THR
3	U	3251[A]	ASP
3	U	3251[B]	ASP
3	U	3254[A]	MET
3	U	3254[B]	MET
3	U	3260[A]	ARG
3	U	3260[B]	ARG

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Mol	Chain	Res	Type
3	U	3267[A]	SER
3	U	3267[B]	SER
3	U	3268[A]	LYS
3	U	3268[B]	LYS
3	U	3271[A]	VAL
3	U	3271[B]	VAL
3	U	3272[A]	HIS
3	U	3272[B]	HIS
3	U	3274[A]	ARG
3	U	3274[B]	ARG
3	U	3276[A]	ASP
3	U	3276[B]	ASP
3	U	3278[A]	HIS
3	U	3278[B]	HIS
3	U	3279[A]	ASP
3	U	3279[B]	ASP
3	U	3283[A]	ILE
3	U	3283[B]	ILE
3	U	3286[A]	THR
3	U	3286[B]	THR
3	U	3287[A]	ILE
3	U	3287[B]	ILE
3	U	3288[A]	MET
3	U	3288[B]	MET
3	U	3290[A]	ILE
3	U	3290[B]	ILE
3	U	3293[A]	LYS
3	U	3293[B]	LYS
3	U	3297[A]	PRO
3	U	3297[B]	PRO
3	U	3299[A]	LEU
3	U	3299[B]	LEU
3	U	3302[A]	SER
3	U	3302[B]	SER
3	U	3304[A]	THR
3	U	3304[B]	THR
3	U	3306[A]	LEU
3	U	3306[B]	LEU
3	U	3308[A]	LYS
3	U	3308[B]	LYS
1	V	4	ARG
1	V	37	ILE

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Mol	Chain	Res	Type
1	V	51	ASP
1	V	64	THR
1	V	67	MET
1	V	70	ARG
1	V	89	ILE
1	V	109	LEU
1	V	111	ILE
1	V	120	LYS
1	V	121	ASN
1	V	132	ASN
1	V	133	LYS
1	V	134	VAL
1	V	149	GLU
1	V	151	GLN
1	V	160	LEU
1	V	163	LEU
1	V	174	GLN
1	V	179	HIS
1	V	185	LEU
1	V	193	SER
1	V	205	LEU
1	V	223	LEU
1	V	235	CYS
1	V	237	LEU
1	V	245	GLU
1	V	249	ARG
1	V	250	ASP
1	V	264	SER
1	V	266	LEU
1	V	282	ASN
1	V	289	LEU
1	V	290	GLU
1	V	293	LEU
1	V	308	LEU
1	V	326	GLU
1	V	336	ASN
1	V	337	ASP
1	V	354	PHE
1	V	365	THR
1	V	386	ILE
1	V	387	ASN
1	V	390	LEU

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Mol	Chain	Res	Type
1	V	391	MET
1	V	393	THR
1	V	395	THR
1	V	407	GLN
1	V	416	ASN
1	V	424	PHE
1	V	434	GLU
1	V	450	LYS
1	V	456	GLN
1	V	464	LEU
1	V	472	ASP
1	V	474	LEU
1	V	494	VAL
1	V	509	ILE
1	V	511	VAL
1	V	518	LYS
1	V	527	LEU
1	V	547	LYS
1	V	560	SER
1	V	564	ASP
1	V	567	LEU
1	V	568	PHE
1	V	570	GLN
1	V	589	GLN
1	V	603	HIS
1	V	625	SER
1	V	650	GLN
1	V	688	VAL
1	V	744	VAL
1	V	749	VAL
1	V	762	VAL
1	V	770	THR
1	V	775	ARG
1	V	776	VAL
1	V	781	ILE
1	V	797	THR
1	V	819	ILE
1	V	830	ASN
1	V	831	VAL
1	V	834	ASP
1	V	841	LYS
1	V	842	ASN

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Mol	Chain	Res	Type
1	V	858	MET
1	V	864	ASP
1	V	865	LYS
1	V	873	VAL
1	V	879	SER
1	V	907	ARG
1	V	909	ILE
1	V	917	LEU
1	V	935	ILE
1	V	941	LEU
1	V	943	LEU
1	V	949	ASP
1	V	951	ASN
1	V	953	GLU
1	V	961	SER
1	V	965	ASP
1	V	979	LEU
1	V	980	TYR
1	V	981	GLU
1	V	984	ASP
1	V	987	LYS
1	V	999	LEU
1	V	1001	GLN
1	V	1002	GLU
1	V	1013	ILE
1	V	1015	HIS
1	V	1017	HIS
1	V	1018	ILE
1	V	1033	LEU
1	V	1041	ILE
1	V	1075	GLU
1	V	1077	LEU
1	V	1078	ARG
1	V	1086	LEU
1	V	1088	SER
1	V	1090	ILE
1	V	1091	ASN
1	V	1118	THR
1	V	1122	ASN
1	V	1126	ILE
1	V	1140	ASN
1	V	1153	LYS

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Mol	Chain	Res	Type
1	V	1157	VAL
1	V	1160	PHE
1	V	1174	GLU
1	V	1181	GLU
1	V	1196	ILE
1	V	1200	MET
1	V	1205	LEU
1	V	1206	HIS
1	V	1207	TYR
1	V	1210	LYS
1	V	1214	GLU
1	V	1215	LEU
1	V	1221	THR
1	V	1226	THR
1	V	1229	LYS
1	V	1230	LEU
1	V	1247	ARG
1	V	1258	ARG
1	V	1260	ARG
1	V	1267	GLU
1	V	1304	ASP
1	V	1309	HIS
1	V	1313	LEU
1	V	1381	LYS
1	V	1394	GLN
1	V	1396	GLU
1	V	1408	LEU
1	V	1415	ASP
1	V	1427	HIS
1	V	1430	ILE
1	V	1433	TRP
1	V	1439	VAL
1	V	1441	SER
1	V	1456	LEU
1	V	1461	VAL
1	V	1484	CYS
1	V	1491	GLN
1	V	1493	MET
1	V	1494	ARG
1	V	1509	THR
1	V	1516	VAL
1	V	1530	LEU

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Mol	Chain	Res	Type
1	V	1541	GLU
1	V	1568	VAL
1	V	1580	GLU
1	V	1620	LEU
1	V	1622	GLN
1	V	1629	GLU
1	V	1632	LEU
1	V	1641	THR
1	V	1643	LYS
1	V	1649	THR
2	W	2089	ARG
2	W	2108	LYS
2	W	2138	LYS
2	W	2143	CYS
2	W	2145	LEU
2	W	2160	VAL
2	W	2184	MET
2	W	2185	THR
2	W	2187	VAL
2	W	2191	LEU
2	W	2205	THR
2	W	2215	SER
2	W	2222	MET
2	W	2237	LEU
2	W	2241	THR
2	W	2260	GLU
2	W	2267	HIS
2	W	2270	ILE
2	W	2274	LEU
2	W	2309	GLN
2	W	2327	GLU
2	W	2328	LEU
2	W	2333	LEU
2	W	2349	THR
2	W	2361	LYS
2	W	2394	VAL
2	W	2403	PHE
2	W	2417	VAL
2	W	2445	MET
2	W	2448	THR
2	W	2480	LEU
2	W	2500	ILE

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Mol	Chain	Res	Type
2	W	2507	ARG
2	W	2533	ASP
2	W	2556	TYR
2	W	2561	HIS
2	W	2572	VAL
2	W	2575	LEU
2	W	2579	GLU
2	W	2581	MET
2	W	2595	TRP
2	W	2597	MET
2	W	2602	LEU
2	W	2617	ASP
2	W	2620	ILE
2	W	2631	TYR
2	W	2644	LEU
2	W	2655	THR
2	W	2680	HIS
2	W	2742	MET
2	W	2746	MET
2	W	2758	THR
2	W	2768	LEU
2	W	2769	PHE
2	W	2772	LYS
2	W	2780	HIS
2	W	2794	LEU
2	W	2800	LYS
2	W	2816	SER
2	W	2825	ILE
2	W	2826	GLU
2	W	2828	ASP
2	W	2830	GLN
2	W	2838	LEU
2	W	2848	PHE
2	W	2851	ASN
2	W	2856	ILE
2	W	2861	LYS
2	W	2865	ILE
2	W	2868	GLU
2	W	2873	HIS
2	W	2876	LYS
2	W	2879	LEU
2	W	2891	LEU

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Mol	Chain	Res	Type
2	W	2895	SER
2	W	2898	LYS
3	X	2929[A]	SER
3	X	2929[B]	SER
3	X	2930[A]	LEU
3	X	2930[B]	LEU
3	X	2931[A]	THR
3	X	2931[B]	THR
3	X	2933[A]	SER
3	X	2933[B]	SER
3	X	2935[A]	ILE
3	X	2935[B]	ILE
3	X	2938[A]	LEU
3	X	2938[B]	LEU
3	X	2942[A]	LEU
3	X	2942[B]	LEU
3	X	2946[A]	GLN
3	X	2946[B]	GLN
3	X	2949[A]	LYS
3	X	2949[B]	LYS
3	X	2954[A]	TYR
3	X	2954[B]	TYR
3	X	2956[A]	LYS
3	X	2956[B]	LYS
3	X	2959[A]	SER
3	X	2959[B]	SER
3	X	2960[A]	PHE
3	X	2960[B]	PHE
3	X	2963[A]	MET
3	X	2963[B]	MET
3	X	2965[A]	LEU
3	X	2965[B]	LEU
3	X	2968[A]	GLN
3	X	2968[B]	GLN
3	X	2973[A]	THR
3	X	2973[B]	THR
3	X	2980[A]	HIS
3	X	2980[B]	HIS
3	X	2982[A]	MET
3	X	2982[B]	MET
3	X	2990[A]	ARG
3	X	2990[B]	ARG

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Mol	Chain	Res	Type
3	X	2995[A]	GLN
3	X	2995[B]	GLN
3	X	2996[A]	MET
3	X	2996[B]	MET
3	X	2997[A]	GLU
3	X	2997[B]	GLU
3	X	3000[A]	LEU
3	X	3000[B]	LEU
3	X	3001[A]	LYS
3	X	3001[B]	LYS
3	X	3019[A]	HIS
3	X	3019[B]	HIS
3	X	3021[A]	LEU
3	X	3021[B]	LEU
3	X	3023[A]	ILE
3	X	3023[B]	ILE
3	X	3024[A]	LEU
3	X	3024[B]	LEU
3	X	3026[A]	THR
3	X	3026[B]	THR
3	X	3029[A]	LYS
3	X	3029[B]	LYS
3	X	3040[A]	VAL
3	X	3040[B]	VAL
3	X	3042[A]	ASP
3	X	3042[B]	ASP
3	X	3044[A]	LYS
3	X	3044[B]	LYS
3	X	3048[A]	ASP
3	X	3048[B]	ASP
3	X	3050[A]	ARG
3	X	3050[B]	ARG
3	X	3063[A]	SER
3	X	3063[B]	SER
3	X	3067[A]	ARG
3	X	3067[B]	ARG
3	X	3077[A]	ASP
3	X	3077[B]	ASP
3	X	3081[A]	PHE
3	X	3081[B]	PHE
3	X	3096[A]	VAL
3	X	3096[B]	VAL

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Mol	Chain	Res	Type
3	X	3105[A]	SER
3	X	3105[B]	SER
3	X	3107[A]	LEU
3	X	3107[B]	LEU
3	X	3110[A]	THR
3	X	3110[B]	THR
3	X	3111[A]	SER
3	X	3111[B]	SER
3	X	3115[A]	LEU
3	X	3115[B]	LEU
3	X	3123[A]	THR
3	X	3123[B]	THR
3	X	3131[A]	GLN
3	X	3131[B]	GLN
3	X	3133[A]	LEU
3	X	3133[B]	LEU
3	X	3134[A]	GLN
3	X	3134[B]	GLN
3	X	3135[A]	LYS
3	X	3135[B]	LYS
3	X	3139[A]	LEU
3	X	3139[B]	LEU
3	X	3141[A]	TYR
3	X	3141[B]	TYR
3	X	3147[A]	GLU
3	X	3147[B]	GLU
3	X	3151[A]	LEU
3	X	3151[B]	LEU
3	X	3156[A]	MET
3	X	3156[B]	MET
3	X	3159[A]	SER
3	X	3159[B]	SER
3	X	3160[A]	SER
3	X	3160[B]	SER
3	X	3161[A]	GLU
3	X	3161[B]	GLU
3	X	3162[A]	ASP
3	X	3162[B]	ASP
3	X	3163[A]	ASN
3	X	3163[B]	ASN
3	X	3169[A]	LYS
3	X	3169[B]	LYS

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Mol	Chain	Res	Type
3	X	3172[A]	SER
3	X	3172[B]	SER
3	X	3176[A]	LYS
3	X	3176[B]	LYS
3	X	3181[A]	GLN
3	X	3181[B]	GLN
3	X	3182[A]	GLN
3	X	3182[B]	GLN
3	X	3183[A]	LEU
3	X	3183[B]	LEU
3	X	3185[A]	TYR
3	X	3185[B]	TYR
3	X	3186[A]	GLU
3	X	3186[B]	GLU
3	X	3188[A]	ASP
3	X	3188[B]	ASP
3	X	3191[A]	ASN
3	X	3191[B]	ASN
3	X	3192[A]	PHE
3	X	3192[B]	PHE
3	X	3193[A]	HIS
3	X	3193[B]	HIS
3	X	3195[A]	MET
3	X	3195[B]	MET
3	X	3196[A]	THR
3	X	3196[B]	THR
3	X	3200[A]	LEU
3	X	3200[B]	LEU
3	X	3201[A]	GLU
3	X	3201[B]	GLU
3	X	3204[A]	LEU
3	X	3204[B]	LEU
3	X	3205[A]	LYS
3	X	3205[B]	LYS
3	X	3210[A]	LYS
3	X	3210[B]	LYS
3	X	3211[A]	ASP
3	X	3211[B]	ASP
3	X	3212[A]	ARG
3	X	3212[B]	ARG
3	X	3218[A]	LEU
3	X	3218[B]	LEU

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Mol	Chain	Res	Type
3	X	3220[A]	ARG
3	X	3220[B]	ARG
3	X	3222[A]	ILE
3	X	3222[B]	ILE
3	X	3224[A]	GLN
3	X	3224[B]	GLN
3	X	3225[A]	SER
3	X	3225[B]	SER
3	X	3230[A]	PHE
3	X	3230[B]	PHE
3	X	3244[A]	THR
3	X	3244[B]	THR
3	X	3251[A]	ASP
3	X	3251[B]	ASP
3	X	3254[A]	MET
3	X	3254[B]	MET
3	X	3260[A]	ARG
3	X	3260[B]	ARG
3	X	3267[A]	SER
3	X	3267[B]	SER
3	X	3268[A]	LYS
3	X	3268[B]	LYS
3	X	3271[A]	VAL
3	X	3271[B]	VAL
3	X	3272[A]	HIS
3	X	3272[B]	HIS
3	X	3274[A]	ARG
3	X	3274[B]	ARG
3	X	3276[A]	ASP
3	X	3276[B]	ASP
3	X	3278[A]	HIS
3	X	3278[B]	HIS
3	X	3279[A]	ASP
3	X	3279[B]	ASP
3	X	3283[A]	ILE
3	X	3283[B]	ILE
3	X	3286[A]	THR
3	X	3286[B]	THR
3	X	3287[A]	ILE
3	X	3287[B]	ILE
3	X	3288[A]	MET
3	X	3288[B]	MET

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Mol	Chain	Res	Type
3	X	3290[A]	ILE
3	X	3290[B]	ILE
3	X	3293[A]	LYS
3	X	3293[B]	LYS
3	X	3297[A]	PRO
3	X	3297[B]	PRO
3	X	3299[A]	LEU
3	X	3299[B]	LEU
3	X	3302[A]	SER
3	X	3302[B]	SER
3	X	3304[A]	THR
3	X	3304[B]	THR
3	X	3306[A]	LEU
3	X	3306[B]	LEU
3	X	3308[A]	LYS
3	X	3308[B]	LYS
1	Y	2	LEU
1	Y	4	ARG
1	Y	19	GLN
1	Y	57	CYS
1	Y	62	MET
1	Y	67	MET
1	Y	70	ARG
1	Y	86	THR
1	Y	104	LEU
1	Y	109	LEU
1	Y	116	LYS
1	Y	117	LYS
1	Y	119	LYS
1	Y	133	LYS
1	Y	140	ASP
1	Y	152	LYS
1	Y	163	LEU
1	Y	167	ASP
1	Y	179	HIS
1	Y	182	ILE
1	Y	185	LEU
1	Y	193	SER
1	Y	194	MET
1	Y	205	LEU
1	Y	214	GLU
1	Y	221	GLN

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Mol	Chain	Res	Type
1	Y	226	HIS
1	Y	235	CYS
1	Y	238	ASN
1	Y	239	LEU
1	Y	249	ARG
1	Y	264	SER
1	Y	265	SER
1	Y	266	LEU
1	Y	281	LEU
1	Y	285	THR
1	Y	289	LEU
1	Y	308	LEU
1	Y	325	THR
1	Y	329	ARG
1	Y	330	GLN
1	Y	336	ASN
1	Y	350	MET
1	Y	365	THR
1	Y	371	LEU
1	Y	386	ILE
1	Y	387	ASN
1	Y	391	MET
1	Y	407	GLN
1	Y	411	ASP
1	Y	413	ASN
1	Y	415	VAL
1	Y	418	ASP
1	Y	424	PHE
1	Y	444	GLU
1	Y	448	SER
1	Y	450	LYS
1	Y	467	LYS
1	Y	476	ARG
1	Y	499	GLU
1	Y	509	ILE
1	Y	515	ASP
1	Y	527	LEU
1	Y	557	VAL
1	Y	560	SER
1	Y	565	GLU
1	Y	567	LEU
1	Y	569	LYS

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Mol	Chain	Res	Type
1	Y	570	GLN
1	Y	575	ASP
1	Y	578	PHE
1	Y	597	VAL
1	Y	603	HIS
1	Y	609	TRP
1	Y	610	THR
1	Y	619	SER
1	Y	624	THR
1	Y	633	HIS
1	Y	692	VAL
1	Y	696	GLN
1	Y	714	ARG
1	Y	720	VAL
1	Y	722	GLU
1	Y	729	VAL
1	Y	736	MET
1	Y	738	ILE
1	Y	739	GLN
1	Y	744	VAL
1	Y	749	VAL
1	Y	788	LEU
1	Y	797	THR
1	Y	805	VAL
1	Y	806	ASN
1	Y	819	ILE
1	Y	826	ILE
1	Y	832	LYS
1	Y	836	GLN
1	Y	865	LYS
1	Y	866	GLU
1	Y	896	HIS
1	Y	901	THR
1	Y	909	ILE
1	Y	912	ASN
1	Y	917	LEU
1	Y	930	ASP
1	Y	935	ILE
1	Y	948	THR
1	Y	965	ASP
1	Y	967	ILE
1	Y	973	ARG

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Mol	Chain	Res	Type
1	Y	979	LEU
1	Y	981	GLU
1	Y	987	LYS
1	Y	989	THR
1	Y	991	LEU
1	Y	995	ILE
1	Y	999	LEU
1	Y	1001	GLN
1	Y	1015	HIS
1	Y	1017	HIS
1	Y	1025	THR
1	Y	1030	MET
1	Y	1033	LEU
1	Y	1041	ILE
1	Y	1075	GLU
1	Y	1077	LEU
1	Y	1086	LEU
1	Y	1090	ILE
1	Y	1093	ASP
1	Y	1097	ARG
1	Y	1105	VAL
1	Y	1118	THR
1	Y	1121	LEU
1	Y	1122	ASN
1	Y	1142	VAL
1	Y	1145	THR
1	Y	1154	SER
1	Y	1157	VAL
1	Y	1160	PHE
1	Y	1161	ILE
1	Y	1164	ASP
1	Y	1168	GLN
1	Y	1170	MET
1	Y	1200	MET
1	Y	1213	VAL
1	Y	1228	LEU
1	Y	1230	LEU
1	Y	1231	VAL
1	Y	1232	THR
1	Y	1245	GLU
1	Y	1247	ARG
1	Y	1258	ARG

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Mol	Chain	Res	Type
1	Y	1260	ARG
1	Y	1286	ARG
1	Y	1304	ASP
1	Y	1307	MET
1	Y	1331	GLU
1	Y	1341	VAL
1	Y	1354	GLU
1	Y	1369	THR
1	Y	1372	ILE
1	Y	1381	LYS
1	Y	1396	GLU
1	Y	1401	ARG
1	Y	1421	VAL
1	Y	1427	HIS
1	Y	1430	ILE
1	Y	1471	LEU
1	Y	1488	LEU
1	Y	1494	ARG
1	Y	1506	LEU
1	Y	1516	VAL
1	Y	1541	GLU
1	Y	1543	ILE
1	Y	1559	LEU
1	Y	1568	VAL
1	Y	1578	ILE
1	Y	1581	GLU
1	Y	1583	CYS
1	Y	1597	THR
1	Y	1621	ASN
1	Y	1622	GLN
1	Y	1629	GLU
1	Y	1632	LEU
1	Y	1642	GLN
1	Y	1656	ASP
2	Z	2089	ARG
2	Z	2104	ILE
2	Z	2108	LYS
2	Z	2117	ASP
2	Z	2131	LEU
2	Z	2132	CYS
2	Z	2134	ASN
2	Z	2143	CYS

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Mol	Chain	Res	Type
2	Z	2145	LEU
2	Z	2160	VAL
2	Z	2168	ARG
2	Z	2180	TRP
2	Z	2184	MET
2	Z	2187	VAL
2	Z	2190	LEU
2	Z	2191	LEU
2	Z	2205	THR
2	Z	2221	THR
2	Z	2227	VAL
2	Z	2233	GLU
2	Z	2237	LEU
2	Z	2241	THR
2	Z	2249	LEU
2	Z	2260	GLU
2	Z	2267	HIS
2	Z	2270	ILE
2	Z	2282	LEU
2	Z	2309	GLN
2	Z	2327	GLU
2	Z	2333	LEU
2	Z	2345	ASN
2	Z	2359	ASN
2	Z	2361	LYS
2	Z	2373	MET
2	Z	2381	LEU
2	Z	2394	VAL
2	Z	2425	HIS
2	Z	2441	ARG
2	Z	2445	MET
2	Z	2457	LYS
2	Z	2460	SER
2	Z	2469	VAL
2	Z	2495	ASN
2	Z	2502	LEU
2	Z	2507	ARG
2	Z	2548	CYS
2	Z	2556	TYR
2	Z	2558	CYS
2	Z	2560	LEU
2	Z	2561	HIS

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Mol	Chain	Res	Type
2	Z	2565	THR
2	Z	2572	VAL
2	Z	2579	GLU
2	Z	2595	TRP
2	Z	2600	ASP
2	Z	2608	ASP
2	Z	2620	ILE
2	Z	2630	LYS
2	Z	2637	VAL
2	Z	2643	GLU
2	Z	2647	LEU
2	Z	2653	GLU
2	Z	2662	LEU
2	Z	2674	VAL
2	Z	2680	HIS
2	Z	2758	THR
2	Z	2768	LEU
2	Z	2769	PHE
2	Z	2772	LYS
2	Z	2780	HIS
2	Z	2781	LEU
2	Z	2809	LEU
2	Z	2813	ILE
2	Z	2825	ILE
2	Z	2828	ASP
2	Z	2835	ILE
2	Z	2838	LEU
2	Z	2848	PHE
2	Z	2850	ARG
2	Z	2851	ASN
2	Z	2856	ILE
2	Z	2863	ARG
2	Z	2868	GLU
2	Z	2870	LEU
2	Z	2873	HIS
2	Z	2876	LYS
2	Z	2878	ARG
2	Z	2884	LYS
2	Z	2891	LEU
2	Z	2895	SER
2	Z	2898	LYS
2	Z	2900	SER

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Mol	Chain	Res	Type
3	a	2929[A]	SER
3	a	2929[B]	SER
3	a	2930[A]	LEU
3	a	2930[B]	LEU
3	a	2931[A]	THR
3	a	2931[B]	THR
3	a	2933[A]	SER
3	a	2933[B]	SER
3	a	2935[A]	ILE
3	a	2935[B]	ILE
3	a	2938[A]	LEU
3	a	2938[B]	LEU
3	a	2942[A]	LEU
3	a	2942[B]	LEU
3	a	2946[A]	GLN
3	a	2946[B]	GLN
3	a	2949[A]	LYS
3	a	2949[B]	LYS
3	a	2954[A]	TYR
3	a	2954[B]	TYR
3	a	2956[A]	LYS
3	a	2956[B]	LYS
3	a	2959[A]	SER
3	a	2959[B]	SER
3	a	2960[A]	PHE
3	a	2960[B]	PHE
3	a	2963[A]	MET
3	a	2963[B]	MET
3	a	2965[A]	LEU
3	a	2965[B]	LEU
3	a	2968[A]	GLN
3	a	2968[B]	GLN
3	a	2973[A]	THR
3	a	2973[B]	THR
3	a	2980[A]	HIS
3	a	2980[B]	HIS
3	a	2982[A]	MET
3	a	2982[B]	MET
3	a	2990[A]	ARG
3	a	2990[B]	ARG
3	a	2995[A]	GLN
3	a	2995[B]	GLN

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Mol	Chain	Res	Type
3	a	2996[A]	MET
3	a	2996[B]	MET
3	a	2997[A]	GLU
3	a	2997[B]	GLU
3	a	3000[A]	LEU
3	a	3000[B]	LEU
3	a	3001[A]	LYS
3	a	3001[B]	LYS
3	a	3019[A]	HIS
3	a	3019[B]	HIS
3	a	3021[A]	LEU
3	a	3021[B]	LEU
3	a	3023[A]	ILE
3	a	3023[B]	ILE
3	a	3024[A]	LEU
3	a	3024[B]	LEU
3	a	3026[A]	THR
3	a	3026[B]	THR
3	a	3029[A]	LYS
3	a	3029[B]	LYS
3	a	3040[A]	VAL
3	a	3040[B]	VAL
3	a	3042[A]	ASP
3	a	3042[B]	ASP
3	a	3044[A]	LYS
3	a	3044[B]	LYS
3	a	3048[A]	ASP
3	a	3048[B]	ASP
3	a	3050[A]	ARG
3	a	3050[B]	ARG
3	a	3063[A]	SER
3	a	3063[B]	SER
3	a	3067[A]	ARG
3	a	3067[B]	ARG
3	a	3077[A]	ASP
3	a	3077[B]	ASP
3	a	3081[A]	PHE
3	a	3081[B]	PHE
3	a	3096[A]	VAL
3	a	3096[B]	VAL
3	a	3105[A]	SER
3	a	3105[B]	SER

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Mol	Chain	Res	Type
3	a	3107[A]	LEU
3	a	3107[B]	LEU
3	a	3110[A]	THR
3	a	3110[B]	THR
3	a	3111[A]	SER
3	a	3111[B]	SER
3	a	3115[A]	LEU
3	a	3115[B]	LEU
3	a	3123[A]	THR
3	a	3123[B]	THR
3	a	3131[A]	GLN
3	a	3131[B]	GLN
3	a	3133[A]	LEU
3	a	3133[B]	LEU
3	a	3134[A]	GLN
3	a	3134[B]	GLN
3	a	3135[A]	LYS
3	a	3135[B]	LYS
3	a	3139[A]	LEU
3	a	3139[B]	LEU
3	a	3141[A]	TYR
3	a	3141[B]	TYR
3	a	3147[A]	GLU
3	a	3147[B]	GLU
3	a	3151[A]	LEU
3	a	3151[B]	LEU
3	a	3156[A]	MET
3	a	3156[B]	MET
3	a	3159[A]	SER
3	a	3159[B]	SER
3	a	3160[A]	SER
3	a	3160[B]	SER
3	a	3161[A]	GLU
3	a	3161[B]	GLU
3	a	3162[A]	ASP
3	a	3162[B]	ASP
3	a	3163[A]	ASN
3	a	3163[B]	ASN
3	a	3169[A]	LYS
3	a	3169[B]	LYS
3	a	3172[A]	SER
3	a	3172[B]	SER

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Mol	Chain	Res	Type
3	a	3176[A]	LYS
3	a	3176[B]	LYS
3	a	3181[A]	GLN
3	a	3181[B]	GLN
3	a	3182[A]	GLN
3	a	3182[B]	GLN
3	a	3183[A]	LEU
3	a	3183[B]	LEU
3	a	3185[A]	TYR
3	a	3185[B]	TYR
3	a	3186[A]	GLU
3	a	3186[B]	GLU
3	a	3188[A]	ASP
3	a	3188[B]	ASP
3	a	3191[A]	ASN
3	a	3191[B]	ASN
3	a	3192[A]	PHE
3	a	3192[B]	PHE
3	a	3193[A]	HIS
3	a	3193[B]	HIS
3	a	3195[A]	MET
3	a	3195[B]	MET
3	a	3196[A]	THR
3	a	3196[B]	THR
3	a	3200[A]	LEU
3	a	3200[B]	LEU
3	a	3201[A]	GLU
3	a	3201[B]	GLU
3	a	3204[A]	LEU
3	a	3204[B]	LEU
3	a	3205[A]	LYS
3	a	3205[B]	LYS
3	a	3210[A]	LYS
3	a	3210[B]	LYS
3	a	3211[A]	ASP
3	a	3211[B]	ASP
3	a	3212[A]	ARG
3	a	3212[B]	ARG
3	a	3218[A]	LEU
3	a	3218[B]	LEU
3	a	3220[A]	ARG
3	a	3220[B]	ARG

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Mol	Chain	Res	Type
3	a	3222[A]	ILE
3	a	3222[B]	ILE
3	a	3224[A]	GLN
3	a	3224[B]	GLN
3	a	3225[A]	SER
3	a	3225[B]	SER
3	a	3230[A]	PHE
3	a	3230[B]	PHE
3	a	3244[A]	THR
3	a	3244[B]	THR
3	a	3251[A]	ASP
3	a	3251[B]	ASP
3	a	3254[A]	MET
3	a	3254[B]	MET
3	a	3260[A]	ARG
3	a	3260[B]	ARG
3	a	3267[A]	SER
3	a	3267[B]	SER
3	a	3268[A]	LYS
3	a	3268[B]	LYS
3	a	3271[A]	VAL
3	a	3271[B]	VAL
3	a	3272[A]	HIS
3	a	3272[B]	HIS
3	a	3274[A]	ARG
3	a	3274[B]	ARG
3	a	3276[A]	ASP
3	a	3276[B]	ASP
3	a	3278[A]	HIS
3	a	3278[B]	HIS
3	a	3279[A]	ASP
3	a	3279[B]	ASP
3	a	3283[A]	ILE
3	a	3283[B]	ILE
3	a	3286[A]	THR
3	a	3286[B]	THR
3	a	3287[A]	ILE
3	a	3287[B]	ILE
3	a	3288[A]	MET
3	a	3288[B]	MET
3	a	3290[A]	ILE
3	a	3290[B]	ILE

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Mol	Chain	Res	Type
3	a	3293[A]	LYS
3	a	3293[B]	LYS
3	a	3297[A]	PRO
3	a	3297[B]	PRO
3	a	3299[A]	LEU
3	a	3299[B]	LEU
3	a	3302[A]	SER
3	a	3302[B]	SER
3	a	3304[A]	THR
3	a	3304[B]	THR
3	a	3306[A]	LEU
3	a	3306[B]	LEU
3	a	3308[A]	LYS
3	a	3308[B]	LYS
1	b	2	LEU
1	b	4	ARG
1	b	17	ASN
1	b	19	GLN
1	b	25	MET
1	b	26	GLN
1	b	35	GLN
1	b	53	SER
1	b	55	ILE
1	b	56	VAL
1	b	62	MET
1	b	67	MET
1	b	89	ILE
1	b	119	LYS
1	b	120	LYS
1	b	127	GLU
1	b	128	ILE
1	b	129	LYS
1	b	130	PHE
1	b	148	GLN
1	b	163	LEU
1	b	179	HIS
1	b	185	LEU
1	b	205	LEU
1	b	213	VAL
1	b	214	GLU
1	b	219	LEU
1	b	223	LEU

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Mol	Chain	Res	Type
1	b	235	CYS
1	b	237	LEU
1	b	238	ASN
1	b	239	LEU
1	b	244	MET
1	b	249	ARG
1	b	266	LEU
1	b	279	LEU
1	b	281	LEU
1	b	285	THR
1	b	289	LEU
1	b	308	LEU
1	b	329	ARG
1	b	371	LEU
1	b	376	ASN
1	b	384	THR
1	b	387	ASN
1	b	391	MET
1	b	407	GLN
1	b	411	ASP
1	b	420	SER
1	b	423	ARG
1	b	424	PHE
1	b	448	SER
1	b	456	GLN
1	b	474	LEU
1	b	476	ARG
1	b	494	VAL
1	b	509	ILE
1	b	516	TRP
1	b	520	PHE
1	b	527	LEU
1	b	557	VAL
1	b	560	SER
1	b	561	ARG
1	b	564	ASP
1	b	569	LYS
1	b	572	SER
1	b	573	LYS
1	b	579	LEU
1	b	603	HIS
1	b	677	LEU

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Mol	Chain	Res	Type
1	b	687	SER
1	b	688	VAL
1	b	692	VAL
1	b	695	TYR
1	b	722	GLU
1	b	739	GLN
1	b	744	VAL
1	b	749	VAL
1	b	753	ASN
1	b	762	VAL
1	b	797	THR
1	b	819	ILE
1	b	821	ILE
1	b	830	ASN
1	b	836	GLN
1	b	838	ARG
1	b	877	HIS
1	b	883	CYS
1	b	885	SER
1	b	896	HIS
1	b	901	THR
1	b	909	ILE
1	b	930	ASP
1	b	935	ILE
1	b	955	LYS
1	b	965	ASP
1	b	967	ILE
1	b	979	LEU
1	b	980	TYR
1	b	982	LYS
1	b	984	ASP
1	b	987	LYS
1	b	999	LEU
1	b	1001	GLN
1	b	1013	ILE
1	b	1015	HIS
1	b	1017	HIS
1	b	1033	LEU
1	b	1041	ILE
1	b	1053	TRP
1	b	1067	TYR
1	b	1068	ASN

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Mol	Chain	Res	Type
1	b	1075	GLU
1	b	1077	LEU
1	b	1109	LYS
1	b	1118	THR
1	b	1153	LYS
1	b	1157	VAL
1	b	1160	PHE
1	b	1161	ILE
1	b	1167	ASP
1	b	1182	ASN
1	b	1183	GLU
1	b	1196	ILE
1	b	1200	MET
1	b	1209	ASP
1	b	1213	VAL
1	b	1221	THR
1	b	1224	GLU
1	b	1227	ASP
1	b	1230	LEU
1	b	1233	SER
1	b	1247	ARG
1	b	1258	ARG
1	b	1260	ARG
1	b	1284	GLU
1	b	1331	GLU
1	b	1368	ARG
1	b	1372	ILE
1	b	1381	LYS
1	b	1396	GLU
1	b	1401	ARG
1	b	1427	HIS
1	b	1430	ILE
1	b	1439	VAL
1	b	1441	SER
1	b	1494	ARG
1	b	1500	THR
1	b	1509	THR
1	b	1516	VAL
1	b	1541	GLU
1	b	1543	ILE
1	b	1568	VAL
1	b	1578	ILE

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Mol	Chain	Res	Type
1	b	1580	GLU
1	b	1581	GLU
1	b	1596	GLU
1	b	1598	GLU
1	b	1620	LEU
1	b	1622	GLN
1	b	1632	LEU
1	b	1640	ILE
1	b	1641	THR
1	b	1642	GLN
2	c	2089	ARG
2	c	2131	LEU
2	c	2132	CYS
2	c	2145	LEU
2	c	2160	VAL
2	c	2180	TRP
2	c	2185	THR
2	c	2187	VAL
2	c	2203	ILE
2	c	2221	THR
2	c	2226	GLU
2	c	2227	VAL
2	c	2234	GLN
2	c	2241	THR
2	c	2249	LEU
2	c	2252	GLU
2	c	2255	ASP
2	c	2267	HIS
2	c	2270	ILE
2	c	2277	LYS
2	c	2326	ILE
2	c	2327	GLU
2	c	2333	LEU
2	c	2344	LEU
2	c	2361	LYS
2	c	2373	MET
2	c	2394	VAL
2	c	2406	SER
2	c	2445	MET
2	c	2448	THR
2	c	2452	GLN
2	c	2480	LEU

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Mol	Chain	Res	Type
2	c	2495	ASN
2	c	2497	GLU
2	c	2498	VAL
2	c	2500	ILE
2	c	2507	ARG
2	c	2546	LEU
2	c	2548	CYS
2	c	2552	GLU
2	c	2556	TYR
2	c	2561	HIS
2	c	2563	MET
2	c	2565	THR
2	c	2572	VAL
2	c	2575	LEU
2	c	2579	GLU
2	c	2581	MET
2	c	2595	TRP
2	c	2597	MET
2	c	2602	LEU
2	c	2608	ASP
2	c	2616	THR
2	c	2620	ILE
2	c	2630	LYS
2	c	2631	TYR
2	c	2640	ILE
2	c	2649	GLU
2	c	2653	GLU
2	c	2662	LEU
2	c	2680	HIS
2	c	2683	ILE
2	c	2742	MET
2	c	2750	ILE
2	c	2758	THR
2	c	2763	SER
2	c	2769	PHE
2	c	2772	LYS
2	c	2782	ASN
2	c	2786	MET
2	c	2809	LEU
2	c	2823	ILE
2	c	2828	ASP
2	c	2830	GLN

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Mol	Chain	Res	Type
2	c	2848	PHE
2	c	2850	ARG
2	c	2851	ASN
2	c	2855	ASP
2	c	2856	ILE
2	c	2860	LEU
2	c	2865	ILE
2	c	2870	LEU
2	c	2874	ASP
2	c	2879	LEU
2	c	2882	GLU
2	c	2891	LEU
2	c	2892	ASP
2	c	2898	LYS
2	c	2900	SER
2	c	2901	LEU
3	d	2929[A]	SER
3	d	2929[B]	SER
3	d	2930[A]	LEU
3	d	2930[B]	LEU
3	d	2931[A]	THR
3	d	2931[B]	THR
3	d	2933[A]	SER
3	d	2933[B]	SER
3	d	2935[A]	ILE
3	d	2935[B]	ILE
3	d	2938[A]	LEU
3	d	2938[B]	LEU
3	d	2942[A]	LEU
3	d	2942[B]	LEU
3	d	2946[A]	GLN
3	d	2946[B]	GLN
3	d	2949[A]	LYS
3	d	2949[B]	LYS
3	d	2954[A]	TYR
3	d	2954[B]	TYR
3	d	2956[A]	LYS
3	d	2956[B]	LYS
3	d	2959[A]	SER
3	d	2959[B]	SER
3	d	2960[A]	PHE
3	d	2960[B]	PHE

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Mol	Chain	Res	Type
3	d	2963[A]	MET
3	d	2963[B]	MET
3	d	2965[A]	LEU
3	d	2965[B]	LEU
3	d	2968[A]	GLN
3	d	2968[B]	GLN
3	d	2973[A]	THR
3	d	2973[B]	THR
3	d	2980[A]	HIS
3	d	2980[B]	HIS
3	d	2982[A]	MET
3	d	2982[B]	MET
3	d	2990[A]	ARG
3	d	2990[B]	ARG
3	d	2995[A]	GLN
3	d	2995[B]	GLN
3	d	2996[A]	MET
3	d	2996[B]	MET
3	d	2997[A]	GLU
3	d	2997[B]	GLU
3	d	3000[A]	LEU
3	d	3000[B]	LEU
3	d	3001[A]	LYS
3	d	3001[B]	LYS
3	d	3019[A]	HIS
3	d	3019[B]	HIS
3	d	3021[A]	LEU
3	d	3021[B]	LEU
3	d	3023[A]	ILE
3	d	3023[B]	ILE
3	d	3024[A]	LEU
3	d	3024[B]	LEU
3	d	3026[A]	THR
3	d	3026[B]	THR
3	d	3029[A]	LYS
3	d	3029[B]	LYS
3	d	3040[A]	VAL
3	d	3040[B]	VAL
3	d	3042[A]	ASP
3	d	3042[B]	ASP
3	d	3044[A]	LYS
3	d	3044[B]	LYS

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Mol	Chain	Res	Type
3	d	3048[A]	ASP
3	d	3048[B]	ASP
3	d	3050[A]	ARG
3	d	3050[B]	ARG
3	d	3063[A]	SER
3	d	3063[B]	SER
3	d	3067[A]	ARG
3	d	3067[B]	ARG
3	d	3077[A]	ASP
3	d	3077[B]	ASP
3	d	3081[A]	PHE
3	d	3081[B]	PHE
3	d	3096[A]	VAL
3	d	3096[B]	VAL
3	d	3105[A]	SER
3	d	3105[B]	SER
3	d	3107[A]	LEU
3	d	3107[B]	LEU
3	d	3110[A]	THR
3	d	3110[B]	THR
3	d	3111[A]	SER
3	d	3111[B]	SER
3	d	3115[A]	LEU
3	d	3115[B]	LEU
3	d	3123[A]	THR
3	d	3123[B]	THR
3	d	3131[A]	GLN
3	d	3131[B]	GLN
3	d	3133[A]	LEU
3	d	3133[B]	LEU
3	d	3134[A]	GLN
3	d	3134[B]	GLN
3	d	3135[A]	LYS
3	d	3135[B]	LYS
3	d	3139[A]	LEU
3	d	3139[B]	LEU
3	d	3141[A]	TYR
3	d	3141[B]	TYR
3	d	3147[A]	GLU
3	d	3147[B]	GLU
3	d	3151[A]	LEU
3	d	3151[B]	LEU

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Mol	Chain	Res	Type
3	d	3156[A]	MET
3	d	3156[B]	MET
3	d	3159[A]	SER
3	d	3159[B]	SER
3	d	3160[A]	SER
3	d	3160[B]	SER
3	d	3161[A]	GLU
3	d	3161[B]	GLU
3	d	3162[A]	ASP
3	d	3162[B]	ASP
3	d	3163[A]	ASN
3	d	3163[B]	ASN
3	d	3169[A]	LYS
3	d	3169[B]	LYS
3	d	3172[A]	SER
3	d	3172[B]	SER
3	d	3176[A]	LYS
3	d	3176[B]	LYS
3	d	3181[A]	GLN
3	d	3181[B]	GLN
3	d	3182[A]	GLN
3	d	3182[B]	GLN
3	d	3183[A]	LEU
3	d	3183[B]	LEU
3	d	3185[A]	TYR
3	d	3185[B]	TYR
3	d	3186[A]	GLU
3	d	3186[B]	GLU
3	d	3188[A]	ASP
3	d	3188[B]	ASP
3	d	3191[A]	ASN
3	d	3191[B]	ASN
3	d	3192[A]	PHE
3	d	3192[B]	PHE
3	d	3193[A]	HIS
3	d	3193[B]	HIS
3	d	3195[A]	MET
3	d	3195[B]	MET
3	d	3196[A]	THR
3	d	3196[B]	THR
3	d	3200[A]	LEU
3	d	3200[B]	LEU

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Mol	Chain	Res	Type
3	d	3201[A]	GLU
3	d	3201[B]	GLU
3	d	3204[A]	LEU
3	d	3204[B]	LEU
3	d	3205[A]	LYS
3	d	3205[B]	LYS
3	d	3210[A]	LYS
3	d	3210[B]	LYS
3	d	3211[A]	ASP
3	d	3211[B]	ASP
3	d	3212[A]	ARG
3	d	3212[B]	ARG
3	d	3218[A]	LEU
3	d	3218[B]	LEU
3	d	3220[A]	ARG
3	d	3220[B]	ARG
3	d	3222[A]	ILE
3	d	3222[B]	ILE
3	d	3224[A]	GLN
3	d	3224[B]	GLN
3	d	3225[A]	SER
3	d	3225[B]	SER
3	d	3230[A]	PHE
3	d	3230[B]	PHE
3	d	3244[A]	THR
3	d	3244[B]	THR
3	d	3251[A]	ASP
3	d	3251[B]	ASP
3	d	3254[A]	MET
3	d	3254[B]	MET
3	d	3260[A]	ARG
3	d	3260[B]	ARG
3	d	3267[A]	SER
3	d	3267[B]	SER
3	d	3268[A]	LYS
3	d	3268[B]	LYS
3	d	3271[A]	VAL
3	d	3271[B]	VAL
3	d	3272[A]	HIS
3	d	3272[B]	HIS
3	d	3274[A]	ARG
3	d	3274[B]	ARG

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Mol	Chain	Res	Type
3	d	3276[A]	ASP
3	d	3276[B]	ASP
3	d	3278[A]	HIS
3	d	3278[B]	HIS
3	d	3279[A]	ASP
3	d	3279[B]	ASP
3	d	3283[A]	ILE
3	d	3283[B]	ILE
3	d	3286[A]	THR
3	d	3286[B]	THR
3	d	3287[A]	ILE
3	d	3287[B]	ILE
3	d	3288[A]	MET
3	d	3288[B]	MET
3	d	3290[A]	ILE
3	d	3290[B]	ILE
3	d	3293[A]	LYS
3	d	3293[B]	LYS
3	d	3297[A]	PRO
3	d	3297[B]	PRO
3	d	3299[A]	LEU
3	d	3299[B]	LEU
3	d	3302[A]	SER
3	d	3302[B]	SER
3	d	3304[A]	THR
3	d	3304[B]	THR
3	d	3306[A]	LEU
3	d	3306[B]	LEU
3	d	3308[A]	LYS
3	d	3308[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (420) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	100	GLN
1	A	106	GLN
1	A	121	ASN
1	A	151	GLN
1	A	165	GLN
1	A	180	ASN
1	A	183	HIS

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Mol	Chain	Res	Type
1	A	238	ASN
1	A	376	ASN
1	A	416	ASN
1	A	497	GLN
1	A	636	GLN
1	A	648	GLN
1	A	696	GLN
1	A	779	HIS
1	A	836	GLN
1	A	871	GLN
1	A	877	HIS
1	A	897	HIS
1	A	912	ASN
1	A	1001	GLN
1	A	1045	HIS
1	A	1366	ASN
1	A	1400	ASN
1	A	1490	ASN
1	A	1524	HIS
1	A	1548	GLN
1	A	1622	GLN
2	B	2086	ASN
2	B	2161	GLN
2	B	2169	HIS
2	B	2240	GLN
2	B	2268	ASN
2	B	2297	HIS
2	B	2343	ASN
2	B	2345	ASN
2	B	2461	HIS
2	B	2780	HIS
2	B	2851	ASN
2	B	2894	ASN
1	D	100	GLN
1	D	106	GLN
1	D	151	GLN
1	D	153	ASN
1	D	192	HIS
1	D	340	GLN
1	D	353	ASN
1	D	482	HIS
1	D	500	ASN

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Mol	Chain	Res	Type
1	D	570	GLN
1	D	636	GLN
1	D	645	GLN
1	D	648	GLN
1	D	650	GLN
1	D	679	ASN
1	D	696	GLN
1	D	753	ASN
1	D	904	HIS
1	D	1017	HIS
1	D	1057	GLN
1	D	1071	ASN
1	D	1107	ASN
1	D	1212	HIS
1	D	1242	ASN
1	D	1321	HIS
1	D	1366	ASN
1	D	1400	ASN
1	D	1520	GLN
1	D	1524	HIS
1	D	1531	ASN
1	D	1582	ASN
1	D	1647	ASN
2	E	2169	HIS
2	E	2210	ASN
2	E	2213	HIS
2	E	2230	HIS
2	E	2283	ASN
2	E	2297	HIS
2	E	2365	HIS
2	E	2412	GLN
2	E	2425	HIS
2	E	2471	HIS
2	E	2495	ASN
2	E	2568	HIS
2	E	2584	HIS
2	E	2651	GLN
2	E	2873	HIS
2	E	2894	ASN
1	G	161	ASN
1	G	180	ASN
1	G	224	GLN

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Mol	Chain	Res	Type
1	G	558	HIS
1	G	679	ASN
1	G	877	HIS
1	G	881	GLN
1	G	897	HIS
1	G	957	ASN
1	G	1045	HIS
1	G	1140	ASN
1	G	1182	ASN
1	G	1242	ASN
1	G	1280	GLN
1	G	1321	HIS
1	G	1440	HIS
1	G	1457	HIS
1	G	1460	ASN
1	G	1524	HIS
1	G	1547	ASN
1	G	1642	GLN
2	H	2101	ASN
2	H	2141	HIS
2	H	2213	HIS
2	H	2230	HIS
2	H	2312	GLN
2	H	2390	GLN
2	H	2471	HIS
2	H	2675	GLN
2	H	2684	HIS
2	H	2782	ASN
2	H	2873	HIS
1	J	121	ASN
1	J	145	GLN
1	J	148	GLN
1	J	151	GLN
1	J	192	HIS
1	J	216	HIS
1	J	224	GLN
1	J	226	HIS
1	J	330	GLN
1	J	348	ASN
1	J	353	ASN
1	J	376	ASN
1	J	407	GLN

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Mol	Chain	Res	Type
1	J	416	ASN
1	J	475	ASN
1	J	497	GLN
1	J	558	HIS
1	J	562	GLN
1	J	598	GLN
1	J	622	HIS
1	J	678	ASN
1	J	679	ASN
1	J	717	GLN
1	J	836	GLN
1	J	837	HIS
1	J	881	GLN
1	J	897	HIS
1	J	1010	GLN
1	J	1017	HIS
1	J	1122	ASN
1	J	1128	GLN
1	J	1168	GLN
1	J	1182	ASN
1	J	1242	ASN
1	J	1276	ASN
1	J	1280	GLN
1	J	1400	ASN
1	J	1440	HIS
1	J	1457	HIS
1	J	1502	ASN
1	J	1560	HIS
1	J	1585	ASN
1	J	1602	GLN
1	J	1621	ASN
1	J	1623	ASN
1	J	1625	HIS
2	K	2101	ASN
2	K	2111	GLN
2	K	2240	GLN
2	K	2283	ASN
2	K	2284	HIS
2	K	2312	GLN
2	K	2343	ASN
2	K	2345	ASN
2	K	2359	ASN

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Mol	Chain	Res	Type
2	K	2390	GLN
2	K	2584	HIS
2	K	2811	HIS
1	M	17	ASN
1	M	19	GLN
1	M	106	GLN
1	M	165	GLN
1	M	174	GLN
1	M	180	ASN
1	M	192	HIS
1	M	216	HIS
1	M	221	GLN
1	M	336	ASN
1	M	598	GLN
1	M	717	GLN
1	M	743	ASN
1	M	877	HIS
1	M	881	GLN
1	M	896	HIS
1	M	897	HIS
1	M	1001	GLN
1	M	1017	HIS
1	M	1068	ASN
1	M	1071	ASN
1	M	1128	GLN
1	M	1168	GLN
1	M	1206	HIS
1	M	1276	ASN
1	M	1280	GLN
1	M	1321	HIS
1	M	1406	HIS
1	M	1457	HIS
1	M	1480	ASN
1	M	1520	GLN
1	M	1524	HIS
2	N	2098	GLN
2	N	2161	GLN
2	N	2230	HIS
2	N	2246	ASN
2	N	2297	HIS
2	N	2374	ASN
2	N	2495	ASN

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Mol	Chain	Res	Type
2	N	2510	ASN
2	N	2568	HIS
2	N	2798	GLN
1	P	106	GLN
1	P	192	HIS
1	P	226	HIS
1	P	353	ASN
1	P	407	GLN
1	P	416	ASN
1	P	475	ASN
1	P	686	HIS
1	P	830	ASN
1	P	836	GLN
1	P	897	HIS
1	P	957	ASN
1	P	1017	HIS
1	P	1045	HIS
1	P	1128	GLN
1	P	1140	ASN
1	P	1276	ASN
1	P	1280	GLN
1	P	1321	HIS
1	P	1457	HIS
1	P	1520	GLN
1	P	1547	ASN
1	P	1621	ASN
2	Q	2111	GLN
2	Q	2297	HIS
2	Q	2374	ASN
2	Q	2387	GLN
2	Q	2503	ASN
2	Q	2537	GLN
2	Q	2568	HIS
2	Q	2732	HIS
2	Q	2873	HIS
2	Q	2894	ASN
1	S	165	GLN
1	S	241	HIS
1	S	340	GLN
1	S	348	ASN
1	S	353	ASN
1	S	394	GLN

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Mol	Chain	Res	Type
1	S	562	GLN
1	S	696	GLN
1	S	830	ASN
1	S	871	GLN
1	S	897	HIS
1	S	904	HIS
1	S	912	ASN
1	S	957	ASN
1	S	1107	ASN
1	S	1128	GLN
1	S	1212	HIS
1	S	1276	ASN
1	S	1371	GLN
1	S	1520	GLN
1	S	1524	HIS
1	S	1585	ASN
1	S	1647	ASN
2	T	2211	HIS
2	T	2230	HIS
2	T	2240	GLN
2	T	2365	HIS
2	T	2387	GLN
2	T	2461	HIS
2	T	2537	GLN
2	T	2576	HIS
2	T	2584	HIS
2	T	2741	GLN
2	T	2756	ASN
2	T	2811	HIS
1	V	17	ASN
1	V	19	GLN
1	V	78	GLN
1	V	121	ASN
1	V	145	GLN
1	V	180	ASN
1	V	260	ASN
1	V	348	ASN
1	V	360	HIS
1	V	416	ASN
1	V	500	ASN
1	V	570	GLN
1	V	679	ASN

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Mol	Chain	Res	Type
1	V	837	HIS
1	V	871	GLN
1	V	890	GLN
1	V	897	HIS
1	V	912	ASN
1	V	1001	GLN
1	V	1068	ASN
1	V	1071	ASN
1	V	1140	ASN
1	V	1242	ASN
1	V	1309	HIS
1	V	1400	ASN
1	V	1428	ASN
1	V	1457	HIS
1	V	1460	ASN
1	V	1520	GLN
1	V	1524	HIS
1	V	1560	HIS
1	V	1582	ASN
2	W	2098	GLN
2	W	2240	GLN
2	W	2297	HIS
2	W	2380	GLN
2	W	2387	GLN
2	W	2425	HIS
2	W	2510	ASN
2	W	2741	GLN
2	W	2784	HIS
2	W	2830	GLN
2	W	2873	HIS
1	Y	35	GLN
1	Y	106	GLN
1	Y	153	ASN
1	Y	305	ASN
1	Y	353	ASN
1	Y	360	HIS
1	Y	413	ASN
1	Y	570	GLN
1	Y	679	ASN
1	Y	696	GLN
1	Y	871	GLN
1	Y	890	GLN

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Mol	Chain	Res	Type
1	Y	897	HIS
1	Y	912	ASN
1	Y	920	ASN
1	Y	951	ASN
1	Y	957	ASN
1	Y	1057	GLN
1	Y	1091	ASN
1	Y	1140	ASN
1	Y	1206	HIS
1	Y	1299	GLN
1	Y	1406	HIS
1	Y	1428	ASN
1	Y	1440	HIS
1	Y	1457	HIS
1	Y	1483	ASN
1	Y	1510	ASN
1	Y	1524	HIS
1	Y	1582	ASN
1	Y	1621	ASN
1	Y	1642	GLN
2	Z	2134	ASN
2	Z	2141	HIS
2	Z	2284	HIS
2	Z	2309	GLN
2	Z	2312	GLN
2	Z	2495	ASN
2	Z	2561	HIS
2	Z	2568	HIS
2	Z	2651	GLN
2	Z	2741	GLN
1	b	145	GLN
1	b	260	ASN
1	b	348	ASN
1	b	353	ASN
1	b	376	ASN
1	b	407	GLN
1	b	416	ASN
1	b	475	ASN
1	b	558	HIS
1	b	570	GLN
1	b	633	HIS
1	b	743	ASN

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Mol	Chain	Res	Type
1	b	779	HIS
1	b	881	GLN
1	b	897	HIS
1	b	912	ASN
1	b	951	ASN
1	b	1045	HIS
1	b	1122	ASN
1	b	1140	ASN
1	b	1182	ASN
1	b	1242	ASN
1	b	1276	ASN
1	b	1299	GLN
1	b	1321	HIS
1	b	1394	GLN
1	b	1400	ASN
1	b	1457	HIS
1	b	1510	ASN
1	b	1524	HIS
1	b	1621	ASN
2	c	2146	HIS
2	c	2211	HIS
2	c	2240	GLN
2	c	2297	HIS
2	c	2374	ASN
2	c	2390	GLN
2	c	2425	HIS
2	c	2495	ASN
2	c	2510	ASN
2	c	2576	HIS
2	c	2780	HIS
2	c	2798	GLN
2	c	2830	GLN
2	c	2847	HIS
2	c	2894	ASN

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 ⓘ

130 monosaccharides 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$
8	NAG	0	1	8,1	14,14,15	0.75	1 (7%)	17,19,21	1.50	2 (11%)
8	NAG	0	2	8	14,14,15	0.53	0	17,19,21	1.52	4 (23%)
8	BMA	0	3	8	11,11,12	0.23	0	15,15,17	1.75	3 (20%)
8	MAN	0	4	8	11,11,12	0.31	0	15,15,17	0.83	1 (6%)
4	NAG	1	1	4,1	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
4	NAG	1	2	4	14,14,15	0.44	0	17,19,21	1.15	2 (11%)
4	NAG	2	1	2,4	14,14,15	1.14	1 (7%)	17,19,21	1.42	2 (11%)
4	NAG	2	2	4	14,14,15	0.33	0	17,19,21	0.69	0
6	NAG	3	1	6,1	14,14,15	1.04	1 (7%)	17,19,21	1.44	2 (11%)
6	NAG	3	2	6	14,14,15	0.42	0	17,19,21	0.76	0
6	BMA	3	3	6	11,11,12	0.25	0	15,15,17	0.55	0
4	NAG	4	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	1.25	2 (11%)
4	NAG	4	2	4	14,14,15	0.41	0	17,19,21	1.17	3 (17%)
6	NAG	5	1	6,1	14,14,15	0.74	0	17,19,21	1.28	1 (5%)
6	NAG	5	2	6	14,14,15	0.30	0	17,19,21	1.03	1 (5%)
6	BMA	5	3	6	11,11,12	0.27	0	15,15,17	1.24	2 (13%)
4	NAG	6	1	4,1	14,14,15	0.97	1 (7%)	17,19,21	1.95	2 (11%)
4	NAG	6	2	4	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
4	NAG	7	1	2,4	14,14,15	0.86	1 (7%)	17,19,21	1.46	2 (11%)
4	NAG	7	2	4	14,14,15	0.43	0	17,19,21	1.08	2 (11%)
4	NAG	8	1	4,1	14,14,15	1.00	1 (7%)	17,19,21	1.88	2 (11%)
4	NAG	8	2	4	14,14,15	0.40	0	17,19,21	0.70	1 (5%)
4	NAG	9	1	4,1	14,14,15	0.96	1 (7%)	17,19,21	1.35	3 (17%)
4	NAG	9	2	4	14,14,15	0.28	0	17,19,21	0.77	1 (5%)
5	NAG	AA	1	5,1	14,14,15	0.69	0	17,19,21	1.18	3 (17%)
5	NAG	AA	2	5	14,14,15	0.42	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	AA	3	5	11,11,12	0.29	0	15,15,17	1.74	3 (20%)
5	MAN	AA	4	5	11,11,12	0.23	0	15,15,17	0.43	0
4	NAG	BA	1	4,1	14,14,15	0.75	1 (7%)	17,19,21	1.34	2 (11%)
4	NAG	BA	2	4	14,14,15	0.57	0	17,19,21	1.12	1 (5%)
6	NAG	CA	1	2,6	14,14,15	1.12	1 (7%)	17,19,21	1.55	2 (11%)
6	NAG	CA	2	6	14,14,15	0.33	0	17,19,21	0.95	1 (5%)
6	BMA	CA	3	6	11,11,12	0.22	0	15,15,17	0.56	0
6	NAG	DA	1	6,1	14,14,15	0.80	1 (7%)	17,19,21	1.17	1 (5%)
6	NAG	DA	2	6	14,14,15	0.31	0	17,19,21	1.22	2 (11%)
6	BMA	DA	3	6	11,11,12	0.25	0	15,15,17	0.88	1 (6%)
6	NAG	EA	1	6,1	14,14,15	0.84	1 (7%)	17,19,21	1.37	2 (11%)
6	NAG	EA	2	6	14,14,15	0.36	0	17,19,21	2.22	4 (23%)
6	BMA	EA	3	6	11,11,12	0.22	0	15,15,17	0.70	0
5	NAG	FA	1	5,1	14,14,15	0.82	1 (7%)	17,19,21	1.37	2 (11%)
5	NAG	FA	2	5	14,14,15	0.50	0	17,19,21	0.91	1 (5%)
5	BMA	FA	3	5	11,11,12	0.59	0	15,15,17	1.26	2 (13%)
5	MAN	FA	4	5	11,11,12	0.21	0	15,15,17	1.09	1 (6%)
6	NAG	GA	1	6,1	14,14,15	0.75	1 (7%)	17,19,21	1.33	1 (5%)
6	NAG	GA	2	6	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
6	BMA	GA	3	6	11,11,12	0.31	0	15,15,17	0.86	0
4	NAG	HA	1	2,4	14,14,15	0.72	1 (7%)	17,19,21	1.20	1 (5%)
4	NAG	HA	2	4	14,14,15	0.31	0	17,19,21	0.57	0
4	NAG	IA	1	4,1	14,14,15	0.85	1 (7%)	17,19,21	1.52	2 (11%)
4	NAG	IA	2	4	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
4	NAG	JA	1	4,1	14,14,15	0.85	1 (7%)	17,19,21	1.24	1 (5%)
4	NAG	JA	2	4	14,14,15	0.35	0	17,19,21	0.77	0
5	NAG	KA	1	5,1	14,14,15	0.75	0	17,19,21	1.88	5 (29%)
5	NAG	KA	2	5	14,14,15	0.38	0	17,19,21	1.31	2 (11%)
5	BMA	KA	3	5	11,11,12	0.29	0	15,15,17	1.29	1 (6%)
5	MAN	KA	4	5	11,11,12	0.41	0	15,15,17	1.70	2 (13%)
6	NAG	LA	1	6,1	14,14,15	1.06	1 (7%)	17,19,21	2.37	4 (23%)
6	NAG	LA	2	6	14,14,15	0.46	0	17,19,21	1.15	2 (11%)
6	BMA	LA	3	6	11,11,12	0.21	0	15,15,17	0.64	0
4	NAG	MA	1	2,4	14,14,15	1.06	1 (7%)	17,19,21	2.42	3 (17%)
4	NAG	MA	2	4	14,14,15	0.33	0	17,19,21	1.73	3 (17%)
6	NAG	NA	1	6,1	14,14,15	0.76	1 (7%)	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	NA	2	6	14,14,15	0.37	0	17,19,21	0.84	0
6	BMA	NA	3	6	11,11,12	0.24	0	15,15,17	0.86	1 (6%)
4	NAG	OA	1	4,1	14,14,15	1.27	1 (7%)	17,19,21	1.60	2 (11%)
4	NAG	OA	2	4	14,14,15	0.54	0	17,19,21	0.99	1 (5%)
5	NAG	PA	1	5,1	14,14,15	0.67	0	17,19,21	1.14	1 (5%)
5	NAG	PA	2	5	14,14,15	0.37	0	17,19,21	0.94	1 (5%)
5	BMA	PA	3	5	11,11,12	0.60	0	15,15,17	2.08	4 (26%)
5	MAN	PA	4	5	11,11,12	0.26	0	15,15,17	0.74	0
4	NAG	QA	1	4,1	14,14,15	0.57	0	17,19,21	2.46	5 (29%)
4	NAG	QA	2	4	14,14,15	0.24	0	17,19,21	0.68	0
4	NAG	RA	1	2,4	14,14,15	1.22	1 (7%)	17,19,21	2.17	2 (11%)
4	NAG	RA	2	4	14,14,15	0.45	0	17,19,21	0.72	0
4	NAG	e	1	4,1	14,14,15	0.64	0	17,19,21	1.68	4 (23%)
4	NAG	e	2	4	14,14,15	0.34	0	17,19,21	0.49	0
4	NAG	f	1	4,1	14,14,15	0.97	1 (7%)	17,19,21	1.43	2 (11%)
4	NAG	f	2	4	14,14,15	0.25	0	17,19,21	1.00	1 (5%)
5	NAG	g	1	5,1	14,14,15	0.61	0	17,19,21	1.53	2 (11%)
5	NAG	g	2	5	14,14,15	0.52	0	17,19,21	1.04	0
5	BMA	g	3	5	11,11,12	0.47	0	15,15,17	1.99	4 (26%)
5	MAN	g	4	5	11,11,12	0.24	0	15,15,17	0.57	0
6	NAG	h	1	6,1	14,14,15	0.66	0	17,19,21	1.15	3 (17%)
6	NAG	h	2	6	14,14,15	0.57	0	17,19,21	1.10	1 (5%)
6	BMA	h	3	6	11,11,12	0.25	0	15,15,17	1.02	2 (13%)
4	NAG	i	1	2,4	14,14,15	1.15	1 (7%)	17,19,21	1.23	2 (11%)
4	NAG	i	2	4	14,14,15	0.44	0	17,19,21	0.88	1 (5%)
4	NAG	j	1	4,1	14,14,15	1.08	1 (7%)	17,19,21	1.66	2 (11%)
4	NAG	j	2	4	14,14,15	0.50	0	17,19,21	1.35	3 (17%)
6	NAG	k	1	6,1	14,14,15	0.85	1 (7%)	17,19,21	1.11	1 (5%)
6	NAG	k	2	6	14,14,15	0.28	0	17,19,21	0.67	1 (5%)
6	BMA	k	3	6	11,11,12	0.25	0	15,15,17	0.44	0
5	NAG	l	1	5,1	14,14,15	0.69	0	17,19,21	1.21	1 (5%)
5	NAG	l	2	5	14,14,15	0.27	0	17,19,21	0.58	0
5	BMA	l	3	5	11,11,12	0.27	0	15,15,17	0.72	0
5	MAN	l	4	5	11,11,12	0.27	0	15,15,17	0.85	1 (6%)
4	NAG	m	1	4,1	14,14,15	0.39	0	17,19,21	0.93	1 (5%)
4	NAG	m	2	4	14,14,15	0.37	0	17,19,21	0.88	1 (5%)
4	NAG	n	1	2,4	14,14,15	0.52	0	17,19,21	1.59	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	n	2	4	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
4	NAG	o	1	4,1	14,14,15	0.61	0	17,19,21	1.02	1 (5%)
4	NAG	o	2	4	14,14,15	0.45	0	17,19,21	1.06	1 (5%)
4	NAG	p	1	4	14,14,15	0.95	1 (7%)	17,19,21	1.94	4 (23%)
4	NAG	p	2	4	14,14,15	0.32	0	17,19,21	0.64	0
4	NAG	q	1	4,1	14,14,15	0.56	0	17,19,21	1.19	2 (11%)
4	NAG	q	2	4	14,14,15	0.51	0	17,19,21	0.88	1 (5%)
6	NAG	r	1	6,1	14,14,15	0.73	1 (7%)	17,19,21	1.75	3 (17%)
6	NAG	r	2	6	14,14,15	0.59	0	17,19,21	1.01	0
6	BMA	r	3	6	11,11,12	0.23	0	15,15,17	0.54	0
4	NAG	s	1	2,4	14,14,15	0.85	1 (7%)	17,19,21	1.24	2 (11%)
4	NAG	s	2	4	14,14,15	0.34	0	17,19,21	0.75	0
4	NAG	t	1	4,1	14,14,15	0.68	0	17,19,21	1.51	3 (17%)
4	NAG	t	2	4	14,14,15	0.32	0	17,19,21	0.49	0
4	NAG	u	1	4,1	14,14,15	0.89	1 (7%)	17,19,21	1.68	3 (17%)
4	NAG	u	2	4	14,14,15	0.33	0	17,19,21	0.77	0
4	NAG	v	1	4,1	14,14,15	0.59	0	17,19,21	1.12	1 (5%)
4	NAG	v	2	4	14,14,15	0.36	0	17,19,21	0.95	1 (5%)
6	NAG	w	1	6,1	14,14,15	0.75	1 (7%)	17,19,21	1.89	4 (23%)
6	NAG	w	2	6	14,14,15	0.43	0	17,19,21	1.16	2 (11%)
6	BMA	w	3	6	11,11,12	0.30	0	15,15,17	0.70	0
4	NAG	x	1	2,4	14,14,15	0.50	0	17,19,21	0.94	0
4	NAG	x	2	4	14,14,15	0.51	0	17,19,21	1.00	1 (5%)
6	NAG	y	1	6,1	14,14,15	0.92	1 (7%)	17,19,21	1.17	1 (5%)
6	NAG	y	2	6	14,14,15	0.34	0	17,19,21	1.91	3 (17%)
6	BMA	y	3	6	11,11,12	0.22	0	15,15,17	1.11	2 (13%)
7	NAG	z	1	7,1	14,14,15	1.15	1 (7%)	17,19,21	2.12	3 (17%)
7	NAG	z	2	7	14,14,15	0.58	0	17,19,21	1.56	3 (17%)
7	BMA	z	3	7	11,11,12	0.45	0	15,15,17	2.53	5 (33%)
7	MAN	z	4	7	11,11,12	0.41	0	15,15,17	1.89	4 (26%)
7	MAN	z	5	7	11,11,12	0.22	0	15,15,17	0.49	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
8	NAG	0	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	0	2	8	-	2/6/23/26	0/1/1/1
8	BMA	0	3	8	-	0/2/19/22	0/1/1/1
8	MAN	0	4	8	-	0/2/19/22	0/1/1/1
4	NAG	1	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	1	2	4	-	0/6/23/26	0/1/1/1
4	NAG	2	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	2	2	4	-	0/6/23/26	0/1/1/1
6	NAG	3	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	3	2	6	-	0/6/23/26	0/1/1/1
6	BMA	3	3	6	-	2/2/19/22	0/1/1/1
4	NAG	4	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	4	2	4	-	4/6/23/26	0/1/1/1
6	NAG	5	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	5	2	6	-	2/6/23/26	0/1/1/1
6	BMA	5	3	6	-	2/2/19/22	0/1/1/1
4	NAG	6	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	6	2	4	-	0/6/23/26	0/1/1/1
4	NAG	7	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	7	2	4	-	4/6/23/26	0/1/1/1
4	NAG	8	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	8	2	4	-	0/6/23/26	0/1/1/1
4	NAG	9	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	9	2	4	-	0/6/23/26	0/1/1/1
5	NAG	AA	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	AA	2	5	-	4/6/23/26	0/1/1/1
5	BMA	AA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	AA	4	5	-	0/2/19/22	0/1/1/1
4	NAG	BA	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	BA	2	4	-	4/6/23/26	0/1/1/1
6	NAG	CA	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	CA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	CA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	DA	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	DA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	DA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	EA	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	EA	2	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	EA	3	6	-	0/2/19/22	0/1/1/1
5	NAG	FA	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	FA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	FA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	FA	4	5	-	0/2/19/22	0/1/1/1
6	NAG	GA	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	GA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	GA	3	6	-	0/2/19/22	0/1/1/1
4	NAG	HA	1	2,4	-	5/6/23/26	0/1/1/1
4	NAG	HA	2	4	-	0/6/23/26	0/1/1/1
4	NAG	IA	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	IA	2	4	-	4/6/23/26	0/1/1/1
4	NAG	JA	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	JA	2	4	-	4/6/23/26	0/1/1/1
5	NAG	KA	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	KA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	KA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	KA	4	5	-	0/2/19/22	0/1/1/1
6	NAG	LA	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	LA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	LA	3	6	-	0/2/19/22	0/1/1/1
4	NAG	MA	1	2,4	-	5/6/23/26	0/1/1/1
4	NAG	MA	2	4	-	1/6/23/26	0/1/1/1
6	NAG	NA	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	NA	2	6	-	3/6/23/26	0/1/1/1
6	BMA	NA	3	6	-	0/2/19/22	0/1/1/1
4	NAG	OA	1	4,1	-	6/6/23/26	0/1/1/1
4	NAG	OA	2	4	-	4/6/23/26	0/1/1/1
5	NAG	PA	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	PA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	PA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	PA	4	5	-	0/2/19/22	0/1/1/1
4	NAG	QA	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	QA	2	4	-	0/6/23/26	0/1/1/1
4	NAG	RA	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	RA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	e	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	f	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	f	2	4	-	0/6/23/26	0/1/1/1
5	NAG	g	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	g	2	5	-	3/6/23/26	0/1/1/1
5	BMA	g	3	5	-	2/2/19/22	0/1/1/1
5	MAN	g	4	5	-	0/2/19/22	0/1/1/1
6	NAG	h	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	h	2	6	-	0/6/23/26	0/1/1/1
6	BMA	h	3	6	-	0/2/19/22	0/1/1/1
4	NAG	i	1	2,4	-	6/6/23/26	0/1/1/1
4	NAG	i	2	4	-	0/6/23/26	0/1/1/1
4	NAG	j	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	j	2	4	-	5/6/23/26	0/1/1/1
6	NAG	k	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	k	2	6	-	0/6/23/26	0/1/1/1
6	BMA	k	3	6	-	0/2/19/22	0/1/1/1
5	NAG	l	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	l	2	5	-	0/6/23/26	0/1/1/1
5	BMA	l	3	5	-	0/2/19/22	0/1/1/1
5	MAN	l	4	5	-	0/2/19/22	0/1/1/1
4	NAG	m	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	m	2	4	-	6/6/23/26	0/1/1/1
4	NAG	n	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	n	2	4	-	0/6/23/26	0/1/1/1
4	NAG	o	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	o	2	4	-	2/6/23/26	0/1/1/1
4	NAG	p	1	4	-	2/6/23/26	0/1/1/1
4	NAG	p	2	4	-	0/6/23/26	0/1/1/1
4	NAG	q	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	q	2	4	-	4/6/23/26	0/1/1/1
6	NAG	r	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	r	2	6	-	4/6/23/26	0/1/1/1
6	BMA	r	3	6	-	0/2/19/22	0/1/1/1
4	NAG	s	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	s	2	4	-	3/6/23/26	0/1/1/1
4	NAG	t	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	t	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	u	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	u	2	4	-	0/6/23/26	0/1/1/1
4	NAG	v	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	v	2	4	-	2/6/23/26	0/1/1/1
6	NAG	w	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	w	2	6	-	1/6/23/26	0/1/1/1
6	BMA	w	3	6	-	0/2/19/22	0/1/1/1
4	NAG	x	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	x	2	4	-	0/6/23/26	0/1/1/1
6	NAG	y	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	y	2	6	-	0/6/23/26	0/1/1/1
6	BMA	y	3	6	-	0/2/19/22	0/1/1/1
7	NAG	z	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	z	2	7	-	0/6/23/26	0/1/1/1
7	BMA	z	3	7	-	2/2/19/22	0/1/1/1
7	MAN	z	4	7	-	1/2/19/22	0/1/1/1
7	MAN	z	5	7	-	1/2/19/22	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	OA	1	NAG	C1-C2	4.47	1.58	1.52
4	2	1	NAG	C1-C2	4.11	1.57	1.52
4	i	1	NAG	C1-C2	4.08	1.57	1.52
4	RA	1	NAG	C1-C2	4.06	1.57	1.52
7	z	1	NAG	C1-C2	3.99	1.57	1.52
6	CA	1	NAG	C1-C2	3.86	1.57	1.52
4	j	1	NAG	C1-C2	3.76	1.57	1.52
6	3	1	NAG	C1-C2	3.67	1.57	1.52
6	LA	1	NAG	C1-C2	3.58	1.57	1.52
4	MA	1	NAG	C1-C2	3.45	1.57	1.52
4	f	1	NAG	C1-C2	3.42	1.57	1.52
4	9	1	NAG	C1-C2	3.25	1.56	1.52
4	6	1	NAG	C1-C2	3.23	1.56	1.52
4	p	1	NAG	C1-C2	3.11	1.56	1.52
6	k	1	NAG	C1-C2	3.01	1.56	1.52
4	8	1	NAG	C1-C2	2.95	1.56	1.52
4	u	1	NAG	C1-C2	2.91	1.56	1.52
4	s	1	NAG	C1-C2	2.86	1.56	1.52
6	y	1	NAG	C1-C2	2.83	1.56	1.52
6	EA	1	NAG	C1-C2	2.62	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7	1	NAG	C1-C2	2.55	1.55	1.52
4	IA	1	NAG	C1-C2	2.47	1.55	1.52
5	FA	1	NAG	C1-C2	2.46	1.55	1.52
6	NA	1	NAG	C1-C2	2.35	1.55	1.52
4	4	1	NAG	C1-C2	2.32	1.55	1.52
6	w	1	NAG	C1-C2	2.31	1.55	1.52
6	DA	1	NAG	C1-C2	2.25	1.55	1.52
8	0	1	NAG	C1-C2	2.24	1.55	1.52
4	JA	1	NAG	C1-C2	2.20	1.55	1.52
4	BA	1	NAG	C1-C2	2.11	1.55	1.52
4	HA	1	NAG	C1-C2	2.09	1.55	1.52
6	GA	1	NAG	C1-C2	2.04	1.55	1.52
6	r	1	NAG	C1-C2	2.01	1.55	1.52

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	LA	1	NAG	C1-O5-C5	8.10	123.04	112.19
4	MA	1	NAG	C1-O5-C5	8.02	122.94	112.19
4	QA	1	NAG	C2-N2-C7	-7.79	112.46	122.90
4	RA	1	NAG	C1-O5-C5	7.46	122.19	112.19
7	z	1	NAG	C1-O5-C5	7.17	121.79	112.19
7	z	3	BMA	C1-O5-C5	6.90	121.43	112.19
4	6	1	NAG	C1-O5-C5	6.40	120.76	112.19
6	EA	2	NAG	C1-O5-C5	6.33	120.68	112.19
4	8	1	NAG	C1-O5-C5	5.95	120.16	112.19
4	j	1	NAG	C1-O5-C5	5.59	119.67	112.19
5	KA	1	NAG	C1-O5-C5	5.42	119.44	112.19
6	CA	1	NAG	C1-O5-C5	5.31	119.31	112.19
4	MA	2	NAG	C2-N2-C7	5.20	129.87	122.90
7	z	3	BMA	C2-C3-C4	-5.15	101.81	110.86
5	g	3	BMA	C1-C2-C3	5.11	117.08	109.64
5	PA	3	BMA	C1-C2-C3	4.95	116.85	109.64
4	OA	1	NAG	C1-O5-C5	4.81	118.63	112.19
8	0	3	BMA	C1-O5-C5	4.81	118.63	112.19
6	y	2	NAG	O4-C4-C3	-4.77	99.14	110.38
8	0	1	NAG	C1-O5-C5	4.65	118.42	112.19
4	p	1	NAG	C1-O5-C5	4.65	118.41	112.19
4	u	1	NAG	C1-O5-C5	4.58	118.32	112.19
6	EA	2	NAG	O4-C4-C3	-4.50	99.78	110.38
7	z	4	MAN	C1-O5-C5	4.47	118.17	112.19
6	r	1	NAG	C1-O5-C5	4.40	118.08	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	KA	4	MAN	C1-O5-C5	4.34	118.01	112.19
4	7	1	NAG	C1-O5-C5	4.30	117.95	112.19
6	y	2	NAG	C1-O5-C5	4.26	117.89	112.19
5	KA	2	NAG	C1-O5-C5	4.25	117.89	112.19
5	AA	3	BMA	C1-C2-C3	4.23	115.81	109.64
6	w	1	NAG	O4-C4-C3	4.14	120.13	110.38
4	2	1	NAG	C1-O5-C5	4.13	117.72	112.19
7	z	2	NAG	C1-O5-C5	4.10	117.68	112.19
4	MA	1	NAG	C2-N2-C7	-4.00	117.54	122.90
5	g	1	NAG	O5-C1-C2	-3.91	105.23	111.29
5	g	1	NAG	C1-O5-C5	3.91	117.42	112.19
5	AA	3	BMA	O3-C3-C2	-3.88	102.13	110.05
5	FA	1	NAG	C1-O5-C5	3.87	117.38	112.19
6	w	1	NAG	C1-O5-C5	3.85	117.35	112.19
5	g	3	BMA	C1-O5-C5	3.82	117.31	112.19
4	f	1	NAG	C1-O5-C5	3.81	117.29	112.19
5	KA	4	MAN	C1-C2-C3	3.80	115.18	109.64
4	t	1	NAG	C1-O5-C5	3.78	117.26	112.19
4	IA	1	NAG	C1-O5-C5	3.77	117.24	112.19
4	s	1	NAG	C2-N2-C7	-3.67	117.98	122.90
4	e	1	NAG	C2-N2-C7	-3.64	118.02	122.90
6	w	1	NAG	C3-C4-C5	-3.61	103.69	110.23
6	y	2	NAG	O4-C4-C5	3.59	118.16	109.32
6	5	3	BMA	C1-O5-C5	3.56	116.95	112.19
6	3	1	NAG	O4-C4-C3	-3.54	102.03	110.38
6	GA	1	NAG	C1-O5-C5	3.51	116.89	112.19
4	j	2	NAG	C2-N2-C7	-3.50	118.20	122.90
6	5	1	NAG	C1-O5-C5	3.44	116.80	112.19
4	QA	1	NAG	C6-C5-C4	-3.42	104.63	113.02
4	n	1	NAG	C2-N2-C7	-3.41	118.33	122.90
4	HA	1	NAG	C2-N2-C7	-3.37	118.38	122.90
5	KA	3	BMA	C1-C2-C3	3.37	114.55	109.64
8	0	2	NAG	O5-C1-C2	-3.36	106.09	111.29
4	QA	1	NAG	O5-C5-C6	3.35	114.18	107.66
4	e	1	NAG	O4-C4-C3	-3.34	102.50	110.38
4	u	1	NAG	C2-N2-C7	-3.34	118.43	122.90
4	IA	1	NAG	C2-N2-C7	-3.31	118.47	122.90
4	t	1	NAG	C2-N2-C7	-3.30	118.47	122.90
4	p	1	NAG	O5-C1-C2	-3.29	106.20	111.29
6	h	1	NAG	C1-O5-C5	3.28	116.59	112.19
4	p	1	NAG	C4-C3-C2	3.28	115.83	111.02
4	n	1	NAG	O4-C4-C3	-3.27	102.67	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	DA	2	NAG	O4-C4-C3	-3.26	102.69	110.38
6	3	1	NAG	C1-O5-C5	3.23	116.51	112.19
5	PA	3	BMA	C1-O5-C5	3.21	116.48	112.19
7	z	4	MAN	C3-C4-C5	3.21	116.05	110.23
6	EA	2	NAG	O5-C5-C6	-3.18	101.47	107.66
6	r	1	NAG	C2-N2-C7	-3.17	118.65	122.90
4	9	1	NAG	O5-C5-C6	3.17	113.83	107.66
6	DA	2	NAG	C1-O5-C5	3.16	116.42	112.19
4	v	1	NAG	C1-O5-C5	3.15	116.41	112.19
4	6	1	NAG	C3-C4-C5	-3.14	104.53	110.23
7	z	2	NAG	C4-C3-C2	-3.13	106.43	111.02
6	r	1	NAG	C4-C3-C2	-3.11	106.46	111.02
6	EA	1	NAG	C1-O5-C5	3.08	116.32	112.19
4	q	1	NAG	O5-C1-C2	-3.08	106.53	111.29
7	z	4	MAN	C1-C2-C3	3.07	114.12	109.64
5	PA	3	BMA	C2-C3-C4	3.04	116.22	110.86
6	CA	2	NAG	C1-O5-C5	3.04	116.27	112.19
6	h	2	NAG	O5-C1-C2	-3.04	106.59	111.29
7	z	1	NAG	C3-C4-C5	-3.04	104.73	110.23
4	f	2	NAG	C1-O5-C5	3.03	116.25	112.19
4	8	1	NAG	C2-N2-C7	-3.02	118.85	122.90
4	RA	1	NAG	C2-N2-C7	-3.02	118.85	122.90
5	KA	1	NAG	C2-N2-C7	-3.00	118.88	122.90
8	0	2	NAG	C1-O5-C5	2.96	116.16	112.19
4	JA	1	NAG	C4-C3-C2	2.95	115.35	111.02
6	5	2	NAG	O5-C1-C2	-2.95	106.73	111.29
7	z	2	NAG	O4-C4-C5	2.95	116.58	109.32
5	PA	3	BMA	C3-C4-C5	2.92	115.53	110.23
4	i	1	NAG	C1-O5-C5	2.92	116.10	112.19
5	FA	3	BMA	C1-C2-C3	2.91	113.89	109.64
6	LA	1	NAG	C3-C4-C5	-2.91	104.96	110.23
5	FA	2	NAG	C1-O5-C5	2.83	115.98	112.19
6	EA	2	NAG	O4-C4-C5	2.82	116.27	109.32
5	l	1	NAG	O5-C1-C2	-2.81	106.94	111.29
4	o	2	NAG	C1-O5-C5	-2.81	108.42	112.19
5	PA	2	NAG	O4-C4-C5	-2.79	102.46	109.32
4	x	2	NAG	C1-O5-C5	2.78	115.91	112.19
4	n	1	NAG	O5-C1-C2	-2.75	107.04	111.29
4	e	1	NAG	C1-O5-C5	2.74	115.86	112.19
8	0	2	NAG	C2-N2-C7	-2.72	119.26	122.90
5	KA	1	NAG	O5-C1-C2	-2.72	107.09	111.29
6	y	1	NAG	C1-O5-C5	2.70	115.80	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	FA	1	NAG	O5-C1-C2	-2.69	107.13	111.29
4	OA	2	NAG	O5-C1-C2	-2.68	107.14	111.29
5	AA	1	NAG	C1-O5-C5	2.67	115.76	112.19
6	LA	1	NAG	C4-C3-C2	2.65	114.91	111.02
6	y	3	BMA	C1-O5-C5	2.64	115.73	112.19
7	z	3	BMA	C6-C5-C4	-2.62	106.59	113.02
7	z	3	BMA	O5-C5-C4	2.61	117.17	110.83
8	0	3	BMA	C1-C2-C3	-2.59	105.87	109.64
7	z	3	BMA	C1-C2-C3	2.58	113.40	109.64
8	0	4	MAN	C1-O5-C5	-2.58	108.73	112.19
4	4	1	NAG	O4-C4-C3	-2.55	104.37	110.38
4	BA	1	NAG	C4-C3-C2	2.55	114.75	111.02
4	MA	2	NAG	O7-C7-N2	2.53	126.45	121.98
6	EA	1	NAG	O5-C1-C2	-2.51	107.41	111.29
6	y	3	BMA	C1-C2-C3	2.50	113.28	109.64
7	z	4	MAN	C6-C5-C4	-2.49	106.90	113.02
4	7	2	NAG	C2-N2-C7	-2.48	119.57	122.90
6	h	3	BMA	C1-O5-C5	2.46	115.48	112.19
4	4	2	NAG	C1-C2-N2	-2.45	106.57	110.43
5	AA	2	NAG	O5-C1-C2	-2.45	107.50	111.29
4	q	1	NAG	C2-N2-C7	-2.44	119.64	122.90
4	e	1	NAG	C4-C3-C2	2.43	114.59	111.02
8	0	3	BMA	C6-C5-C4	-2.42	107.08	113.02
6	DA	1	NAG	O4-C4-C3	-2.41	104.69	110.38
5	KA	2	NAG	O4-C4-C3	-2.40	104.72	110.38
5	g	3	BMA	O3-C3-C2	-2.40	105.16	110.05
4	9	2	NAG	C1-O5-C5	2.38	115.38	112.19
4	t	1	NAG	O4-C4-C3	-2.38	104.76	110.38
4	MA	1	NAG	C3-C4-C5	-2.37	105.93	110.23
6	w	2	NAG	C8-C7-N2	2.37	120.05	116.12
4	MA	2	NAG	C1-C2-N2	-2.37	106.70	110.43
5	AA	1	NAG	O5-C1-C2	-2.36	107.64	111.29
4	OA	1	NAG	O5-C1-C2	-2.35	107.65	111.29
6	LA	1	NAG	C2-N2-C7	-2.35	119.75	122.90
4	v	2	NAG	C2-N2-C7	-2.34	119.77	122.90
4	1	2	NAG	C8-C7-N2	2.34	119.99	116.12
4	6	2	NAG	C8-C7-N2	2.34	119.99	116.12
6	NA	3	BMA	C1-O5-C5	-2.32	109.08	112.19
4	i	1	NAG	C4-C3-C2	-2.32	107.62	111.02
5	AA	1	NAG	C2-N2-C7	-2.31	119.81	122.90
4	2	1	NAG	C3-C4-C5	-2.31	106.05	110.23
4	j	1	NAG	C3-C4-C5	-2.30	106.06	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	GA	2	NAG	C8-C7-N2	2.30	119.92	116.12
4	q	2	NAG	C1-C2-N2	-2.29	106.82	110.43
4	m	2	NAG	C1-O5-C5	2.29	115.26	112.19
4	4	1	NAG	O5-C1-C2	-2.29	107.75	111.29
4	1	1	NAG	C1-O5-C5	2.27	115.23	112.19
4	BA	2	NAG	C1-C2-N2	-2.27	106.86	110.43
5	PA	1	NAG	O5-C1-C2	-2.26	107.80	111.29
6	LA	2	NAG	C2-N2-C7	-2.25	119.88	122.90
5	FA	3	BMA	C3-C4-C5	2.25	114.31	110.23
6	LA	2	NAG	O4-C4-C3	-2.24	105.10	110.38
7	z	1	NAG	C4-C3-C2	2.23	114.28	111.02
4	7	1	NAG	C3-C4-C5	-2.23	106.19	110.23
5	AA	3	BMA	C1-O5-C5	2.23	115.17	112.19
5	g	3	BMA	O3-C3-C4	2.23	115.62	110.38
4	n	2	NAG	C1-O5-C5	-2.21	109.23	112.19
4	o	1	NAG	C2-N2-C7	-2.21	119.94	122.90
8	0	1	NAG	C3-C4-C5	-2.20	106.24	110.23
6	GA	2	NAG	C2-N2-C7	-2.19	119.96	122.90
4	7	2	NAG	C1-O5-C5	2.19	115.12	112.19
4	BA	1	NAG	O5-C1-C2	-2.19	107.91	111.29
4	6	2	NAG	C2-N2-C7	-2.19	119.97	122.90
8	0	2	NAG	C3-C4-C5	-2.19	106.27	110.23
4	IA	2	NAG	C2-N2-C7	-2.18	119.98	122.90
6	w	1	NAG	C2-N2-C7	-2.17	120.00	122.90
5	l	4	MAN	C1-C2-C3	2.16	112.79	109.64
4	4	2	NAG	O5-C5-C4	-2.16	105.58	110.83
4	j	2	NAG	C4-C3-C2	-2.15	107.87	111.02
4	u	1	NAG	C3-C4-C5	-2.14	106.35	110.23
5	KA	1	NAG	C3-C4-C5	-2.13	106.36	110.23
4	9	1	NAG	C1-O5-C5	2.13	115.04	112.19
4	1	2	NAG	C2-N2-C7	-2.13	120.05	122.90
4	p	1	NAG	O5-C5-C6	-2.13	103.52	107.66
6	h	1	NAG	C2-N2-C7	-2.12	120.06	122.90
6	k	2	NAG	C1-O5-C5	2.12	115.02	112.19
4	QA	1	NAG	O5-C5-C4	2.11	115.97	110.83
6	w	2	NAG	C2-N2-C7	-2.11	120.07	122.90
6	DA	3	BMA	C1-C2-C3	2.10	112.70	109.64
6	h	3	BMA	C1-C2-C3	2.08	112.67	109.64
6	5	3	BMA	C1-C2-C3	2.07	112.66	109.64
6	k	1	NAG	C1-O5-C5	2.06	114.95	112.19
4	m	1	NAG	O5-C1-C2	-2.06	108.10	111.29
4	9	1	NAG	C3-C4-C5	-2.06	106.50	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	8	2	NAG	C1-O5-C5	2.06	114.94	112.19
4	QA	1	NAG	O4-C4-C3	-2.05	105.55	110.38
6	CA	1	NAG	C2-N2-C7	-2.05	120.16	122.90
4	j	2	NAG	C1-O5-C5	2.04	114.93	112.19
4	f	1	NAG	C3-C4-C5	-2.04	106.53	110.23
4	i	2	NAG	C1-C2-N2	2.04	113.65	110.43
6	h	1	NAG	O5-C5-C4	2.03	115.77	110.83
6	NA	1	NAG	C4-C3-C2	2.03	113.99	111.02
4	4	2	NAG	O5-C1-C2	2.03	114.43	111.29
5	FA	4	MAN	C2-C3-C4	-2.02	107.30	110.86
5	KA	1	NAG	O4-C4-C3	-2.02	105.62	110.38
4	s	1	NAG	C4-C3-C2	-2.00	108.08	111.02

There are no chirality outliers.

All (239) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	e	1	NAG	C8-C7-N2-C2
4	e	1	NAG	O7-C7-N2-C2
4	f	1	NAG	C1-C2-N2-C7
4	i	1	NAG	C1-C2-N2-C7
4	j	1	NAG	C3-C2-N2-C7
4	j	1	NAG	C8-C7-N2-C2
4	j	1	NAG	O7-C7-N2-C2
4	n	1	NAG	C8-C7-N2-C2
4	n	1	NAG	O7-C7-N2-C2
4	o	1	NAG	O7-C7-N2-C2
4	q	2	NAG	C3-C2-N2-C7
4	q	2	NAG	C8-C7-N2-C2
4	q	2	NAG	O7-C7-N2-C2
4	t	1	NAG	C8-C7-N2-C2
4	t	1	NAG	O7-C7-N2-C2
4	u	1	NAG	C8-C7-N2-C2
4	u	1	NAG	O7-C7-N2-C2
4	2	1	NAG	C1-C2-N2-C7
4	4	2	NAG	C8-C7-N2-C2
4	4	2	NAG	O7-C7-N2-C2
4	7	1	NAG	O7-C7-N2-C2
4	BA	1	NAG	C3-C2-N2-C7
4	BA	1	NAG	C8-C7-N2-C2
4	BA	1	NAG	O7-C7-N2-C2
4	IA	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	IA	1	NAG	O7-C7-N2-C2
4	JA	2	NAG	C1-C2-N2-C7
4	MA	1	NAG	C8-C7-N2-C2
4	MA	1	NAG	O7-C7-N2-C2
4	MA	2	NAG	C3-C2-N2-C7
4	OA	1	NAG	C1-C2-N2-C7
4	OA	1	NAG	O7-C7-N2-C2
6	k	1	NAG	C1-C2-N2-C7
6	k	1	NAG	C8-C7-N2-C2
6	k	1	NAG	O7-C7-N2-C2
6	w	1	NAG	C8-C7-N2-C2
6	w	1	NAG	O7-C7-N2-C2
6	3	1	NAG	C1-C2-N2-C7
6	GA	1	NAG	C1-C2-N2-C7
6	LA	2	NAG	C1-C2-N2-C7
6	NA	1	NAG	C8-C7-N2-C2
6	NA	1	NAG	O7-C7-N2-C2
6	NA	2	NAG	C8-C7-N2-C2
6	NA	2	NAG	O7-C7-N2-C2
4	j	2	NAG	C8-C7-N2-C2
4	o	1	NAG	C8-C7-N2-C2
4	7	1	NAG	C8-C7-N2-C2
4	7	2	NAG	C8-C7-N2-C2
4	7	2	NAG	O7-C7-N2-C2
4	OA	1	NAG	C8-C7-N2-C2
5	AA	1	NAG	C8-C7-N2-C2
5	AA	1	NAG	O7-C7-N2-C2
6	r	1	NAG	C8-C7-N2-C2
6	r	1	NAG	O7-C7-N2-C2
6	r	2	NAG	C8-C7-N2-C2
6	r	2	NAG	O7-C7-N2-C2
4	x	1	NAG	O5-C5-C6-O6
4	i	1	NAG	O5-C5-C6-O6
4	u	1	NAG	O5-C5-C6-O6
4	8	1	NAG	O5-C5-C6-O6
4	HA	1	NAG	O5-C5-C6-O6
6	k	1	NAG	O5-C5-C6-O6
6	y	1	NAG	O5-C5-C6-O6
6	5	3	BMA	O5-C5-C6-O6
4	j	2	NAG	O5-C5-C6-O6
6	3	1	NAG	O5-C5-C6-O6
6	5	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	g	3	BMA	C4-C5-C6-O6
4	j	2	NAG	O7-C7-N2-C2
5	KA	1	NAG	C8-C7-N2-C2
5	KA	1	NAG	O7-C7-N2-C2
4	j	1	NAG	O5-C5-C6-O6
4	s	2	NAG	O5-C5-C6-O6
4	7	1	NAG	O5-C5-C6-O6
4	BA	2	NAG	O5-C5-C6-O6
4	JA	1	NAG	O5-C5-C6-O6
4	MA	1	NAG	O5-C5-C6-O6
4	OA	1	NAG	O5-C5-C6-O6
4	RA	1	NAG	O5-C5-C6-O6
5	l	1	NAG	O5-C5-C6-O6
6	EA	1	NAG	O5-C5-C6-O6
8	0	1	NAG	O5-C5-C6-O6
4	o	1	NAG	O5-C5-C6-O6
4	p	1	NAG	O5-C5-C6-O6
4	IA	1	NAG	O5-C5-C6-O6
6	LA	1	NAG	O5-C5-C6-O6
4	u	1	NAG	C4-C5-C6-O6
4	BA	2	NAG	C4-C5-C6-O6
4	JA	1	NAG	C4-C5-C6-O6
4	n	1	NAG	O5-C5-C6-O6
4	x	1	NAG	C4-C5-C6-O6
4	4	1	NAG	O5-C5-C6-O6
5	FA	1	NAG	O5-C5-C6-O6
4	OA	1	NAG	C4-C5-C6-O6
4	f	1	NAG	O5-C5-C6-O6
4	v	2	NAG	O5-C5-C6-O6
4	7	1	NAG	C4-C5-C6-O6
4	HA	1	NAG	C4-C5-C6-O6
6	k	1	NAG	C4-C5-C6-O6
6	y	1	NAG	C4-C5-C6-O6
8	0	1	NAG	C4-C5-C6-O6
5	KA	1	NAG	O5-C5-C6-O6
4	i	1	NAG	C4-C5-C6-O6
4	p	1	NAG	C4-C5-C6-O6
6	5	1	NAG	C4-C5-C6-O6
4	m	2	NAG	C8-C7-N2-C2
6	DA	1	NAG	C8-C7-N2-C2
6	DA	1	NAG	O7-C7-N2-C2
6	LA	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	LA	1	NAG	O7-C7-N2-C2
8	0	2	NAG	C8-C7-N2-C2
4	JA	2	NAG	O5-C5-C6-O6
6	GA	1	NAG	O5-C5-C6-O6
4	4	2	NAG	O5-C5-C6-O6
5	g	3	BMA	O5-C5-C6-O6
4	j	2	NAG	C4-C5-C6-O6
4	IA	1	NAG	C4-C5-C6-O6
6	LA	1	NAG	C4-C5-C6-O6
4	m	2	NAG	O5-C5-C6-O6
6	r	1	NAG	O5-C5-C6-O6
4	IA	2	NAG	O5-C5-C6-O6
5	PA	1	NAG	O5-C5-C6-O6
4	v	2	NAG	C4-C5-C6-O6
4	4	2	NAG	C4-C5-C6-O6
5	FA	1	NAG	C4-C5-C6-O6
6	5	3	BMA	C4-C5-C6-O6
4	o	1	NAG	C4-C5-C6-O6
4	s	1	NAG	C4-C5-C6-O6
5	l	1	NAG	C4-C5-C6-O6
5	KA	1	NAG	C4-C5-C6-O6
7	z	3	BMA	C4-C5-C6-O6
4	m	2	NAG	O7-C7-N2-C2
4	HA	1	NAG	C8-C7-N2-C2
8	0	2	NAG	O7-C7-N2-C2
6	r	2	NAG	O5-C5-C6-O6
4	f	1	NAG	C4-C5-C6-O6
4	8	1	NAG	C4-C5-C6-O6
4	MA	1	NAG	C4-C5-C6-O6
4	RA	1	NAG	C4-C5-C6-O6
6	EA	1	NAG	C4-C5-C6-O6
4	j	1	NAG	C4-C5-C6-O6
5	PA	1	NAG	C4-C5-C6-O6
6	3	1	NAG	C4-C5-C6-O6
4	q	1	NAG	O5-C5-C6-O6
4	s	2	NAG	C4-C5-C6-O6
4	4	1	NAG	C4-C5-C6-O6
6	GA	1	NAG	C4-C5-C6-O6
4	RA	2	NAG	O5-C5-C6-O6
4	s	1	NAG	C8-C7-N2-C2
4	BA	2	NAG	C8-C7-N2-C2
4	HA	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	GA	1	NAG	C8-C7-N2-C2
5	AA	2	NAG	O5-C5-C6-O6
4	n	1	NAG	C4-C5-C6-O6
4	IA	2	NAG	C4-C5-C6-O6
4	JA	2	NAG	C4-C5-C6-O6
6	r	2	NAG	C4-C5-C6-O6
4	m	2	NAG	C4-C5-C6-O6
6	5	2	NAG	O5-C5-C6-O6
6	5	2	NAG	C4-C5-C6-O6
4	s	1	NAG	O5-C5-C6-O6
6	GA	1	NAG	O7-C7-N2-C2
4	1	1	NAG	C4-C5-C6-O6
4	v	1	NAG	O5-C5-C6-O6
4	s	1	NAG	O7-C7-N2-C2
4	4	1	NAG	C8-C7-N2-C2
4	8	1	NAG	C8-C7-N2-C2
4	BA	2	NAG	O7-C7-N2-C2
4	1	1	NAG	O5-C5-C6-O6
7	z	3	BMA	O5-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
4	i	1	NAG	C8-C7-N2-C2
4	m	1	NAG	O5-C5-C6-O6
4	BA	1	NAG	C4-C5-C6-O6
6	3	3	BMA	O5-C5-C6-O6
5	g	1	NAG	O5-C5-C6-O6
4	4	1	NAG	O7-C7-N2-C2
5	AA	1	NAG	O5-C5-C6-O6
4	q	1	NAG	C4-C5-C6-O6
4	8	1	NAG	O7-C7-N2-C2
4	OA	2	NAG	O5-C5-C6-O6
4	OA	2	NAG	C4-C5-C6-O6
4	q	2	NAG	O5-C5-C6-O6
4	s	2	NAG	C3-C2-N2-C7
4	2	1	NAG	C3-C2-N2-C7
4	JA	2	NAG	C3-C2-N2-C7
4	OA	1	NAG	C3-C2-N2-C7
4	OA	2	NAG	C3-C2-N2-C7
6	LA	2	NAG	C3-C2-N2-C7
6	NA	1	NAG	C3-C2-N2-C7
6	NA	2	NAG	C3-C2-N2-C7
7	z	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	AA	2	NAG	C4-C5-C6-O6
6	w	1	NAG	O5-C5-C6-O6
5	g	1	NAG	C4-C5-C6-O6
4	i	1	NAG	O7-C7-N2-C2
5	AA	2	NAG	C8-C7-N2-C2
4	9	1	NAG	C4-C5-C6-O6
4	m	2	NAG	C1-C2-N2-C7
4	OA	2	NAG	C1-C2-N2-C7
6	NA	1	NAG	C1-C2-N2-C7
4	v	1	NAG	C4-C5-C6-O6
5	AA	1	NAG	C4-C5-C6-O6
4	7	2	NAG	C4-C5-C6-O6
6	h	1	NAG	C4-C5-C6-O6
5	AA	2	NAG	O7-C7-N2-C2
7	z	4	MAN	O5-C5-C6-O6
4	j	2	NAG	C3-C2-N2-C7
4	m	2	NAG	C3-C2-N2-C7
4	HA	1	NAG	C3-C2-N2-C7
5	g	2	NAG	C3-C2-N2-C7
6	h	1	NAG	C3-C2-N2-C7
4	BA	1	NAG	O5-C5-C6-O6
4	m	1	NAG	C4-C5-C6-O6
6	w	1	NAG	C4-C5-C6-O6
4	RA	2	NAG	C4-C5-C6-O6
4	6	1	NAG	O5-C5-C6-O6
4	m	1	NAG	C8-C7-N2-C2
4	RA	1	NAG	C8-C7-N2-C2
4	q	1	NAG	C8-C7-N2-C2
6	r	1	NAG	C4-C5-C6-O6
4	IA	2	NAG	C8-C7-N2-C2
4	x	1	NAG	C1-C2-N2-C7
4	4	1	NAG	C1-C2-N2-C7
4	MA	1	NAG	C1-C2-N2-C7
6	w	2	NAG	C1-C2-N2-C7
4	9	1	NAG	O5-C5-C6-O6
4	i	1	NAG	C3-C2-N2-C7
4	x	1	NAG	C3-C2-N2-C7
4	6	1	NAG	C4-C5-C6-O6
6	3	3	BMA	C4-C5-C6-O6
4	7	2	NAG	O5-C5-C6-O6
4	m	1	NAG	O7-C7-N2-C2
4	RA	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	IA	2	NAG	O7-C7-N2-C2
4	o	2	NAG	C8-C7-N2-C2
4	o	2	NAG	O7-C7-N2-C2
4	q	1	NAG	O7-C7-N2-C2

There are no ring outliers.

78 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	o	1	NAG	3	0
4	RA	1	NAG	1	0
4	MA	1	NAG	7	0
6	NA	2	NAG	2	0
6	5	2	NAG	2	0
6	CA	1	NAG	2	0
6	GA	3	BMA	2	0
4	RA	2	NAG	1	0
4	s	1	NAG	2	0
5	l	3	BMA	1	0
4	n	1	NAG	1	0
4	MA	2	NAG	5	0
4	HA	2	NAG	2	0
4	9	2	NAG	1	0
4	v	2	NAG	2	0
6	DA	1	NAG	2	0
4	u	1	NAG	6	0
4	t	1	NAG	1	0
4	m	2	NAG	4	0
6	EA	1	NAG	1	0
6	LA	3	BMA	1	0
6	w	1	NAG	2	0
4	j	2	NAG	3	0
6	NA	1	NAG	3	0
5	FA	3	BMA	1	0
6	CA	2	NAG	3	0
6	GA	2	NAG	9	0
4	9	1	NAG	2	0
4	1	1	NAG	1	0
4	QA	1	NAG	4	0
6	5	3	BMA	1	0
6	h	2	NAG	1	0
4	JA	1	NAG	2	0

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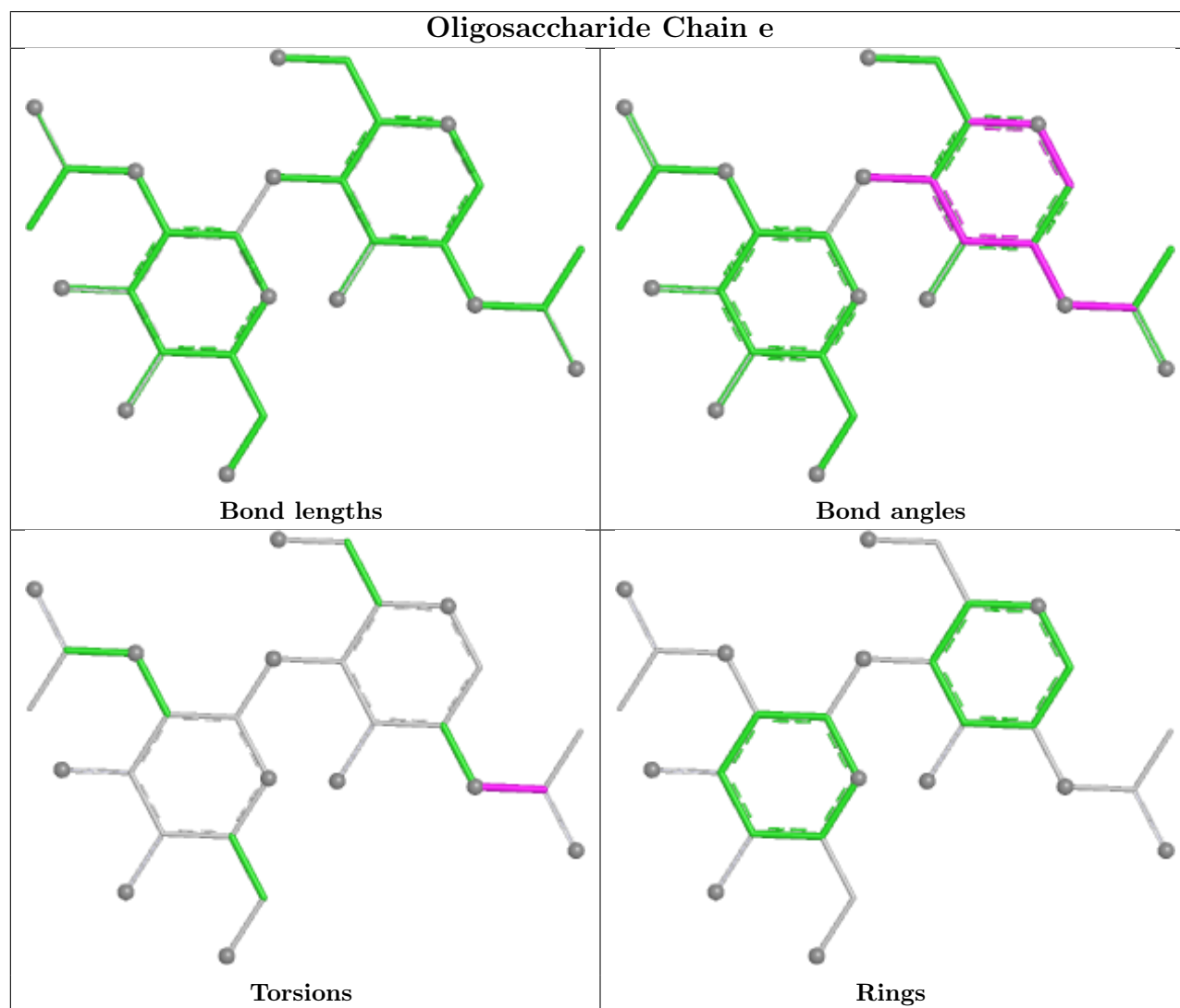
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	r	1	NAG	8	0
6	DA	2	NAG	2	0
4	q	1	NAG	3	0
5	l	1	NAG	1	0
4	i	1	NAG	3	0
4	6	1	NAG	2	0
6	k	1	NAG	4	0
4	OA	1	NAG	2	0
7	z	4	MAN	2	0
8	0	1	NAG	6	0
4	i	2	NAG	1	0
5	l	4	MAN	1	0
5	l	2	NAG	1	0
4	q	2	NAG	7	0
4	2	1	NAG	1	0
6	GA	1	NAG	7	0
8	0	2	NAG	8	0
6	5	1	NAG	1	0
4	v	1	NAG	1	0
8	0	3	BMA	1	0
4	JA	2	NAG	1	0
4	BA	2	NAG	3	0
7	z	3	BMA	2	0
4	BA	1	NAG	3	0
4	HA	1	NAG	4	0
4	OA	2	NAG	1	0
6	LA	1	NAG	3	0
5	FA	1	NAG	1	0
5	PA	1	NAG	1	0
5	FA	4	MAN	1	0
6	r	2	NAG	3	0
4	7	1	NAG	6	0
4	m	1	NAG	9	0
4	f	1	NAG	2	0
5	KA	1	NAG	1	0
4	n	2	NAG	1	0
6	3	2	NAG	1	0
4	7	2	NAG	6	0
6	k	2	NAG	1	0
6	LA	2	NAG	5	0
5	FA	2	NAG	1	0
4	j	1	NAG	4	0

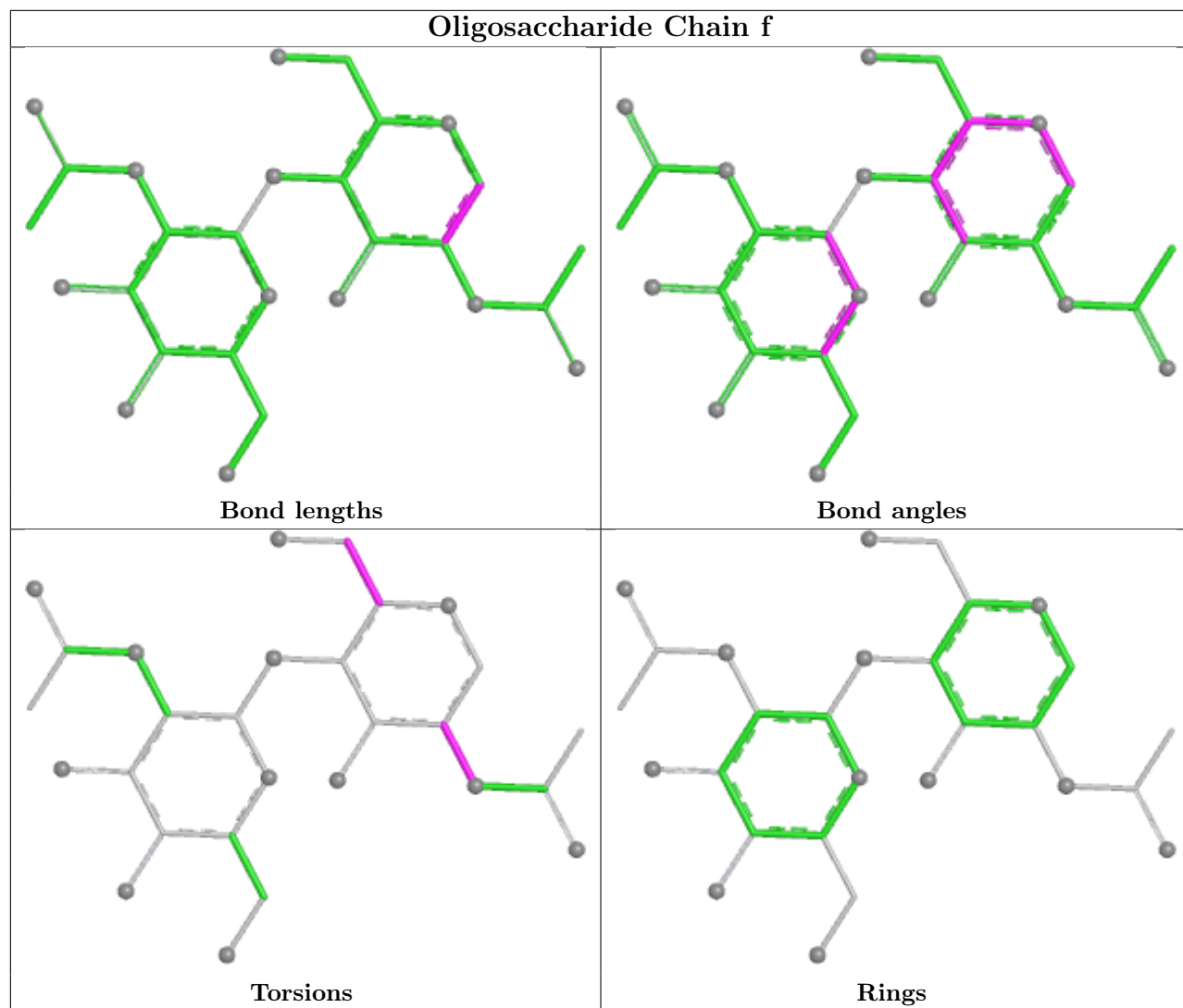
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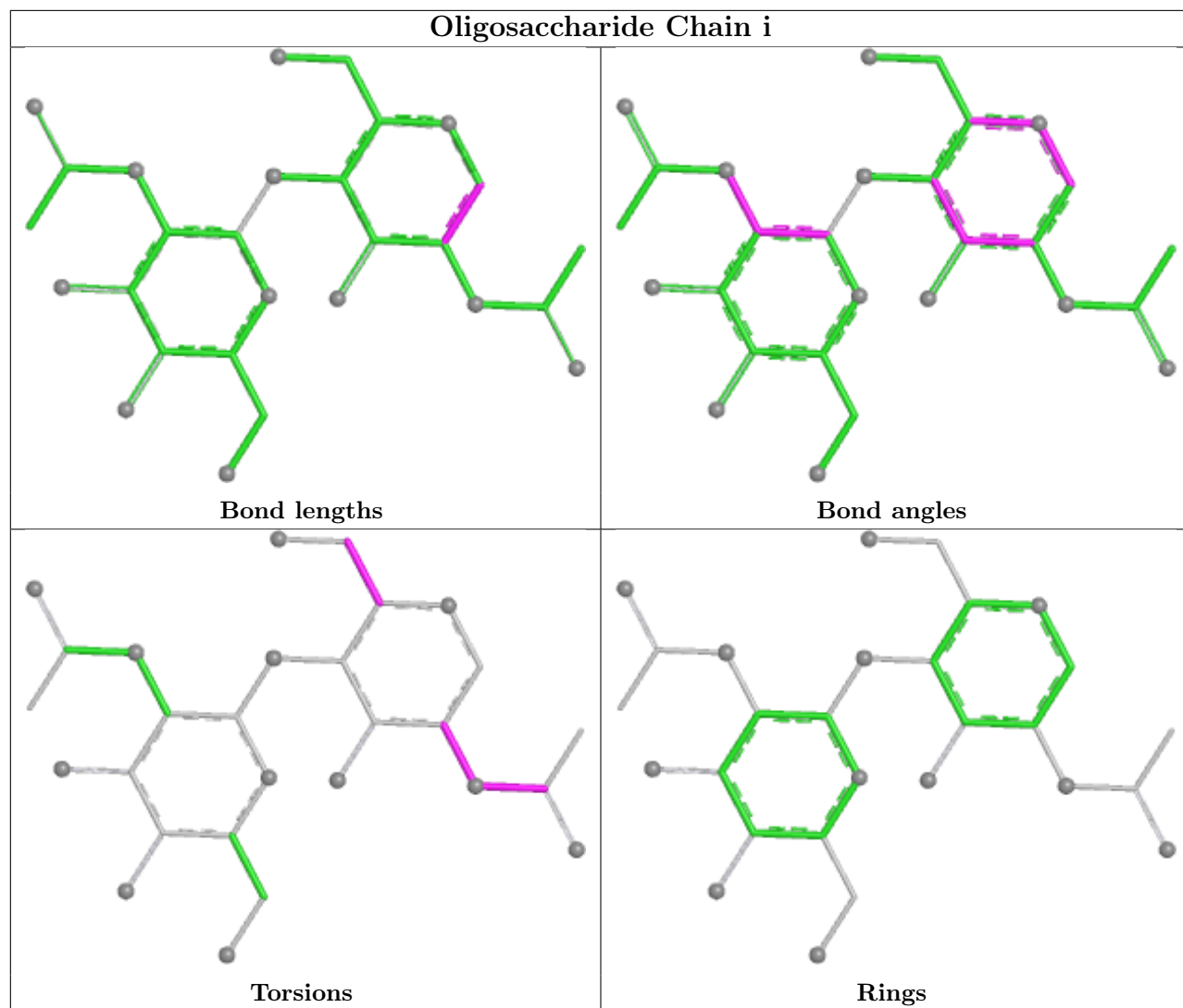
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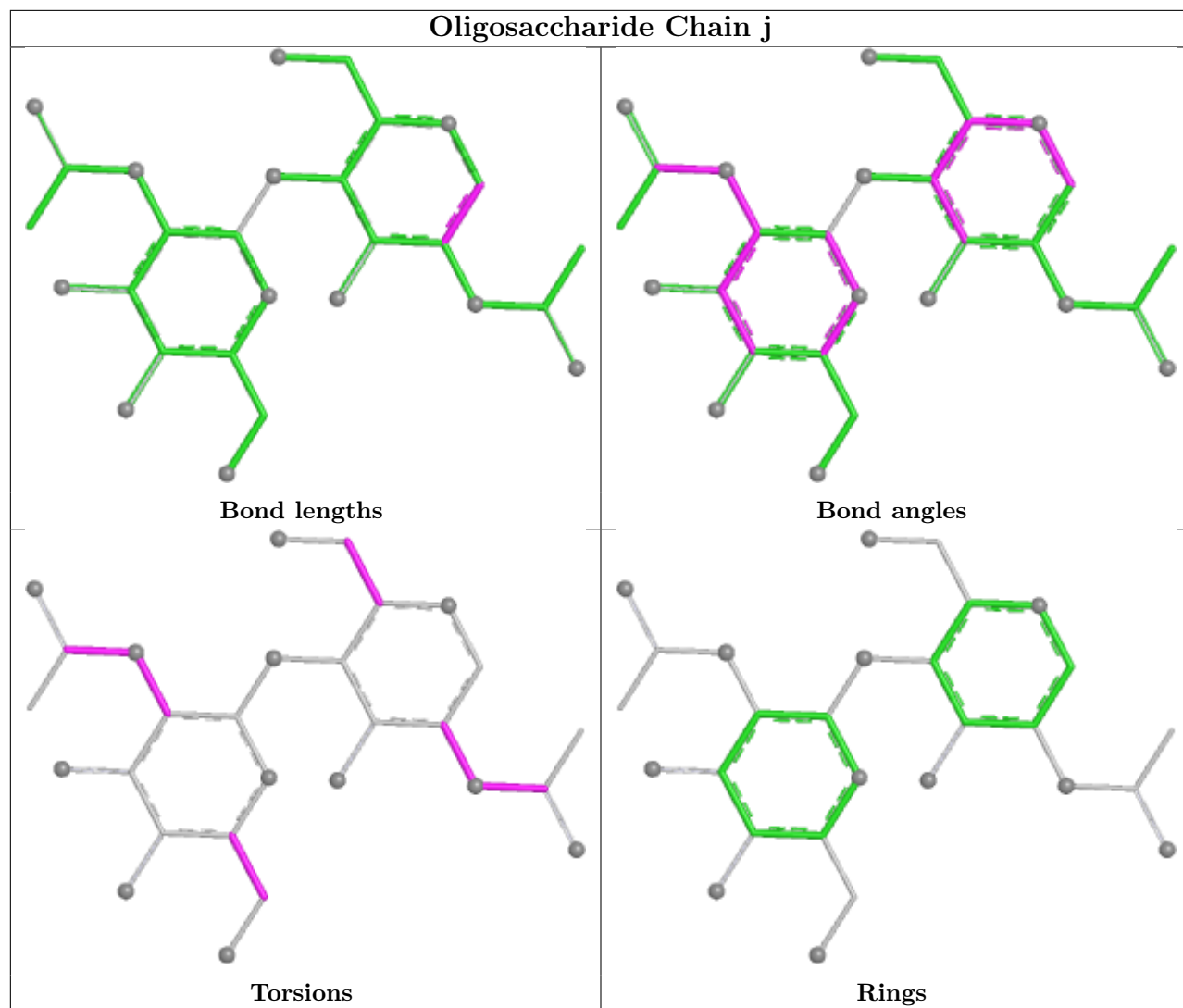
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	3	1	NAG	3	0
5	AA	1	NAG	1	0
5	PA	2	NAG	1	0

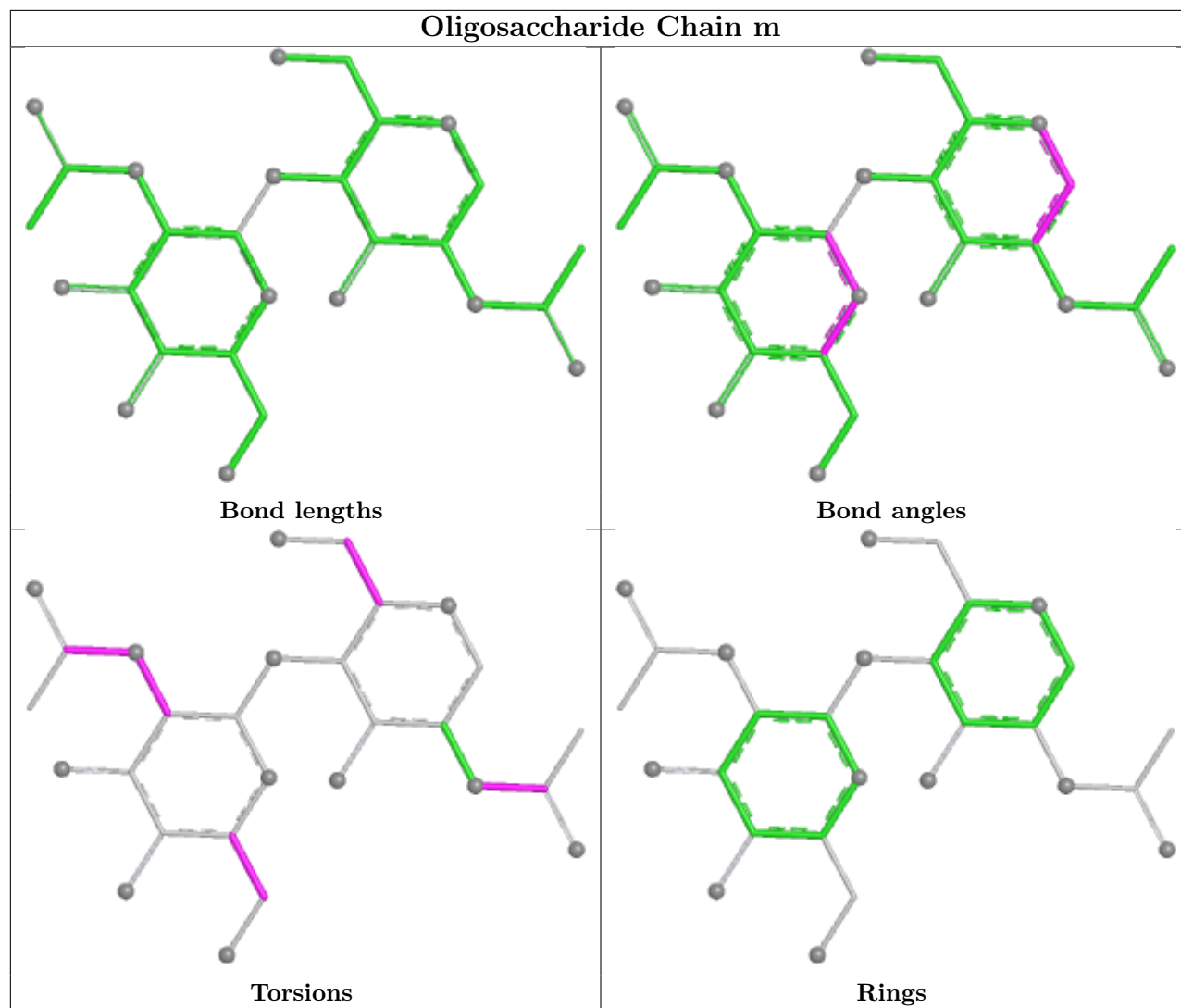
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

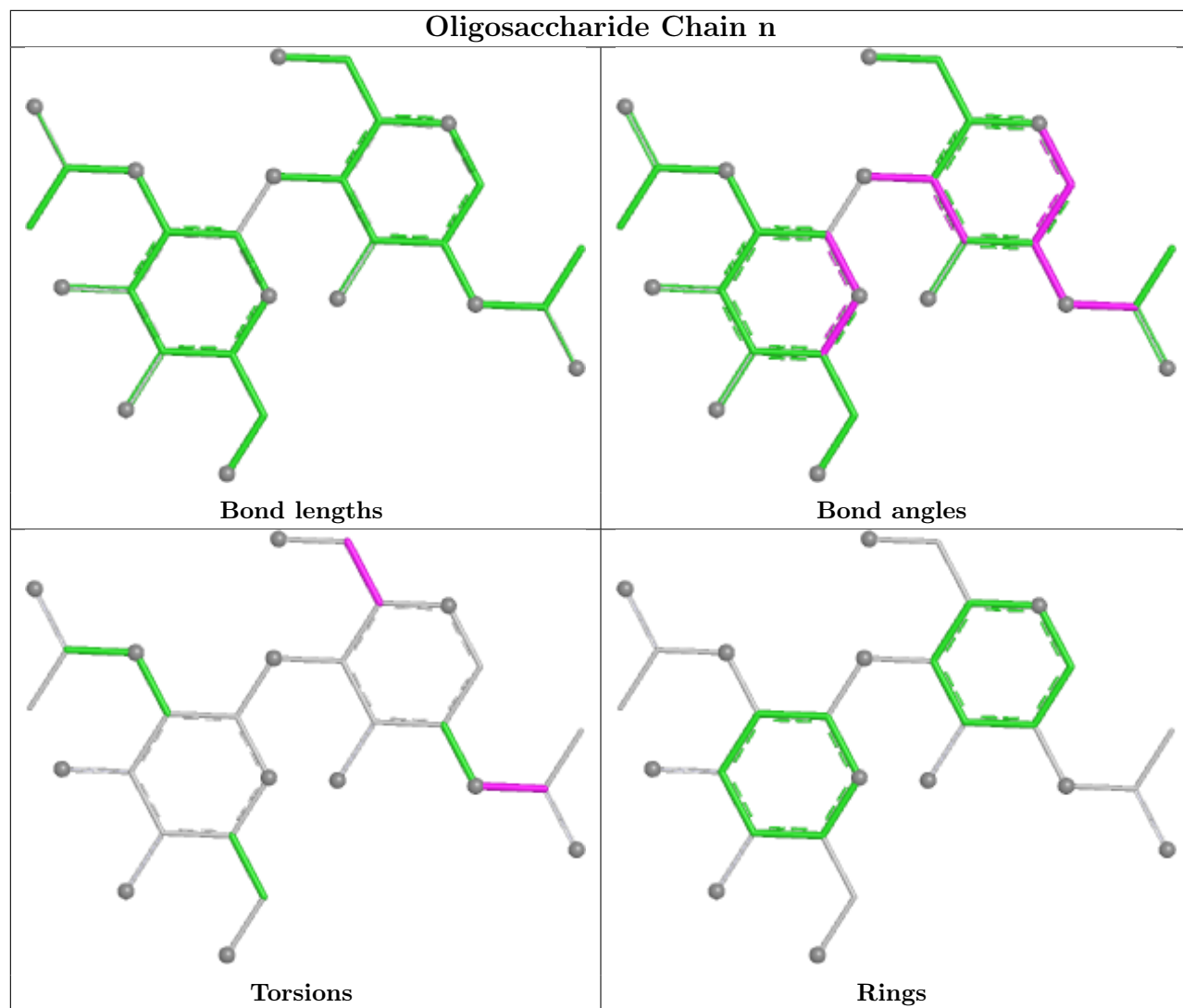


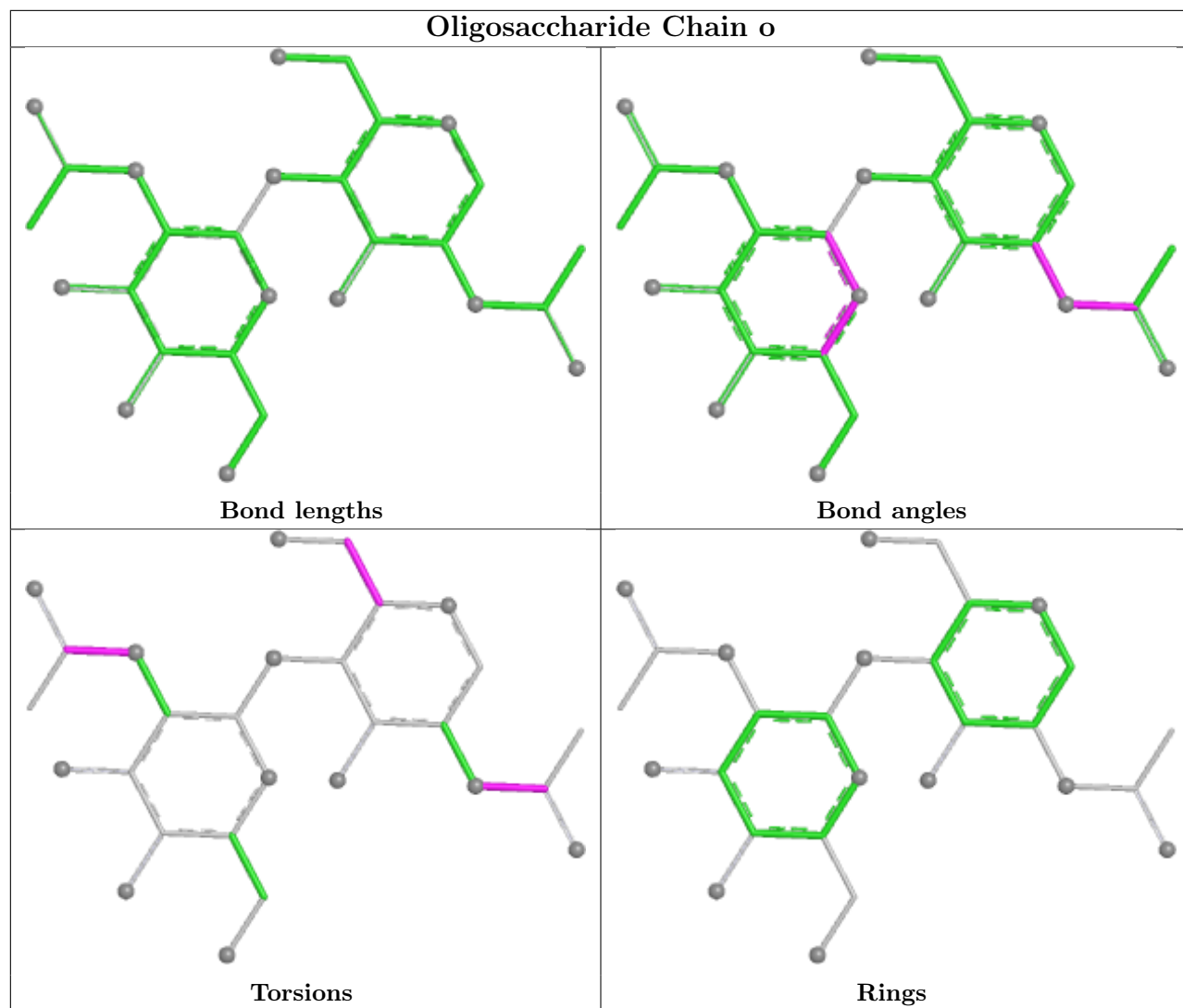


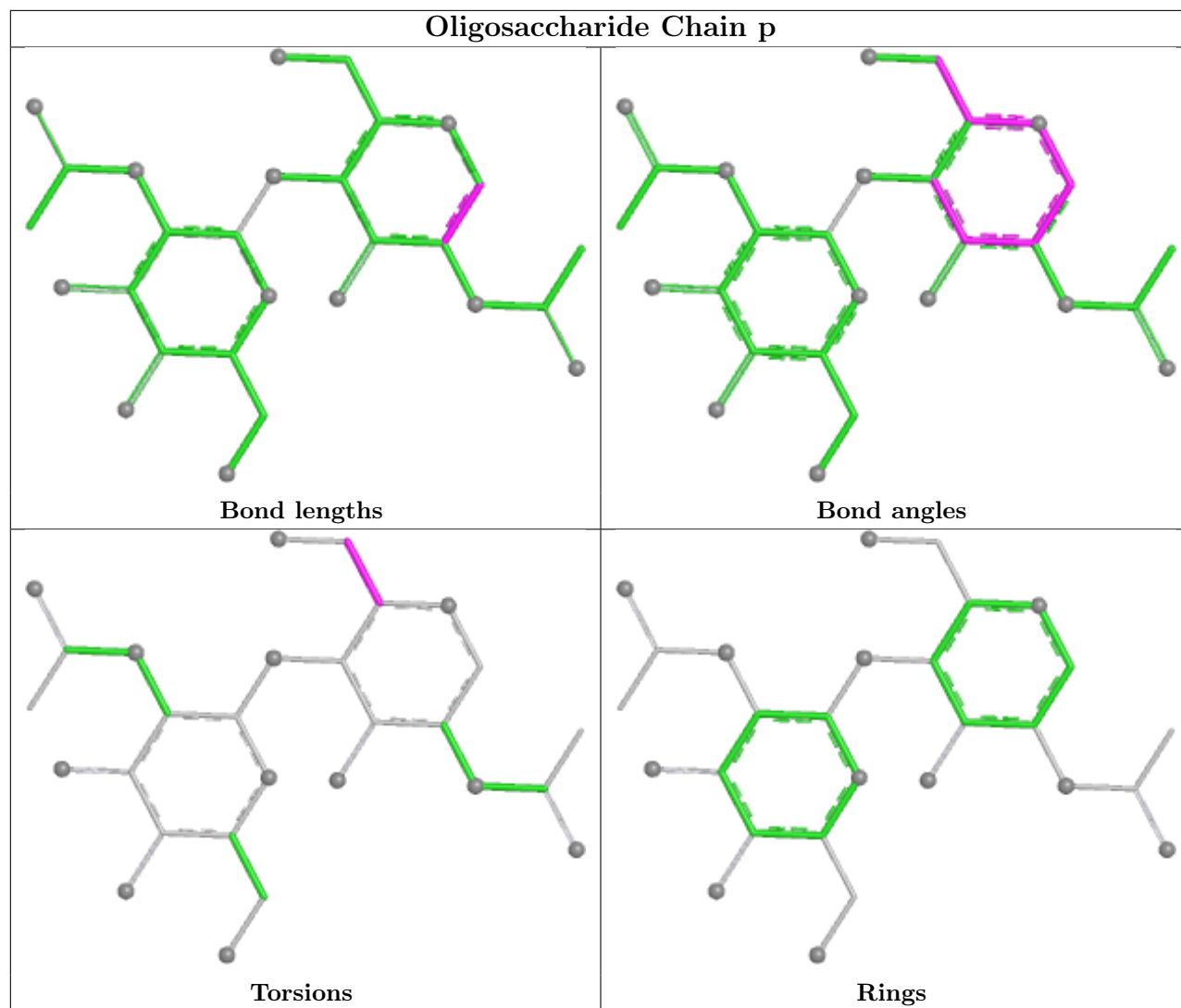


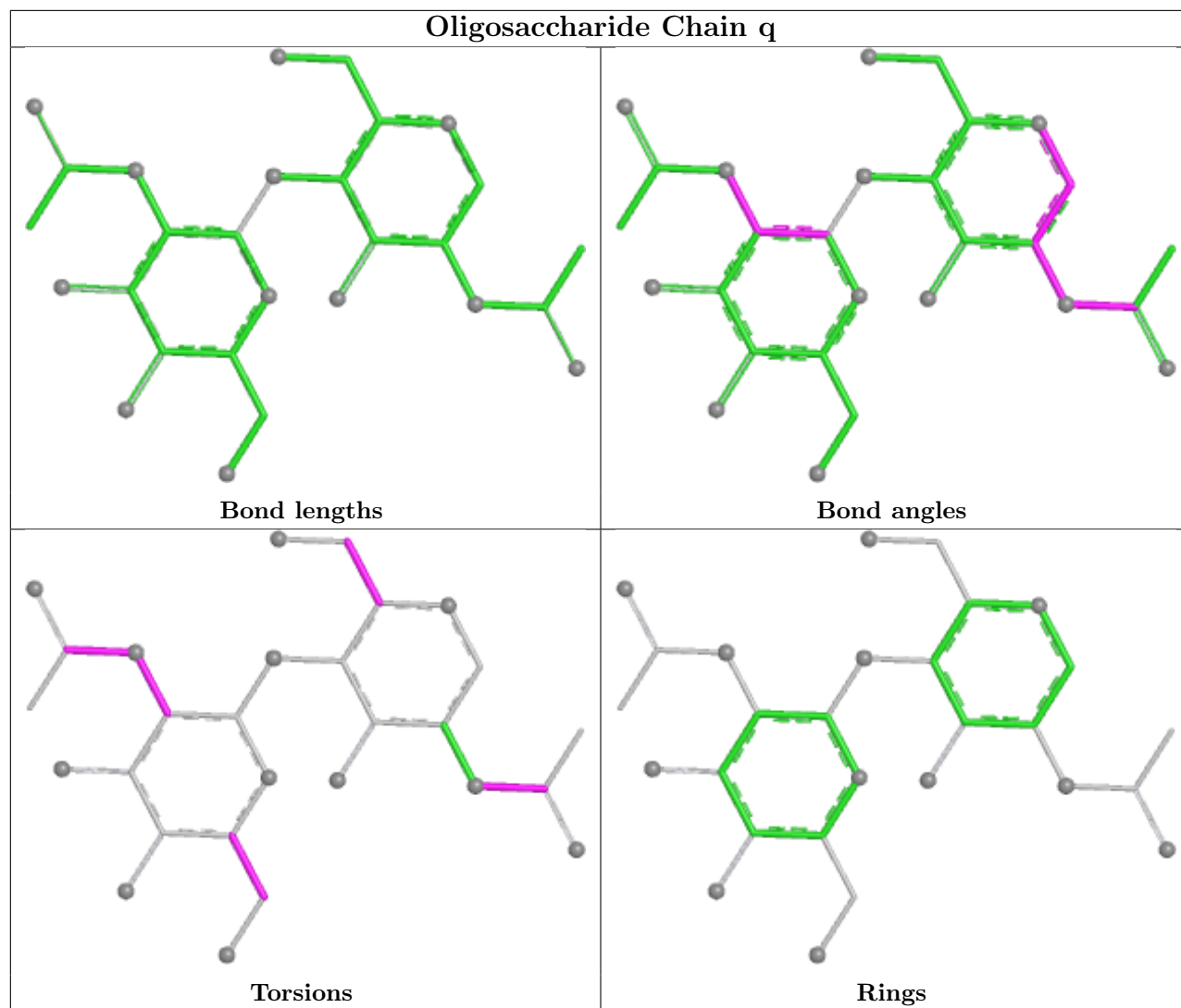


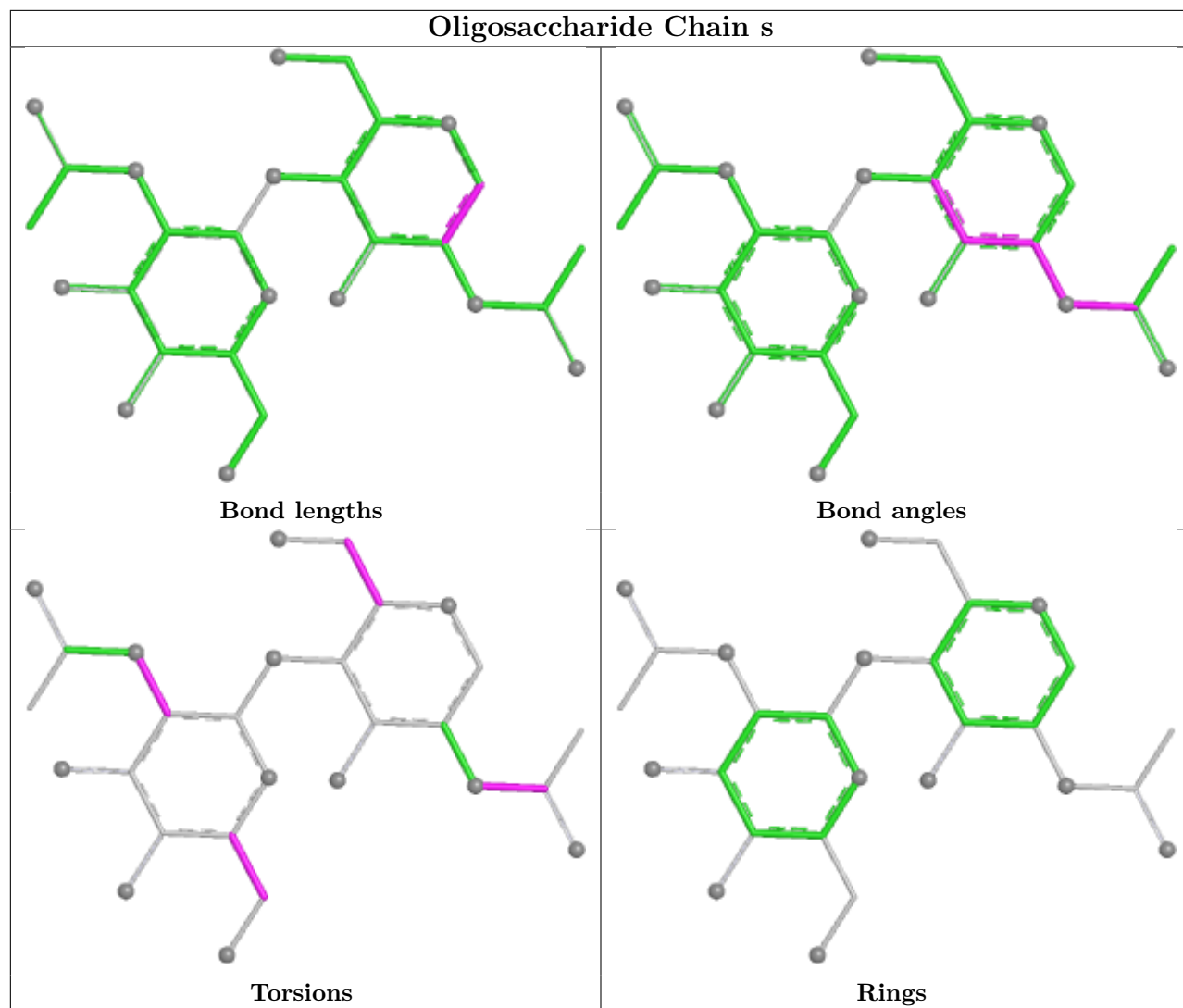


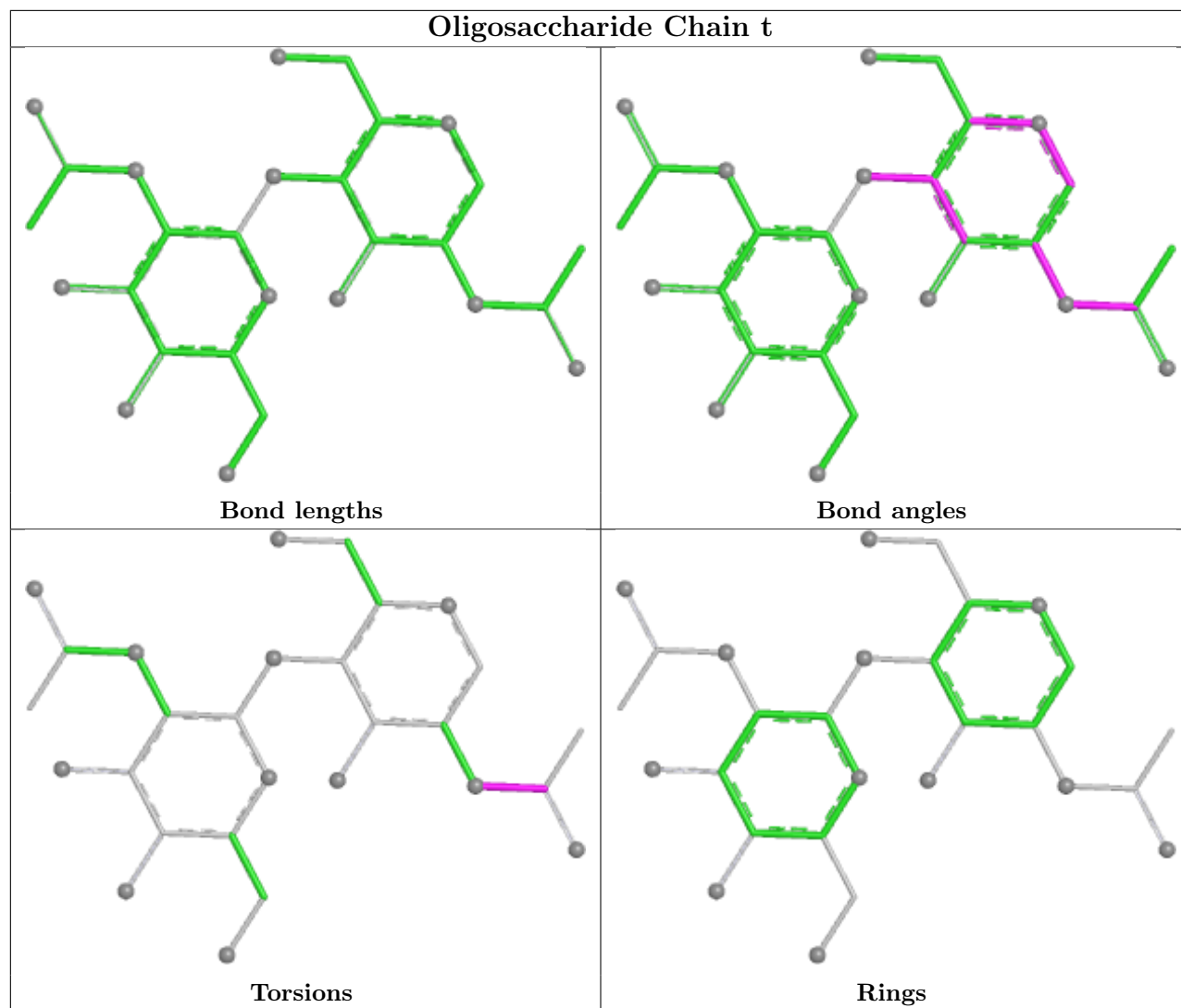


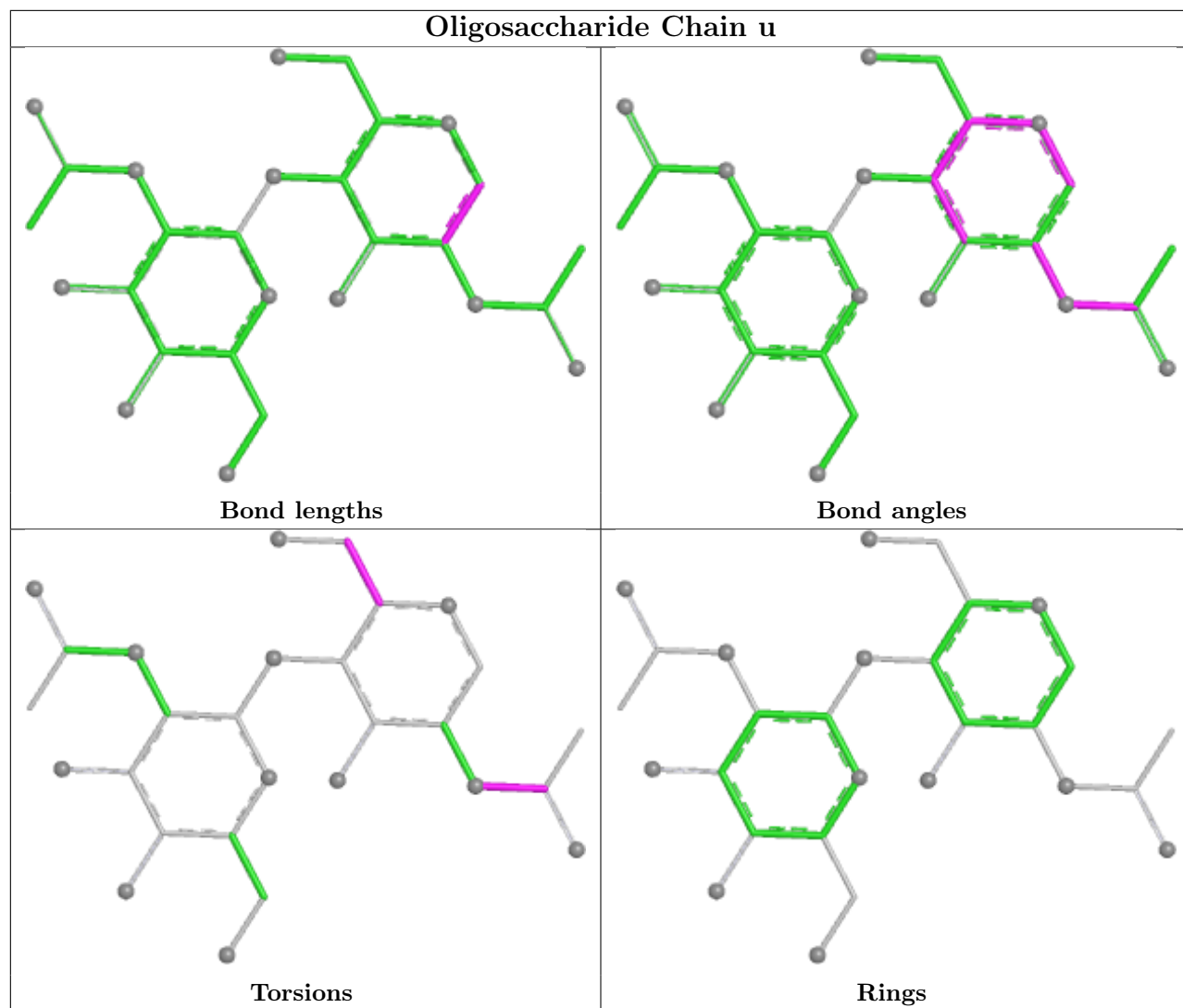


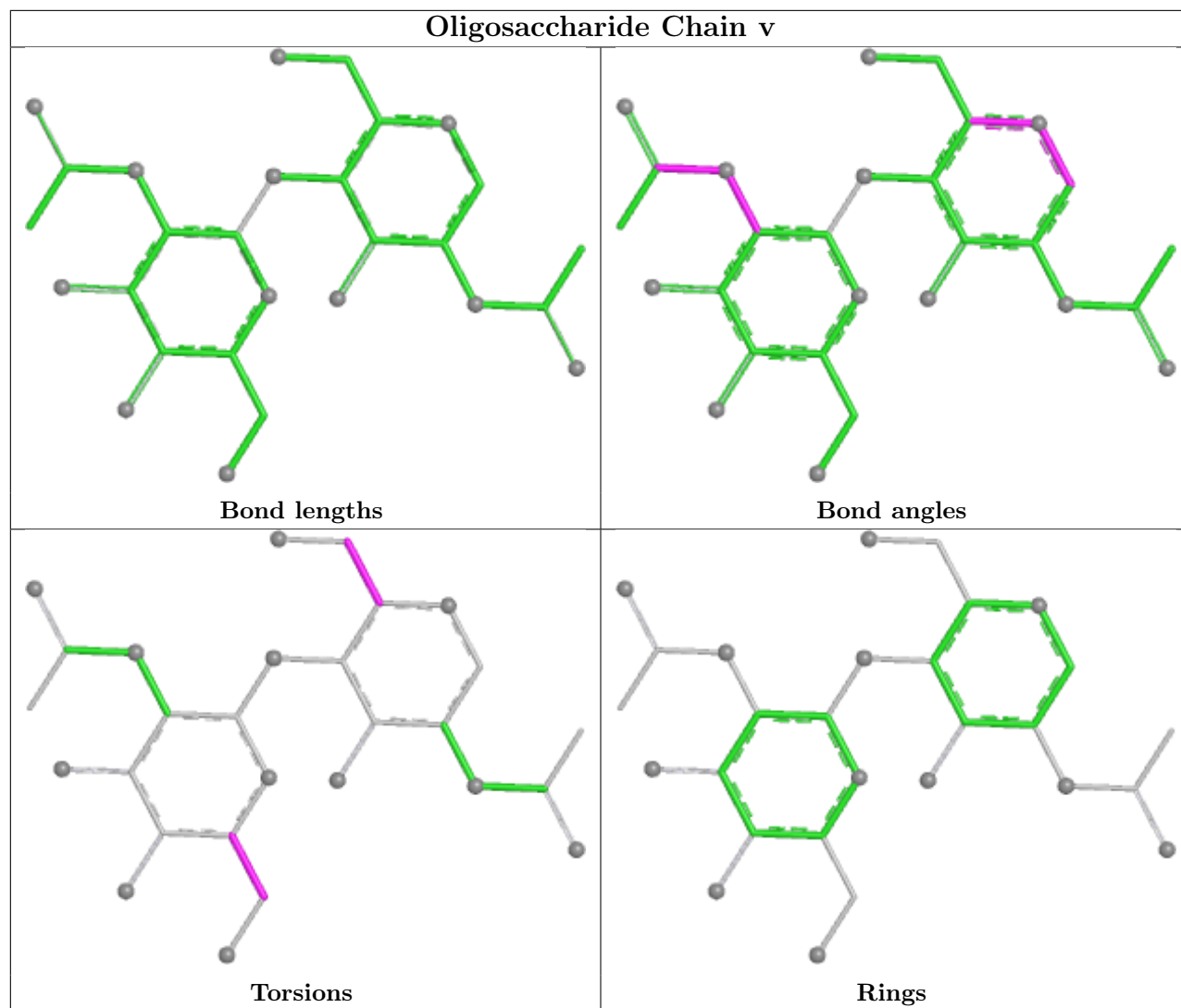


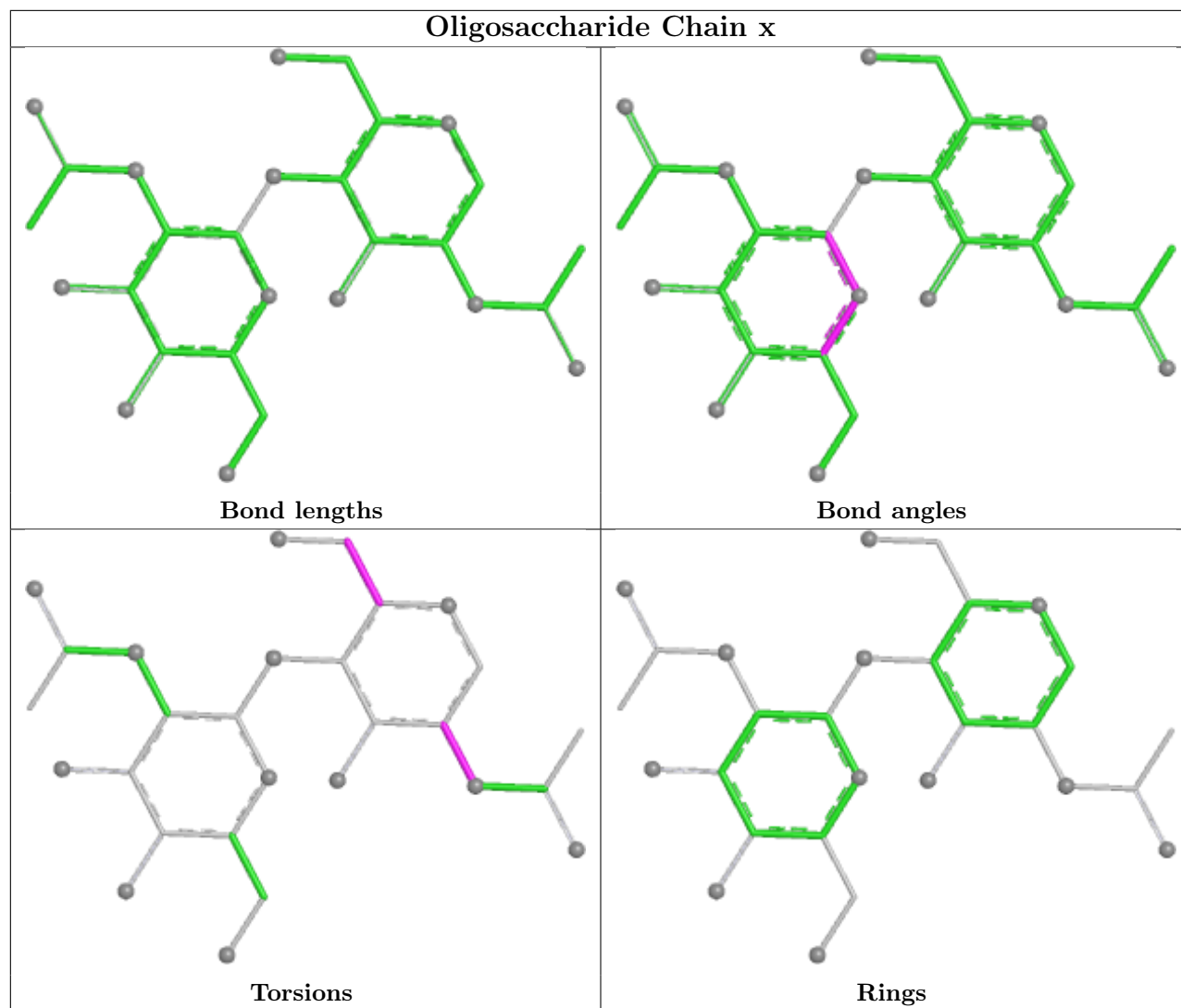


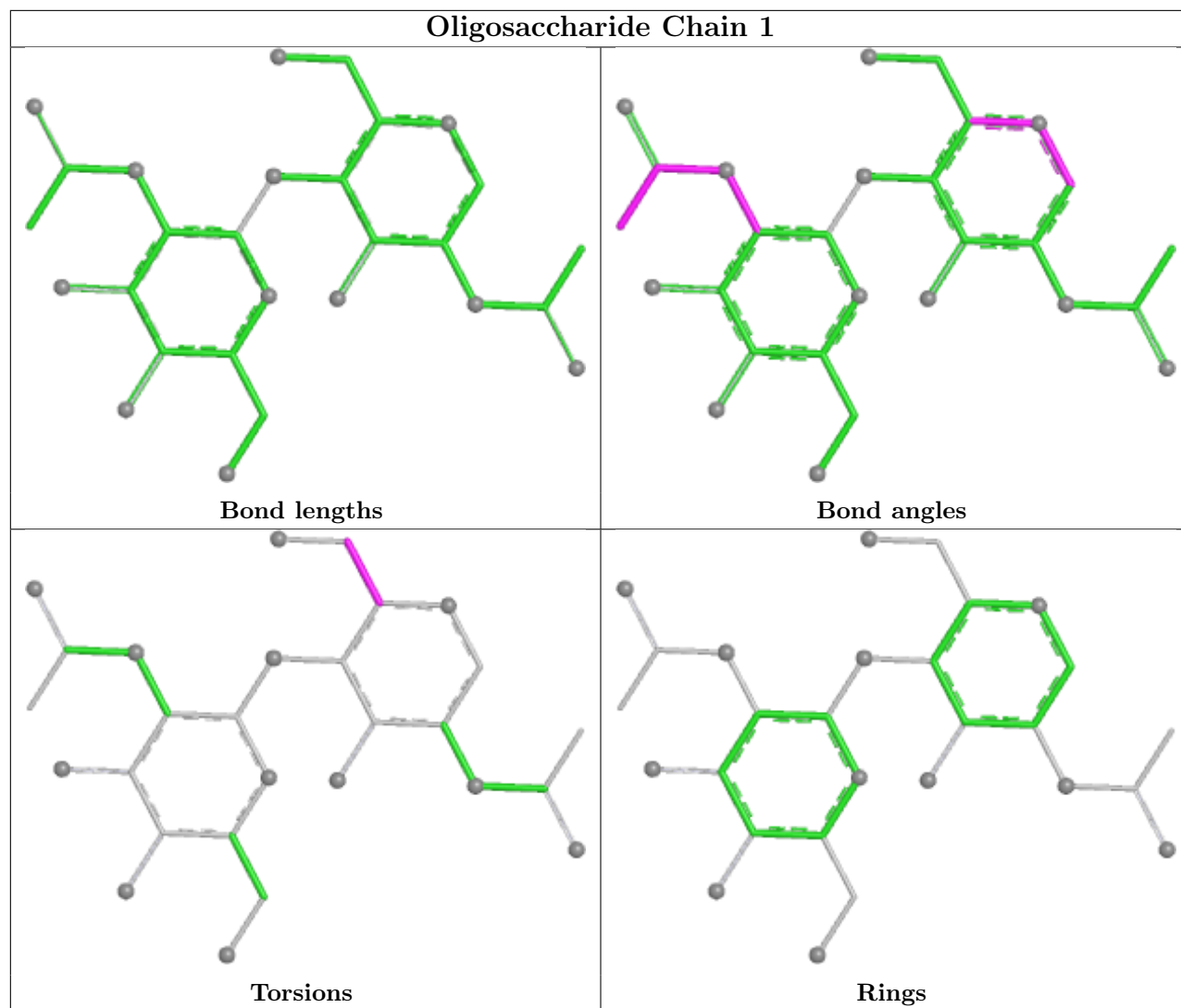


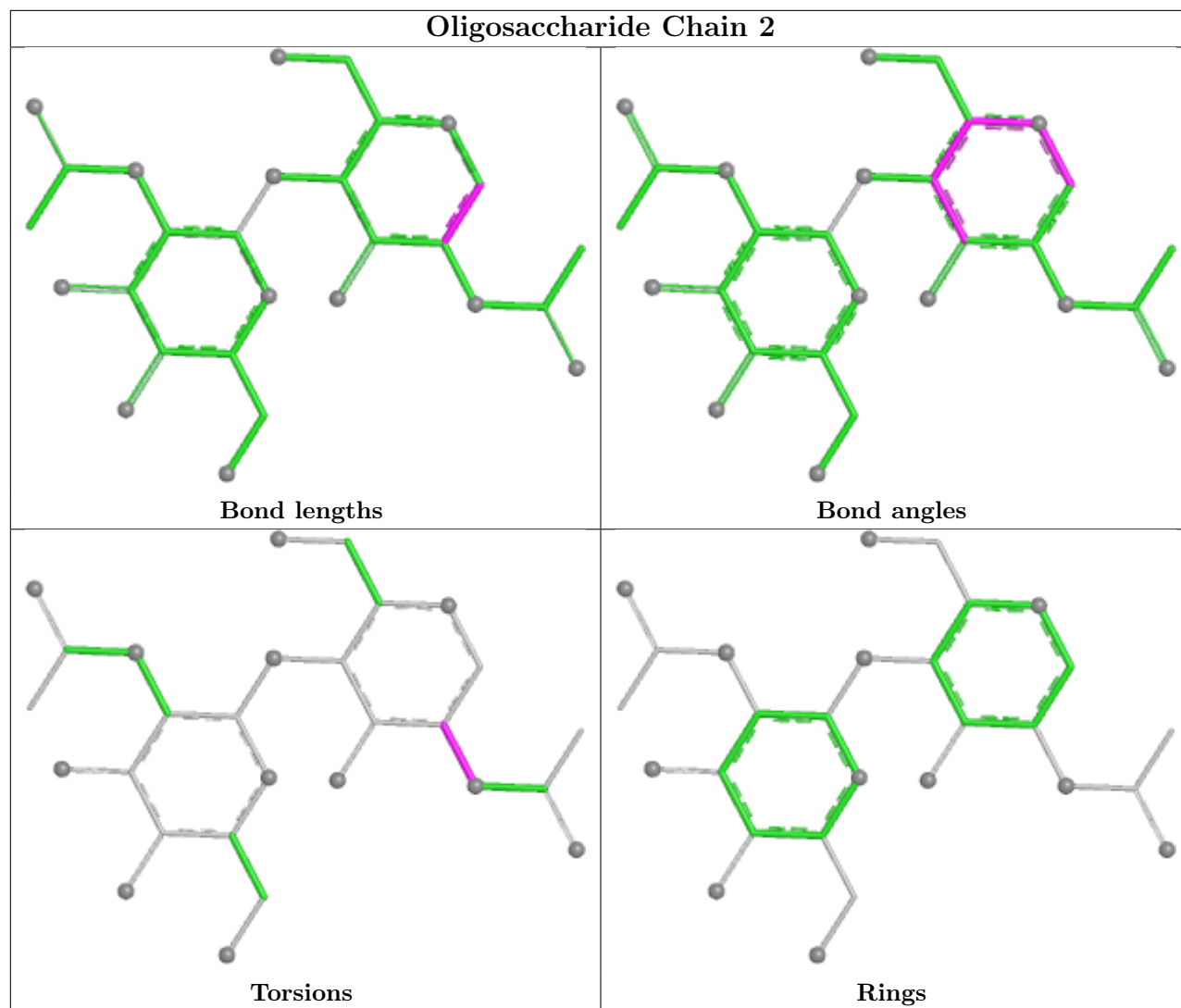


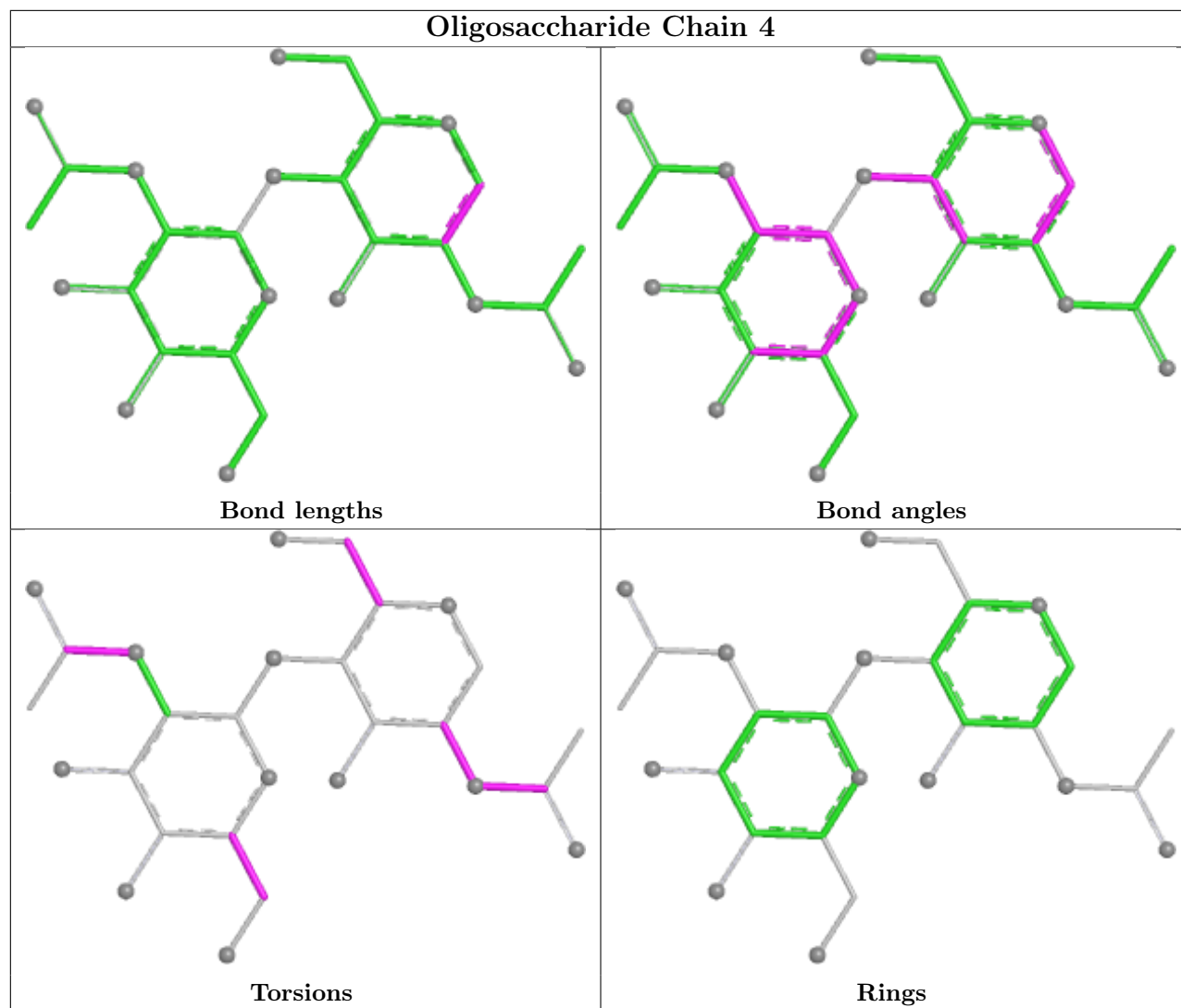


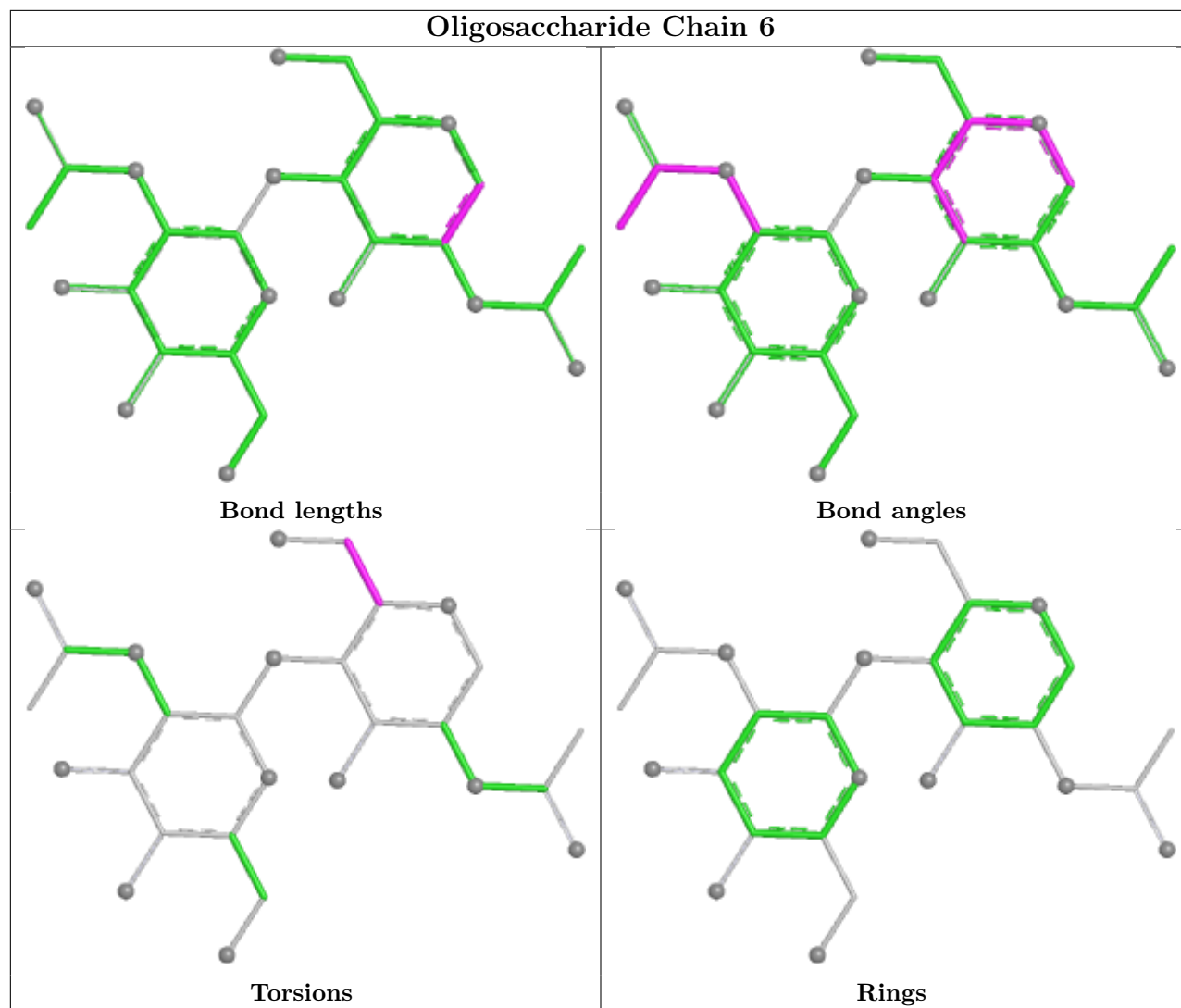


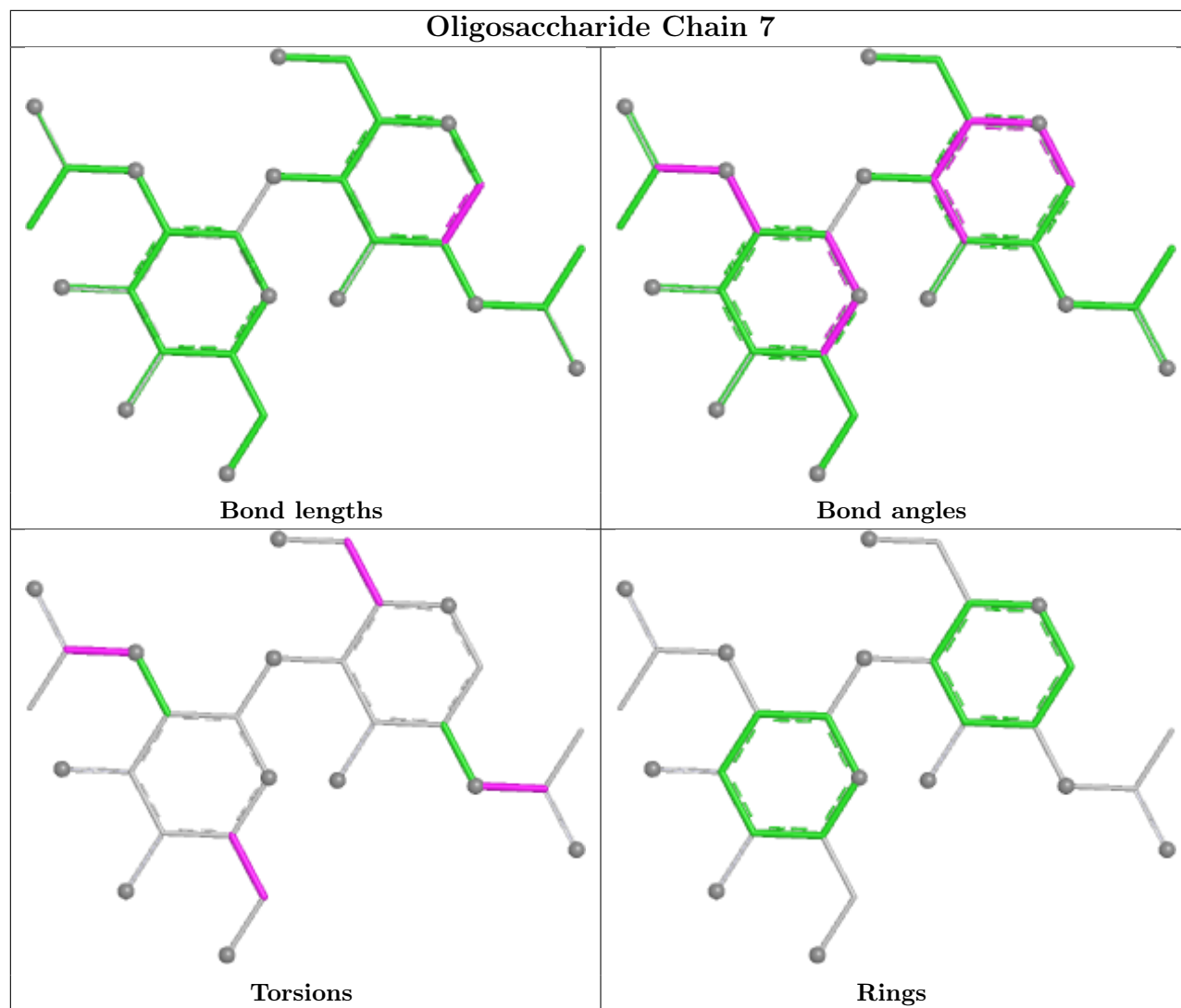


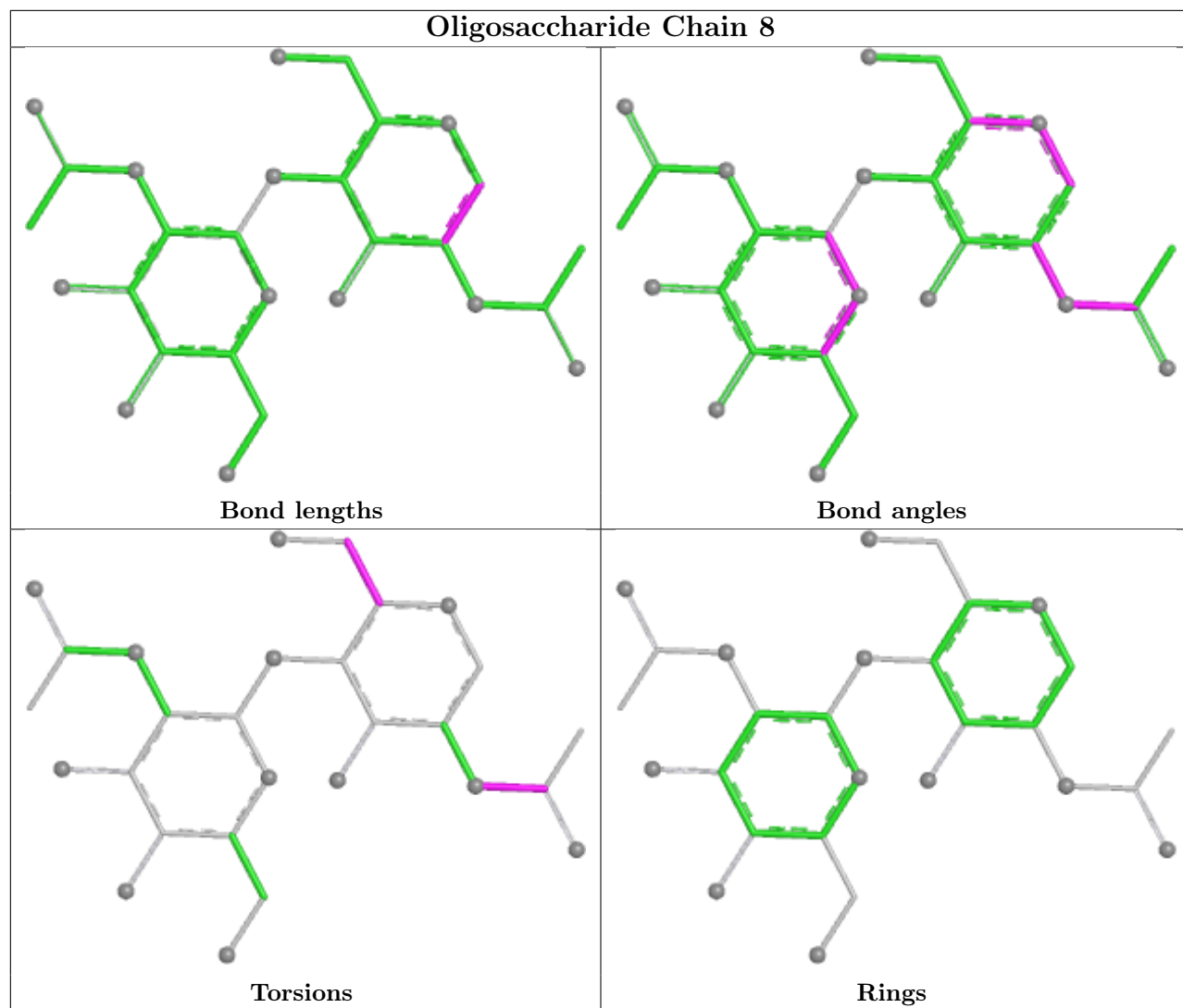


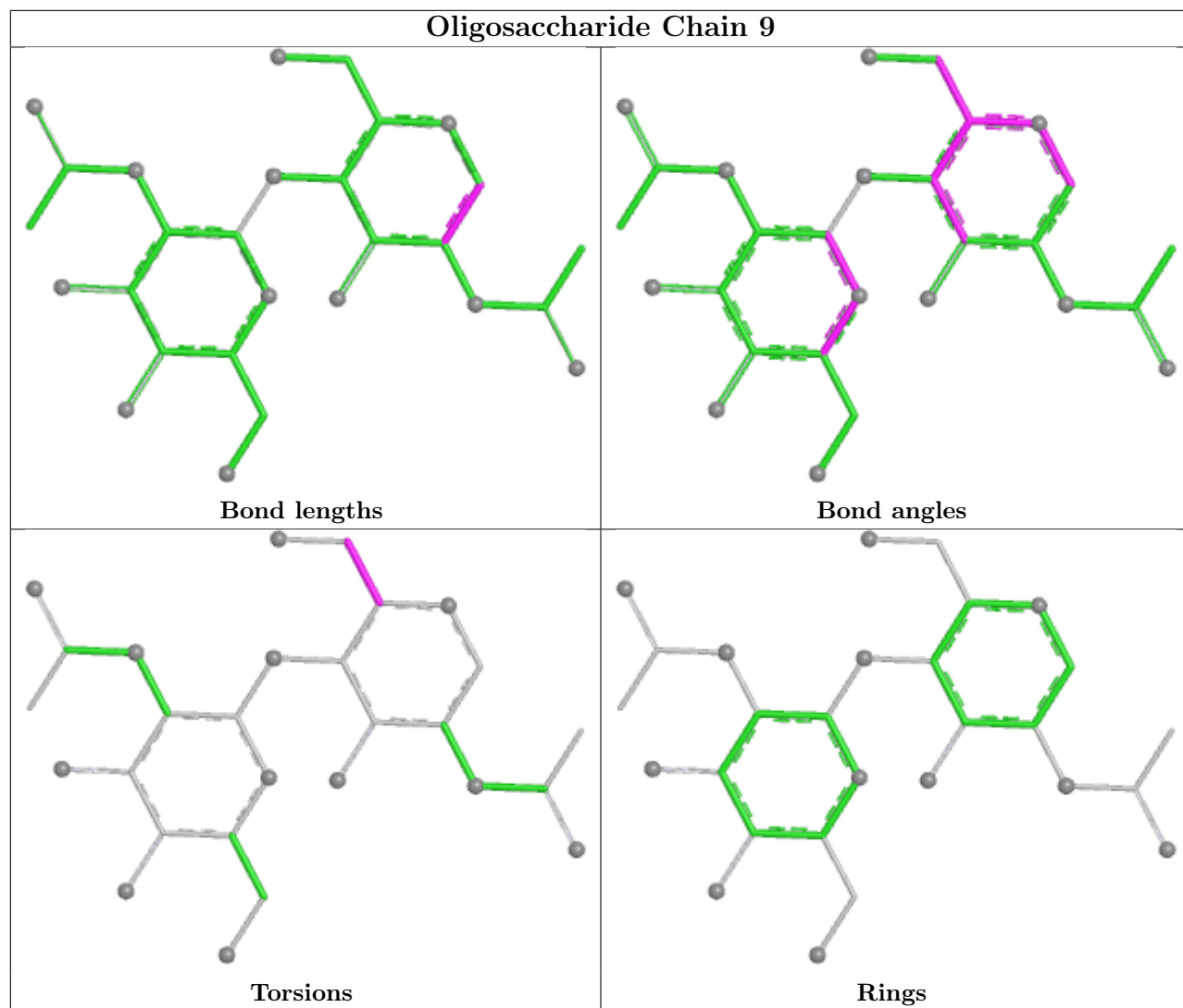


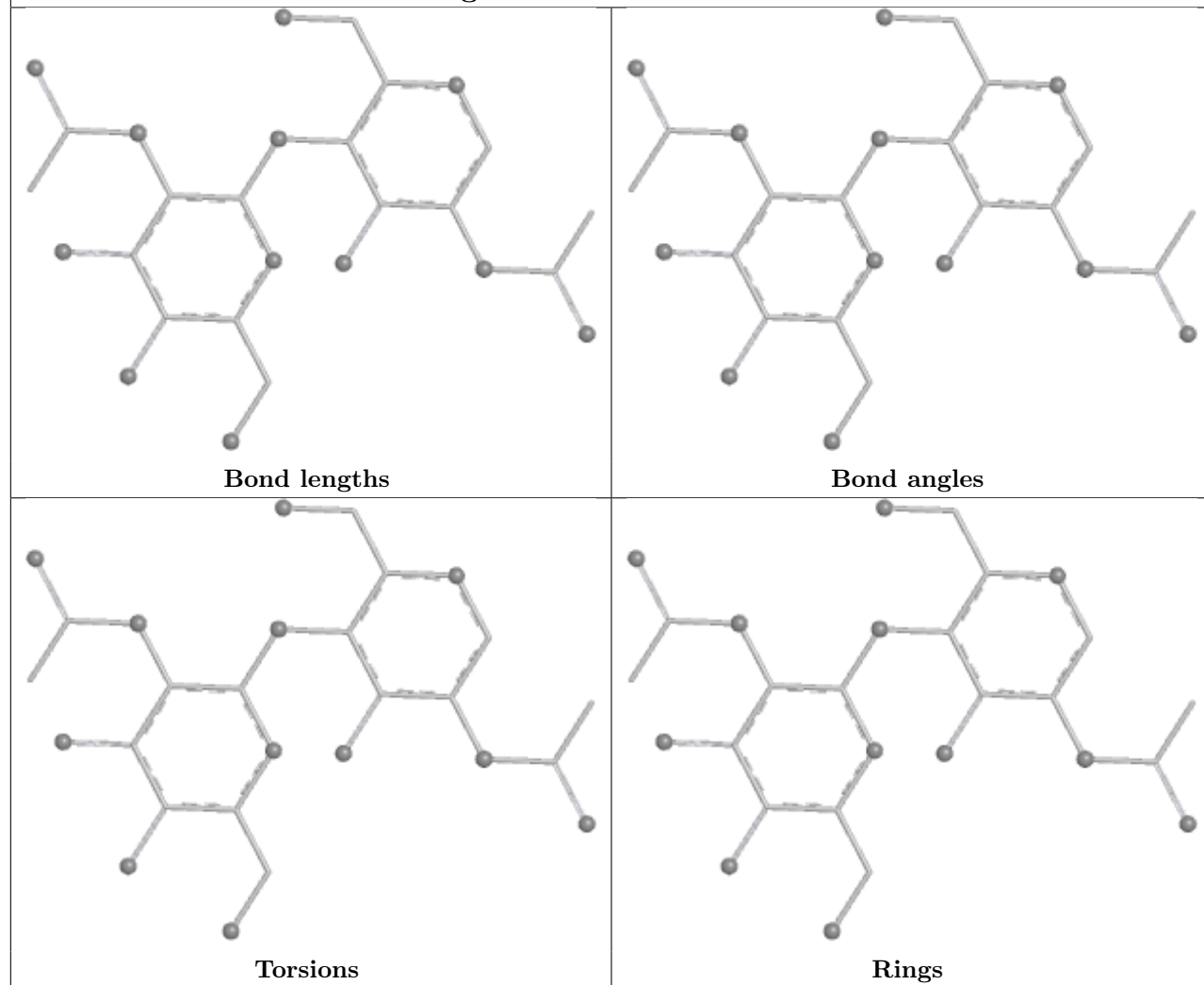


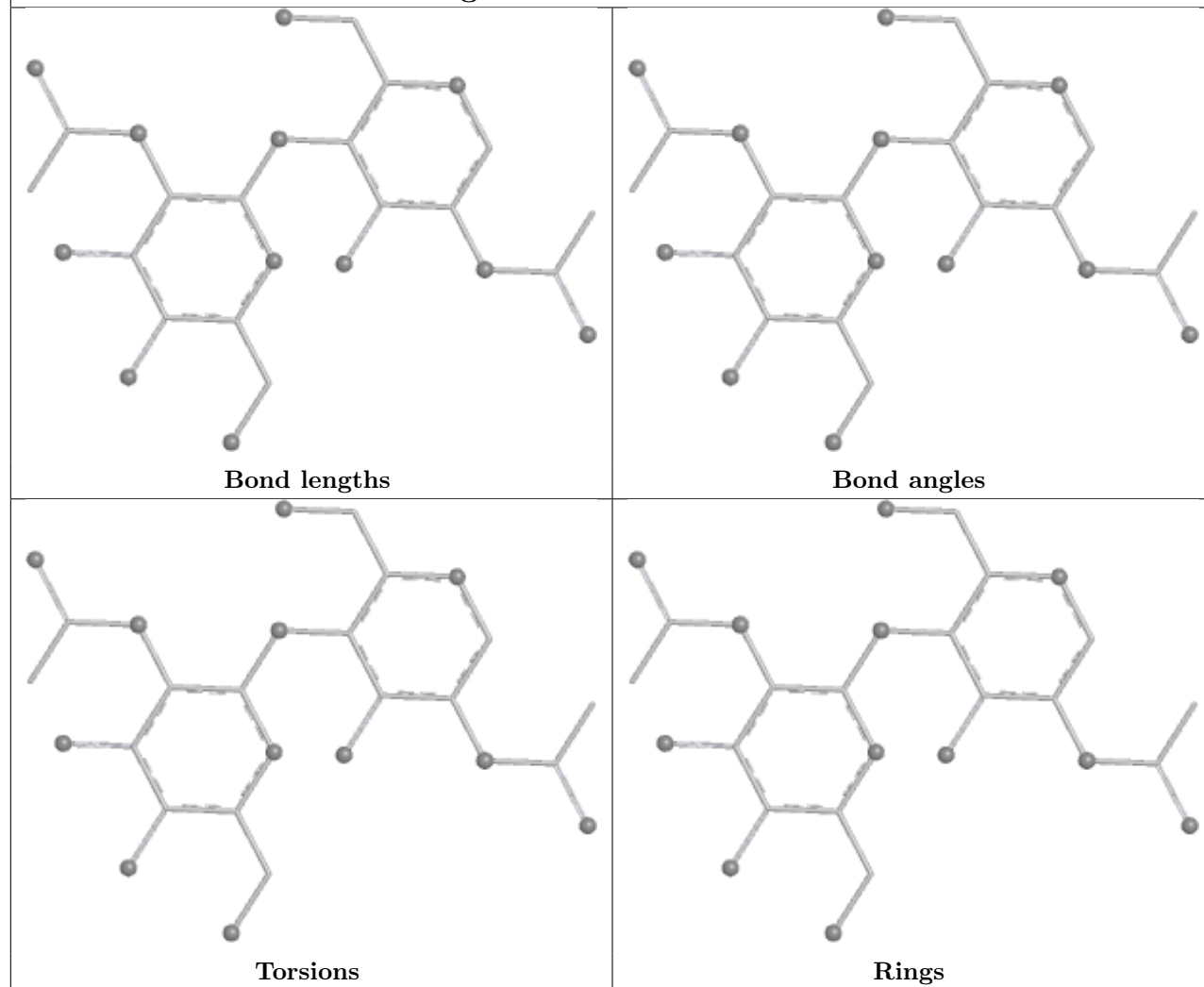




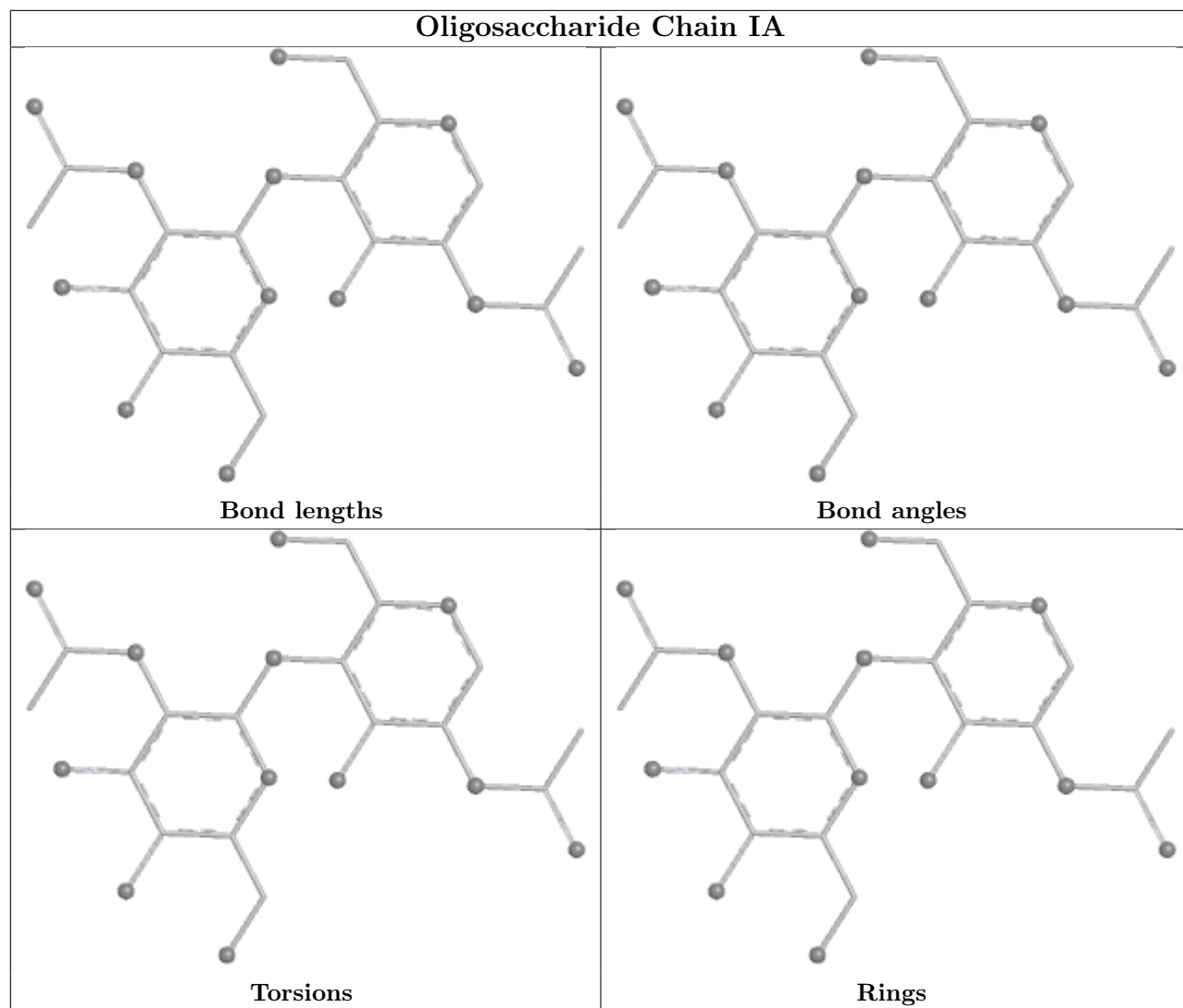




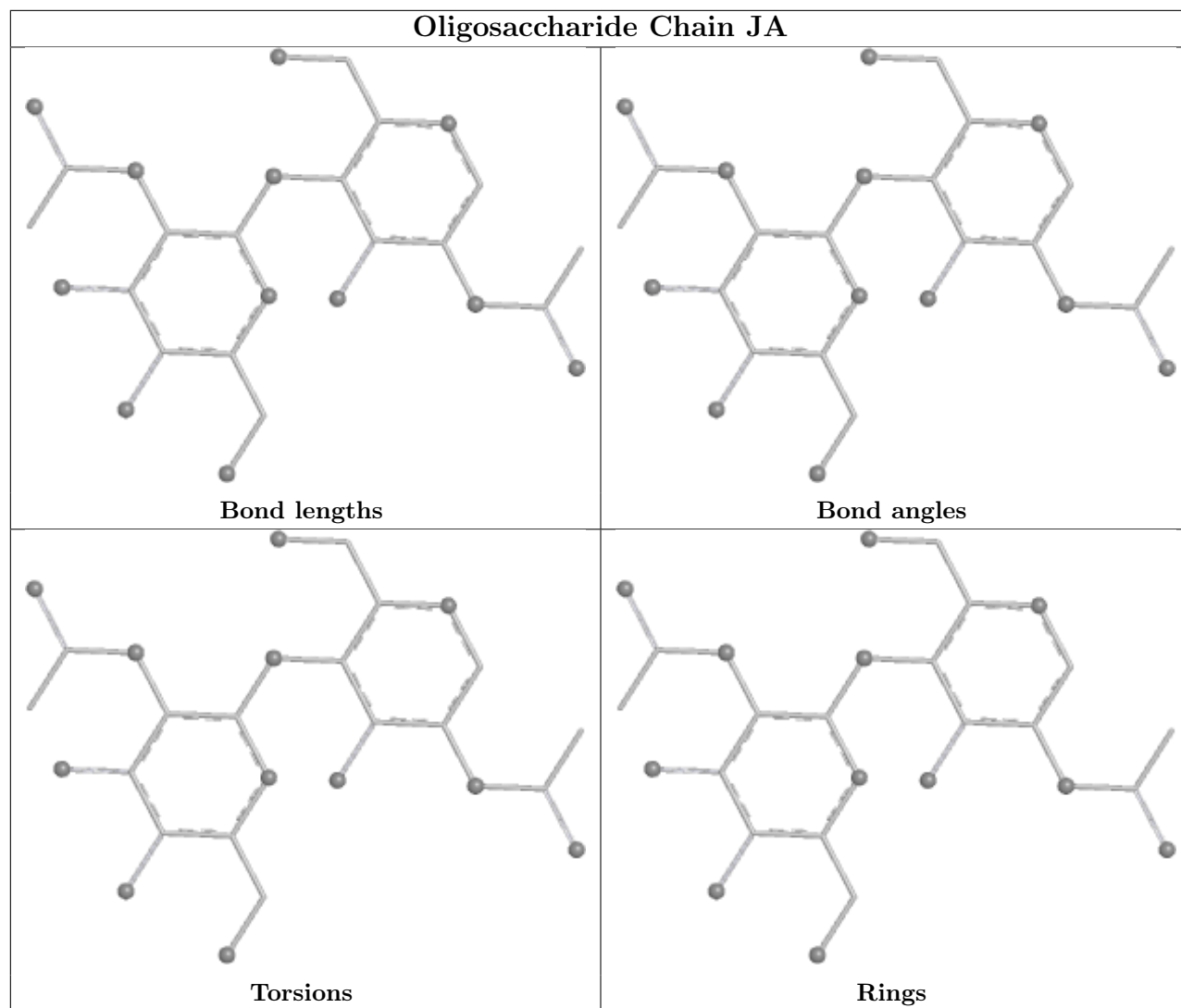
Oligosaccharide Chain BA

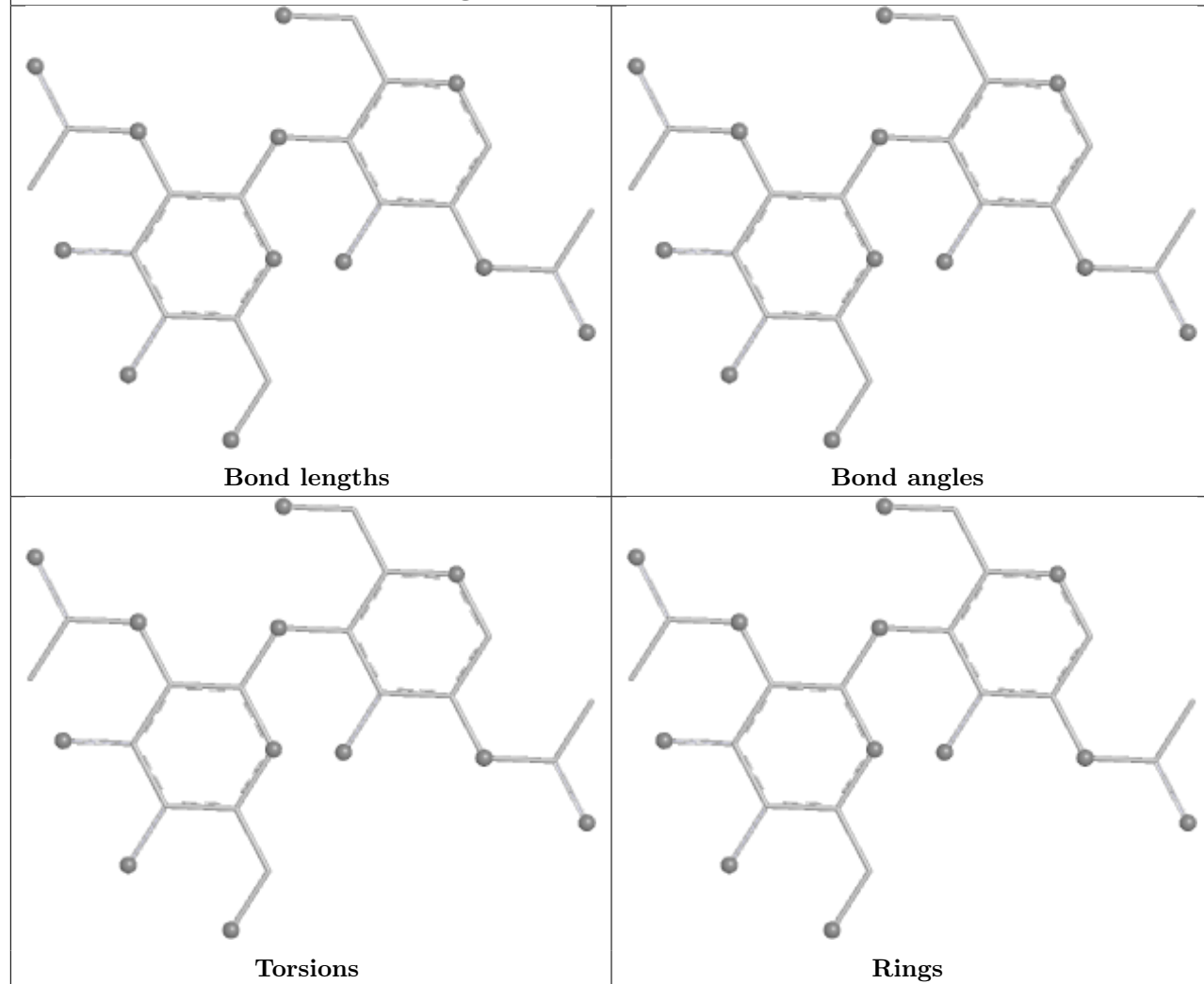
Oligosaccharide Chain HA

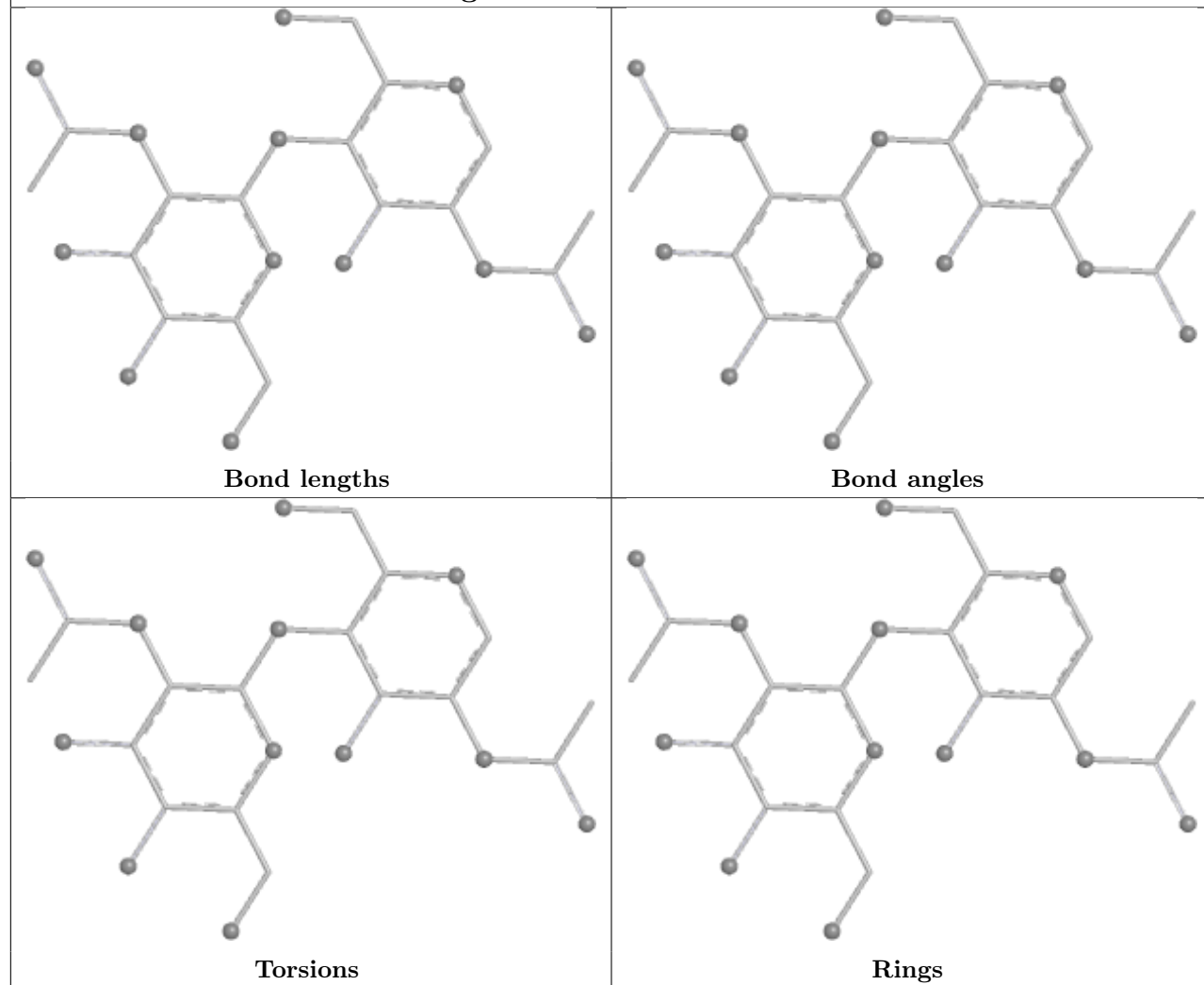
Oligosaccharide Chain IA



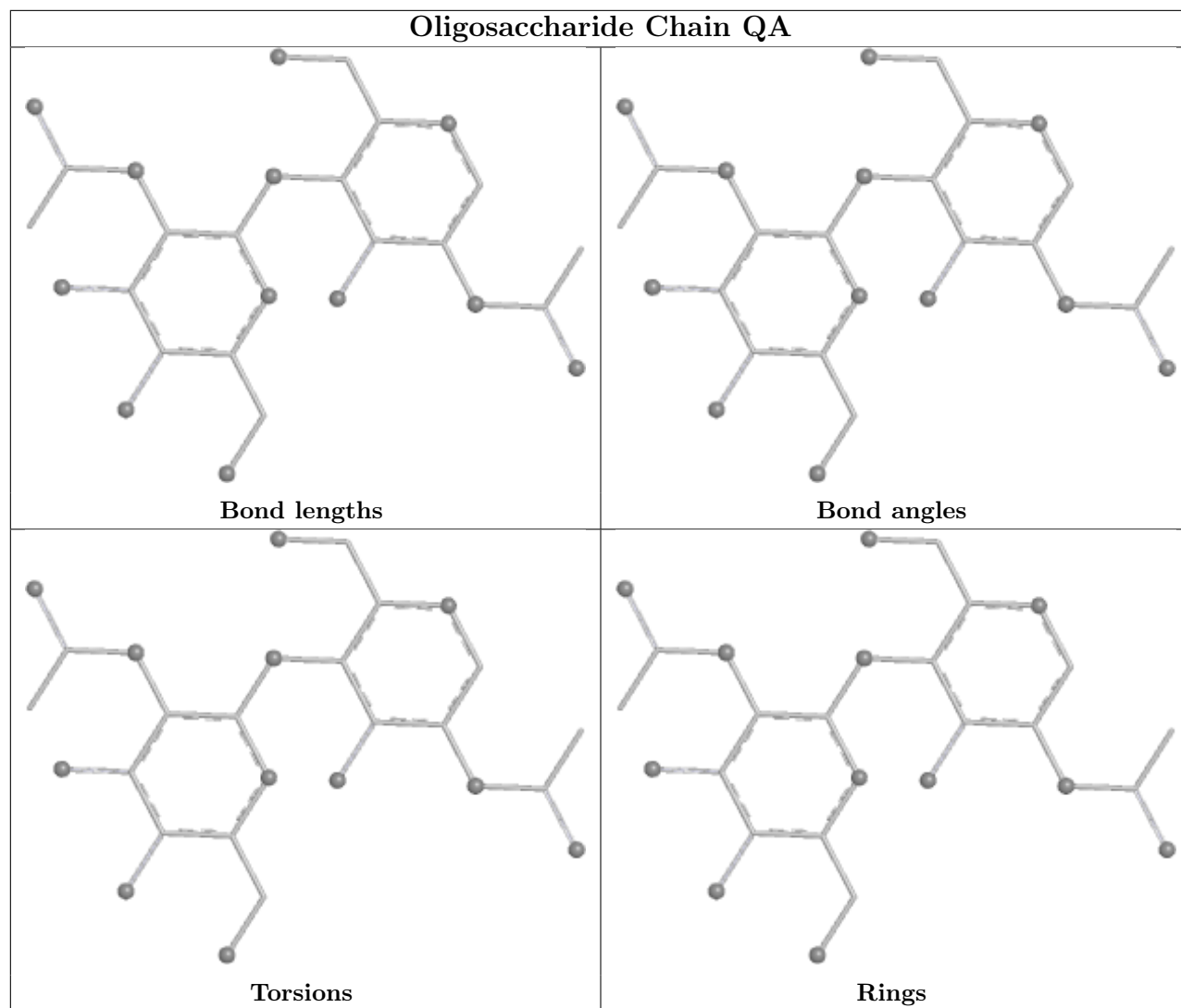
Oligosaccharide Chain JA

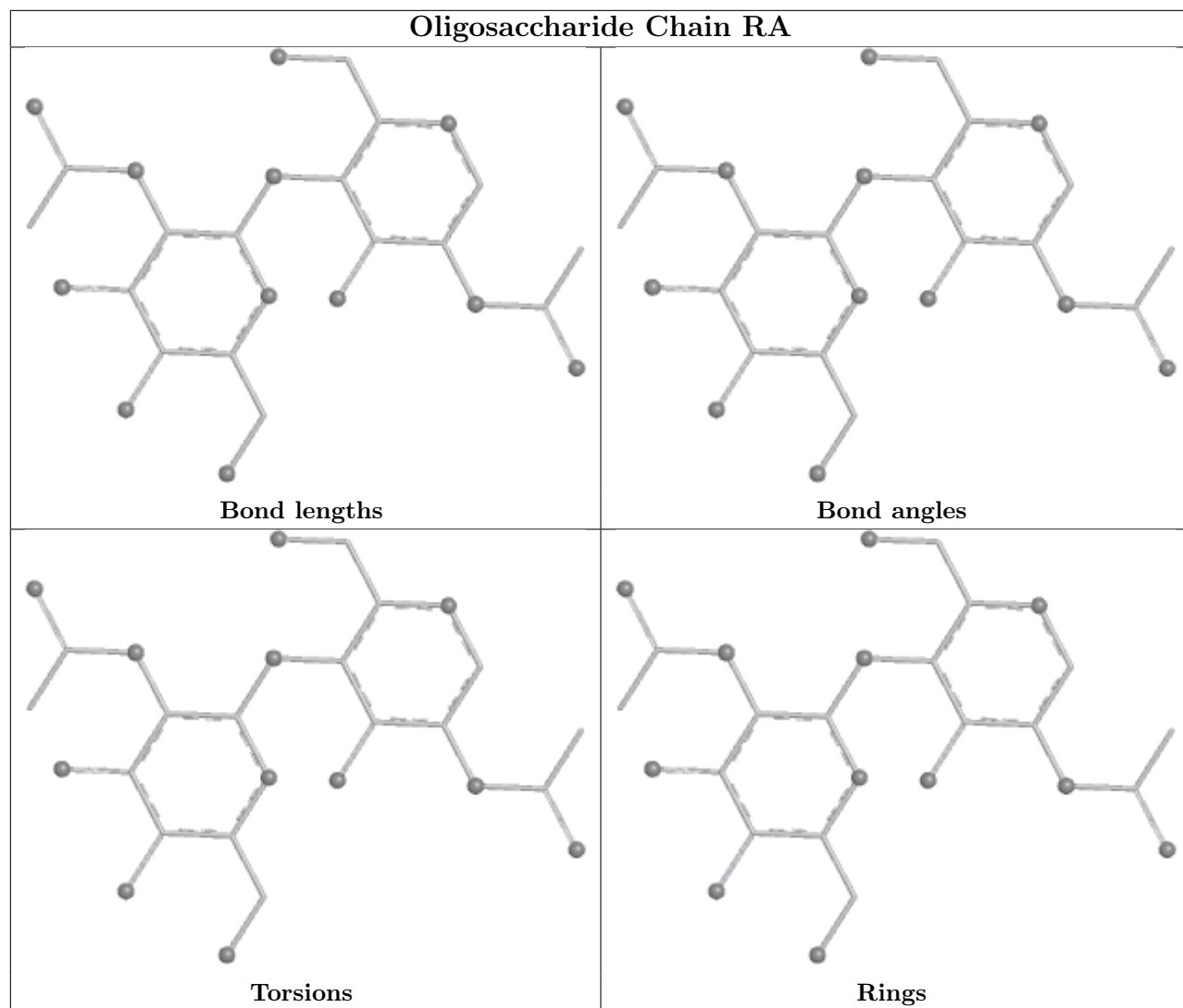


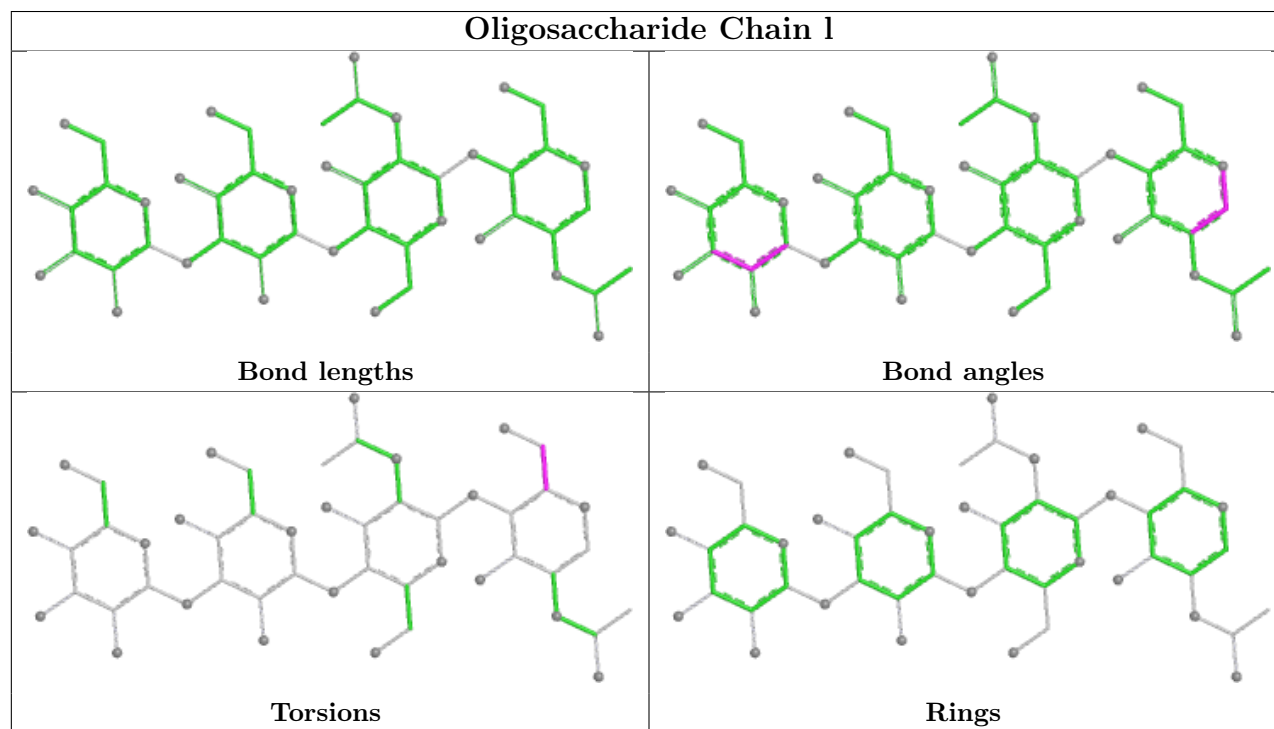
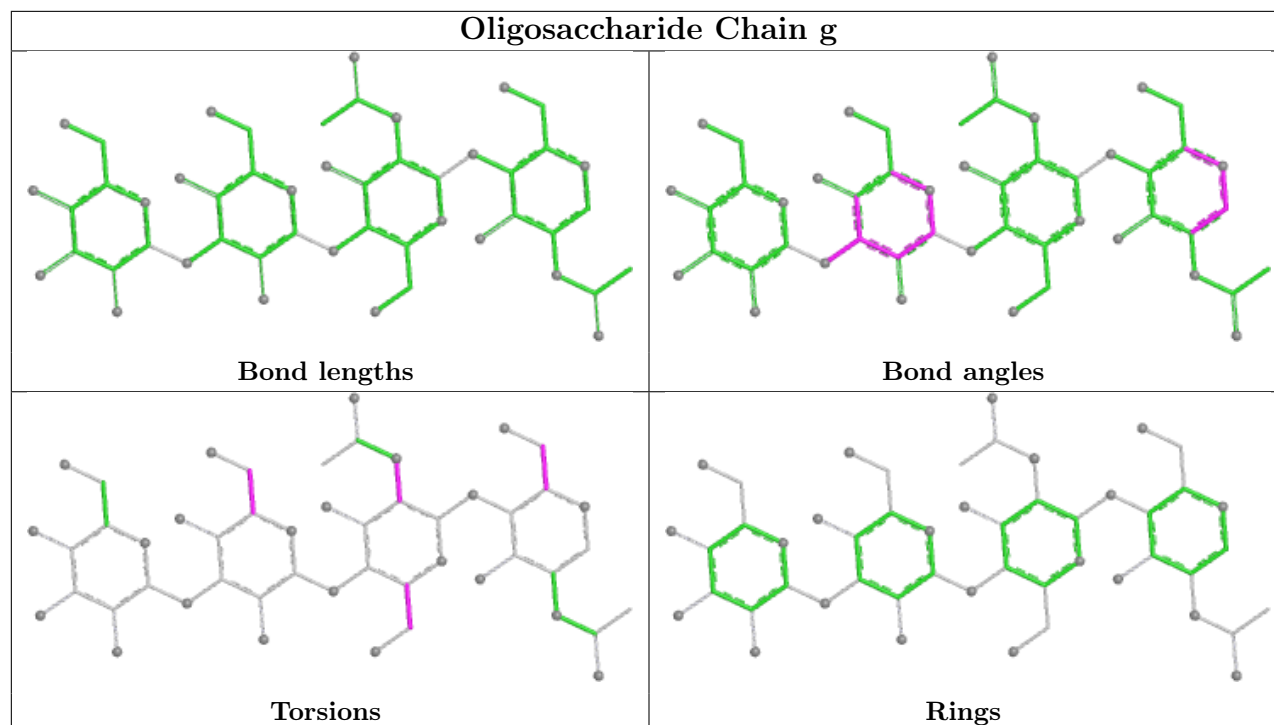
Oligosaccharide Chain MA

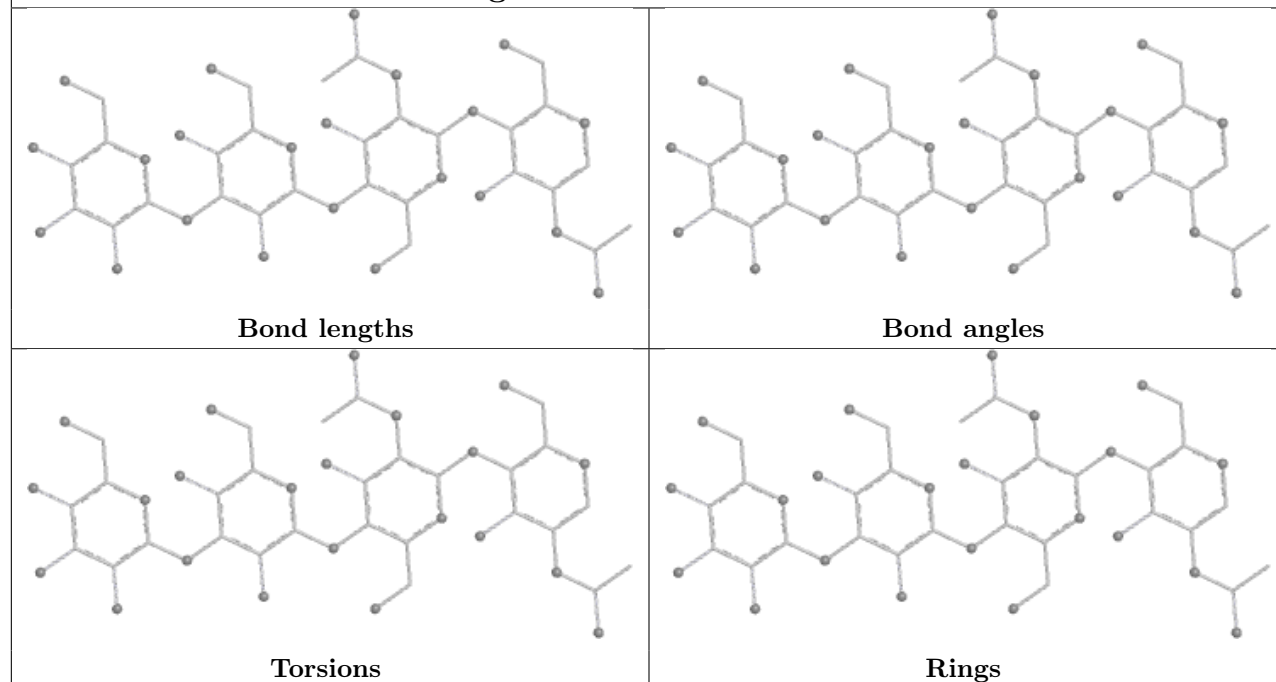
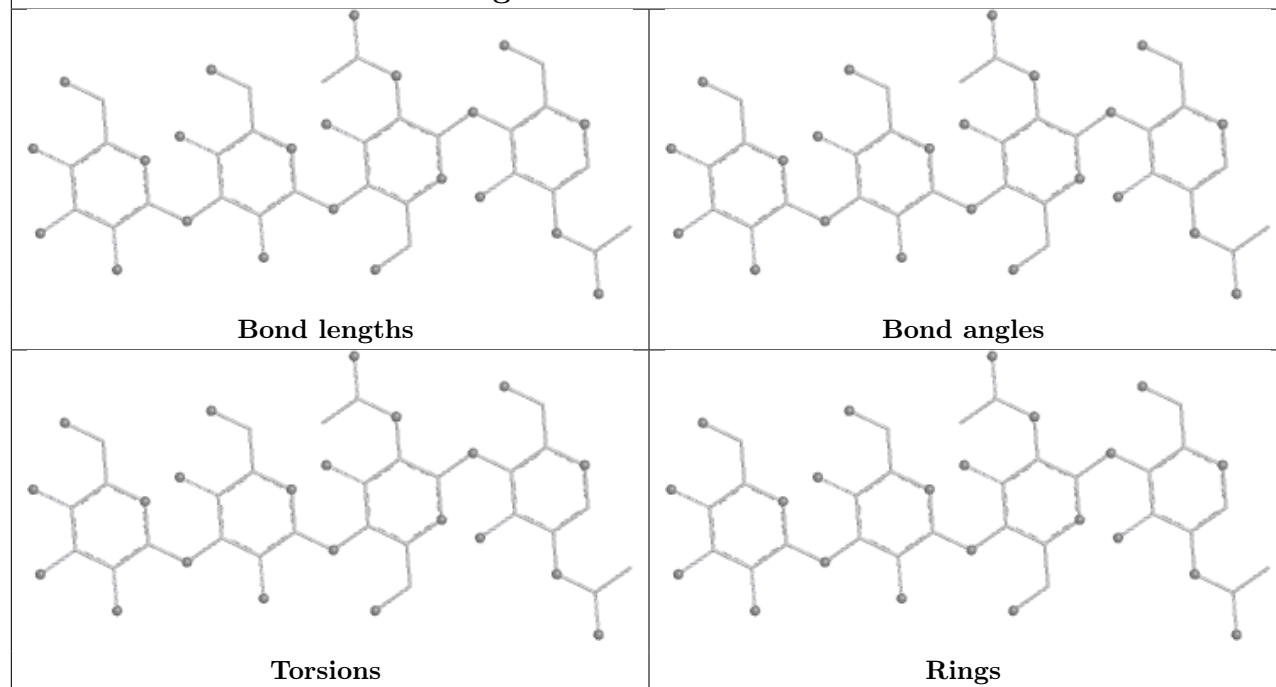
Oligosaccharide Chain OA

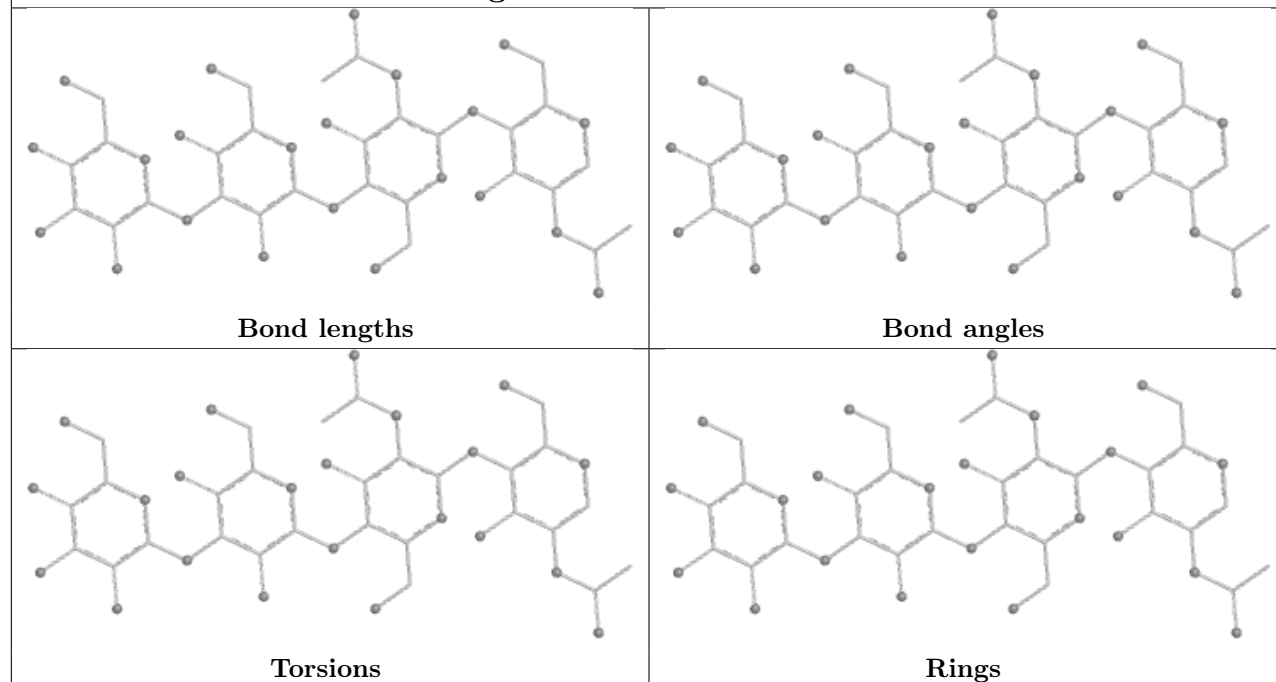
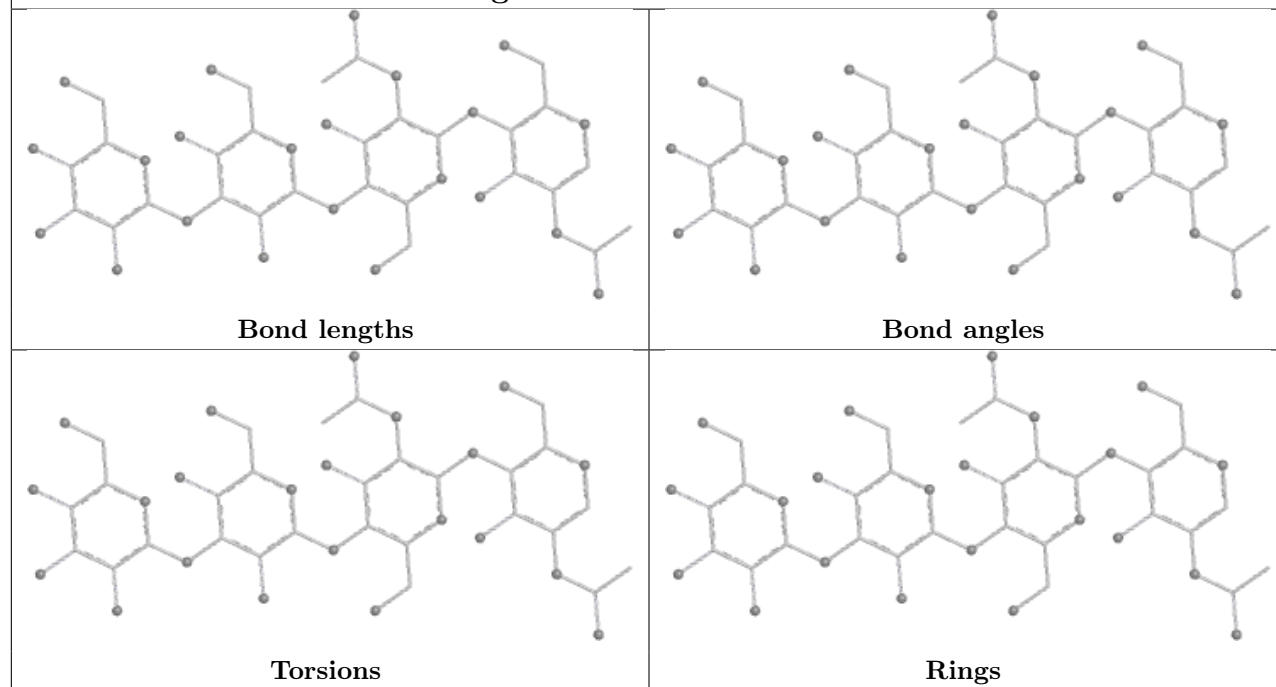
Oligosaccharide Chain QA

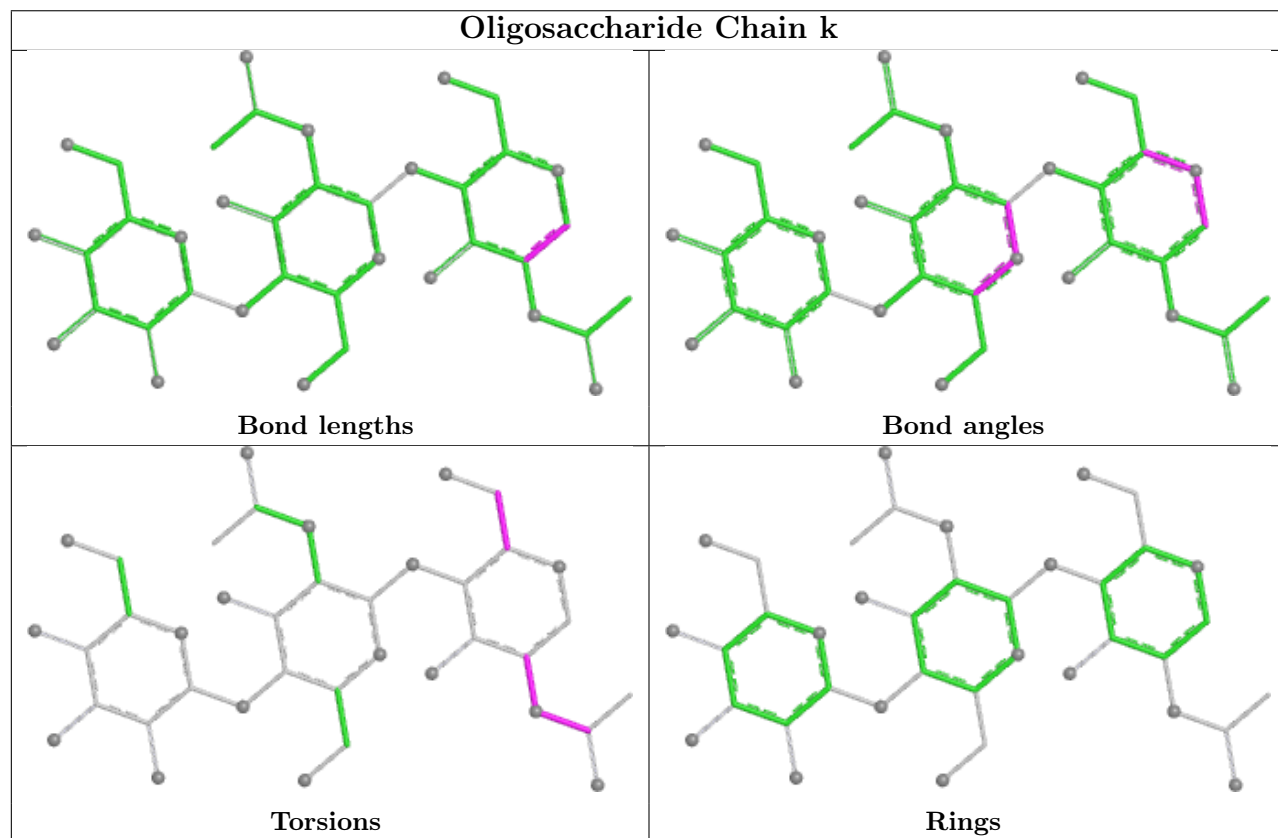
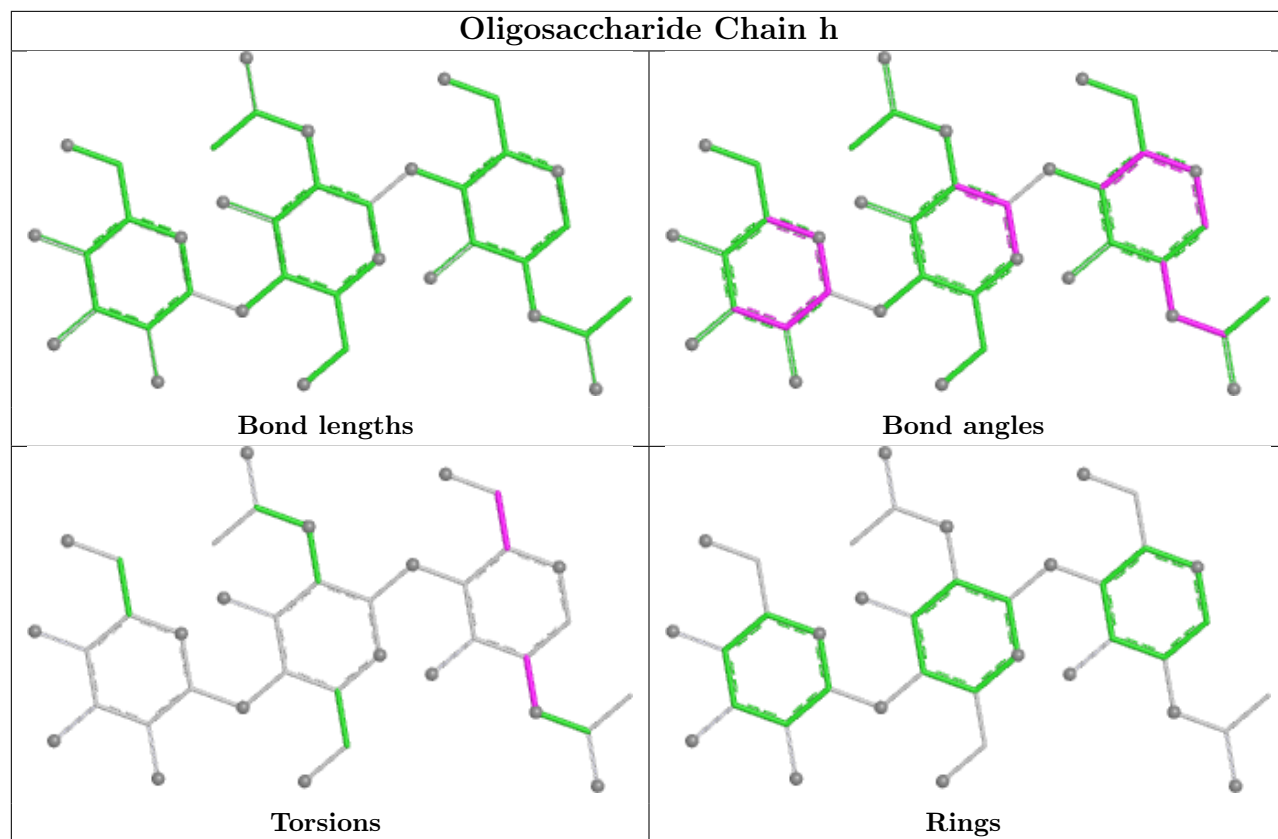


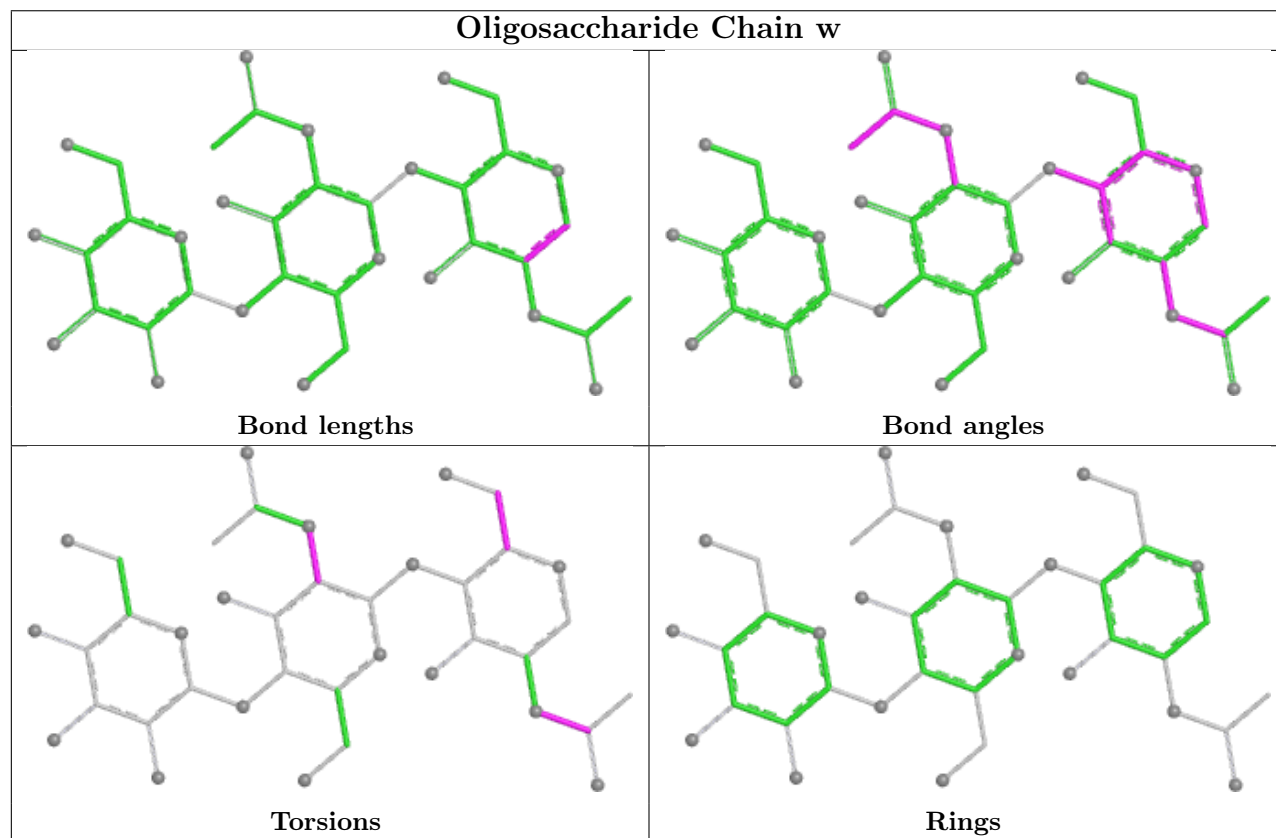
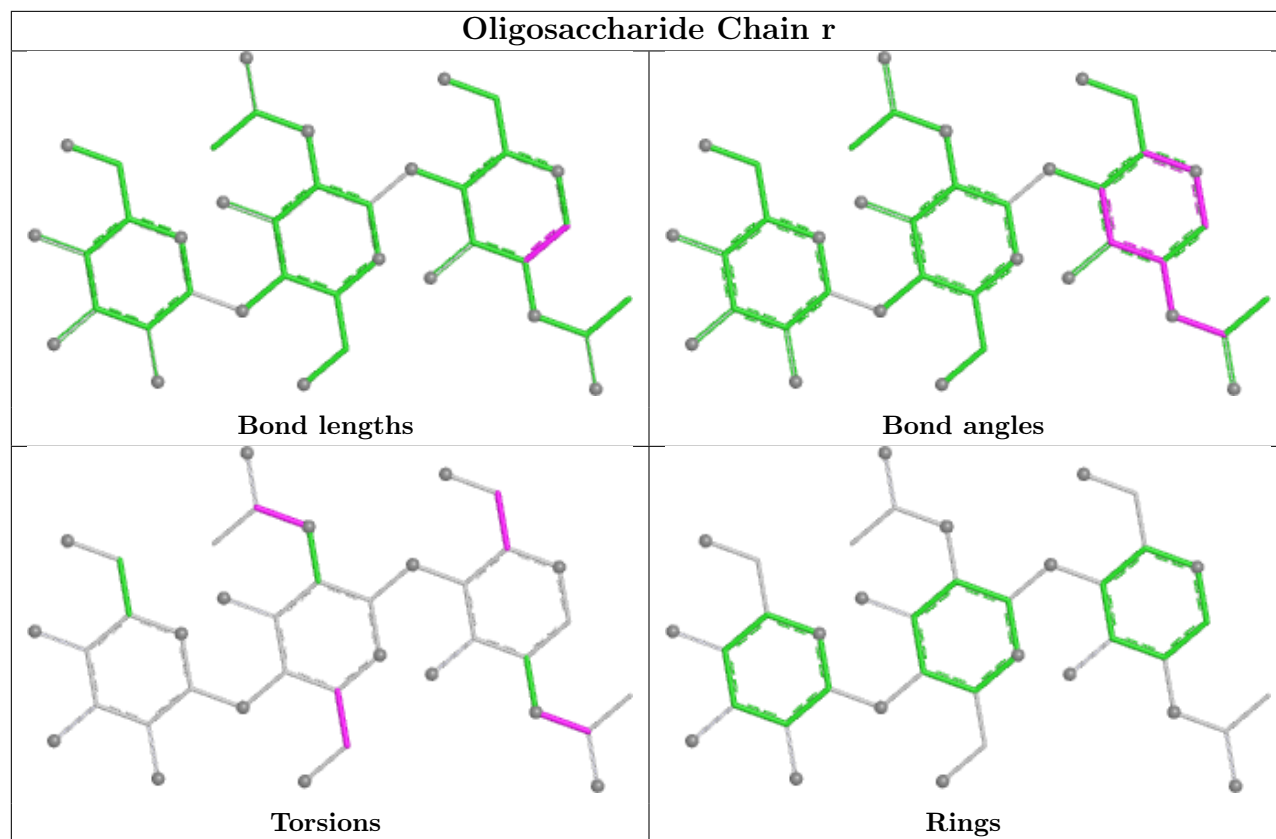


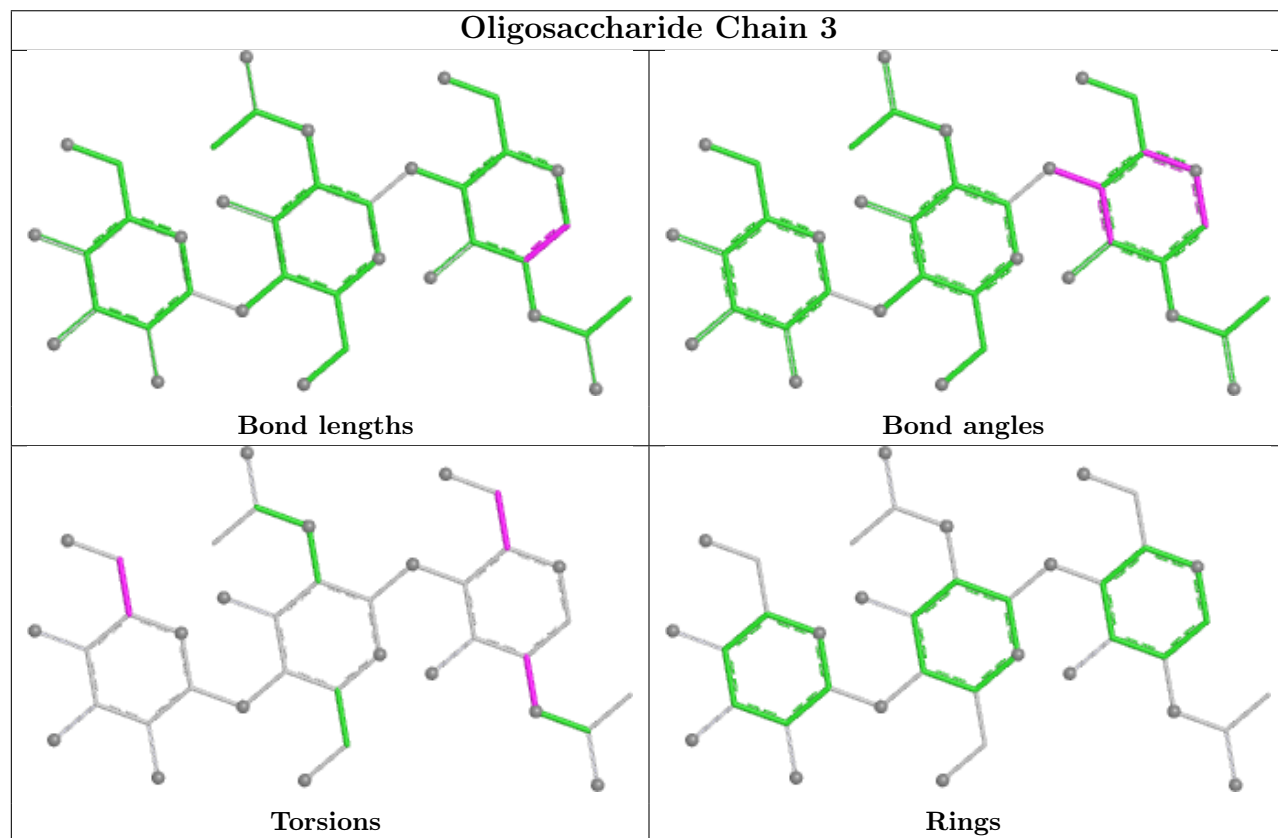
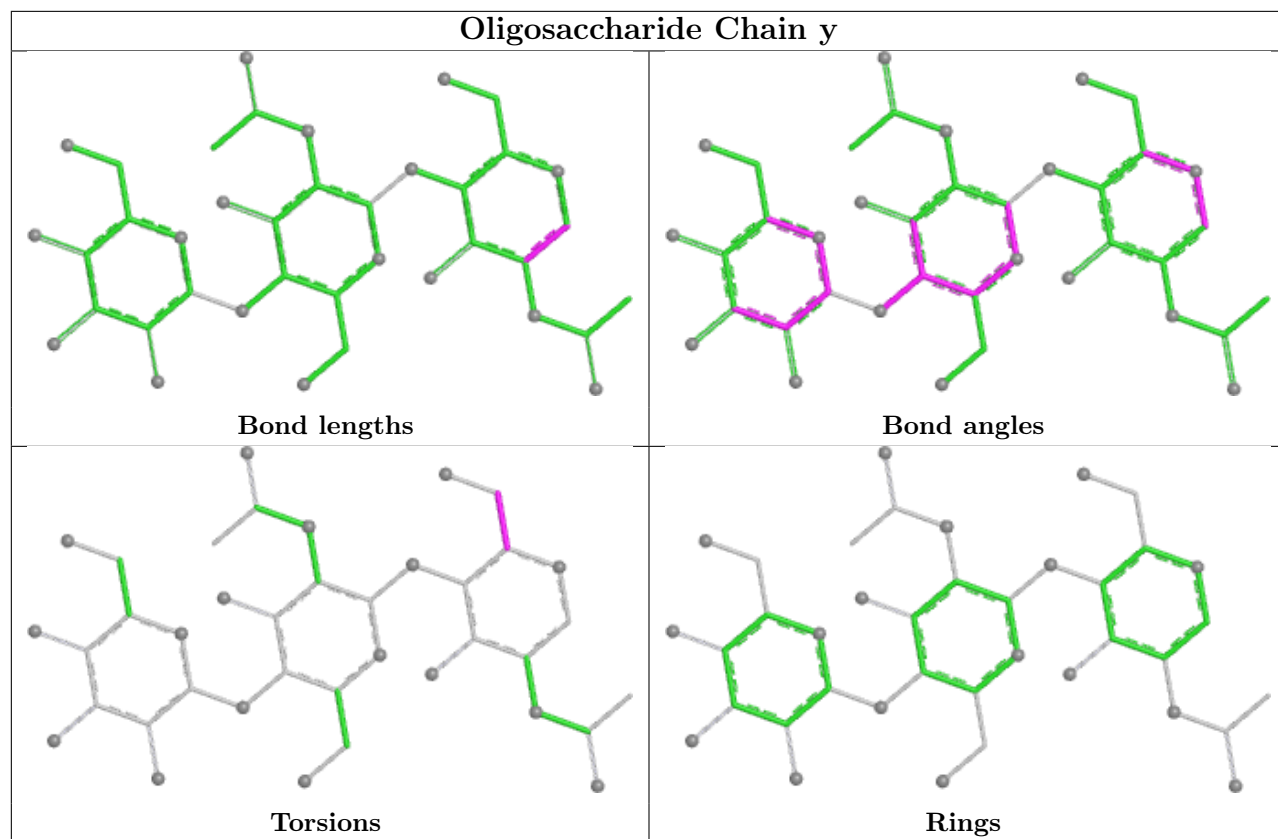


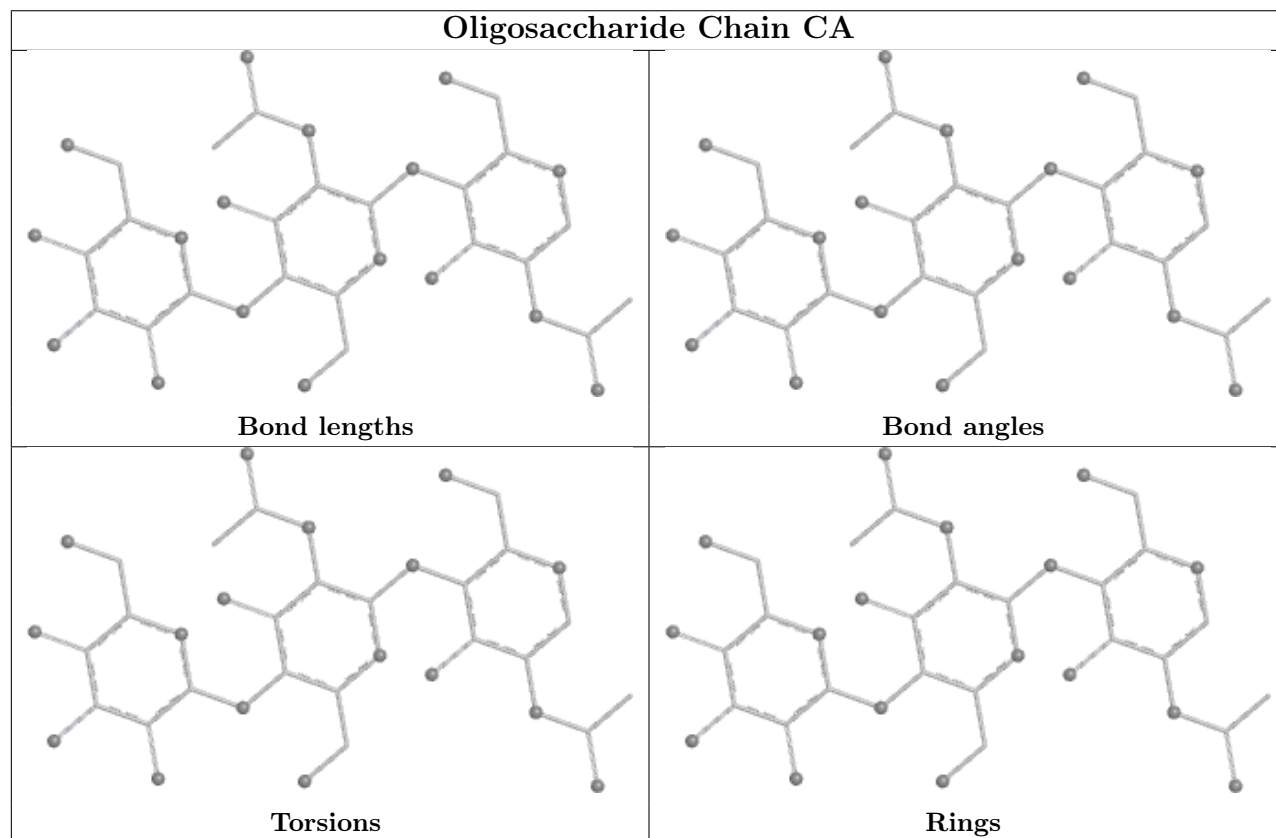
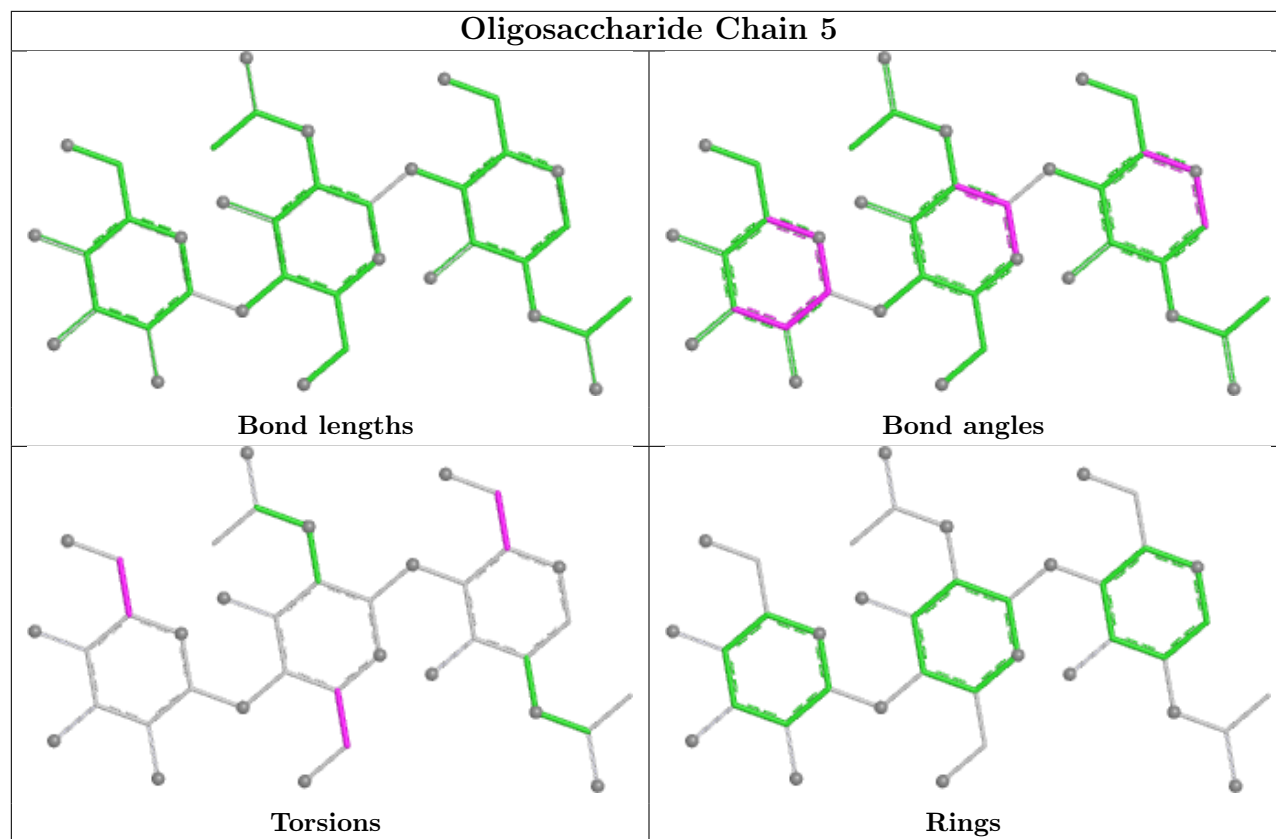
Oligosaccharide Chain AA**Oligosaccharide Chain FA**

Oligosaccharide Chain KA**Oligosaccharide Chain PA**

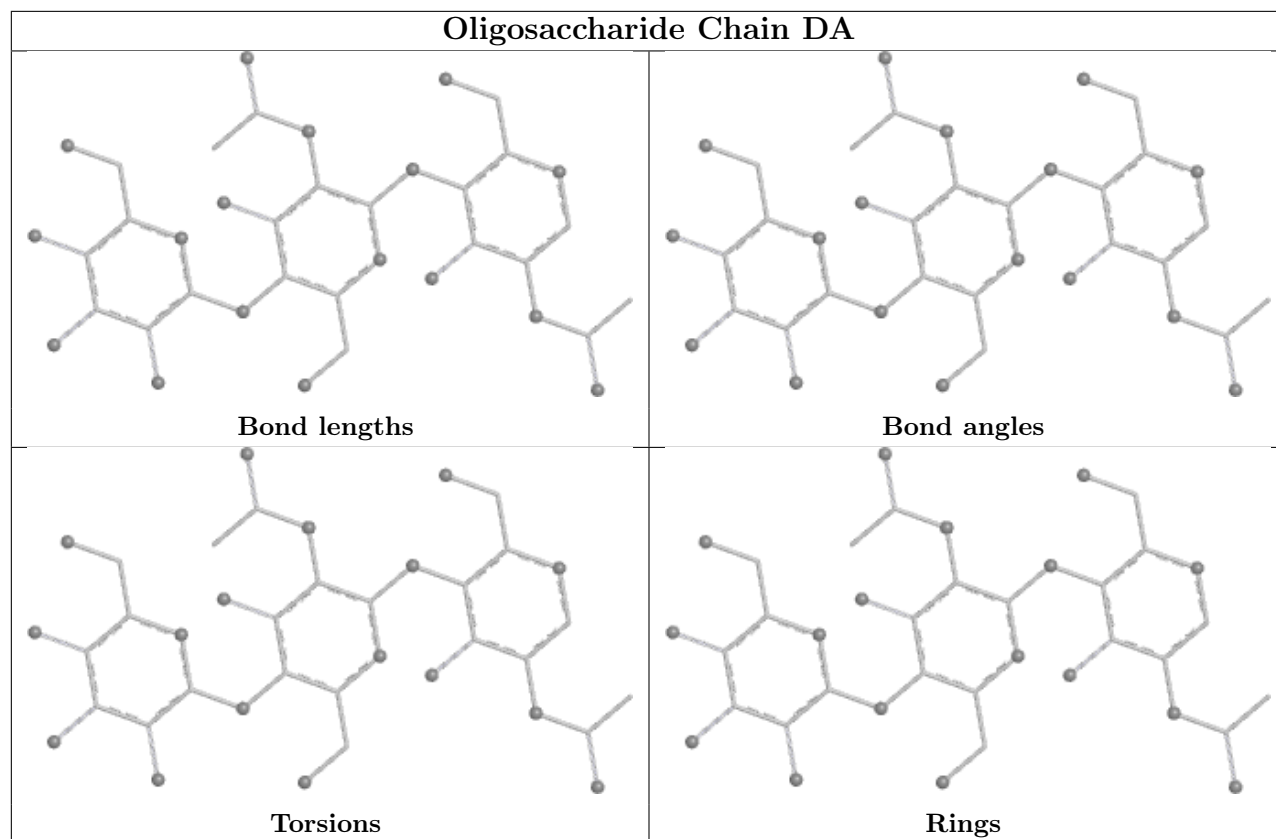




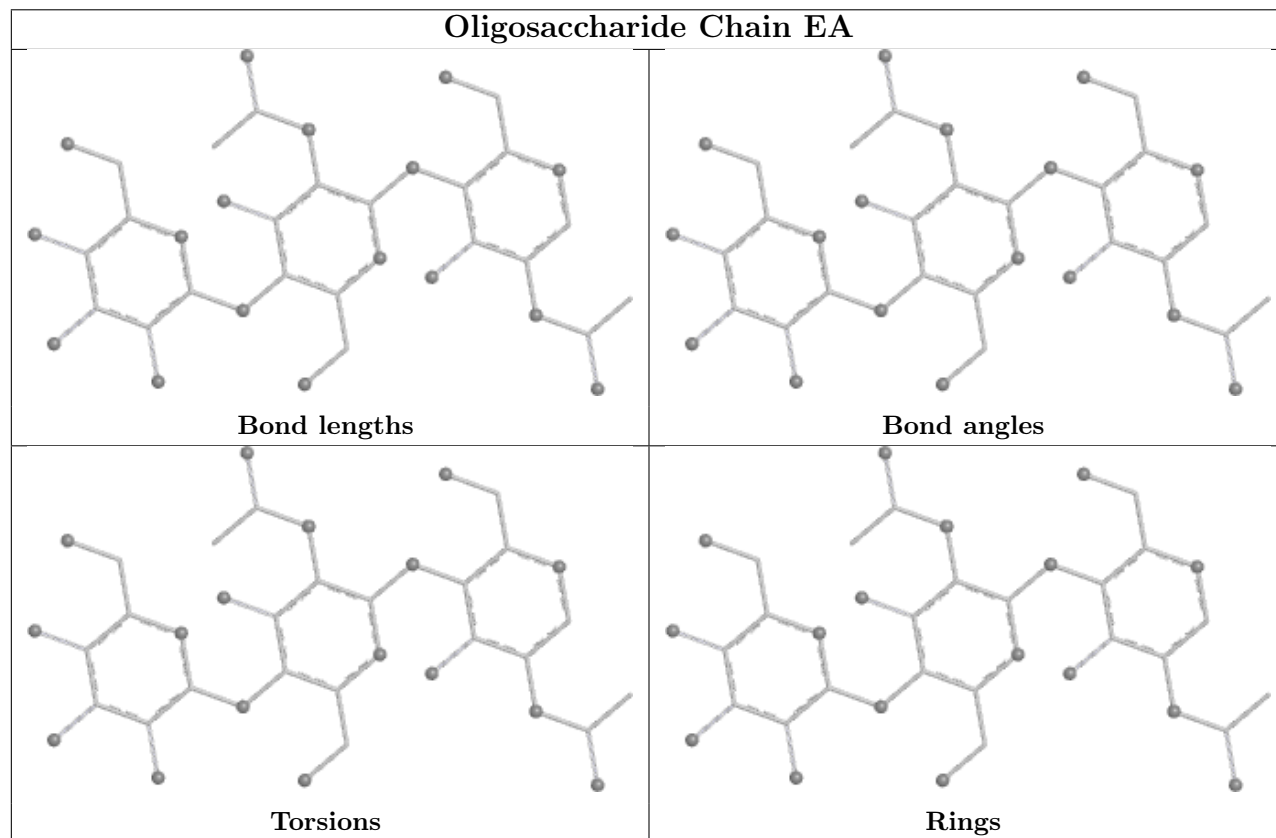




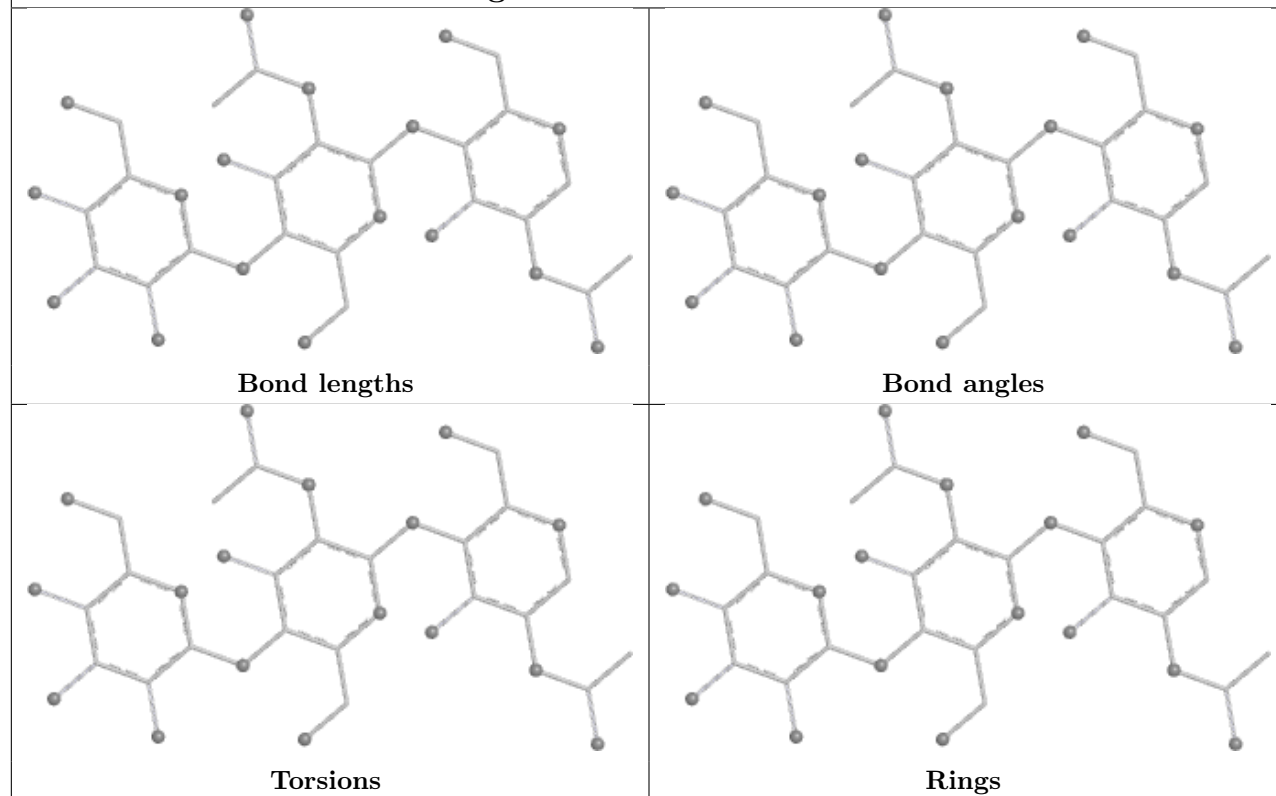
Oligosaccharide Chain DA



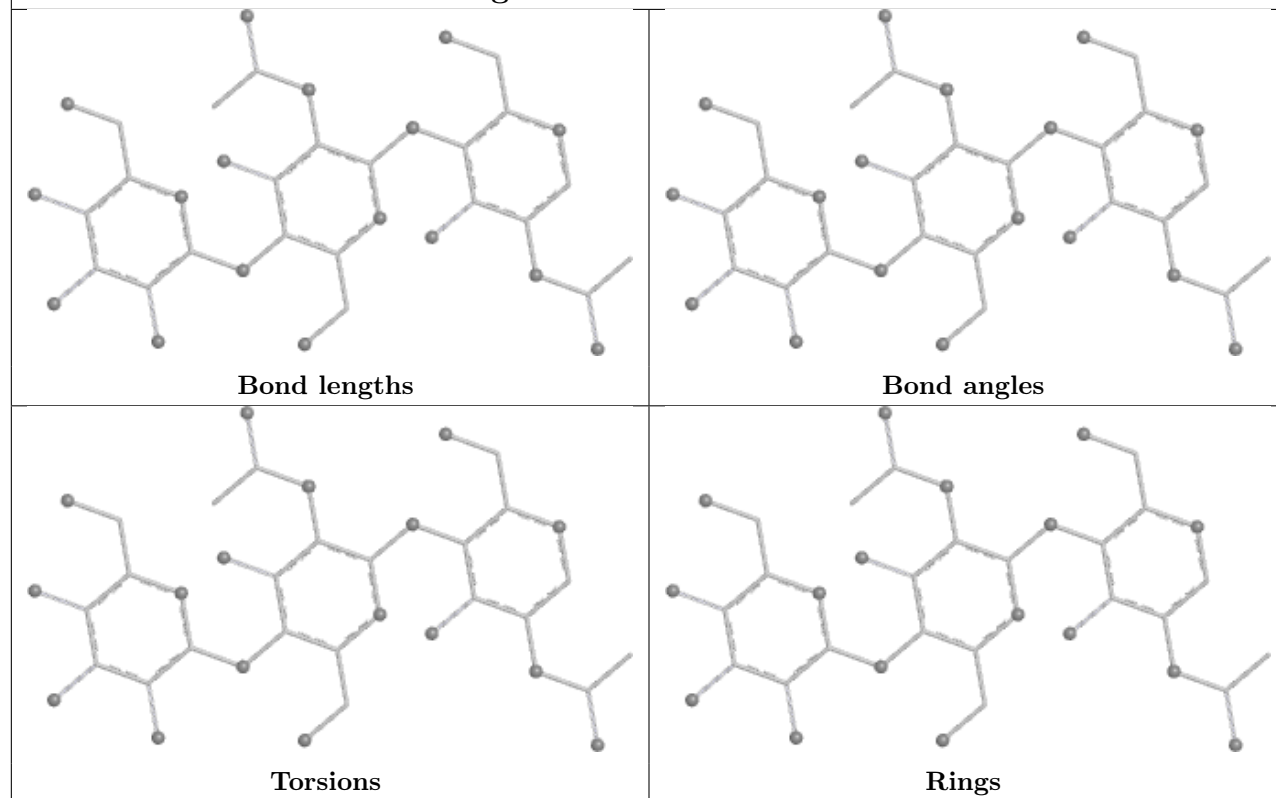
Oligosaccharide Chain EA



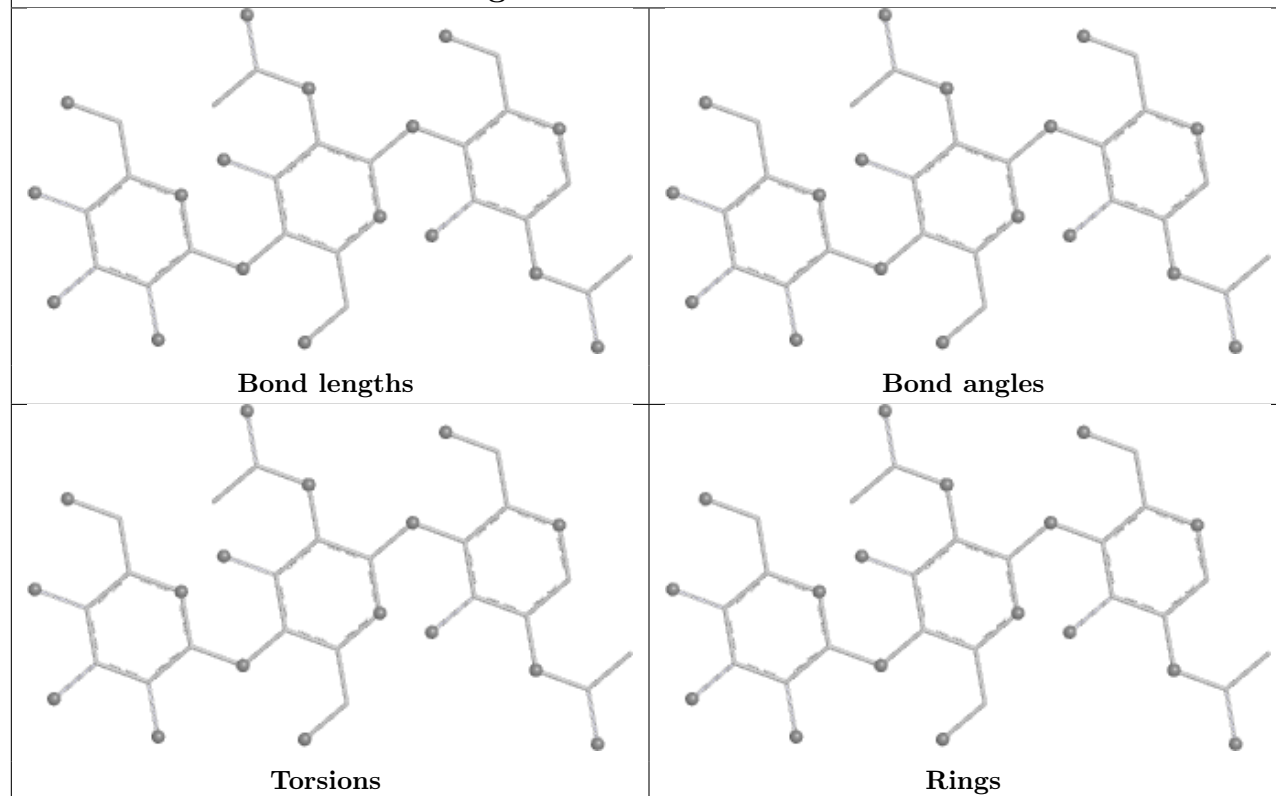
Oligosaccharide Chain GA



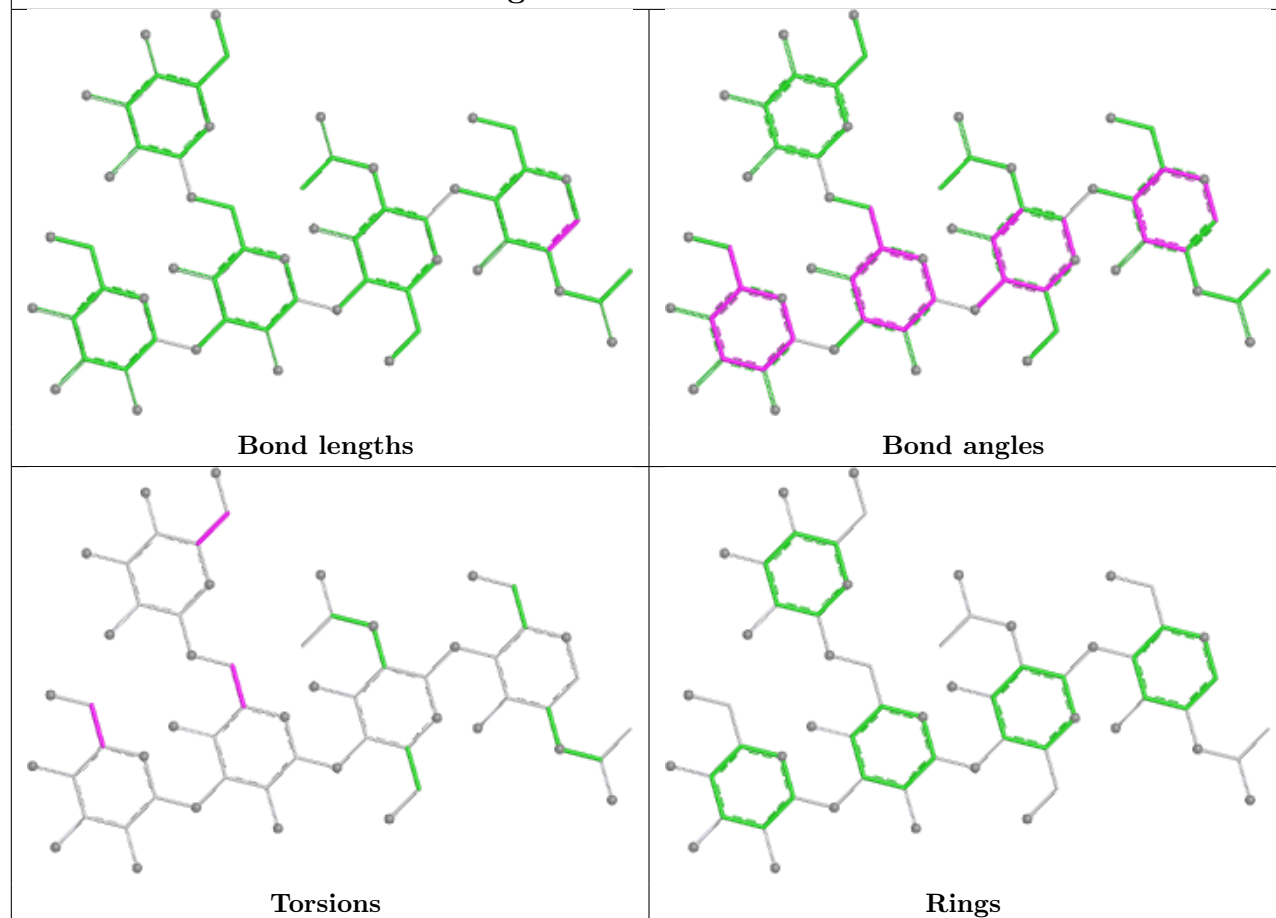
Oligosaccharide Chain LA

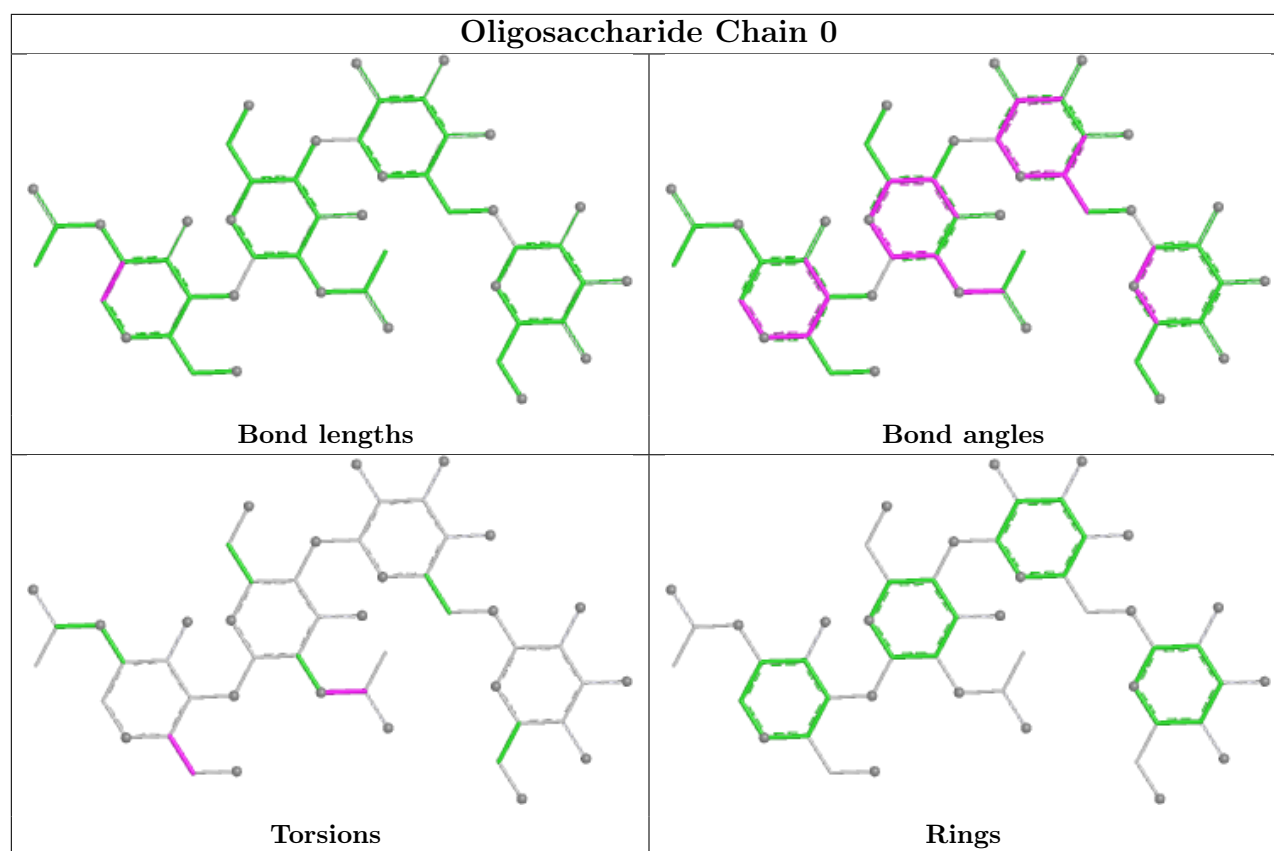


Oligosaccharide Chain NA



Oligosaccharide Chain z





5.6 Ligand geometry [i](#)

100 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	$\# Z > 2$
9	CUO	J	5001	1	0,4,4	-	-	-		
9	CUO	A	5005[C]	-	0,4,4	-	-	-		
9	CUO	P	5003	1	0,4,4	-	-	-		
9	CUO	J	5005[C]	-	0,4,4	-	-	-		
9	CUO	D	5004	1	0,4,4	-	-	-		
9	CUO	P	5005[D]	-	0,4,4	-	-	-		
9	CUO	D	5002	1	0,4,4	-	-	-		
9	CUO	X	3401[A]	3	0,4,4	-	-	-		
9	CUO	V	5003	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CUO	S	2105	1	0,4,4	-	-	-		
9	CUO	U	3401[B]	3	0,4,4	-	-	-		
9	CUO	P	5001	1	0,4,4	-	-	-		
9	CUO	L	3401[A]	3	0,4,4	-	-	-		
9	CUO	F	3401[A]	3	0,4,4	-	-	-		
9	CUO	O	3401[B]	3	0,4,4	-	-	-		
9	CUO	a	3401[B]	3	0,4,4	-	-	-		
9	CUO	R	3401[B]	3	0,4,4	-	-	-		
9	CUO	A	5004	1	0,4,4	-	-	-		
9	CUO	I	3401[A]	3	0,4,4	-	-	-		
9	CUO	A	5001	1	0,4,4	-	-	-		
9	CUO	M	2101[C]	-	0,4,4	-	-	-		
9	CUO	Q	3001	2	0,4,4	-	-	-		
9	CUO	S	2103	1	0,4,4	-	-	-		
9	CUO	V	5001	1	0,4,4	-	-	-		
9	CUO	J	5003	1	0,4,4	-	-	-		
9	CUO	N	3001	2	0,4,4	-	-	-		
9	CUO	J	5002	1	0,4,4	-	-	-		
9	CUO	Y	2101[D]	-	0,4,4	-	-	-		
9	CUO	B	3002	2	0,4,4	-	-	-		
9	CUO	J	5004	1	0,4,4	-	-	-		
9	CUO	K	3001	2	0,4,4	-	-	-		
9	CUO	d	3401[B]	3	0,4,4	-	-	-		
9	CUO	X	3401[B]	3	0,4,4	-	-	-		
9	CUO	V	5002	1	0,4,4	-	-	-		
9	CUO	V	5004	1	0,4,4	-	-	-		
9	CUO	D	5005[D]	-	0,4,4	-	-	-		
9	CUO	Y	2101[C]	-	0,4,4	-	-	-		
9	CUO	C	3401[A]	3	0,4,4	-	-	-		
9	CUO	L	3401[B]	3	0,4,4	-	-	-		
9	CUO	P	5005[C]	-	0,4,4	-	-	-		
9	CUO	F	3401[B]	3	0,4,4	-	-	-		
9	CUO	B	3001	2	0,4,4	-	-	-		
9	CUO	Y	2105	1	0,4,4	-	-	-		
9	CUO	D	5001	1	0,4,4	-	-	-		
9	CUO	M	2103	1	0,4,4	-	-	-		
9	CUO	D	5005[C]	-	0,4,4	-	-	-		
9	CUO	A	5002	1	0,4,4	-	-	-		
9	CUO	S	2102	1	0,4,4	-	-	-		
9	CUO	Y	2104	1	0,4,4	-	-	-		
9	CUO	T	3002	2	0,4,4	-	-	-		
9	CUO	D	5003	1	0,4,4	-	-	-		
9	CUO	G	2105	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CUO	Z	3001	2	0,4,4	-	-	-		
9	CUO	V	5005[D]	-	0,4,4	-	-	-		
9	CUO	H	3001	2	0,4,4	-	-	-		
9	CUO	H	3002	2	0,4,4	-	-	-		
9	CUO	V	5005[C]	-	0,4,4	-	-	-		
9	CUO	U	3401[A]	3	0,4,4	-	-	-		
9	CUO	b	2102	1	0,4,4	-	-	-		
9	CUO	Y	2102	1	0,4,4	-	-	-		
9	CUO	S	2104	1	0,4,4	-	-	-		
9	CUO	M	2104	1	0,4,4	-	-	-		
9	CUO	O	3401[A]	3	0,4,4	-	-	-		
9	CUO	N	3002	2	0,4,4	-	-	-		
9	CUO	W	3002	2	0,4,4	-	-	-		
9	CUO	a	3401[A]	3	0,4,4	-	-	-		
9	CUO	R	3401[A]	3	0,4,4	-	-	-		
9	CUO	M	2102	1	0,4,4	-	-	-		
9	CUO	b	2105	1	0,4,4	-	-	-		
9	CUO	W	3001	2	0,4,4	-	-	-		
9	CUO	P	5002	1	0,4,4	-	-	-		
9	CUO	c	3002	2	0,4,4	-	-	-		
9	CUO	I	3401[B]	3	0,4,4	-	-	-		
9	CUO	J	5005[D]	-	0,4,4	-	-	-		
9	CUO	K	3002	2	0,4,4	-	-	-		
9	CUO	A	5003	1	0,4,4	-	-	-		
9	CUO	d	3401[A]	3	0,4,4	-	-	-		
9	CUO	E	3002	2	0,4,4	-	-	-		
9	CUO	T	3001	2	0,4,4	-	-	-		
9	CUO	G	2102	1	0,4,4	-	-	-		
9	CUO	Z	3002	2	0,4,4	-	-	-		
9	CUO	Q	3002	2	0,4,4	-	-	-		
9	CUO	b	2101[D]	-	0,4,4	-	-	-		
9	CUO	M	2101[D]	-	0,4,4	-	-	-		
9	CUO	b	2103	1	0,4,4	-	-	-		
9	CUO	Y	2103	1	0,4,4	-	-	-		
9	CUO	G	2101[D]	-	0,4,4	-	-	-		
9	CUO	S	2101[D]	-	0,4,4	-	-	-		
9	CUO	E	3001	2	0,4,4	-	-	-		
9	CUO	b	2101[C]	-	0,4,4	-	-	-		
9	CUO	C	3401[B]	3	0,4,4	-	-	-		
9	CUO	P	5004	1	0,4,4	-	-	-		
9	CUO	G	2103	1	0,4,4	-	-	-		
9	CUO	b	2104	1	0,4,4	-	-	-		
9	CUO	G	2101[C]	-	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CUO	A	5005[D]	-	0,4,4	-	-	-		
9	CUO	S	2101[C]	-	0,4,4	-	-	-		
9	CUO	M	2105	1	0,4,4	-	-	-		
9	CUO	c	3001	2	0,4,4	-	-	-		
9	CUO	G	2104	1	0,4,4	-	-	-		

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
9	CUO	J	5001	1	-	-	0/1/1/1
9	CUO	A	5005[C]	-	-	-	0/1/1/1
9	CUO	P	5003	1	-	-	0/1/1/1
9	CUO	J	5005[C]	-	-	-	0/1/1/1
9	CUO	D	5004	1	-	-	0/1/1/1
9	CUO	P	5005[D]	-	-	-	0/1/1/1
9	CUO	D	5002	1	-	-	0/1/1/1
9	CUO	X	3401[A]	3	-	-	0/1/1/1
9	CUO	V	5003	1	-	-	0/1/1/1
9	CUO	S	2105	1	-	-	0/1/1/1
9	CUO	U	3401[B]	3	-	-	0/1/1/1
9	CUO	P	5001	1	-	-	0/1/1/1
9	CUO	L	3401[A]	3	-	-	0/1/1/1
9	CUO	F	3401[A]	3	-	-	0/1/1/1
9	CUO	O	3401[B]	3	-	-	0/1/1/1
9	CUO	a	3401[B]	3	-	-	0/1/1/1
9	CUO	R	3401[B]	3	-	-	0/1/1/1
9	CUO	A	5004	1	-	-	0/1/1/1
9	CUO	I	3401[A]	3	-	-	0/1/1/1
9	CUO	A	5001	1	-	-	0/1/1/1
9	CUO	M	2101[C]	-	-	-	0/1/1/1
9	CUO	Q	3001	2	-	-	0/1/1/1
9	CUO	S	2103	1	-	-	0/1/1/1
9	CUO	V	5001	1	-	-	0/1/1/1
9	CUO	J	5003	1	-	-	0/1/1/1
9	CUO	N	3001	2	-	-	0/1/1/1
9	CUO	J	5002	1	-	-	0/1/1/1
9	CUO	Y	2101[D]	-	-	-	0/1/1/1
9	CUO	B	3002	2	-	-	0/1/1/1
9	CUO	J	5004	1	-	-	0/1/1/1
9	CUO	K	3001	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CUO	d	3401[B]	3	-	-	0/1/1/1
9	CUO	X	3401[B]	3	-	-	0/1/1/1
9	CUO	V	5002	1	-	-	0/1/1/1
9	CUO	V	5004	1	-	-	0/1/1/1
9	CUO	D	5005[D]	-	-	-	0/1/1/1
9	CUO	Y	2101[C]	-	-	-	0/1/1/1
9	CUO	C	3401[A]	3	-	-	0/1/1/1
9	CUO	L	3401[B]	3	-	-	0/1/1/1
9	CUO	P	5005[C]	-	-	-	0/1/1/1
9	CUO	F	3401[B]	3	-	-	0/1/1/1
9	CUO	B	3001	2	-	-	0/1/1/1
9	CUO	Y	2105	1	-	-	0/1/1/1
9	CUO	D	5001	1	-	-	0/1/1/1
9	CUO	M	2103	1	-	-	0/1/1/1
9	CUO	D	5005[C]	-	-	-	0/1/1/1
9	CUO	A	5002	1	-	-	0/1/1/1
9	CUO	S	2102	1	-	-	0/1/1/1
9	CUO	Y	2104	1	-	-	0/1/1/1
9	CUO	T	3002	2	-	-	0/1/1/1
9	CUO	D	5003	1	-	-	0/1/1/1
9	CUO	G	2105	1	-	-	0/1/1/1
9	CUO	Z	3001	2	-	-	0/1/1/1
9	CUO	V	5005[D]	-	-	-	0/1/1/1
9	CUO	H	3001	2	-	-	0/1/1/1
9	CUO	H	3002	2	-	-	0/1/1/1
9	CUO	V	5005[C]	-	-	-	0/1/1/1
9	CUO	U	3401[A]	3	-	-	0/1/1/1
9	CUO	b	2102	1	-	-	0/1/1/1
9	CUO	Y	2102	1	-	-	0/1/1/1
9	CUO	S	2104	1	-	-	0/1/1/1
9	CUO	M	2104	1	-	-	0/1/1/1
9	CUO	O	3401[A]	3	-	-	0/1/1/1
9	CUO	N	3002	2	-	-	0/1/1/1
9	CUO	W	3002	2	-	-	0/1/1/1
9	CUO	a	3401[A]	3	-	-	0/1/1/1
9	CUO	R	3401[A]	3	-	-	0/1/1/1
9	CUO	M	2102	1	-	-	0/1/1/1
9	CUO	b	2105	1	-	-	0/1/1/1
9	CUO	W	3001	2	-	-	0/1/1/1
9	CUO	P	5002	1	-	-	0/1/1/1
9	CUO	c	3002	2	-	-	0/1/1/1
9	CUO	I	3401[B]	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CUO	J	5005[D]	-	-	-	0/1/1/1
9	CUO	K	3002	2	-	-	0/1/1/1
9	CUO	A	5003	1	-	-	0/1/1/1
9	CUO	d	3401[A]	3	-	-	0/1/1/1
9	CUO	E	3002	2	-	-	0/1/1/1
9	CUO	T	3001	2	-	-	0/1/1/1
9	CUO	G	2102	1	-	-	0/1/1/1
9	CUO	Z	3002	2	-	-	0/1/1/1
9	CUO	Q	3002	2	-	-	0/1/1/1
9	CUO	b	2101[D]	-	-	-	0/1/1/1
9	CUO	M	2101[D]	-	-	-	0/1/1/1
9	CUO	b	2103	1	-	-	0/1/1/1
9	CUO	Y	2103	1	-	-	0/1/1/1
9	CUO	G	2101[D]	-	-	-	0/1/1/1
9	CUO	S	2101[D]	-	-	-	0/1/1/1
9	CUO	E	3001	2	-	-	0/1/1/1
9	CUO	b	2101[C]	-	-	-	0/1/1/1
9	CUO	C	3401[B]	3	-	-	0/1/1/1
9	CUO	P	5004	1	-	-	0/1/1/1
9	CUO	G	2103	1	-	-	0/1/1/1
9	CUO	b	2104	1	-	-	0/1/1/1
9	CUO	G	2101[C]	-	-	-	0/1/1/1
9	CUO	A	5005[D]	-	-	-	0/1/1/1
9	CUO	S	2101[C]	-	-	-	0/1/1/1
9	CUO	M	2105	1	-	-	0/1/1/1
9	CUO	c	3001	2	-	-	0/1/1/1
9	CUO	G	2104	1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

38 monomers are involved in 101 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	5001	CUO	1	0
9	D	5004	CUO	1	0
9	X	3401[A]	CUO	5	0
9	V	5003	CUO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	U	3401[B]	CUO	5	0
9	L	3401[A]	CUO	5	0
9	F	3401[A]	CUO	5	0
9	O	3401[B]	CUO	5	0
9	a	3401[B]	CUO	2	0
9	R	3401[B]	CUO	1	0
9	I	3401[A]	CUO	5	0
9	A	5001	CUO	2	0
9	J	5002	CUO	1	0
9	d	3401[B]	CUO	5	0
9	X	3401[B]	CUO	5	0
9	V	5004	CUO	1	0
9	C	3401[A]	CUO	5	0
9	L	3401[B]	CUO	2	0
9	F	3401[B]	CUO	2	0
9	Y	2105	CUO	1	0
9	D	5001	CUO	1	0
9	S	2102	CUO	1	0
9	Y	2104	CUO	1	0
9	T	3002	CUO	1	0
9	U	3401[A]	CUO	5	0
9	Y	2102	CUO	1	0
9	S	2104	CUO	2	0
9	M	2104	CUO	1	0
9	O	3401[A]	CUO	5	0
9	W	3002	CUO	1	0
9	a	3401[A]	CUO	5	0
9	R	3401[A]	CUO	5	0
9	b	2105	CUO	1	0
9	I	3401[B]	CUO	1	0
9	d	3401[A]	CUO	5	0
9	C	3401[B]	CUO	2	0
9	M	2105	CUO	2	0
9	G	2104	CUO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1656/2000 (82%)	-0.43	6 (0%) 88 76	36, 70, 118, 164	0
1	D	1656/2000 (82%)	-0.44	10 (0%) 85 69	37, 67, 114, 176	0
1	G	1656/2000 (82%)	-0.46	6 (0%) 88 76	31, 68, 109, 152	0
1	J	1656/2000 (82%)	-0.46	5 (0%) 90 79	30, 64, 119, 162	0
1	M	1656/2000 (82%)	-0.59	6 (0%) 88 76	29, 56, 109, 157	0
1	P	1656/2000 (82%)	-0.66	10 (0%) 85 69	27, 53, 97, 176	0
1	S	1656/2000 (82%)	-0.58	5 (0%) 90 79	31, 60, 108, 164	0
1	V	1656/2000 (82%)	-0.66	4 (0%) 91 83	26, 55, 105, 154	0
1	Y	1656/2000 (82%)	-0.50	3 (0%) 91 83	31, 66, 112, 160	0
1	b	1656/2000 (82%)	-0.58	7 (0%) 88 76	30, 60, 105, 161	0
2	B	825/920 (89%)	-0.68	0 100 100	32, 57, 101, 140	0
2	E	825/920 (89%)	-0.65	2 (0%) 91 83	30, 59, 106, 137	0
2	H	825/920 (89%)	-0.55	2 (0%) 91 83	31, 63, 112, 147	0
2	K	825/920 (89%)	-0.59	0 100 100	34, 60, 101, 158	0
2	N	825/920 (89%)	-0.80	2 (0%) 91 83	21, 46, 92, 135	0
2	Q	825/920 (89%)	-0.80	1 (0%) 92 86	26, 49, 100, 134	0
2	T	825/920 (89%)	-0.73	1 (0%) 92 86	30, 53, 93, 137	0
2	W	825/920 (89%)	-0.75	1 (0%) 92 86	25, 53, 99, 129	0
2	Z	825/920 (89%)	-0.76	1 (0%) 92 86	25, 52, 95, 130	0
2	c	825/920 (89%)	-0.71	2 (0%) 91 83	26, 55, 103, 135	0
3	C	366/394 (92%)	0.97	49 (13%) 7 4	34, 45, 49, 55	366 (100%)
3	F	366/394 (92%)	0.76	30 (8%) 17 9	28, 39, 44, 54	366 (100%)
3	I	366/394 (92%)	0.72	28 (7%) 19 10	29, 39, 46, 56	366 (100%)
3	L	366/394 (92%)	0.84	30 (8%) 17 9	32, 44, 49, 53	366 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	O	366/394 (92%)	0.76	29 (7%) 18 10	26, 37, 47, 53	366 (100%)
3	R	366/394 (92%)	0.68	23 (6%) 26 13	29, 39, 45, 55	366 (100%)
3	U	366/394 (92%)	0.74	27 (7%) 20 10	26, 37, 47, 51	366 (100%)
3	X	366/394 (92%)	1.27	47 (12%) 7 5	39, 51, 56, 58	366 (100%)
3	a	366/394 (92%)	0.69	22 (6%) 27 14	27, 38, 44, 48	366 (100%)
3	d	366/394 (92%)	1.13	39 (10%) 11 6	41, 49, 53, 56	366 (100%)
All	All	28470/33140 (85%)	-0.41	398 (1%) 73 51	21, 56, 106, 176	3660 (12%)

All (398) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	3282[A]	ASP	6.6
3	F	3216[A]	GLY	6.3
3	X	3088[A]	GLY	5.9
3	O	3101[A]	PRO	5.8
3	X	3108[A]	HIS	5.8
3	I	3002[A]	ALA	5.6
3	L	3302[A]	SER	5.6
3	C	2929[A]	SER	5.6
3	F	3106[A]	THR	5.5
3	F	3282[A]	ASP	5.3
3	d	3282[A]	ASP	5.2
3	X	2931[A]	THR	5.2
3	d	3101[A]	PRO	5.1
3	O	3146[A]	CYS	5.1
3	R	3292[A]	GLY	5.1
3	C	3282[A]	ASP	5.0
3	a	3302[A]	SER	5.0
3	F	3101[A]	PRO	5.0
3	U	2999[A]	ALA	4.9
3	F	3166[A]	GLU	4.8
3	F	3215[A]	ALA	4.8
3	U	3294[A]	SER	4.7
3	O	3097[A]	GLY	4.6
3	X	2952[A]	ALA	4.6
3	F	3085[A]	PHE	4.6
3	L	2986[A]	PRO	4.6
1	D	1165	GLY	4.4
3	X	2979[A]	GLN	4.4
3	O	3220[A]	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
3	d	2977[A]	CYS	4.4
3	R	3282[A]	ASP	4.3
3	L	3079[A]	CYS	4.3
3	F	3283[A]	ILE	4.3
3	X	3040[A]	VAL	4.2
3	C	3285[A]	VAL	4.2
3	X	2953[A]	GLY	4.2
3	a	3243[A]	GLY	4.2
3	d	3221[A]	ALA	4.1
1	S	956	PRO	4.1
1	Y	961	SER	4.0
3	C	2953[A]	GLY	4.0
3	I	3100[A]	SER	4.0
3	L	3248[A]	LEU	4.0
3	L	3303[A]	PRO	4.0
3	I	3288[A]	MET	4.0
3	U	3216[A]	GLY	3.9
3	a	3293[A]	LYS	3.9
3	O	3094[A]	SER	3.9
3	O	2952[A]	ALA	3.9
3	C	3298[A]	ASN	3.9
3	X	2989[A]	HIS	3.9
1	V	1577	GLY	3.8
3	I	3166[A]	GLU	3.8
3	X	3091[A]	ALA	3.8
3	a	3282[A]	ASP	3.8
3	X	3292[A]	GLY	3.8
3	a	2952[A]	ALA	3.7
3	O	3002[A]	ALA	3.7
3	O	3282[A]	ASP	3.7
3	C	3286[A]	THR	3.7
3	R	2931[A]	THR	3.7
1	G	563	ILE	3.7
3	d	2931[A]	THR	3.6
3	U	3293[A]	LYS	3.6
3	U	2953[A]	GLY	3.6
3	I	3289[A]	GLY	3.6
3	a	2953[A]	GLY	3.5
3	U	2932[A]	PRO	3.5
1	J	962	GLY	3.5
1	D	571	PRO	3.5
3	L	3166[A]	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	3088[A]	GLY	3.4
3	U	3002[A]	ALA	3.4
3	F	2932[A]	PRO	3.4
3	U	2952[A]	ALA	3.4
3	a	3114[A]	PRO	3.4
3	C	3302[A]	SER	3.4
3	I	3172[A]	SER	3.4
3	F	2983[A]	VAL	3.4
3	d	3185[A]	TYR	3.4
1	D	956	PRO	3.4
3	O	3183[A]	LEU	3.3
3	X	2965[A]	LEU	3.3
3	U	3100[A]	SER	3.3
3	U	3299[A]	LEU	3.3
3	X	2934[A]	GLU	3.3
1	b	1577	GLY	3.3
3	U	2958[A]	ALA	3.3
3	C	3256[A]	TRP	3.3
3	d	3100[A]	SER	3.3
1	J	873	VAL	3.2
1	A	1023	GLY	3.2
3	L	2953[A]	GLY	3.2
3	C	3094[A]	SER	3.2
3	C	3247[A]	VAL	3.2
3	L	3282[A]	ASP	3.2
3	R	3002[A]	ALA	3.2
3	F	3303[A]	PRO	3.2
3	I	2932[A]	PRO	3.2
3	a	3301[A]	PRO	3.2
2	Z	2548	CYS	3.2
3	C	2958[A]	ALA	3.2
3	O	3216[A]	GLY	3.2
3	I	3297[A]	PRO	3.2
3	I	3282[A]	ASP	3.2
3	C	3299[A]	LEU	3.2
3	C	3283[A]	ILE	3.2
3	F	3220[A]	ARG	3.1
3	C	3226[A]	ALA	3.1
1	b	962	GLY	3.1
3	U	3302[A]	SER	3.1
3	U	3247[A]	VAL	3.1
3	O	2937[A]	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	3086[A]	GLU	3.1
3	C	3092[A]	ILE	3.1
3	X	3104[A]	MET	3.1
3	R	3112[A]	TYR	3.1
2	N	2651	GLN	3.0
3	U	3102[A]	TYR	3.0
3	X	3143[A]	SER	3.0
1	b	419	THR	3.0
3	L	3101[A]	PRO	3.0
3	X	3032[A]	PRO	2.9
3	d	2932[A]	PRO	2.9
1	A	473	ALA	2.9
1	b	1501	ALA	2.9
3	a	2983[A]	VAL	2.9
3	R	2930[A]	LEU	2.9
3	R	2932[A]	PRO	2.9
1	M	964	ILE	2.9
3	d	3091[A]	ALA	2.9
3	I	2979[A]	GLN	2.9
3	F	3179[A]	ASP	2.9
1	P	870	TYR	2.9
3	X	3100[A]	SER	2.9
3	d	3302[A]	SER	2.9
3	C	2932[A]	PRO	2.9
3	R	3173[A]	THR	2.9
2	E	2651	GLN	2.8
3	C	3297[A]	PRO	2.8
3	d	2951[A]	ASP	2.8
3	L	2985[A]	PHE	2.8
3	d	3109[A]	TYR	2.8
3	O	2953[A]	GLY	2.8
3	X	3138[A]	GLY	2.8
3	O	2931[A]	THR	2.8
3	a	2981[A]	GLY	2.8
3	U	2954[A]	TYR	2.8
1	D	1166	THR	2.8
1	A	1167	ASP	2.7
1	P	834	ASP	2.7
1	D	955	LYS	2.7
2	T	2555	GLU	2.7
3	I	3245[A]	PHE	2.7
3	C	3106[A]	THR	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	2951[A]	ASP	2.7
3	O	3288[A]	MET	2.7
1	P	1577	GLY	2.7
3	a	2931[A]	THR	2.7
3	C	3169[A]	LYS	2.7
1	V	834	ASP	2.7
3	L	3090[A]	ASN	2.7
3	U	3101[A]	PRO	2.7
3	X	3028[A]	PRO	2.7
3	X	3048[A]	ASP	2.7
3	O	2932[A]	PRO	2.7
3	d	3301[A]	PRO	2.7
3	a	3094[A]	SER	2.7
3	F	3185[A]	TYR	2.7
3	X	3035[A]	HIS	2.7
3	C	3164[A]	PRO	2.6
3	C	2934[A]	GLU	2.6
3	I	2929[A]	SER	2.6
3	R	2948[A]	ASP	2.6
3	X	3030[A]	ASN	2.6
3	d	3104[A]	MET	2.6
3	L	3114[A]	PRO	2.6
3	R	3101[A]	PRO	2.6
3	U	2982[A]	MET	2.6
3	I	3179[A]	ASP	2.6
1	M	1023	GLY	2.6
3	F	2931[A]	THR	2.6
3	d	3170[A]	ALA	2.6
3	C	3217[A]	PHE	2.6
1	M	1304	ASP	2.6
3	d	3248[A]	LEU	2.6
3	X	3140[A]	PRO	2.6
3	X	3302[A]	SER	2.6
1	A	1086	LEU	2.6
3	R	3040[A]	VAL	2.6
3	d	3286[A]	THR	2.6
3	R	3020[A]	SER	2.5
3	a	3294[A]	SER	2.5
3	I	3107[A]	LEU	2.5
3	R	3248[A]	LEU	2.5
3	O	3077[A]	ASP	2.5
3	C	3252[A]	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	1244	GLY	2.5
3	X	3248[A]	LEU	2.5
2	c	2733	ASP	2.5
3	I	3162[A]	ASP	2.5
3	X	3090[A]	ASN	2.5
3	L	3255[A]	PRO	2.5
3	I	3299[A]	LEU	2.5
3	O	2976[A]	ALA	2.5
3	d	3005[A]	ALA	2.5
1	G	956	PRO	2.5
3	C	3218[A]	LEU	2.5
3	C	3220[A]	ARG	2.5
3	C	2947[A]	ALA	2.5
3	F	3002[A]	ALA	2.5
3	d	2952[A]	ALA	2.5
3	R	3288[A]	MET	2.5
3	X	2963[A]	MET	2.5
3	L	3240[A]	THR	2.5
3	d	3026[A]	THR	2.5
3	L	3032[A]	PRO	2.5
3	a	3299[A]	LEU	2.5
3	C	3100[A]	SER	2.4
3	F	2977[A]	CYS	2.4
3	R	3148[A]	ILE	2.4
2	W	2552	GLU	2.4
1	b	965	ASP	2.4
3	X	3101[A]	PRO	2.4
3	a	2932[A]	PRO	2.4
3	X	2992[A]	TYR	2.4
1	J	1577	GLY	2.4
1	M	972	SER	2.4
3	C	2928[A]	ASN	2.4
3	a	3142[A]	ASN	2.4
1	A	834	ASP	2.4
1	S	834	ASP	2.4
3	L	3040[A]	VAL	2.4
1	P	1002	GLU	2.4
3	d	3161[A]	GLU	2.4
1	J	961	SER	2.4
3	a	2933[A]	SER	2.4
3	C	3244[A]	THR	2.4
3	R	3032[A]	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	X	3097[A]	GLY	2.4
3	C	2935[A]	ILE	2.4
3	C	3101[A]	PRO	2.4
3	F	3164[A]	PRO	2.4
3	X	3106[A]	THR	2.4
3	C	2954[A]	TYR	2.4
1	P	151	GLN	2.4
3	X	2929[A]	SER	2.4
3	I	2983[A]	VAL	2.4
3	O	3114[A]	PRO	2.4
1	D	948	THR	2.3
3	L	2931[A]	THR	2.3
3	F	2976[A]	ALA	2.3
3	I	3293[A]	LYS	2.3
3	L	3170[A]	ALA	2.3
1	V	828	ASP	2.3
3	O	3048[A]	ASP	2.3
3	X	3188[A]	ASP	2.3
3	X	2985[A]	PHE	2.3
1	P	961	SER	2.3
3	F	3032[A]	PRO	2.3
1	b	1025	THR	2.3
3	U	2931[A]	THR	2.3
3	d	3281[A]	PHE	2.3
3	X	2983[A]	VAL	2.3
3	d	3198[A]	PRO	2.3
1	D	419	THR	2.3
3	C	2931[A]	THR	2.3
3	L	3143[A]	SER	2.3
3	O	3106[A]	THR	2.3
3	I	2978[A]	CYS	2.3
3	d	3082[A]	GLU	2.3
3	I	3101[A]	PRO	2.3
3	U	3226[A]	ALA	2.3
3	I	3286[A]	THR	2.3
3	O	3286[A]	THR	2.3
3	U	2979[A]	GLN	2.3
3	X	3029[A]	LYS	2.3
3	C	3232[A]	VAL	2.3
3	U	3232[A]	VAL	2.3
3	d	2934[A]	GLU	2.3
3	X	3005[A]	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	I	2987[A]	HIS	2.3
3	O	2987[A]	HIS	2.3
3	X	3046[A]	THR	2.3
3	F	3230[A]	PHE	2.3
3	X	3111[A]	SER	2.3
1	M	148	GLN	2.3
2	N	2083	VAL	2.3
3	L	2934[A]	GLU	2.2
3	X	2936[A]	GLU	2.2
1	P	956	PRO	2.2
2	E	2889	ALA	2.2
1	G	1576	THR	2.2
3	C	3037[A]	TYR	2.2
1	D	1621	ASN	2.2
3	U	3097[A]	GLY	2.2
3	U	3006[A]	LYS	2.2
3	d	3244[A]	THR	2.2
1	P	331	SER	2.2
3	C	3271[A]	VAL	2.2
3	U	3285[A]	VAL	2.2
3	X	2945[A]	VAL	2.2
1	D	326	GLU	2.2
2	c	2841	GLU	2.2
3	U	3080[A]	ASP	2.2
3	C	3114[A]	PRO	2.2
3	F	2958[A]	ALA	2.2
3	X	2932[A]	PRO	2.2
3	a	3032[A]	PRO	2.2
3	X	3274[A]	ARG	2.2
3	d	2939[A]	ARG	2.2
1	D	870	TYR	2.2
1	V	448	SER	2.2
3	C	3143[A]	SER	2.2
3	O	3100[A]	SER	2.2
3	a	3121[A]	SER	2.2
1	A	562	GLN	2.2
1	S	562	GLN	2.2
3	d	2935[A]	ILE	2.2
1	Y	957	ASN	2.2
1	b	1214	GLU	2.2
3	L	2937[A]	ASN	2.2
3	L	3107[A]	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	2947[A]	ALA	2.2
3	X	3146[A]	CYS	2.2
1	J	887	ASP	2.2
3	R	3153[A]	LYS	2.2
3	I	3168[A]	THR	2.2
3	O	3271[A]	VAL	2.2
1	Y	1638	SER	2.2
3	d	3020[A]	SER	2.2
3	C	3161[A]	GLU	2.2
3	R	3050[A]	ARG	2.2
3	O	2948[A]	ASP	2.2
3	X	3109[A]	TYR	2.1
2	Q	2549	PRO	2.1
3	I	3050[A]	ARG	2.1
3	d	3217[A]	PHE	2.1
3	a	3240[A]	THR	2.1
3	I	3112[A]	TYR	2.1
3	U	3300[A]	LEU	2.1
3	F	3144[A]	ALA	2.1
3	L	2933[A]	SER	2.1
3	a	3039[A]	ASP	2.1
3	L	3007[A]	ILE	2.1
2	H	2555	GLU	2.1
3	F	3217[A]	PHE	2.1
3	C	3248[A]	LEU	2.1
3	F	3280[A]	ASP	2.1
3	L	3150[A]	LYS	2.1
3	L	3162[A]	ASP	2.1
3	O	3123[A]	THR	2.1
3	X	3240[A]	THR	2.1
3	O	3088[A]	GLY	2.1
1	M	571	PRO	2.1
2	H	2549	PRO	2.1
3	I	2934[A]	GLU	2.1
1	G	1257	SER	2.1
3	C	3040[A]	VAL	2.1
3	X	3299[A]	LEU	2.1
3	C	3112[A]	TYR	2.1
3	F	3112[A]	TYR	2.1
3	I	3091[A]	ALA	2.1
3	C	2979[A]	GLN	2.1
3	R	2953[A]	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
3	R	3243[A]	GLY	2.1
3	C	3085[A]	PHE	2.1
3	C	3255[A]	PRO	2.1
3	O	3164[A]	PRO	2.1
3	R	3164[A]	PRO	2.1
1	P	831	VAL	2.0
1	S	1639	LYS	2.0
3	F	3096[A]	VAL	2.0
3	C	3274[A]	ARG	2.0
3	L	3137[A]	ARG	2.0
3	O	3261[A]	LEU	2.0
3	a	3277[A]	ALA	2.0
3	d	3240[A]	THR	2.0
3	d	3098[A]	GLY	2.0
3	d	3206[A]	LYS	2.0
3	L	3274[A]	ARG	2.0
3	d	2930[A]	LEU	2.0
1	G	964	ILE	2.0
3	F	3038[A]	ILE	2.0
3	C	3095[A]	TRP	2.0
3	d	3035[A]	HIS	2.0
3	R	3106[A]	THR	2.0
3	U	2974[A]	ALA	2.0
3	d	3045[A]	THR	2.0
1	P	418	ASP	2.0
3	I	3048[A]	ASP	2.0
3	d	3039[A]	ASP	2.0
3	F	2964[A]	PRO	2.0
3	R	2995[A]	GLN	2.0
1	S	795	GLU	2.0
3	L	3050[A]	ARG	2.0
3	d	3107[A]	LEU	2.0
3	d	3083[A]	ILE	2.0

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

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	e	1	14/15	-	-	62,79,86,94	0
4	NAG	e	2	14/15	-	-	69,83,96,102	0
4	NAG	f	1	14/15	-	-	88,95,105,109	0
4	NAG	f	2	14/15	-	-	106,116,123,129	0
4	NAG	i	1	14/15	-	-	59,68,91,95	0
4	NAG	i	2	14/15	-	-	84,92,107,111	0
4	NAG	j	1	14/15	-	-	59,67,76,76	0
4	NAG	j	2	14/15	-	-	49,57,73,79	0
4	NAG	m	1	14/15	-	-	77,91,99,104	0
4	NAG	m	2	14/15	-	-	80,95,108,108	0
4	NAG	n	1	14/15	-	-	67,77,90,98	0
4	NAG	n	2	14/15	-	-	72,91,105,110	0
4	NAG	o	1	14/15	-	-	61,73,85,88	0
4	NAG	o	2	14/15	-	-	43,67,86,87	0
4	NAG	p	1	14/15	-	-	47,61,75,75	0
4	NAG	p	2	14/15	-	-	54,72,84,88	0
4	NAG	q	1	14/15	-	-	56,67,78,80	0
4	NAG	q	2	14/15	-	-	80,88,92,93	0
4	NAG	s	1	14/15	-	-	71,77,85,90	0
4	NAG	s	2	14/15	-	-	89,102,108,116	0
4	NAG	t	1	14/15	-	-	53,69,82,85	0
4	NAG	t	2	14/15	-	-	50,90,102,103	0
4	NAG	u	1	14/15	-	-	73,78,87,92	0
4	NAG	u	2	14/15	-	-	86,100,114,132	0
4	NAG	v	1	14/15	-	-	64,80,91,91	0
4	NAG	v	2	14/15	-	-	82,97,104,106	0
4	NAG	x	1	14/15	-	-	80,94,105,105	0
4	NAG	x	2	14/15	-	-	104,115,125,125	0
4	NAG	1	1	14/15	-	-	88,96,102,103	0
4	NAG	1	2	14/15	-	-	91,104,121,126	0
4	NAG	2	1	14/15	-	-	41,56,75,80	0
4	NAG	2	2	14/15	-	-	53,71,87,100	0
4	NAG	4	1	14/15	-	-	57,70,74,80	0
4	NAG	4	2	14/15	-	-	78,96,107,116	0
4	NAG	6	1	14/15	-	-	74,81,89,91	0
4	NAG	6	2	14/15	-	-	49,73,85,91	0
4	NAG	7	1	14/15	-	-	57,70,83,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	7	2	14/15	-	-	69,83,101,104	0
4	NAG	8	1	14/15	-	-	57,62,72,81	0
4	NAG	8	2	14/15	-	-	64,84,98,101	0
4	NAG	9	1	14/15	-	-	87,95,100,108	0
4	NAG	9	2	14/15	-	-	73,97,113,113	0
4	NAG	BA	1	14/15	-	-	80,84,96,97	0
4	NAG	BA	2	14/15	-	-	62,82,95,101	0
6	NAG	GA	2	14/15	0.91	0.13	88,108,127,131	0
5	BMA	KA	3	11/12	0.92	0.07	79,99,114,127	0
4	NAG	MA	2	14/15	0.92	0.09	84,93,116,127	0
4	NAG	IA	2	14/15	0.93	0.10	75,89,96,100	0
5	NAG	FA	2	14/15	0.94	0.10	74,88,101,105	0
6	NAG	EA	2	14/15	0.94	0.08	70,82,98,108	0
5	NAG	KA	1	14/15	0.94	0.08	60,66,76,78	0
6	NAG	LA	2	14/15	0.94	0.10	76,89,100,104	0
6	BMA	LA	3	11/12	0.94	0.09	101,110,119,119	0
6	NAG	NA	2	14/15	0.94	0.10	61,80,101,112	0
4	NAG	QA	2	14/15	0.95	0.08	97,115,121,125	0
5	NAG	PA	2	14/15	0.95	0.07	72,80,89,91	0
4	NAG	RA	1	14/15	0.95	0.12	75,83,99,108	0
4	NAG	RA	2	14/15	0.95	0.07	83,92,102,114	0
5	NAG	g	1	14/15	-	-	57,79,95,97	0
5	NAG	g	2	14/15	-	-	99,105,109,109	0
5	BMA	g	3	11/12	-	-	110,124,133,139	0
5	MAN	g	4	11/12	-	-	103,117,133,133	0
5	NAG	l	1	14/15	-	-	52,57,72,76	0
5	NAG	l	2	14/15	-	-	69,84,96,97	0
5	BMA	l	3	11/12	-	-	98,113,119,128	0
5	MAN	l	4	11/12	-	-	114,118,122,128	0
5	NAG	AA	1	14/15	-	-	61,71,75,75	0
5	NAG	AA	2	14/15	-	-	87,92,98,104	0
5	BMA	AA	3	11/12	-	-	112,120,124,127	0
5	MAN	AA	4	11/12	-	-	114,125,132,145	0
6	BMA	GA	3	11/12	0.95	0.09	130,136,142,143	0
4	NAG	MA	1	14/15	0.95	0.10	69,77,85,86	0
5	BMA	FA	3	11/12	-	-	85,101,110,113	0
5	MAN	FA	4	11/12	-	-	94,107,126,132	0
4	NAG	HA	1	14/15	0.95	0.08	56,63,83,93	0
5	NAG	KA	2	14/15	0.95	0.07	67,81,92,93	0
6	NAG	GA	1	14/15	0.96	0.09	79,97,106,109	0
5	MAN	KA	4	11/12	-	-	87,103,122,135	0
6	NAG	EA	1	14/15	0.96	0.07	46,58,71,75	0

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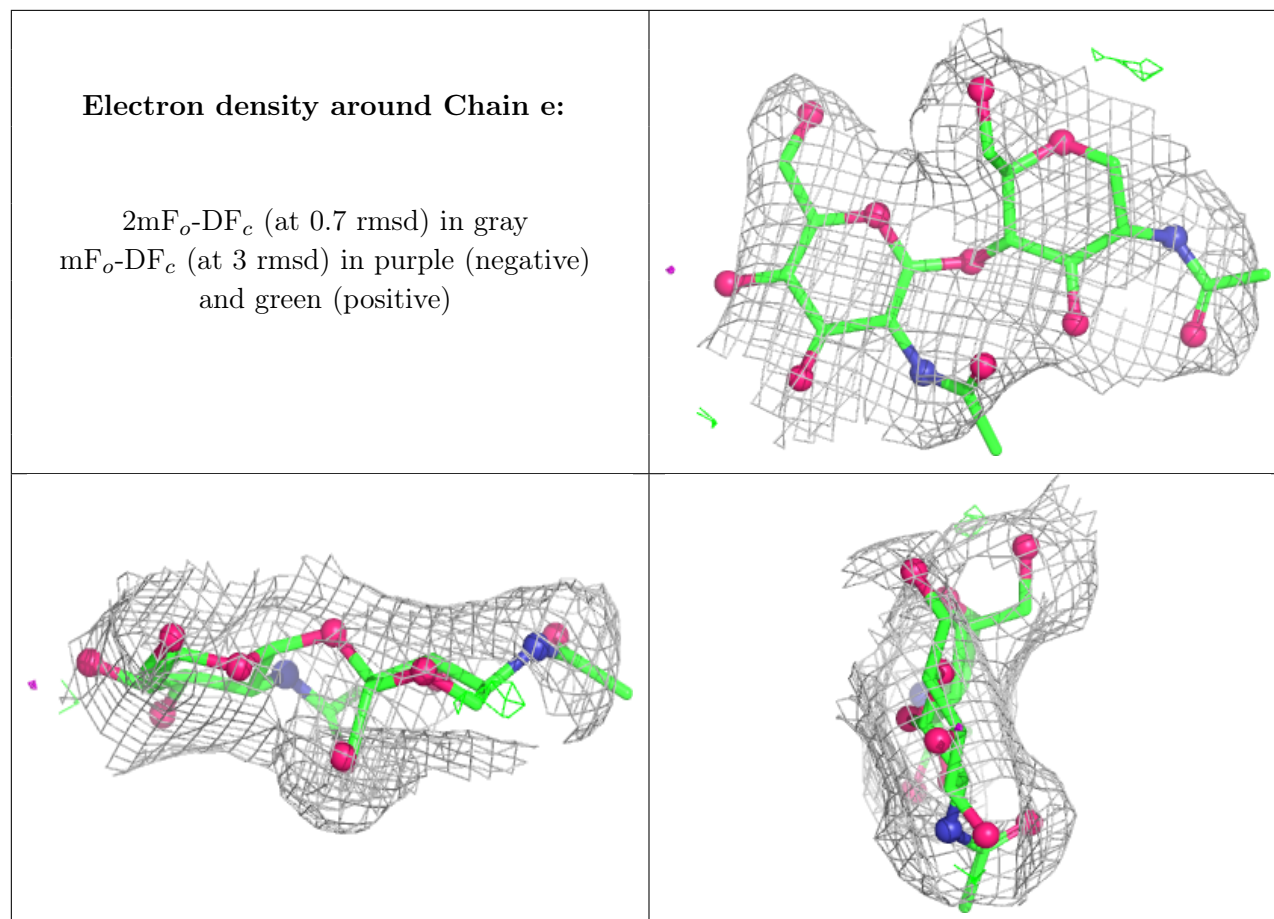
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	OA	1	14/15	0.96	0.09	57,70,80,85	0
5	BMA	PA	3	11/12	-	-	96,97,104,125	0
5	MAN	PA	4	11/12	-	-	107,112,125,133	0
6	NAG	h	1	14/15	-	-	85,93,112,115	0
6	NAG	h	2	14/15	-	-	84,94,107,114	0
6	BMA	h	3	11/12	-	-	108,114,120,126	0
6	NAG	k	1	14/15	-	-	71,83,92,99	0
6	NAG	k	2	14/15	-	-	88,104,119,123	0
6	BMA	k	3	11/12	-	-	110,119,126,133	0
6	NAG	r	1	14/15	-	-	79,88,107,112	0
6	NAG	r	2	14/15	-	-	84,91,98,102	0
6	BMA	r	3	11/12	-	-	111,120,128,129	0
6	NAG	w	1	14/15	-	-	78,100,106,118	0
6	NAG	w	2	14/15	-	-	88,104,108,111	0
6	BMA	w	3	11/12	-	-	107,110,117,128	0
6	NAG	y	1	14/15	-	-	52,67,74,75	0
6	NAG	y	2	14/15	-	-	65,83,94,109	0
6	BMA	y	3	11/12	-	-	102,116,123,123	0
6	NAG	3	1	14/15	-	-	46,67,81,90	0
6	NAG	3	2	14/15	-	-	61,82,96,102	0
6	BMA	3	3	11/12	-	-	114,119,149,149	0
6	NAG	5	1	14/15	-	-	52,60,70,76	0
6	NAG	5	2	14/15	-	-	61,77,95,103	0
6	BMA	5	3	11/12	-	-	98,114,124,127	0
6	NAG	CA	1	14/15	-	-	59,71,83,91	0
6	NAG	CA	2	14/15	-	-	88,97,115,124	0
6	BMA	CA	3	11/12	-	-	96,123,130,130	0
6	NAG	DA	1	14/15	-	-	50,66,77,82	0
6	NAG	DA	2	14/15	-	-	78,91,95,98	0
6	BMA	DA	3	11/12	-	-	82,103,108,108	0
4	NAG	IA	1	14/15	0.97	0.07	51,66,83,92	0
4	NAG	HA	2	14/15	0.97	0.07	71,82,95,107	0
6	BMA	EA	3	11/12	-	-	104,115,132,134	0
6	NAG	LA	1	14/15	0.97	0.07	78,87,93,98	0
4	NAG	JA	1	14/15	0.97	0.05	70,80,88,90	0
4	NAG	OA	2	14/15	0.97	0.08	55,73,85,91	0
6	NAG	NA	1	14/15	0.97	0.07	56,62,71,72	0
4	NAG	JA	2	14/15	0.97	0.05	82,92,100,100	0
5	NAG	PA	1	14/15	0.98	0.06	62,72,77,78	0
4	NAG	QA	1	14/15	0.98	0.07	97,107,114,118	0
5	NAG	FA	1	14/15	0.98	0.06	49,68,77,78	0
6	BMA	NA	3	11/12	-	-	102,117,134,138	0

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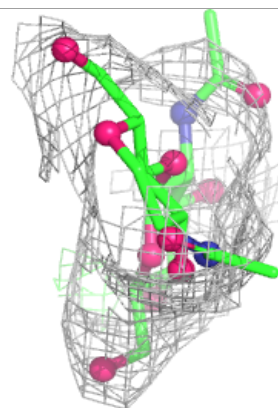
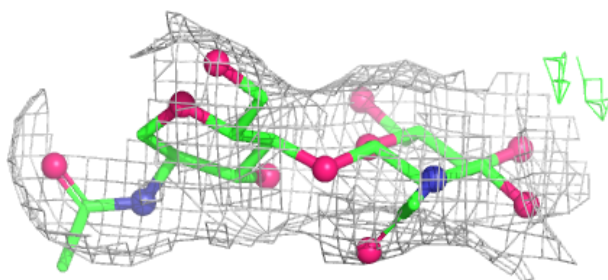
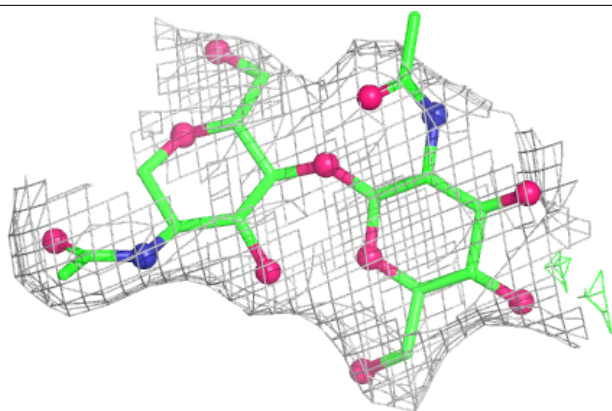
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	z	1	14/15	-	-	79,85,93,96	0
7	NAG	z	2	14/15	-	-	92,105,121,128	0
7	BMA	z	3	11/12	-	-	124,134,140,150	0
7	MAN	z	4	11/12	-	-	135,140,150,154	0
7	MAN	z	5	11/12	-	-	121,135,151,154	0
8	NAG	0	1	14/15	-	-	60,67,72,81	0
8	NAG	0	2	14/15	-	-	58,78,82,90	0
8	BMA	0	3	11/12	-	-	97,112,128,130	0
8	MAN	0	4	11/12	-	-	94,114,123,126	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

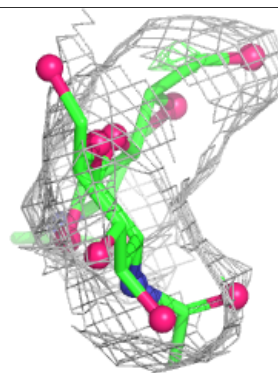
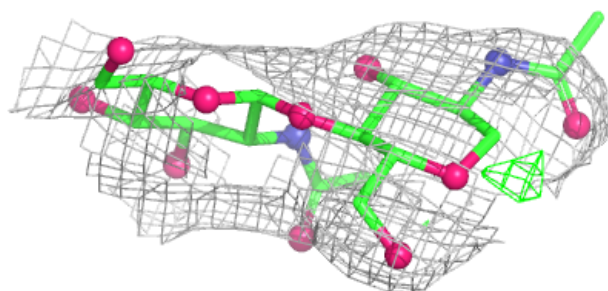
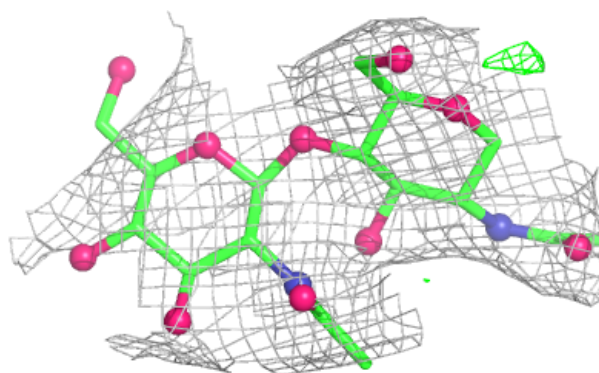


Electron density around Chain f:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

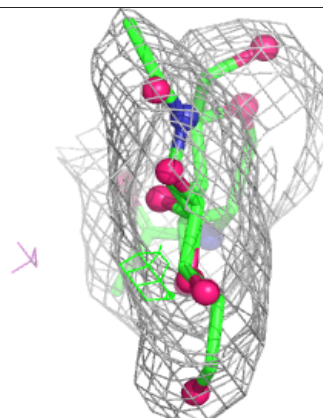
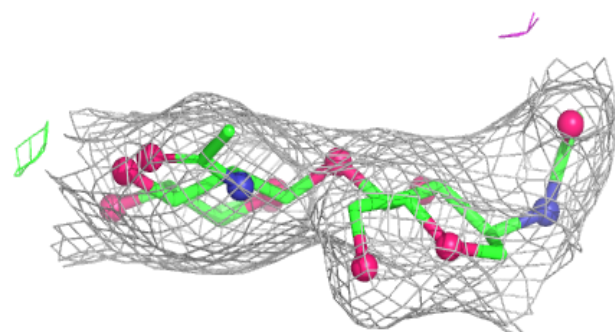
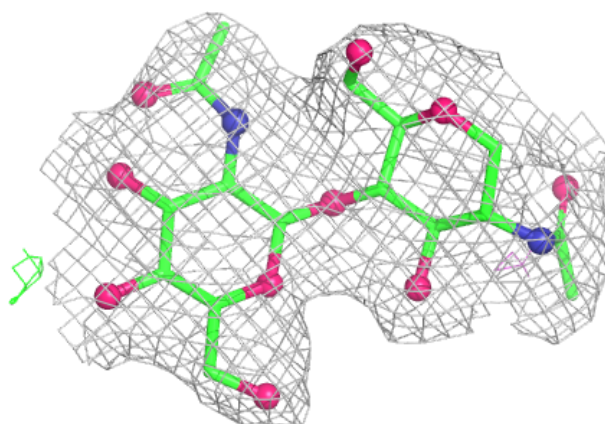
**Electron density around Chain i:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



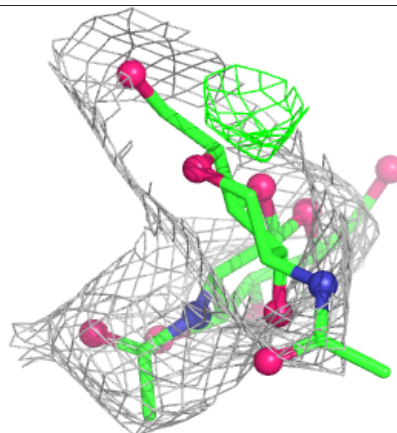
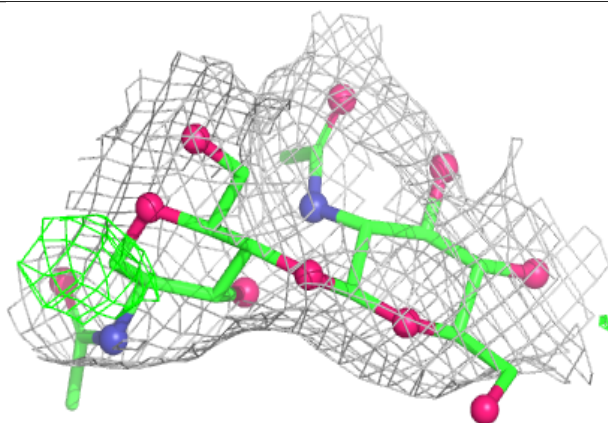
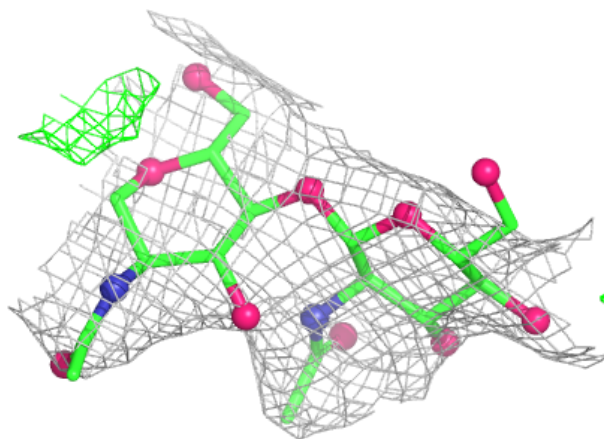
Electron density around Chain j:

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



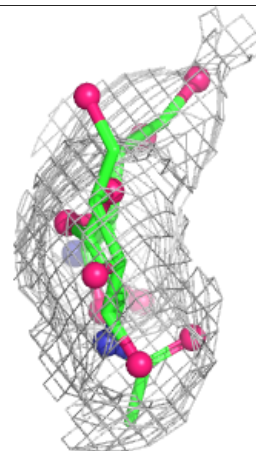
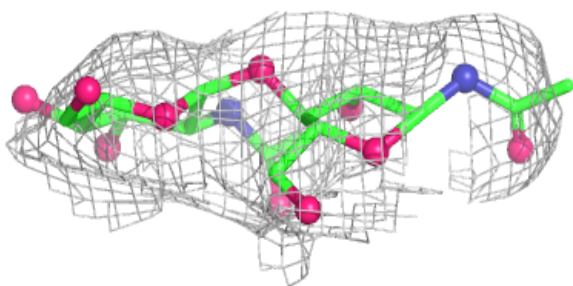
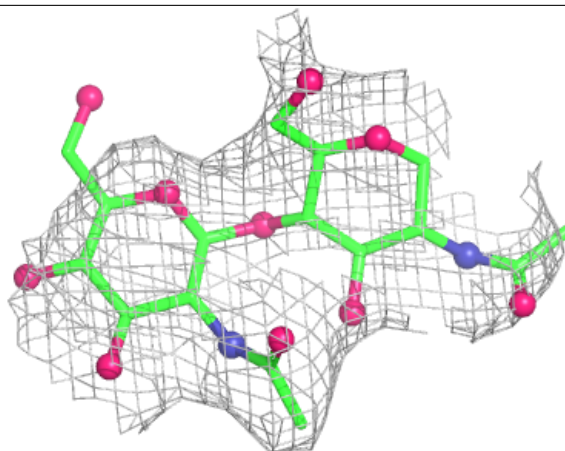
Electron density around Chain m:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



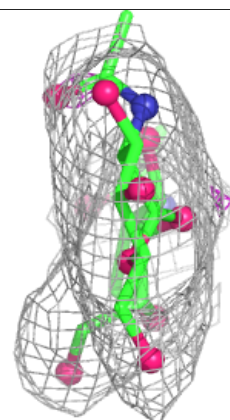
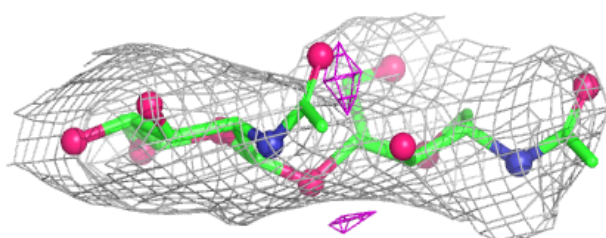
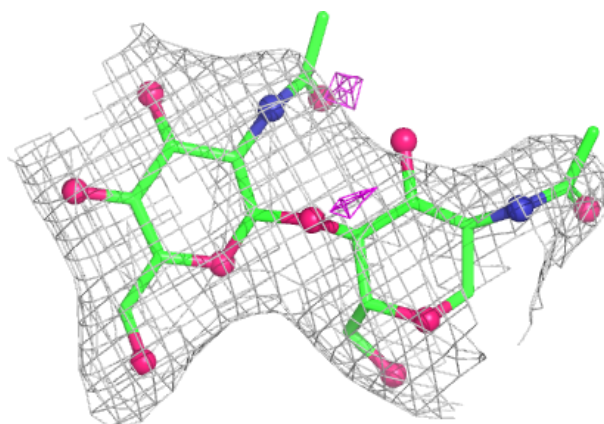
Electron density around Chain n:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

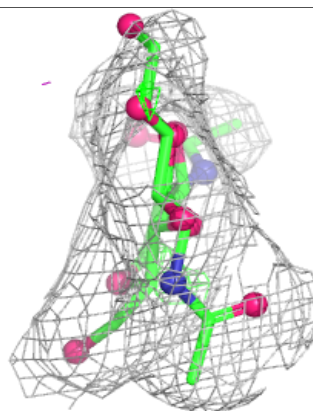
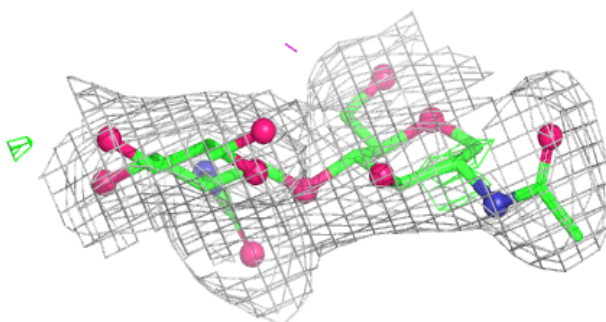
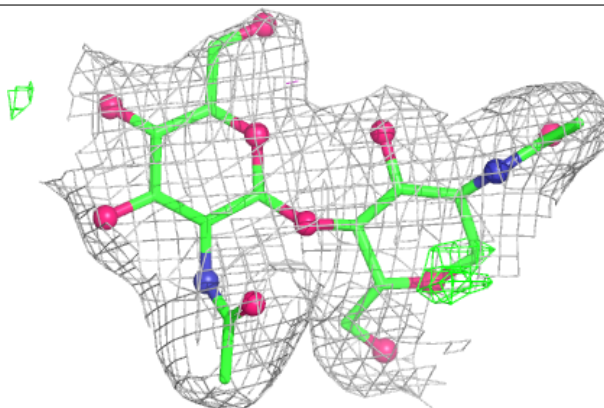


Electron density around Chain o:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

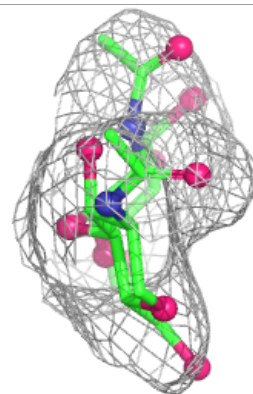
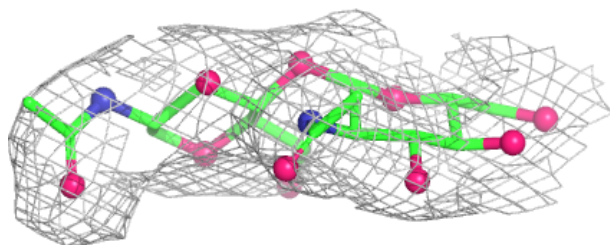
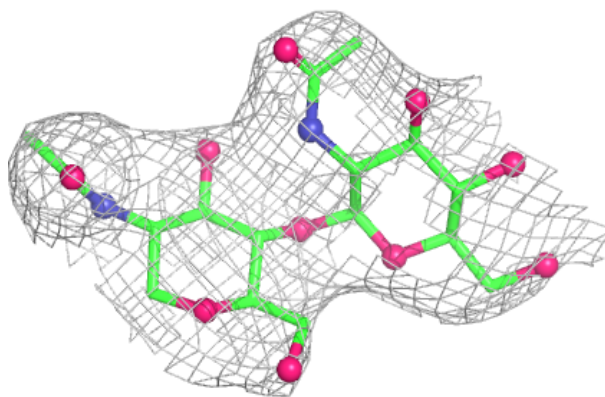
**Electron density around Chain p:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



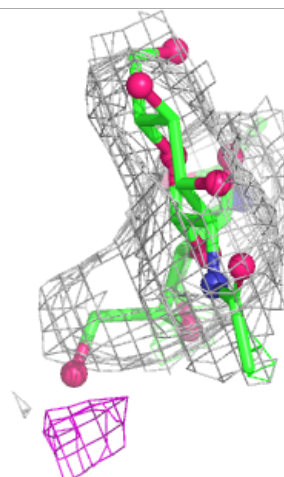
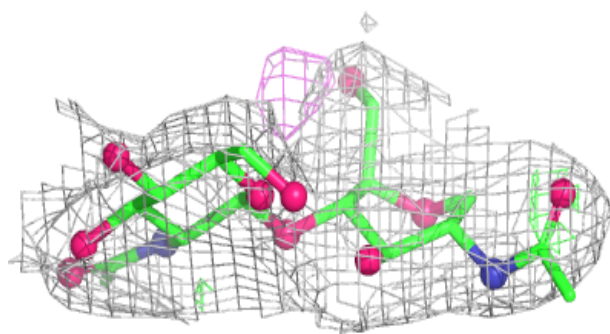
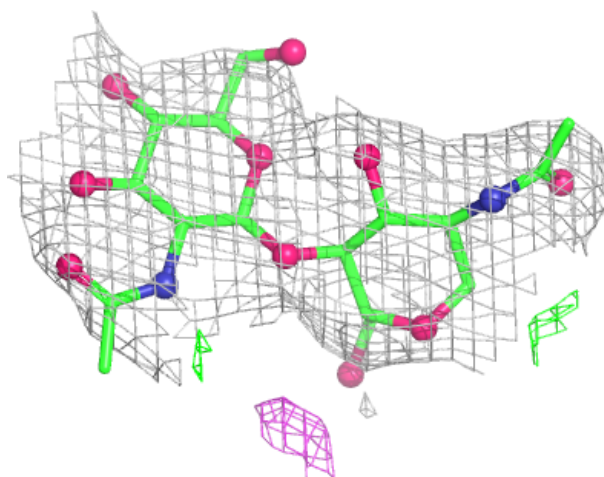
Electron density around Chain q:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



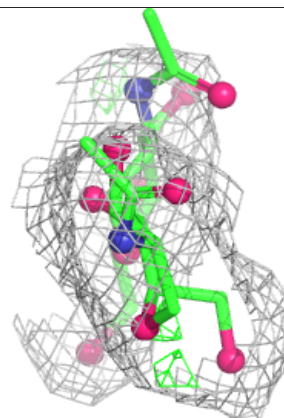
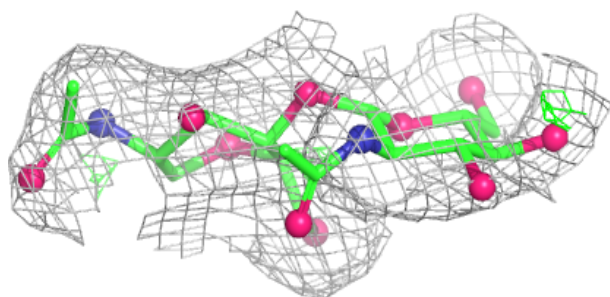
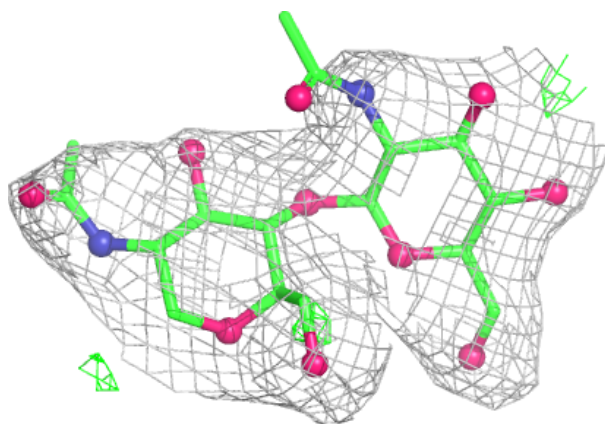
Electron density around Chain s:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



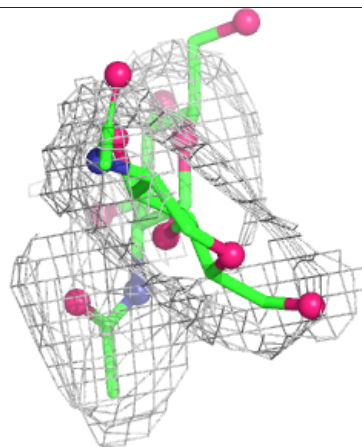
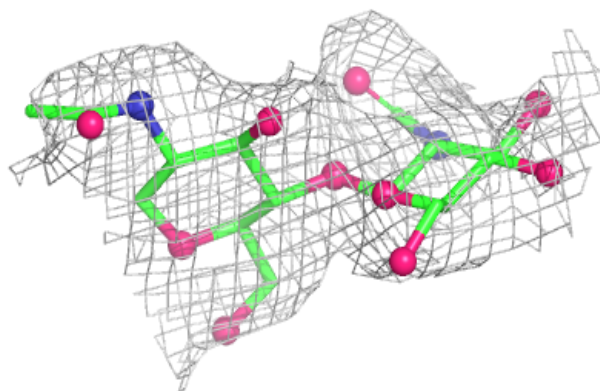
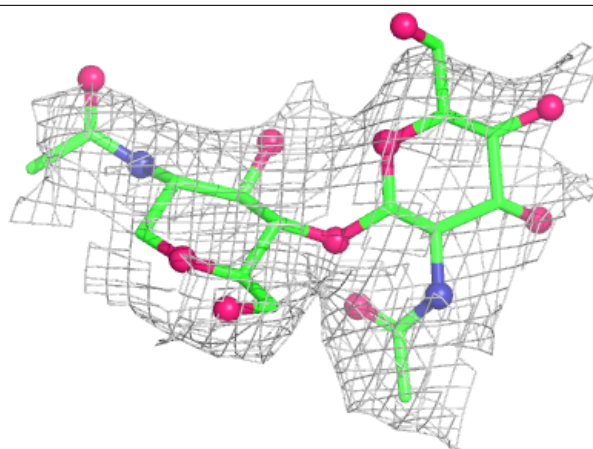
Electron density around Chain t:

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

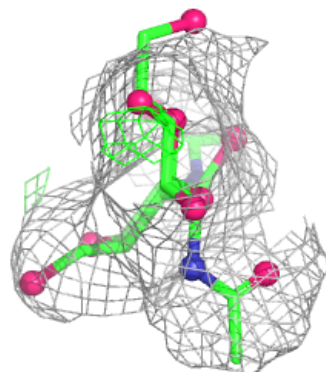
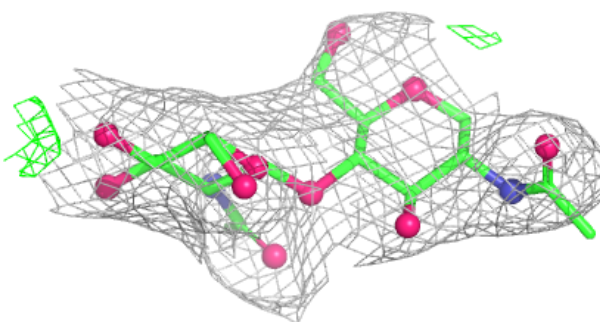
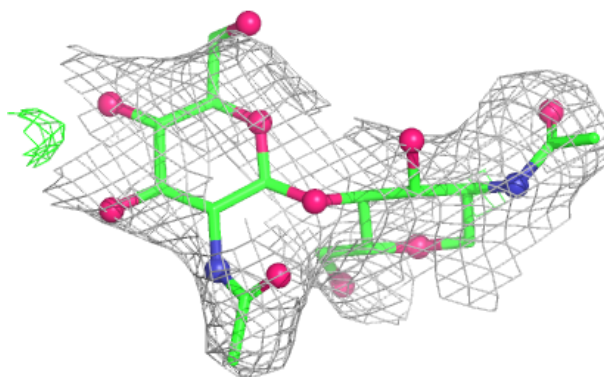


Electron density around Chain u:

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and green (positive)

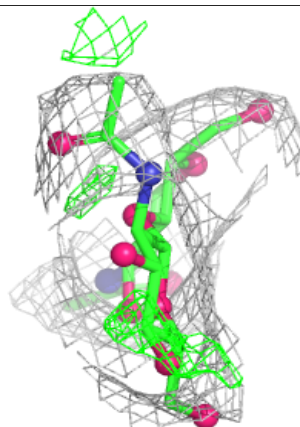
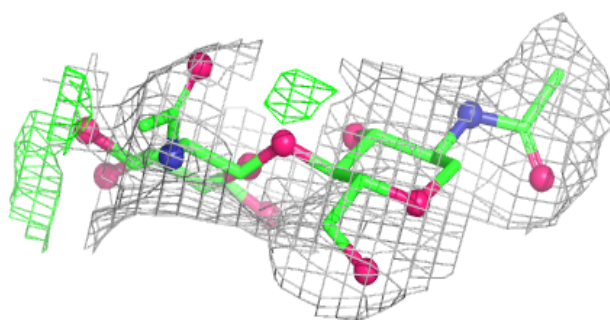
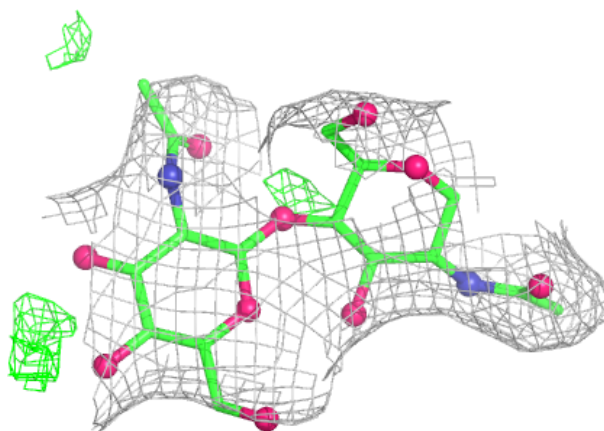
**Electron density around Chain v:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



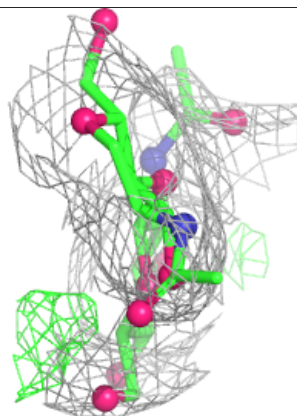
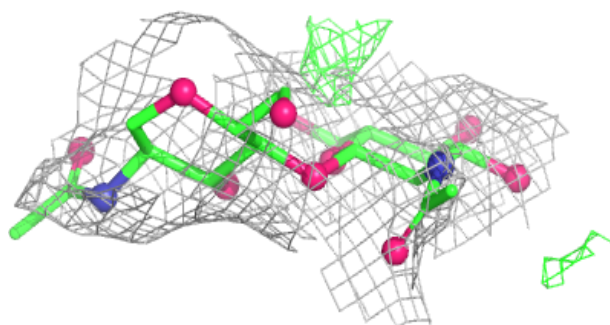
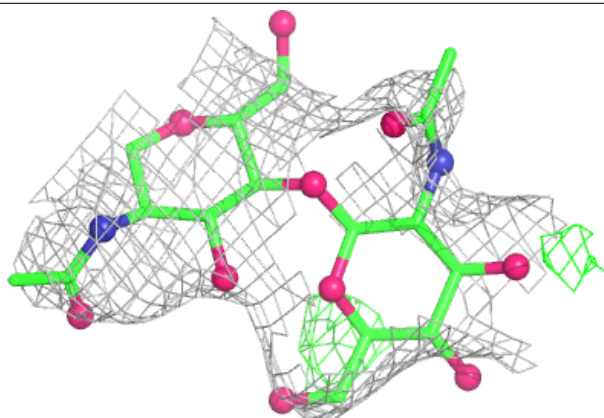
Electron density around Chain x:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)

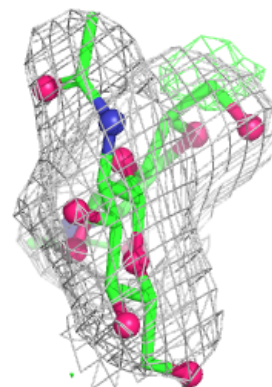
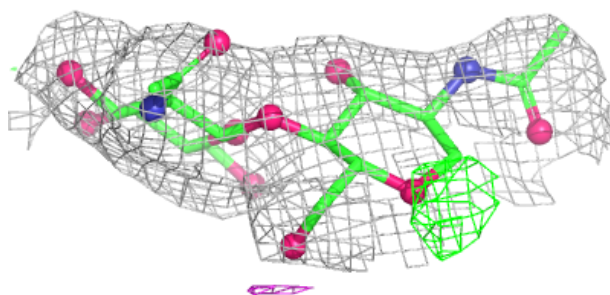
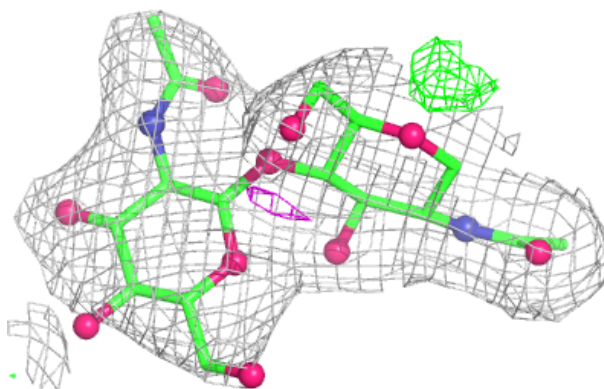


Electron density around Chain 1:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

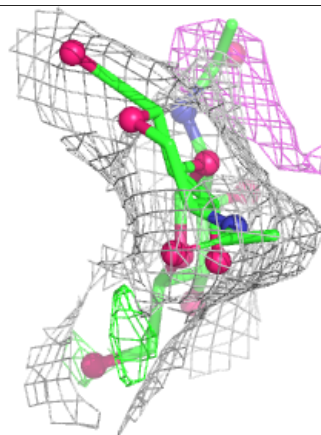
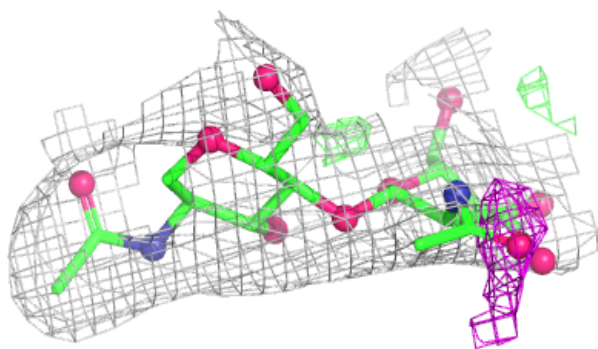
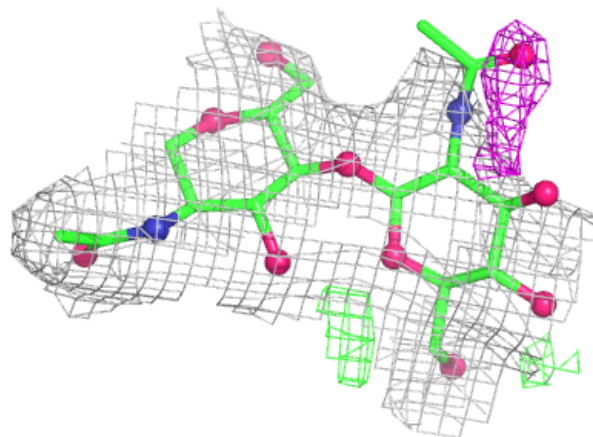
**Electron density around Chain 2:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

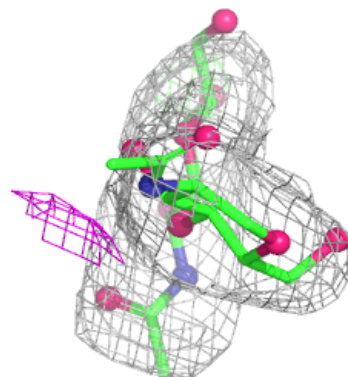
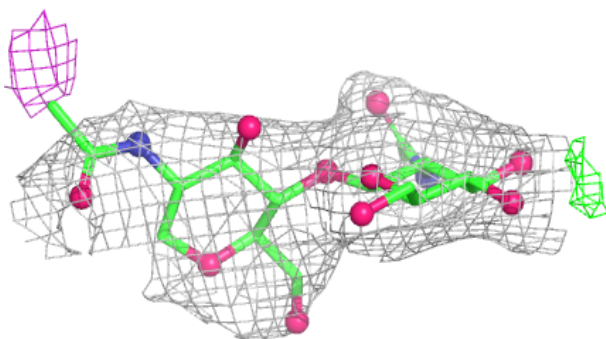
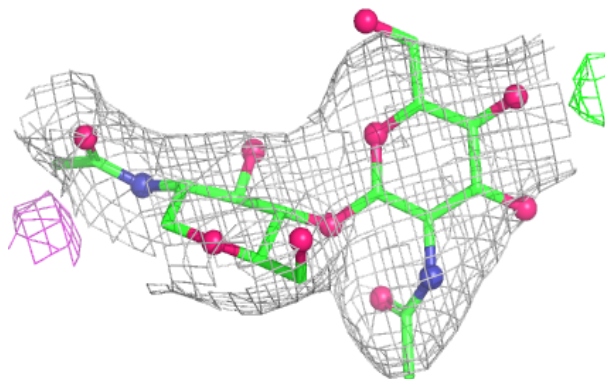


Electron density around Chain 4:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

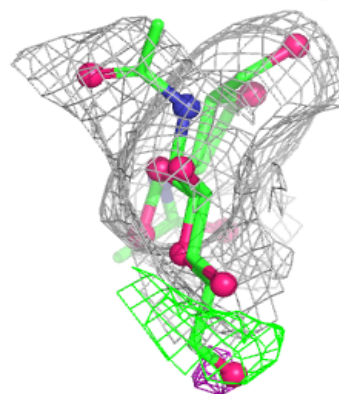
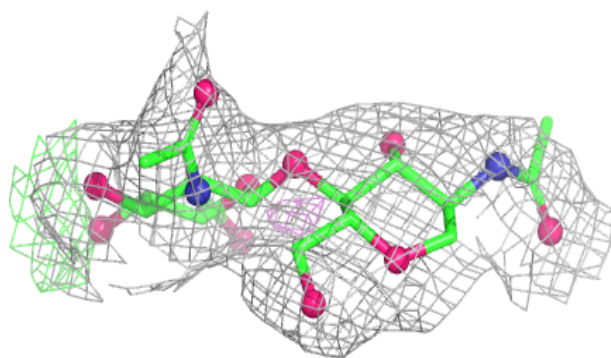
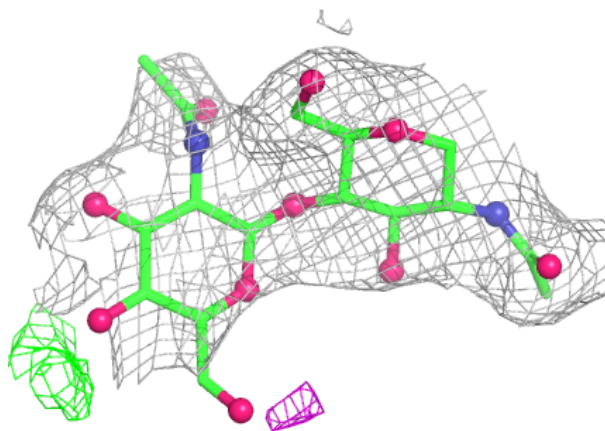
**Electron density around Chain 6:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



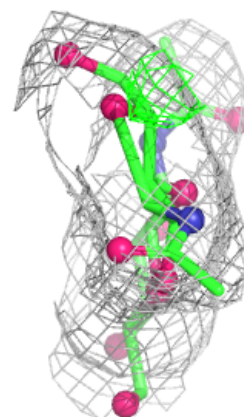
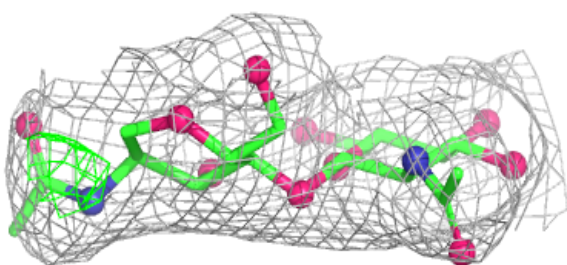
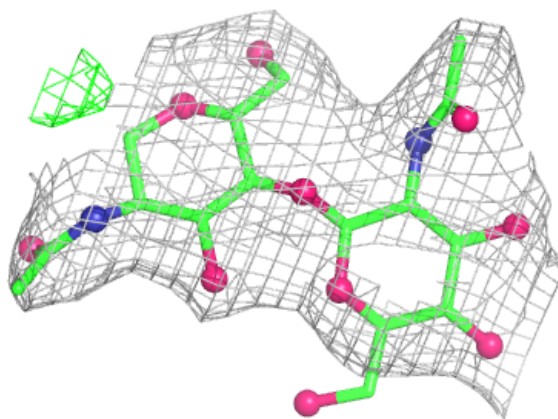
Electron density around Chain 7:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

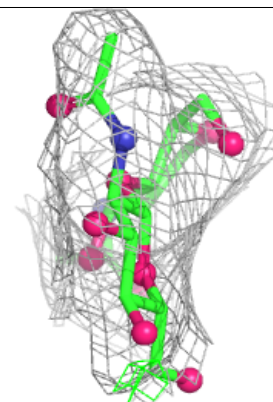
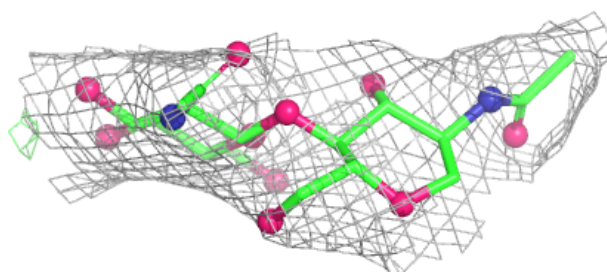
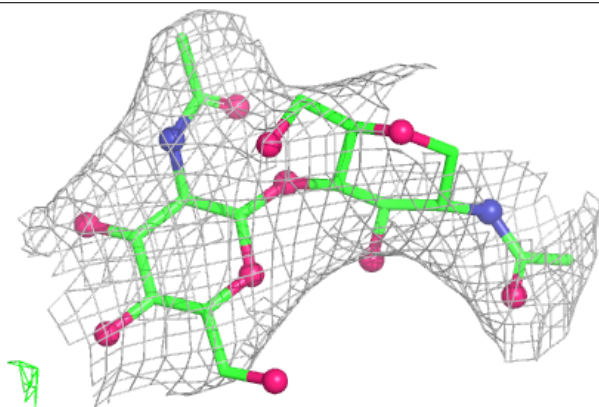


Electron density around Chain 8:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

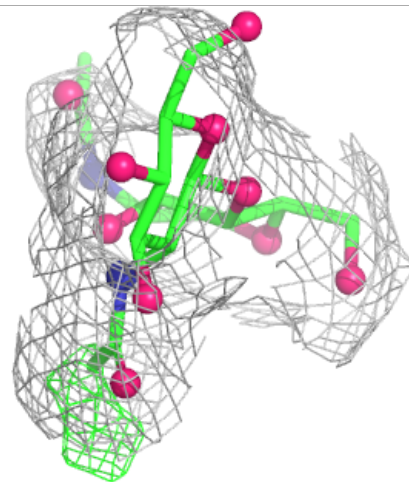
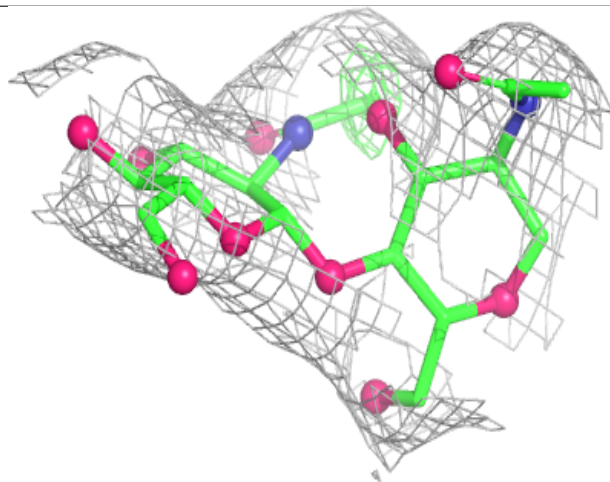
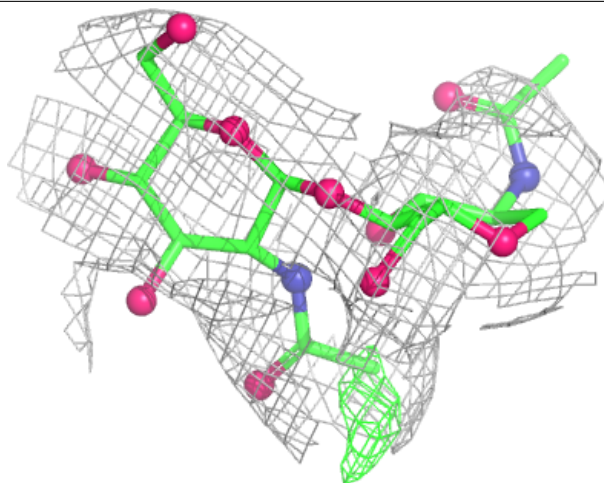
**Electron density around Chain 9:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



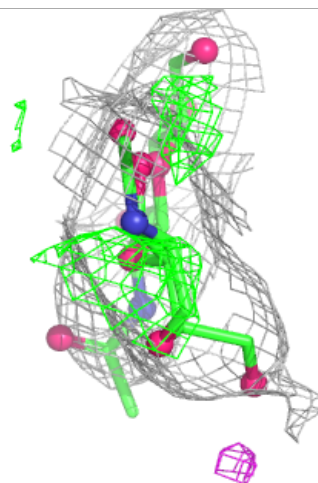
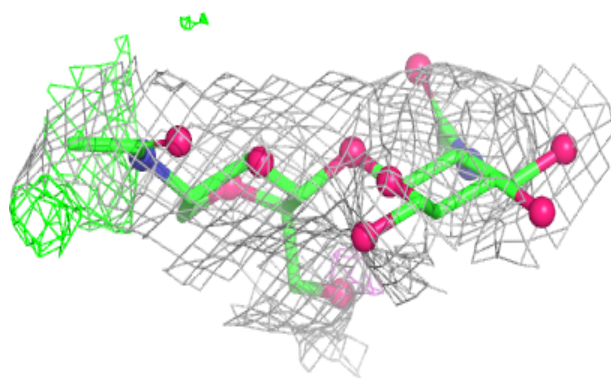
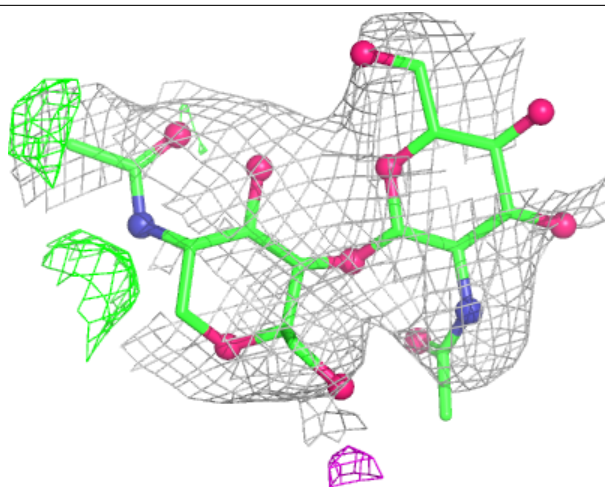
Electron density around Chain BA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



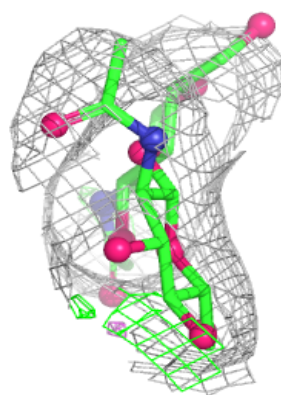
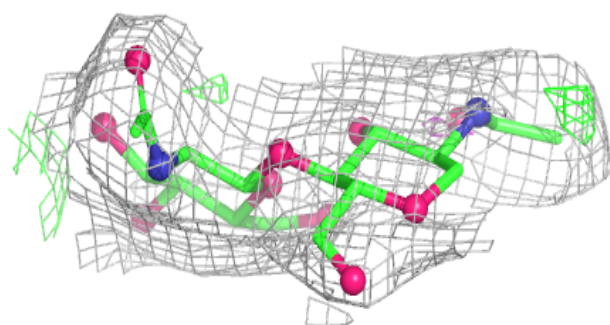
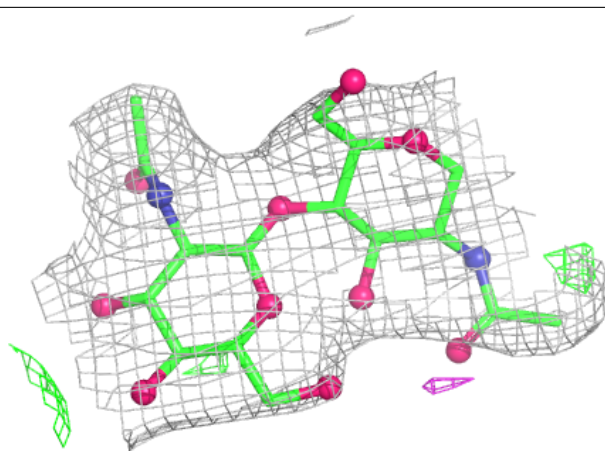
Electron density around Chain HA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



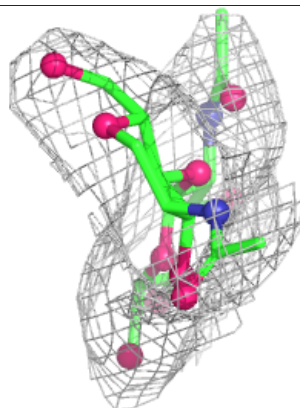
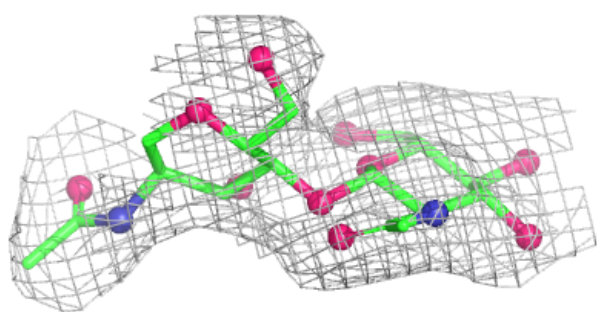
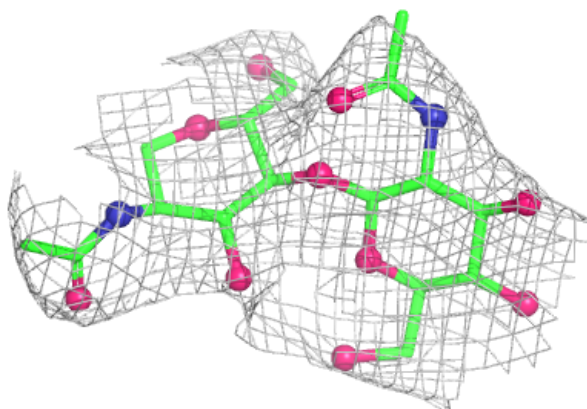
Electron density around Chain IA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

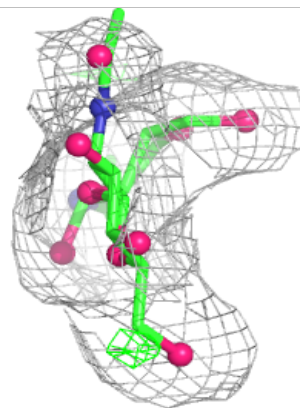
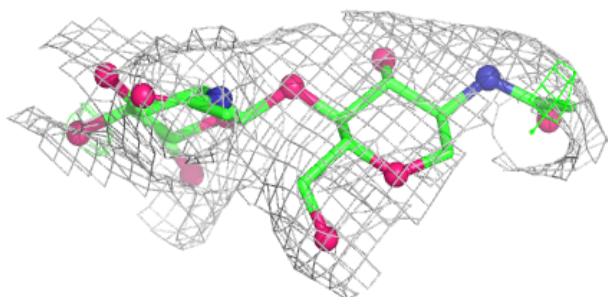
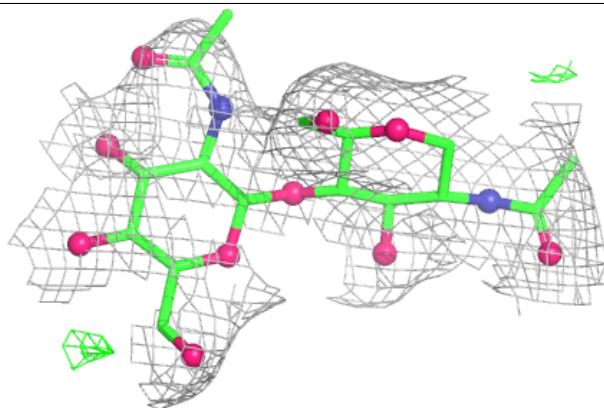


Electron density around Chain JA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

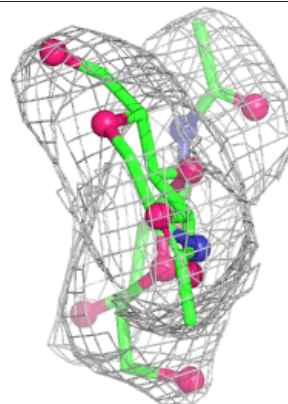
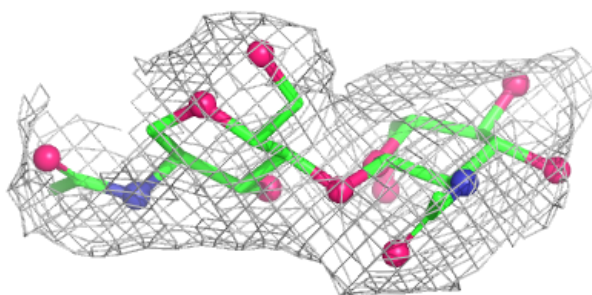
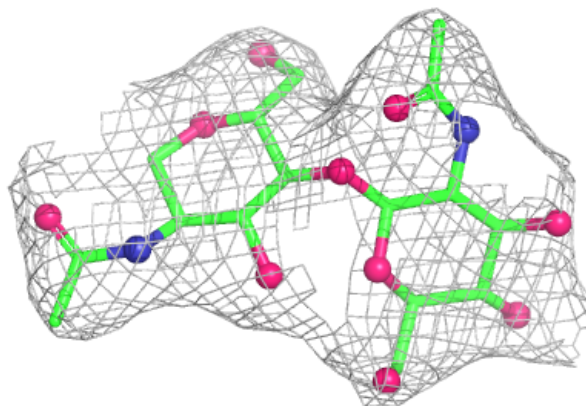
**Electron density around Chain MA:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



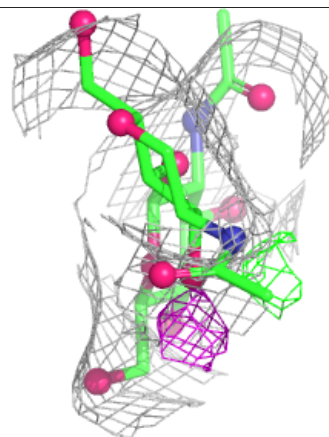
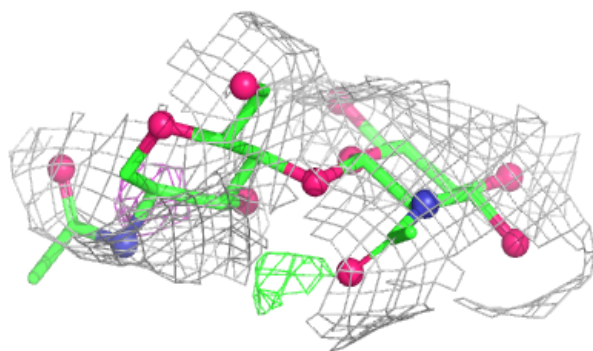
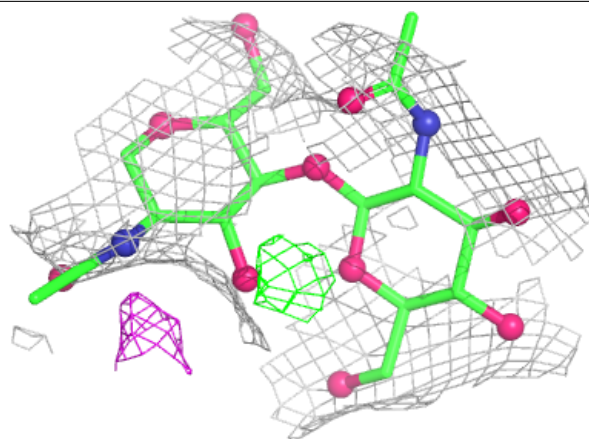
Electron density around Chain OA:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



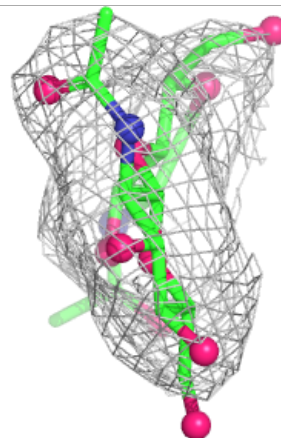
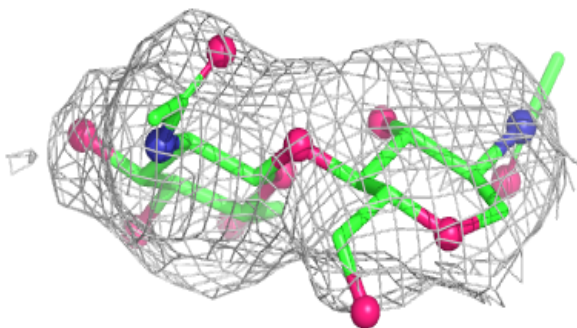
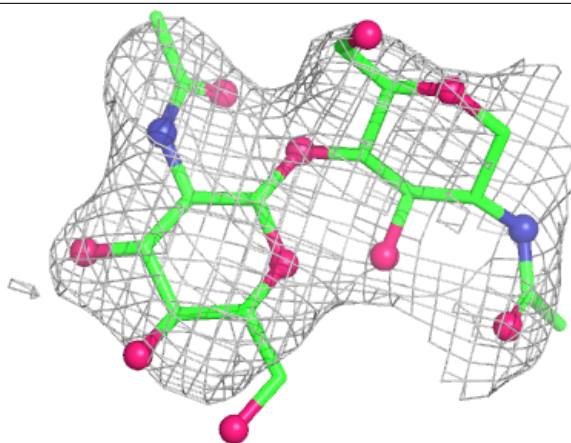
Electron density around Chain QA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



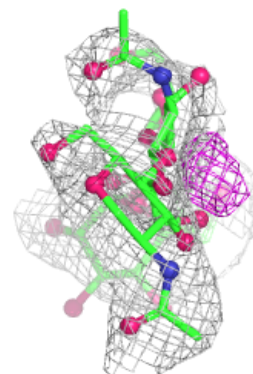
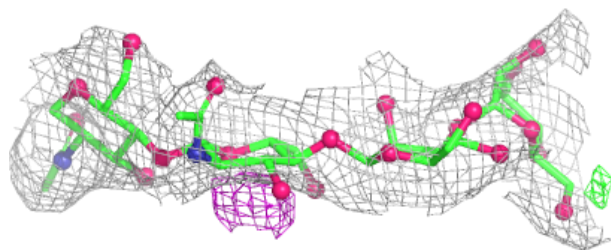
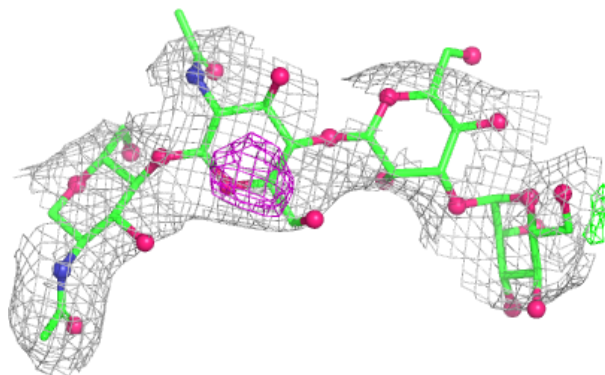
Electron density around Chain RA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

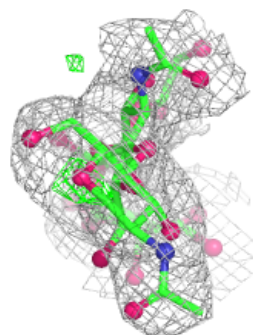
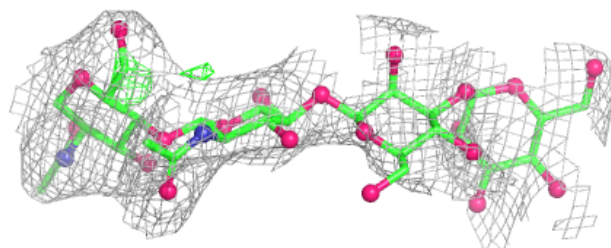
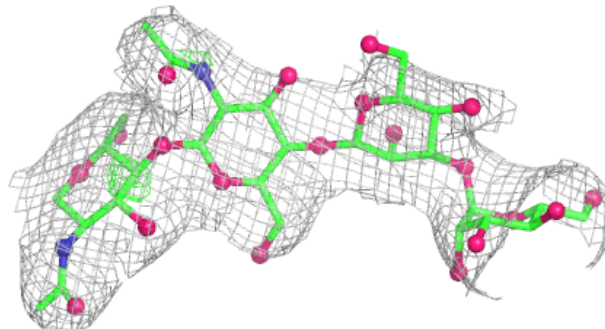


Electron density around Chain g:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

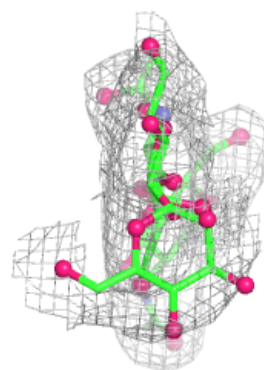
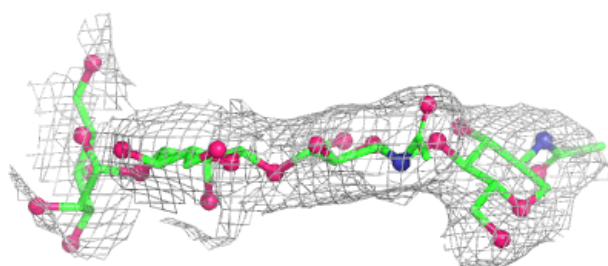
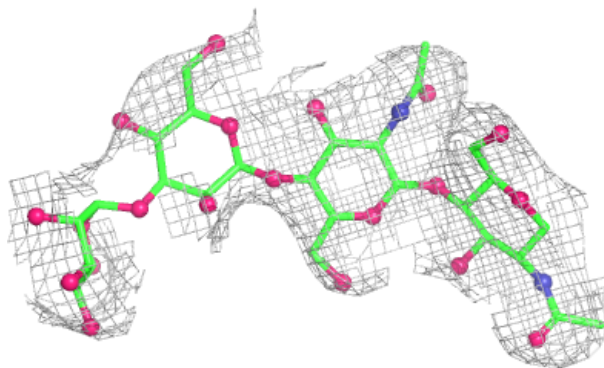
**Electron density around Chain l:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

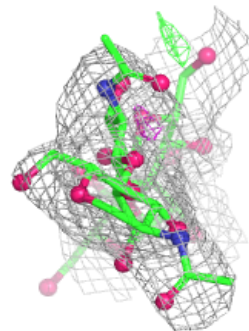
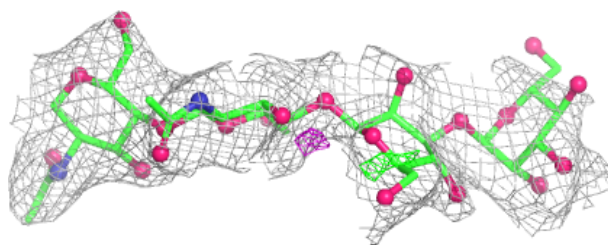
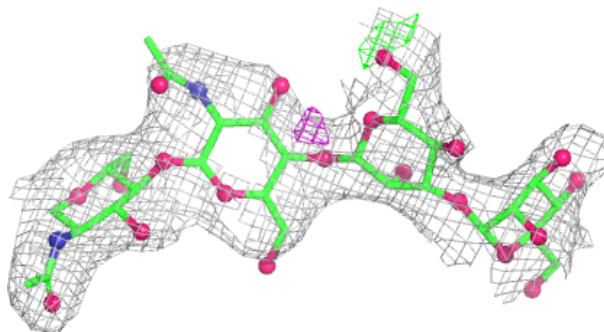


Electron density around Chain AA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

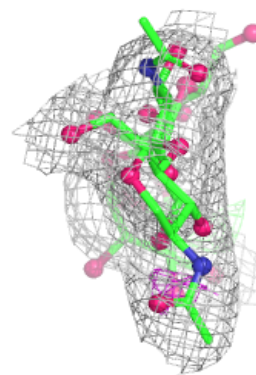
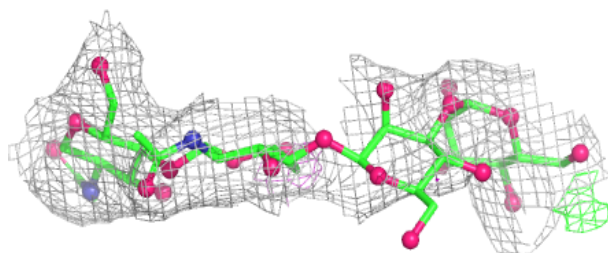
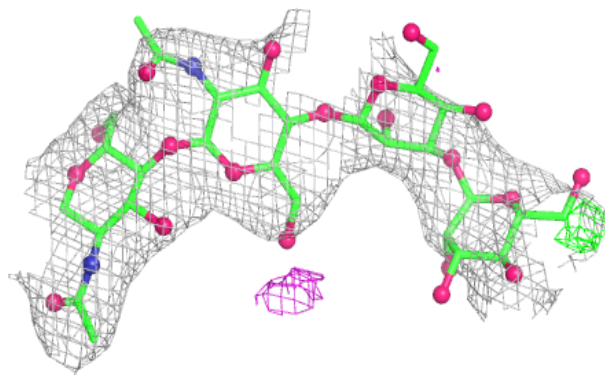
**Electron density around Chain FA:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

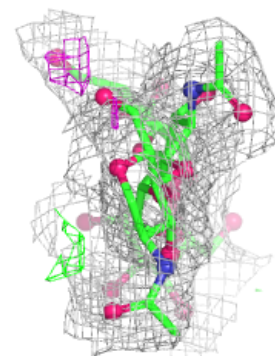
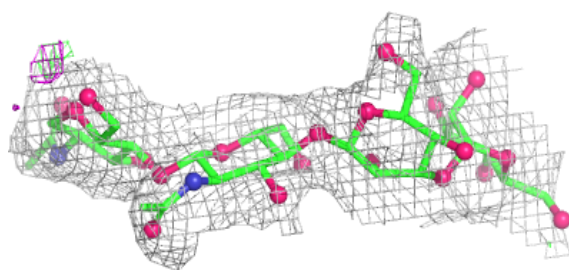
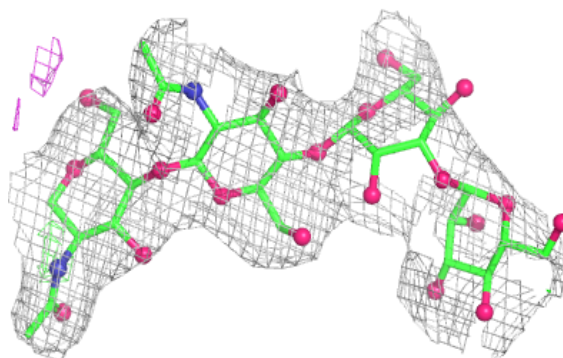


Electron density around Chain KA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

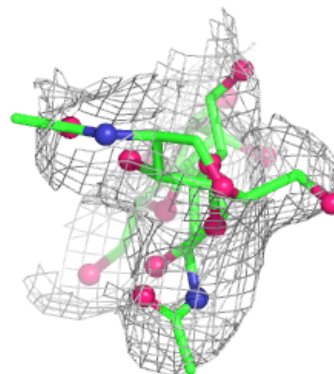
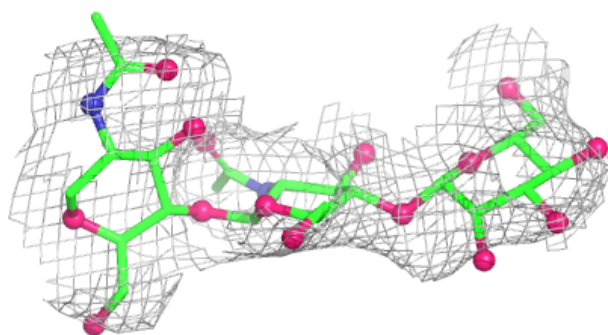
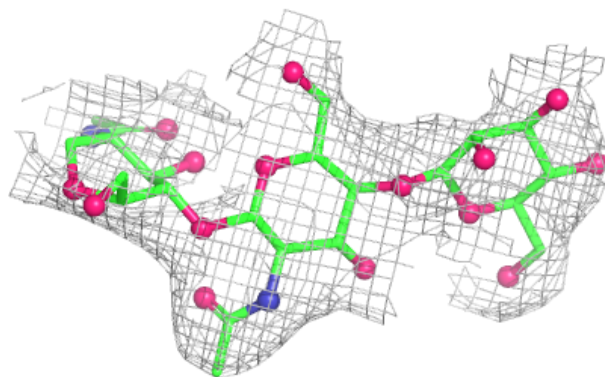
**Electron density around Chain PA:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

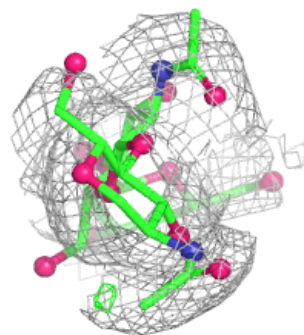
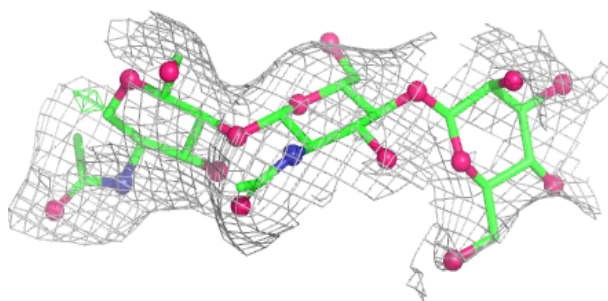
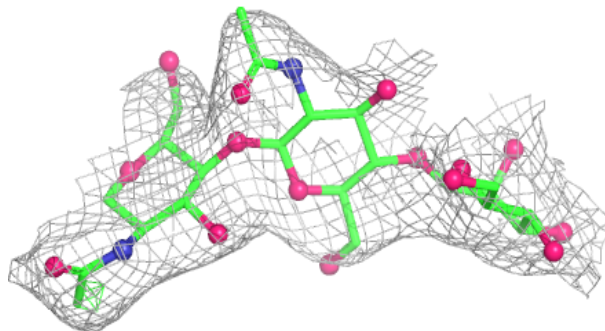


Electron density around Chain h:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

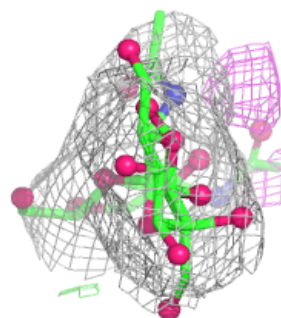
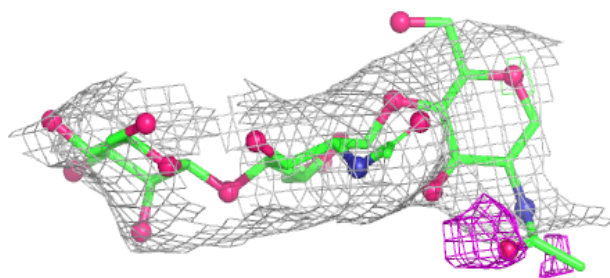
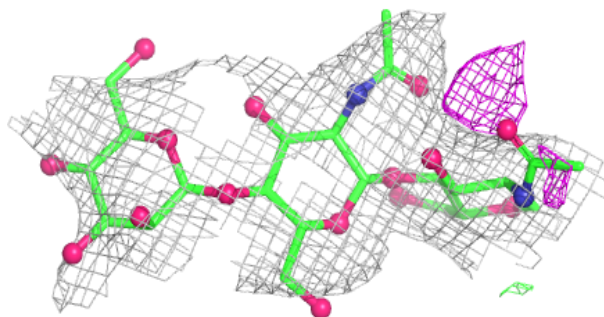
**Electron density around Chain k:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

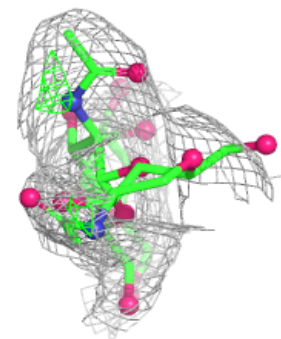
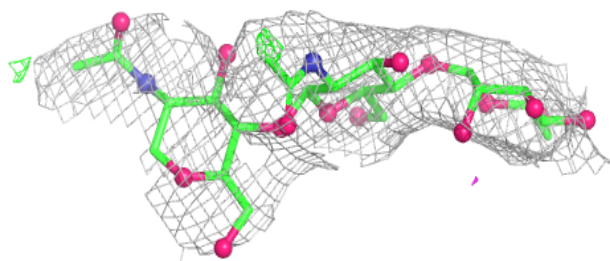
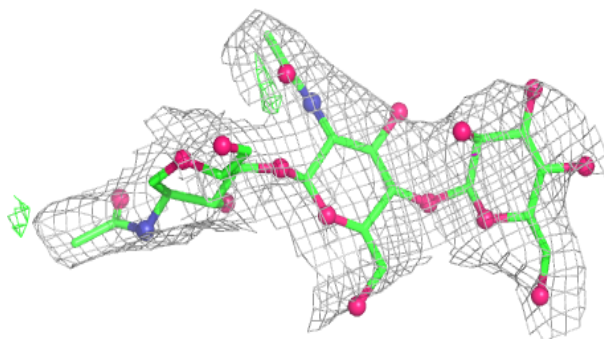


Electron density around Chain r:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

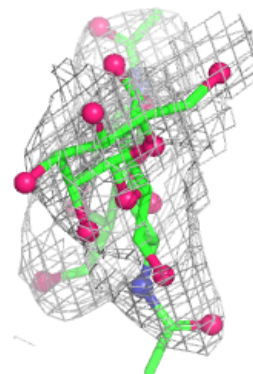
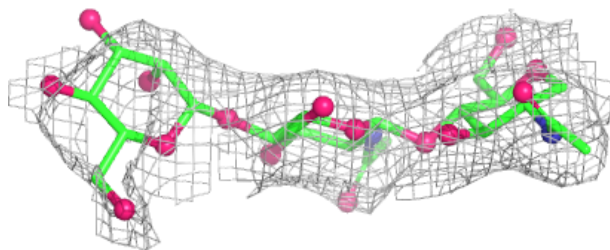
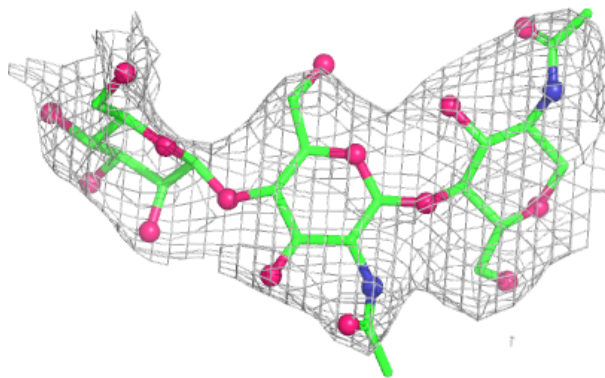
**Electron density around Chain w:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

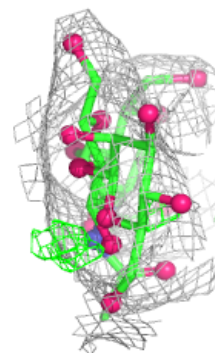
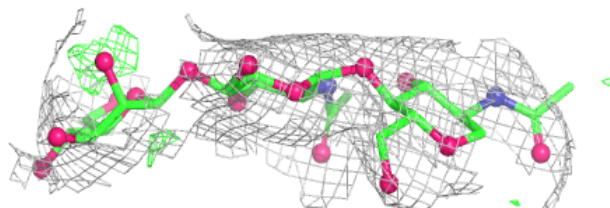
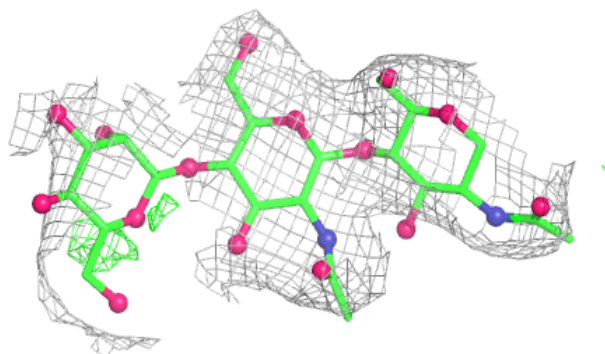


Electron density around Chain y:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

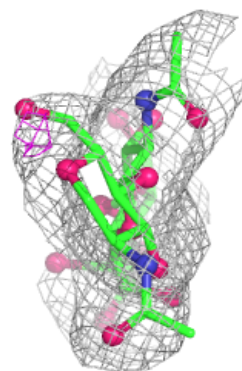
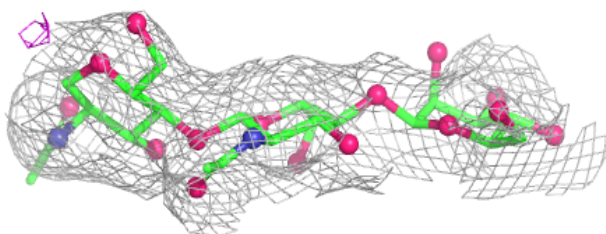
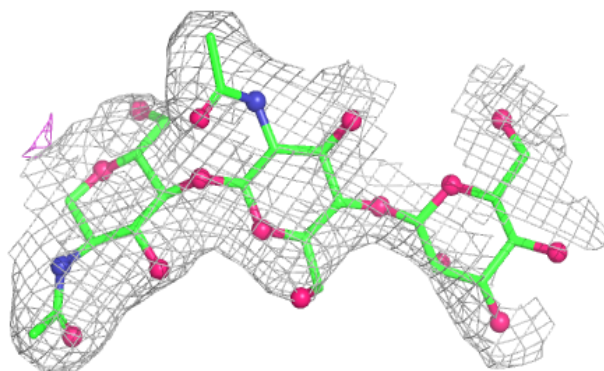
**Electron density around Chain 3:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



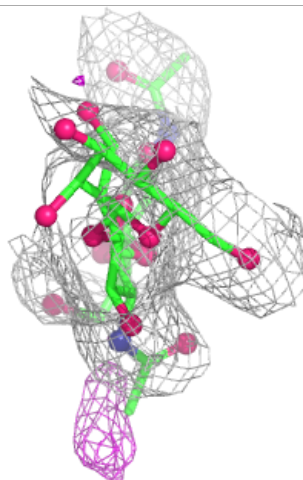
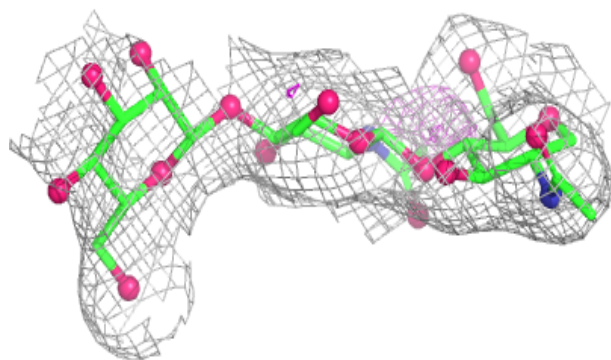
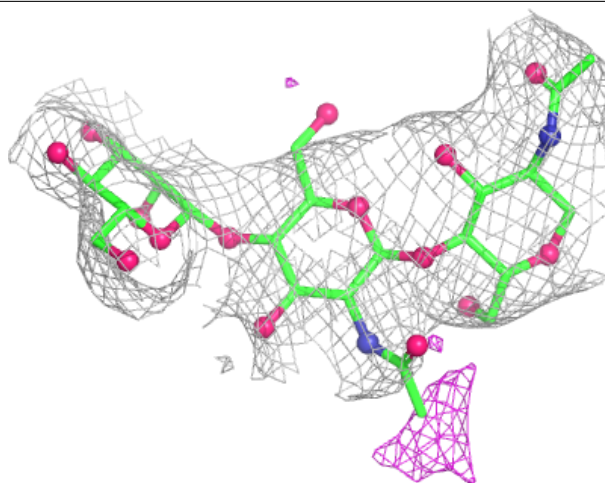
Electron density around Chain 5:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



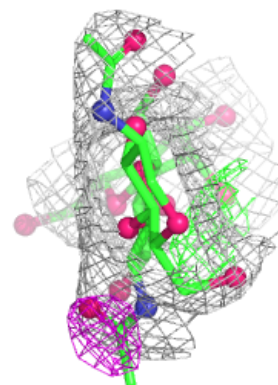
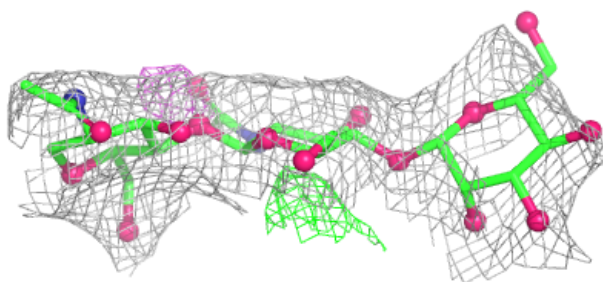
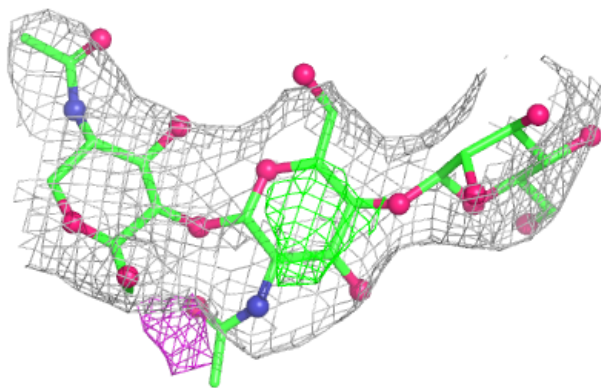
Electron density around Chain CA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



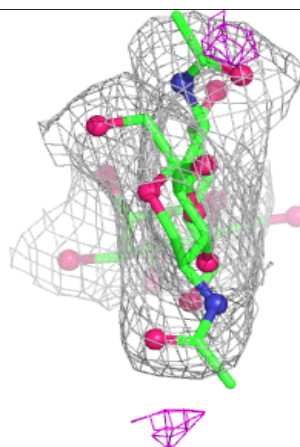
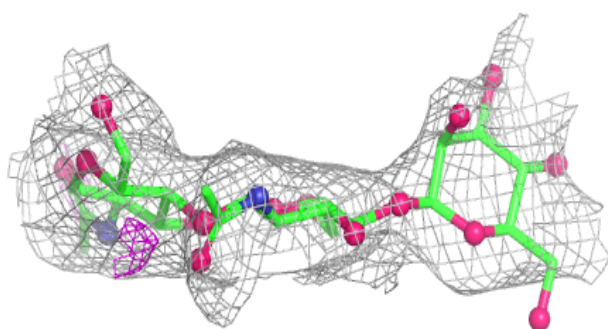
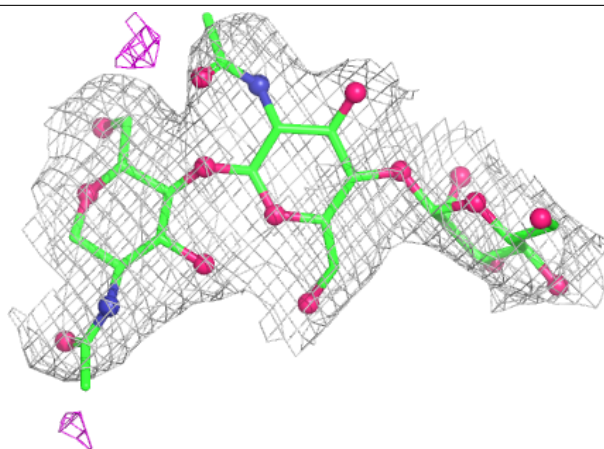
Electron density around Chain DA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

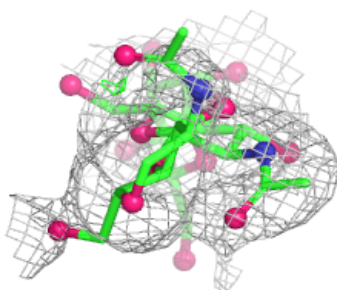
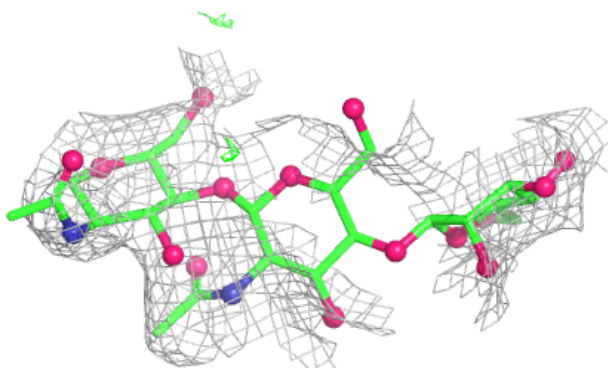
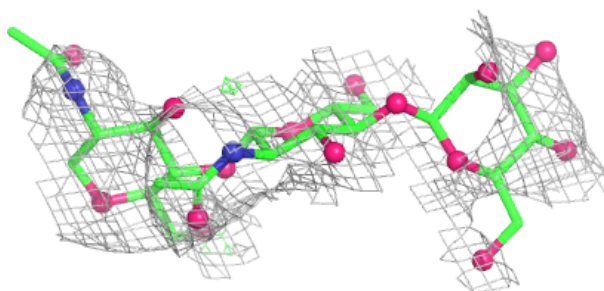


Electron density around Chain EA:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

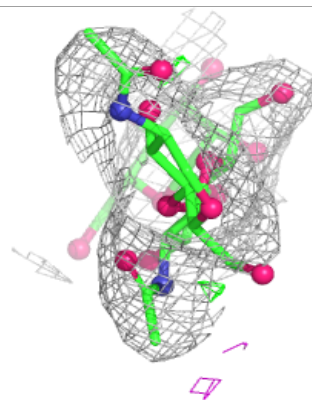
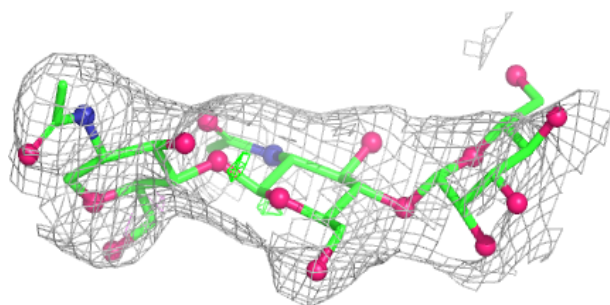
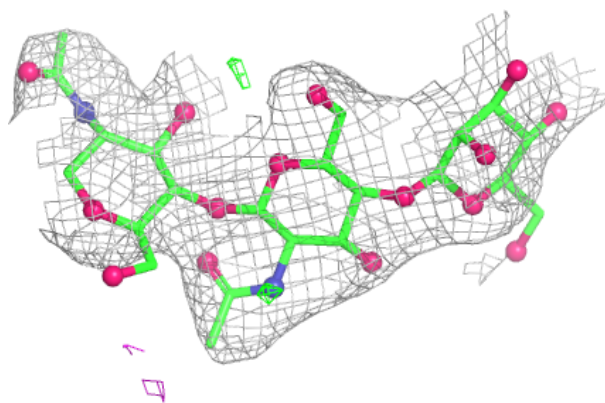
**Electron density around Chain GA:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

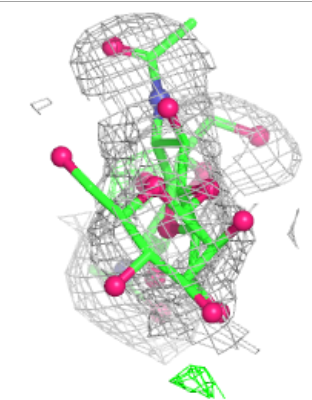
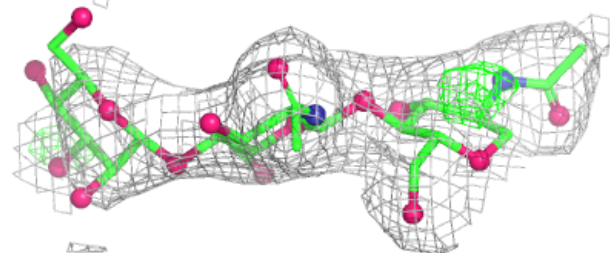
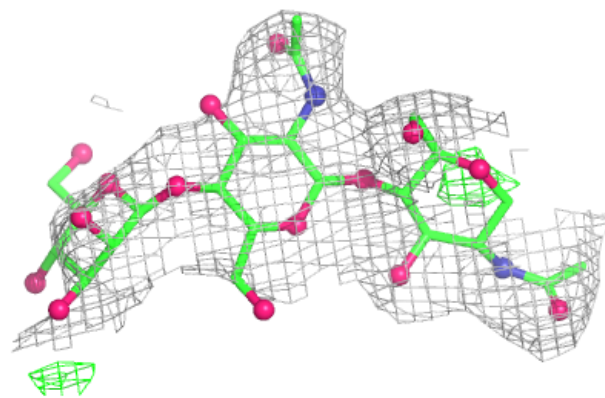


Electron density around Chain LA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

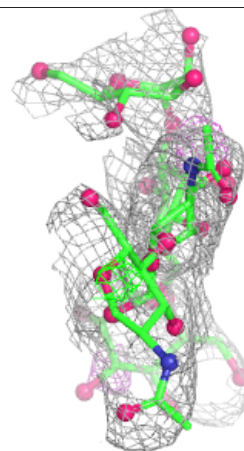
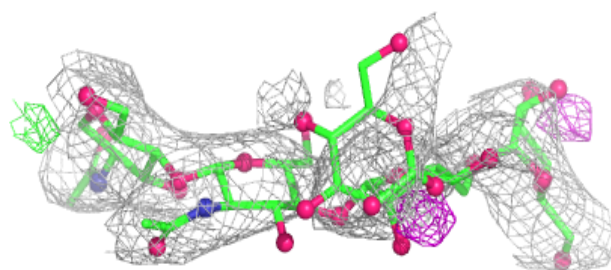
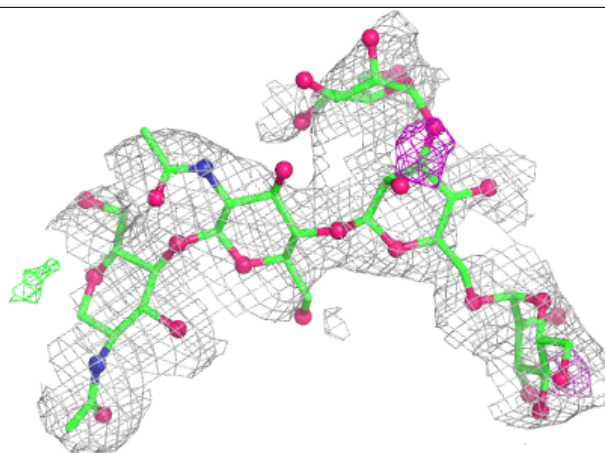
**Electron density around Chain NA:**

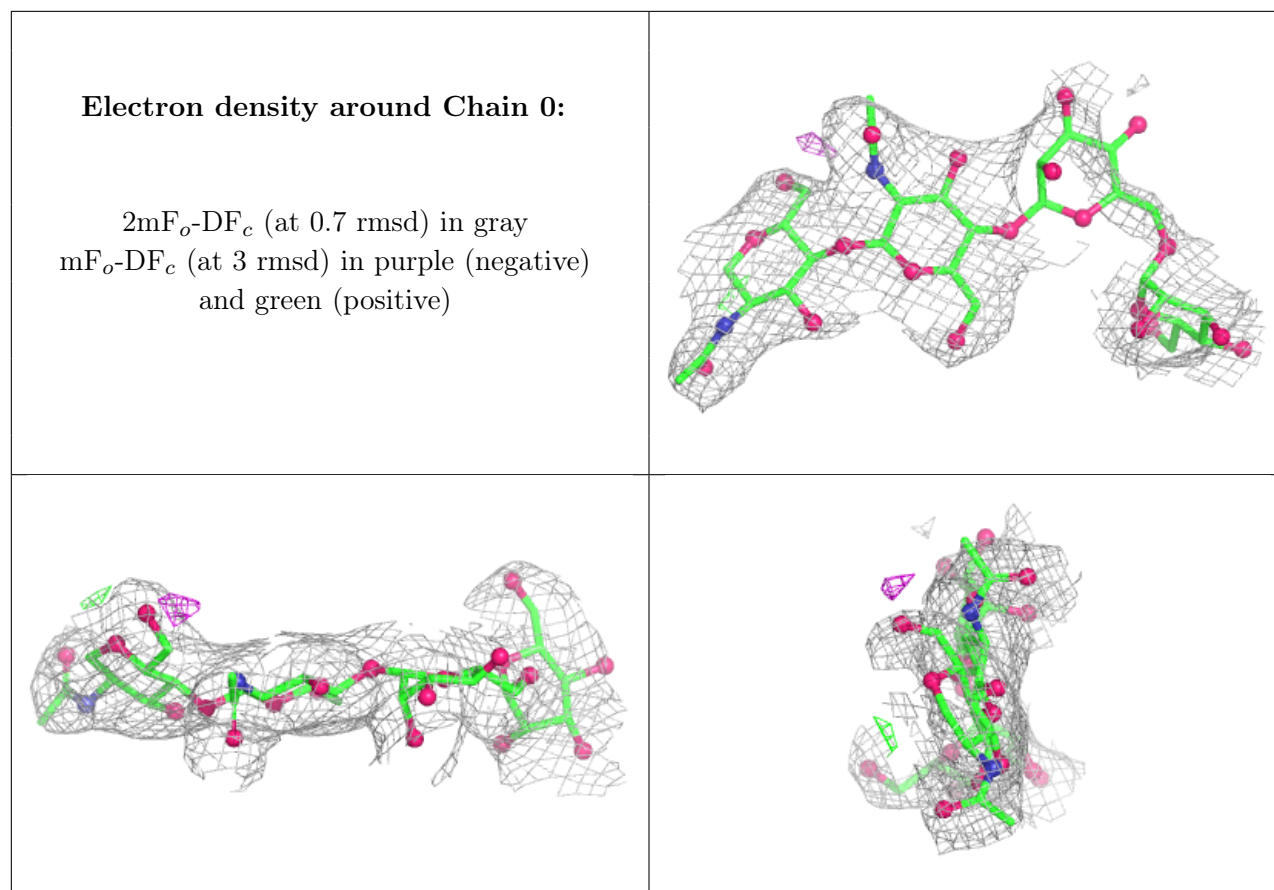
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain z:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	CUO	P	5005[C]	4/4	0.93	0.20	114,114,114,114	4
9	CUO	P	5005[D]	4/4	0.93	0.20	114,114,114,114	4
9	CUO	b	2101[C]	4/4	0.94	0.12	106,106,106,106	4
9	CUO	b	2101[D]	4/4	0.94	0.12	106,106,106,106	4
9	CUO	J	5005[C]	4/4	0.95	0.12	98,98,98,98	4
9	CUO	J	5005[D]	4/4	0.95	0.12	98,98,98,98	4
9	CUO	D	5005[C]	4/4	0.95	0.12	109,109,109,109	4
9	CUO	D	5005[D]	4/4	0.95	0.12	109,109,109,109	4
9	CUO	U	3401[A]	4/4	0.95	0.17	81,81,81,81	4
9	CUO	U	3401[B]	4/4	0.95	0.17	81,81,81,81	4
9	CUO	X	3401[A]	4/4	0.95	0.12	121,121,121,121	4
9	CUO	X	3401[B]	4/4	0.95	0.12	121,121,121,121	4
9	CUO	G	2101[C]	4/4	0.95	0.10	104,104,104,104	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	CUO	G	2101[D]	4/4	0.95	0.10	104,104,104,104	4
9	CUO	O	3401[A]	4/4	0.96	0.11	85,85,85,85	4
9	CUO	O	3401[B]	4/4	0.96	0.11	85,85,85,85	4
9	CUO	C	3401[A]	4/4	0.96	0.09	99,99,99,99	4
9	CUO	C	3401[B]	4/4	0.96	0.09	99,99,99,99	4
9	CUO	S	2101[C]	4/4	0.96	0.12	94,94,94,94	4
9	CUO	S	2101[D]	4/4	0.96	0.12	94,94,94,94	4
9	CUO	I	3401[A]	4/4	0.96	0.11	84,84,84,84	4
9	CUO	I	3401[B]	4/4	0.96	0.11	84,84,84,84	4
9	CUO	F	3401[A]	4/4	0.96	0.12	86,86,86,86	4
9	CUO	F	3401[B]	4/4	0.96	0.12	86,86,86,86	4
9	CUO	Y	2101[C]	4/4	0.96	0.10	99,99,99,99	4
9	CUO	Y	2101[D]	4/4	0.96	0.10	99,99,99,99	4
9	CUO	M	2101[C]	4/4	0.96	0.10	103,103,103,103	4
9	CUO	M	2101[D]	4/4	0.96	0.10	103,103,103,103	4
9	CUO	L	3401[A]	4/4	0.97	0.09	100,100,100,100	4
9	CUO	L	3401[B]	4/4	0.97	0.09	100,100,100,100	4
9	CUO	A	5005[C]	4/4	0.97	0.10	95,95,95,95	4
9	CUO	A	5005[D]	4/4	0.97	0.10	95,95,95,95	4
9	CUO	a	3401[A]	4/4	0.97	0.10	85,85,85,85	4
9	CUO	a	3401[B]	4/4	0.97	0.10	85,85,85,85	4
9	CUO	V	5005[C]	4/4	0.97	0.14	113,113,113,113	4
9	CUO	V	5005[D]	4/4	0.97	0.14	113,113,113,113	4
9	CUO	d	3401[A]	4/4	0.97	0.12	111,111,111,111	4
9	CUO	d	3401[B]	4/4	0.97	0.12	111,111,111,111	4
9	CUO	J	5003	4/4	0.98	0.07	89,96,96,103	0
9	CUO	M	2104	4/4	0.98	0.07	58,70,74,76	0
9	CUO	R	3401[A]	4/4	0.98	0.06	84,84,84,84	4
9	CUO	R	3401[B]	4/4	0.98	0.06	84,84,84,84	4
9	CUO	A	5002	4/4	0.98	0.09	55,75,89,91	0
9	CUO	G	2104	4/4	0.98	0.09	58,85,92,97	0
9	CUO	S	2104	4/4	0.98	0.07	74,79,82,87	0
9	CUO	N	3002	4/4	0.99	0.05	48,51,70,74	0
9	CUO	D	5002	4/4	0.99	0.08	51,60,82,85	0
9	CUO	G	2105	4/4	0.99	0.04	58,60,66,69	0
9	CUO	P	5001	4/4	0.99	0.05	36,38,56,71	0
9	CUO	P	5002	4/4	0.99	0.06	56,59,75,82	0
9	CUO	P	5003	4/4	0.99	0.07	45,54,76,83	0
9	CUO	P	5004	4/4	0.99	0.06	40,48,67,68	0
9	CUO	H	3001	4/4	0.99	0.06	58,60,72,78	0
9	CUO	H	3002	4/4	0.99	0.04	67,79,83,84	0
9	CUO	Q	3001	4/4	0.99	0.07	37,43,64,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CUO	Q	3002	4/4	0.99	0.04	53,62,64,73	0
9	CUO	D	5003	4/4	0.99	0.04	60,62,67,79	0
9	CUO	A	5003	4/4	0.99	0.04	79,87,89,89	0
9	CUO	J	5001	4/4	0.99	0.07	49,52,60,69	0
9	CUO	J	5002	4/4	0.99	0.05	53,56,80,83	0
9	CUO	S	2102	4/4	0.99	0.06	54,65,85,90	0
9	CUO	S	2103	4/4	0.99	0.07	49,52,72,80	0
9	CUO	B	3001	4/4	0.99	0.08	49,55,75,88	0
9	CUO	S	2105	4/4	0.99	0.05	45,45,62,71	0
9	CUO	T	3001	4/4	0.99	0.05	44,59,84,85	0
9	CUO	T	3002	4/4	0.99	0.06	52,69,74,84	0
9	CUO	J	5004	4/4	0.99	0.05	49,58,62,63	0
9	CUO	E	3001	4/4	0.99	0.06	55,55,80,85	0
9	CUO	V	5001	4/4	0.99	0.08	39,39,64,66	0
9	CUO	V	5002	4/4	0.99	0.07	50,61,67,72	0
9	CUO	V	5003	4/4	0.99	0.07	66,79,89,90	0
9	CUO	V	5004	4/4	0.99	0.05	44,50,62,65	0
9	CUO	B	3002	4/4	0.99	0.06	57,58,80,91	0
9	CUO	K	3001	4/4	0.99	0.04	57,73,73,80	0
9	CUO	W	3001	4/4	0.99	0.08	37,41,72,78	0
9	CUO	W	3002	4/4	0.99	0.05	58,62,70,77	0
9	CUO	K	3002	4/4	0.99	0.06	52,69,75,79	0
9	CUO	A	5004	4/4	0.99	0.06	51,60,67,70	0
9	CUO	A	5001	4/4	0.99	0.07	70,73,87,92	0
9	CUO	D	5001	4/4	0.99	0.07	64,68,95,98	0
9	CUO	Y	2102	4/4	0.99	0.06	59,67,69,83	0
9	CUO	Y	2103	4/4	0.99	0.10	58,65,82,85	0
9	CUO	Y	2104	4/4	0.99	0.06	69,75,80,100	0
9	CUO	Y	2105	4/4	0.99	0.05	47,59,61,62	0
9	CUO	Z	3001	4/4	0.99	0.07	46,54,67,69	0
9	CUO	Z	3002	4/4	0.99	0.07	48,68,69,72	0
9	CUO	G	2102	4/4	0.99	0.04	57,62,65,70	0
9	CUO	M	2102	4/4	0.99	0.05	41,52,59,63	0
9	CUO	M	2103	4/4	0.99	0.05	50,59,66,68	0
9	CUO	G	2103	4/4	0.99	0.07	49,58,62,73	0
9	CUO	b	2102	4/4	0.99	0.06	60,63,73,78	0
9	CUO	b	2103	4/4	0.99	0.06	55,59,71,73	0
9	CUO	b	2104	4/4	0.99	0.08	60,75,83,94	0
9	CUO	b	2105	4/4	0.99	0.04	54,57,68,74	0
9	CUO	c	3001	4/4	0.99	0.07	48,56,77,80	0
9	CUO	c	3002	4/4	0.99	0.05	70,71,79,80	0
9	CUO	M	2105	4/4	0.99	0.06	48,60,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CUO	N	3001	4/4	0.99	0.06	36,39,74,80	0
9	CUO	D	5004	4/4	1.00	0.04	52,54,59,62	0
9	CUO	E	3002	4/4	1.00	0.04	57,61,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.