



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:43 pm BST

PDB ID : 2A68  
Title : Crystal structure of the T. thermophilus RNA polymerase holoenzyme in complex with antibiotic rifabutin  
Authors : Artsimovitch, I.; Vassilyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-07-01  
Resolution : 2.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

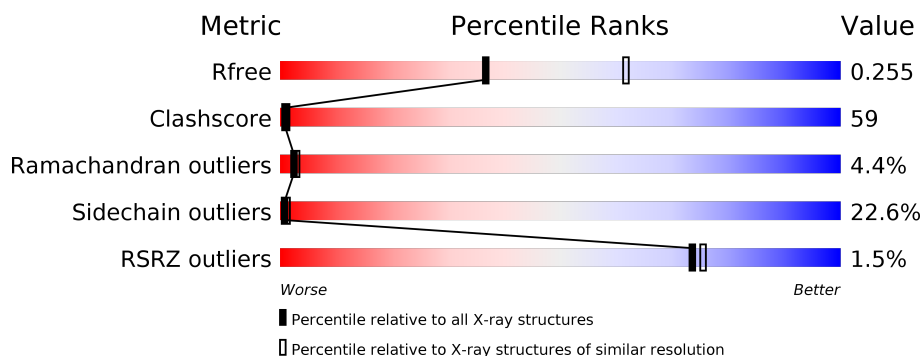
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	315	<div> <div></div> <div>14% 44% 14% 27%</div> </div>
1	B	315	<div> <div>4%</div> <div>20% 41% 11% 27%</div> </div>
1	K	315	<div> <div>%</div> <div>17% 40% 15% 27%</div> </div>
1	L	315	<div> <div>3%</div> <div>20% 42% 11% 27%</div> </div>
2	C	1119	<div> <div>%</div> <div>23% 59% 17%</div> </div>
2	M	1119	<div> <div>%</div> <div>25% 58% 17%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1524	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%23%51%16%•9%</div></div>
3	N	1524	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%25%51%15%•9%</div></div>
4	E	99	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%27%58%11%•</div></div>
4	O	99	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%22%56%17%••</div></div>
5	F	423	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%21%48%11%•18%</div></div>
5	P	423	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%24%47%10%18%</div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 61089 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 DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

- Molecule 2 is a protein called DNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			

- Molecule 4 is a protein called RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

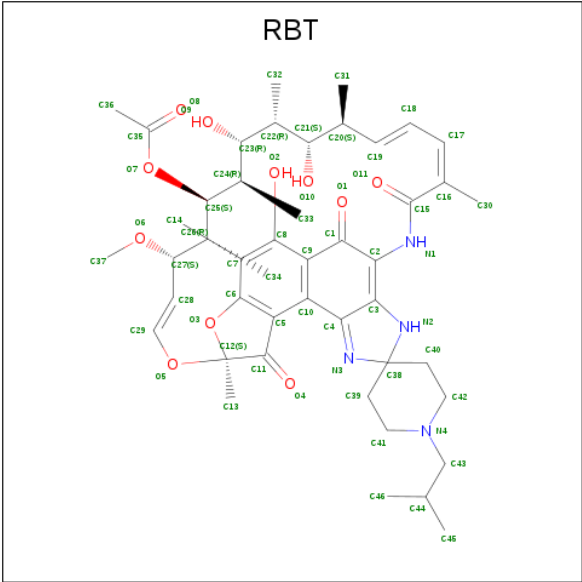
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	20	Total	Mg	0	0
			20	20		
6	D	137	Total	Mg	0	0
			137	137		
6	K	21	Total	Mg	0	0
			21	21		
6	E	10	Total	Mg	0	0
			10	10		
6	B	23	Total	Mg	0	0
			23	23		
6	C	81	Total	Mg	0	0
			81	81		
6	A	31	Total	Mg	0	0
			31	31		
6	N	108	Total	Mg	0	0
			108	108		
6	O	6	Total	Mg	0	0
			6	6		
6	L	25	Total	Mg	0	0
			25	25		
6	F	31	Total	Mg	0	0
			31	31		
6	M	69	Total	Mg	0	0
			69	69		

- Molecule 7 is RIFABUTIN (three-letter code: RBT) (formula: C<sub>46</sub>H<sub>62</sub>N<sub>4</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			61	46	4	11		
7	M	1	Total	C	N	O	0	0
			61	46	4	11		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	N	2	Total	Zn	0	0
			2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	253	Total	O	0	0
			253	253		
9	B	307	Total	O	0	0
			307	307		
9	C	1000	Total	O	0	0
			1000	1000		
9	D	1418	Total	O	0	0
			1418	1418		
9	E	112	Total	O	0	0
			112	112		

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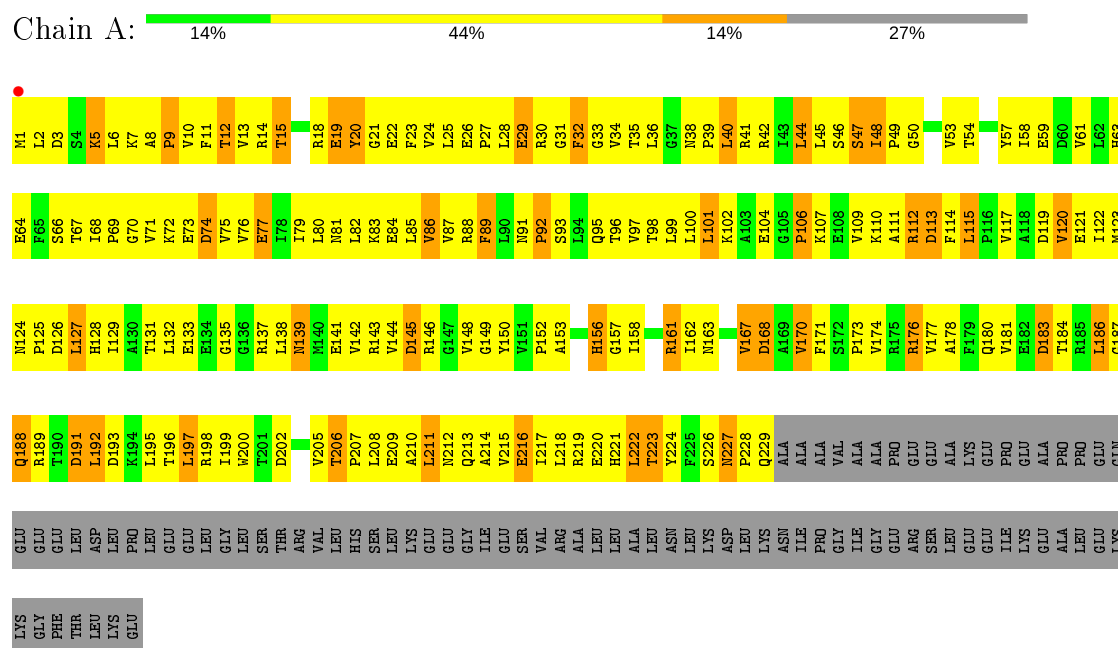
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	456	Total 456	O 456	0	0
9	K	213	Total 213	O 213	0	0
9	L	237	Total 237	O 237	0	0
9	M	998	Total 998	O 998	0	0
9	N	1357	Total 1357	O 1357	0	0
9	O	117	Total 117	O 117	0	0
9	P	377	Total 377	O 377	0	0

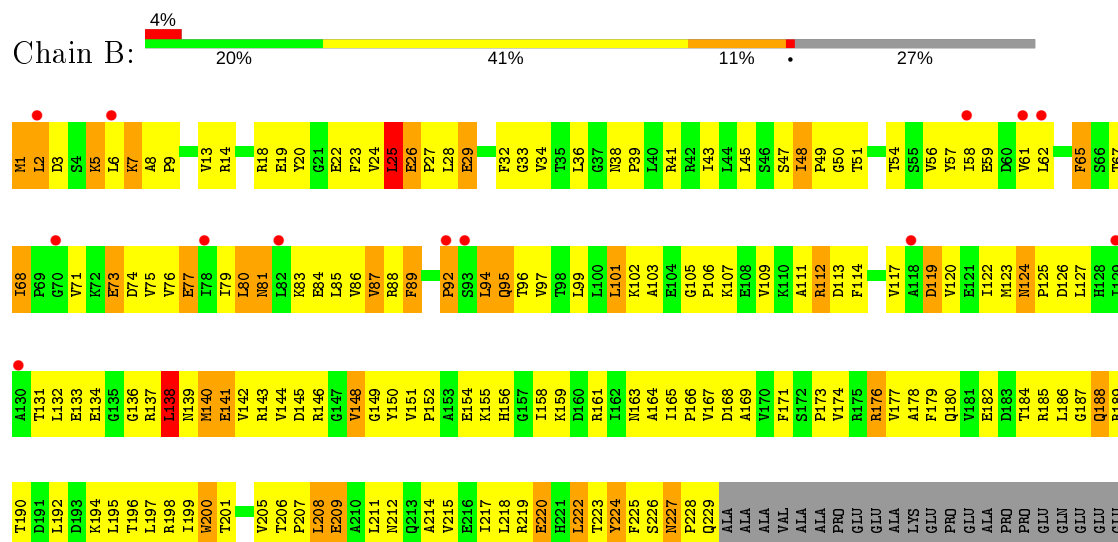
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: DNA-directed RNA polymerase alpha chain



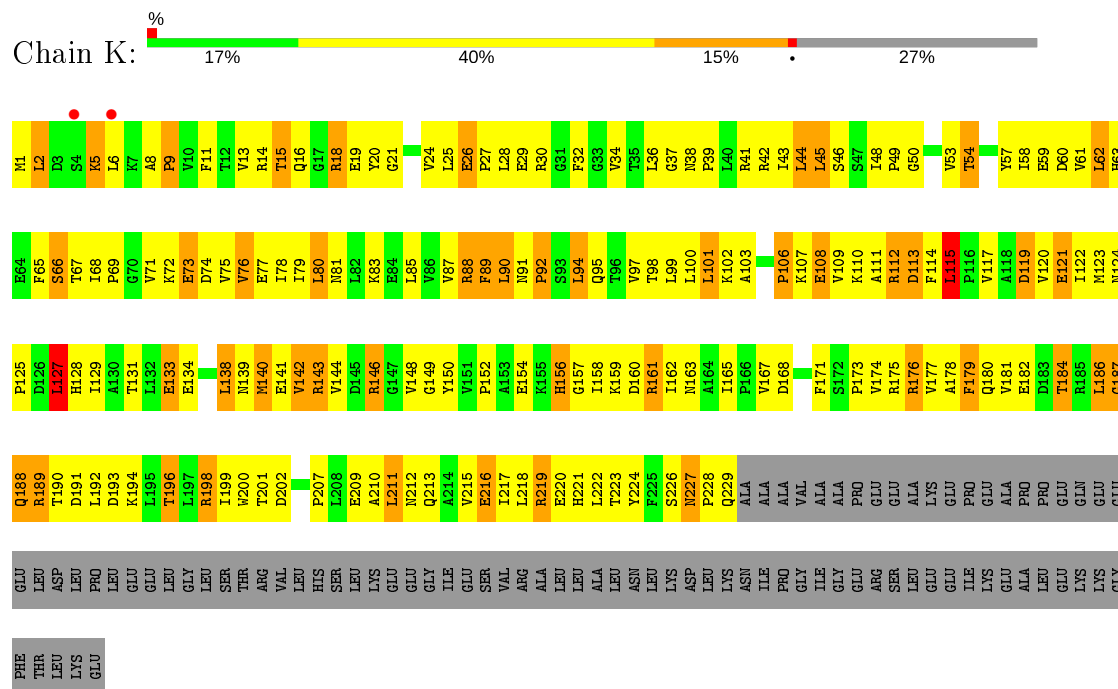
#### • Molecule 1: DNA-directed RNA polymerase alpha chain



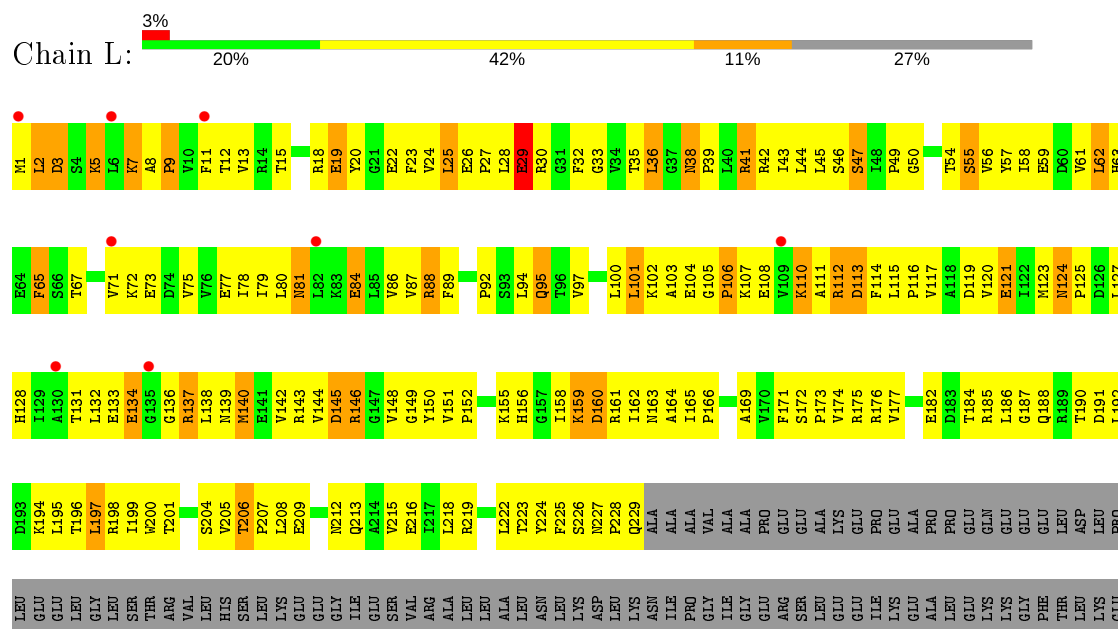


LEU	ASP	LEU	PRO	GLU	GLU	LEU	GLY	SER	THR	ARG	VAL	LEU	HIS	SER	LEU	LYS	GLU	GLY	LEU	LYS	GLY	LYS	PHE
THR	LEU	LYS	GLU																				

• Molecule 1: DNA-directed RNA polymerase alpha chain



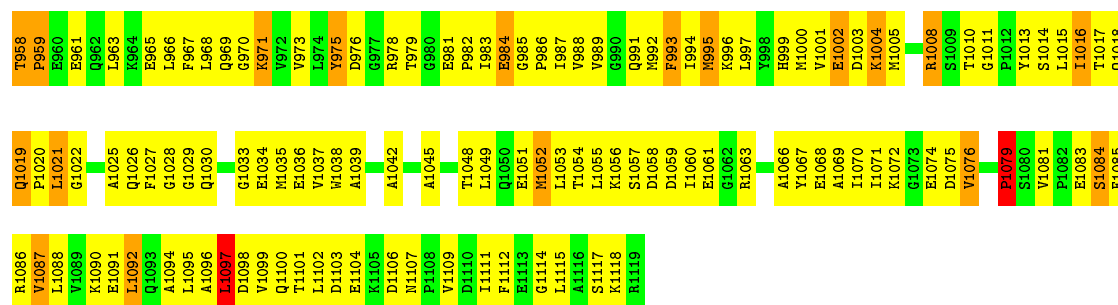
• Molecule 1: DNA-directed RNA polymerase alpha chain



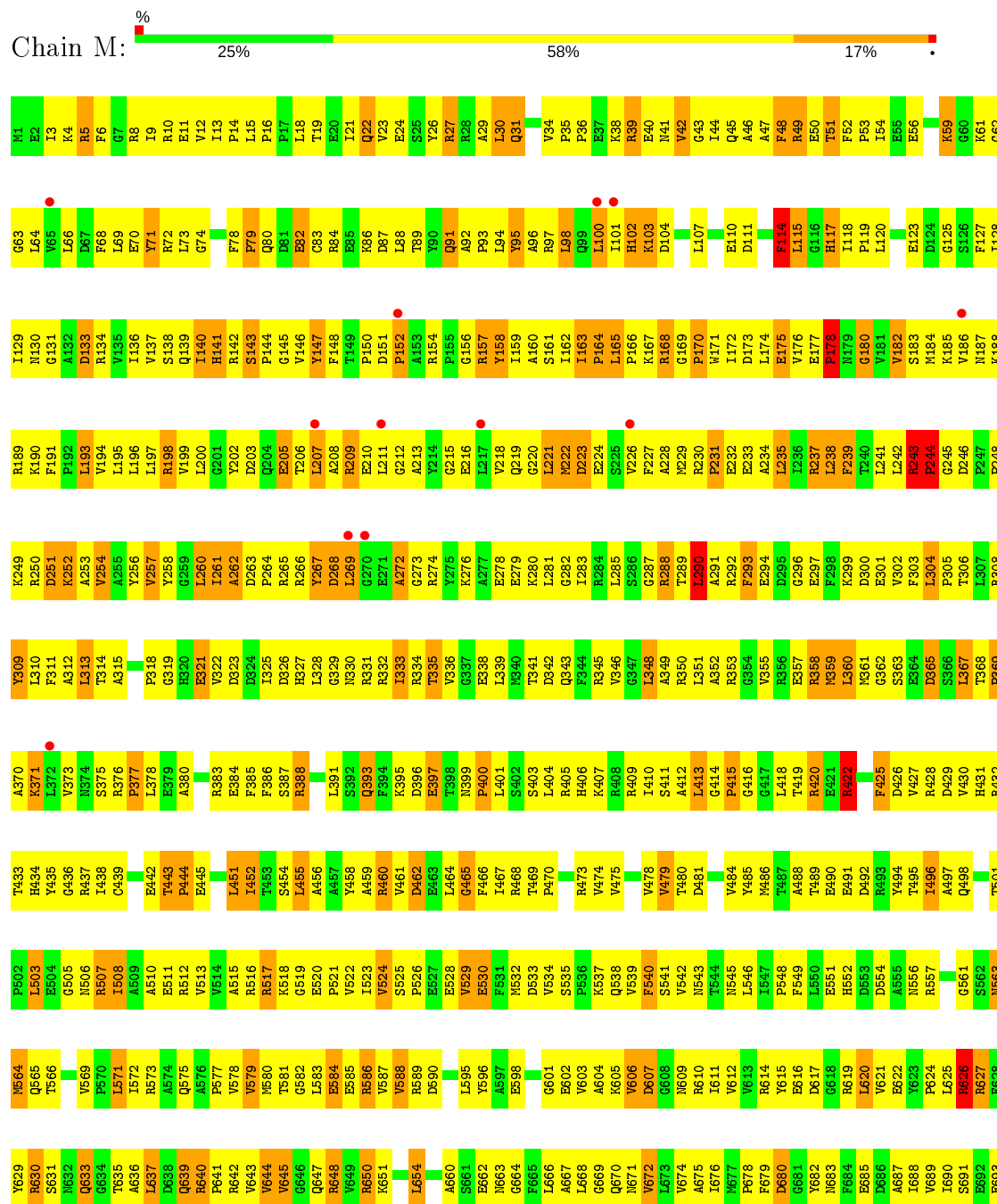
• Molecule 2: DNA-directed RNA polymerase beta chain





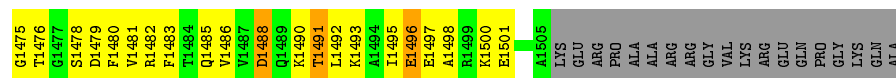


• Molecule 2: DNA-directed RNA polymerase beta chain

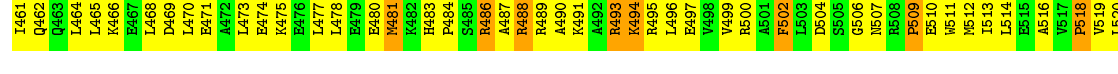
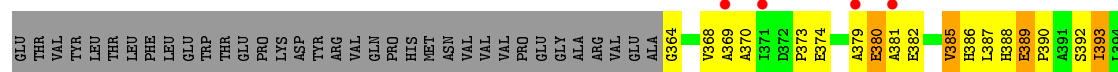
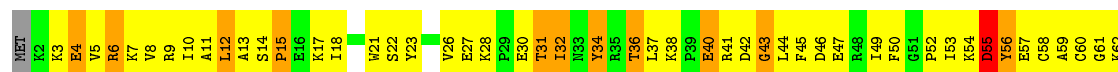


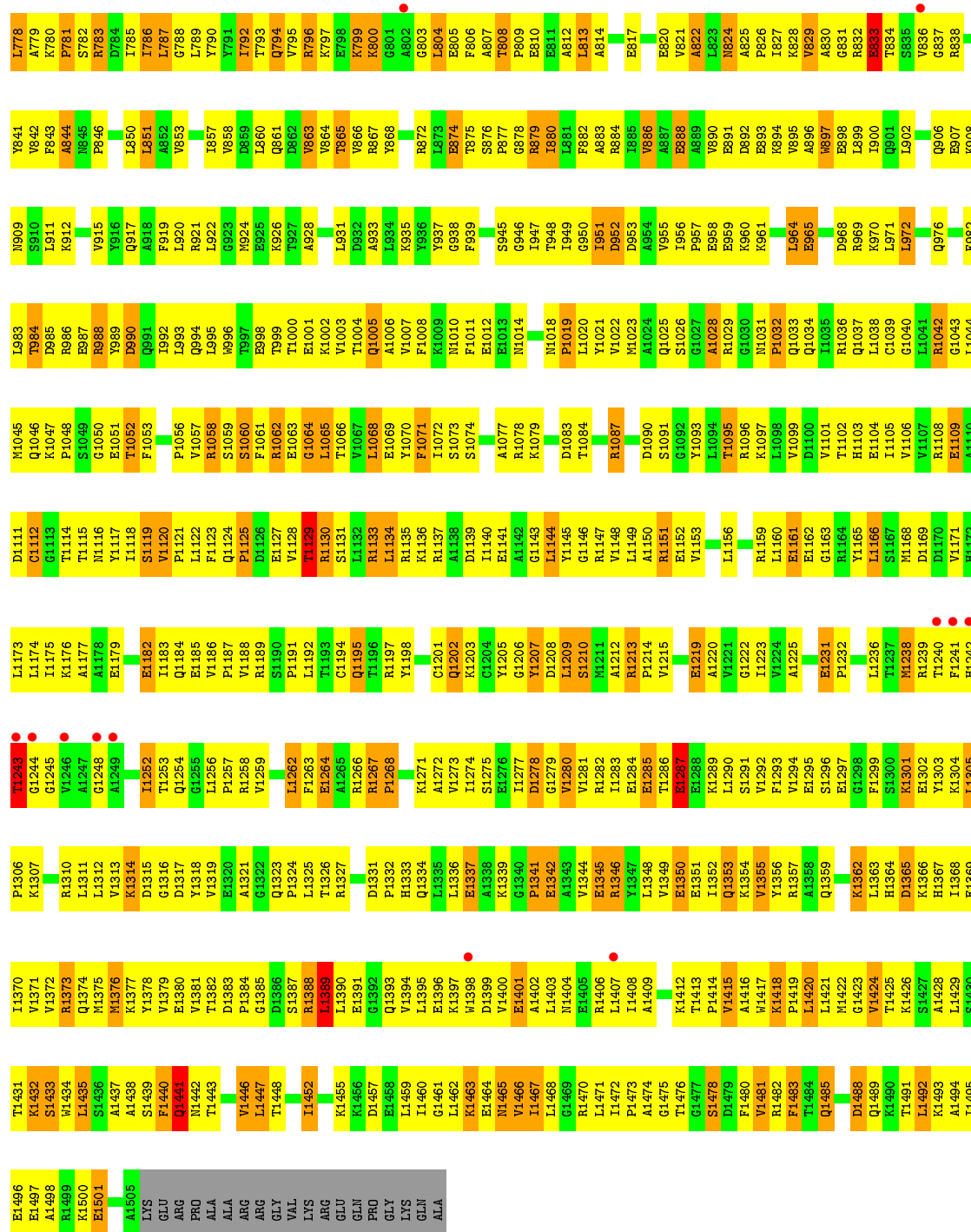






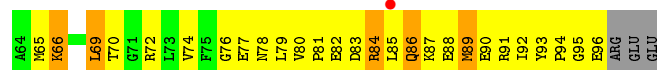
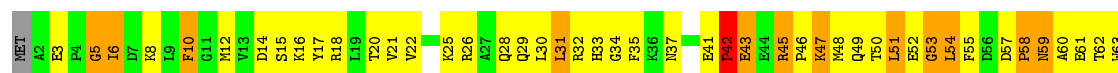
• Molecule 3: DNA-directed RNA polymerase beta' chain



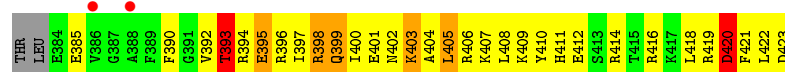
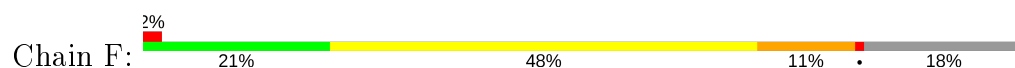




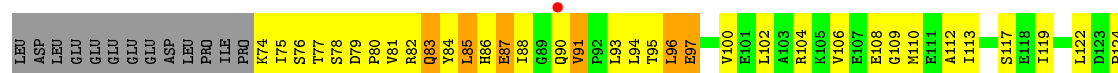
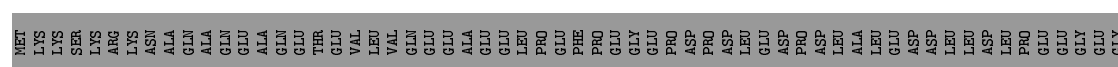
- Molecule 4: RNA polymerase omega chain



- Molecule 5: RNA polymerase sigma factor rpoD



- Molecule 5: RNA polymerase sigma factor rpoD





G391	K325	P261	I188	D125
V392	D326	V262	E189	L126
T393	S327	E263	A190	I127
R394	F328	M264	N191	R128
E395	Y329	V265	L192	E129
R396	G330	E266	R193	V130
I397	D331	T267	L194	V131
R398	F332	I268	V195	A132
Q399	I333	M269	V196	A133
I400	P334	K270	S197	K134
E401	D335	L271	I198	I135
M402	E336	S272	A199	L136
K403	H337	R273	K200	G137
A404	L338	T274	K201	S138
L405		A275	T202	A139
R406	P341	R276	T203	R140
L408	V342	Q277	G204	V141
K409	D343	L278	L207	R142
Y410	A344	Q279	S208	H143
H411	A345	Q280	P209	I144
E412	T346	E281	L210	P145
S413	S348		D211	G146
R414	L349	P286	L212	L147
T415	L350	T287	L213	
R416	S351	Y288	Q214	T150
K417	E352	E289	E215	L151
L418	E353	E290	G216	D152
R419	L354	I291	N217	P153
D420	E355	A292	Q218	K154
F421	K356		G219	T155
L422	A357	K295	L220	V156
D423	L358	G296	I221	
		P297	R232	I159
		W298	Y238	D160
	L361	W299	W242	Q161
	E362	D300	I243	K162
	E363	A301	R244	L163
	R364	K302	Q245	K164
	E365	R303	A246	S165
	A366	V304	I247	L166
	K367	E305	N248	P167
	V368	E306	I251	K168
	L369	T307	A252	E169
	K370	L308	T257	H170
	L371	R309	I260	K171
	R372	I310		R172
	K373	A311		Y173
	G374	Q312		L174
	L375	E313		H175
		P314		I176
	G376	V315		A177
	ARG	S316		R178
	GLU	L317		
	HIS	E318		E181
	THR	T319		A182
	LEU	P320		A183
		I321		R184
	E384	G322		Q185
	E385	D323		H186
		E324		L187
	F390			

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 91.2 (24.85-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.225 , 0.257 0.223 , 0.255	Depositor DCC
$R_{free}$ test set	29386 reflections (5.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 77.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.085 for h,-h-k,-l 0.085 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	61089	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: ZN, RBT, MG

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	0.79	1/1838 (0.1%)	0.86	2/2498 (0.1%)
1	B	0.73	0/1838	0.82	3/2498 (0.1%)
1	K	0.75	0/1838	0.84	2/2498 (0.1%)
1	L	0.71	1/1838 (0.1%)	0.78	0/2498
2	C	0.81	0/8997	0.88	6/12164 (0.0%)
2	M	0.79	0/8997	0.88	8/12164 (0.1%)
3	D	0.82	0/10975	0.93	22/14836 (0.1%)
3	N	0.80	0/10975	0.91	14/14836 (0.1%)
4	E	0.82	0/783	0.98	1/1054 (0.1%)
4	O	0.84	0/783	0.96	1/1054 (0.1%)
5	F	0.73	0/2812	0.82	2/3781 (0.1%)
5	P	0.71	0/2812	0.80	1/3781 (0.0%)
All	All	0.79	2/54486 (0.0%)	0.88	62/73662 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	5.18	1.44	1.34
1	L	172	SER	N-CA	-5.06	1.36	1.46

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	LEU	CA-CB-CG	8.26	134.29	115.30
3	D	199	LEU	CA-CB-CG	-8.08	96.72	115.30
3	N	199	LEU	CA-CB-CG	-7.83	97.28	115.30
3	N	1389	LEU	CA-CB-CG	7.33	132.15	115.30
5	F	361	LEU	CA-CB-CG	7.04	131.49	115.30
3	N	705	ALA	C-N-CD	6.92	142.94	128.40
3	D	637	LEU	CA-CB-CG	6.79	130.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	136	LEU	CA-CB-CG	6.19	129.54	115.30
1	A	192	LEU	CA-CB-CG	6.15	129.44	115.30
2	C	98	LEU	CA-CB-CG	6.07	129.25	115.30
2	M	571	LEU	CA-CB-CG	6.06	129.24	115.30
3	D	80	VAL	C-N-CA	6.02	136.75	121.70
1	K	115	LEU	CA-CB-CG	6.01	129.13	115.30
3	D	73	CYS	CA-CB-SG	5.91	124.64	114.00
3	N	80	VAL	C-N-CA	5.83	136.27	121.70
2	M	243	ARG	C-N-CD	-5.80	107.84	120.60
3	D	1209	LEU	N-CA-C	-5.78	95.39	111.00
3	N	1209	LEU	N-CA-C	-5.77	95.43	111.00
3	D	238	PRO	N-CA-CB	5.76	110.21	103.30
5	F	354	LEU	CA-CB-CG	5.73	128.48	115.30
2	C	260	LEU	CA-CB-CG	5.73	128.47	115.30
3	N	209	ARG	N-CA-C	5.72	126.45	111.00
3	D	1395	LEU	CA-CB-CG	5.72	128.46	115.30
3	D	581	LEU	CA-CB-CG	5.67	128.34	115.30
3	D	208	PRO	CA-N-CD	-5.62	103.63	111.50
3	D	153	LEU	CA-CB-CG	5.61	128.20	115.30
2	M	165	LEU	C-N-CD	-5.57	108.35	120.60
3	N	82	LYS	C-N-CA	-5.57	107.79	121.70
3	D	1134	LEU	CA-CB-CG	5.52	127.99	115.30
3	N	554	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	115	LEU	CA-CB-CG	5.50	127.95	115.30
2	M	100	LEU	CA-CB-CG	5.50	127.95	115.30
1	B	25	LEU	CA-CB-CG	5.49	127.93	115.30
3	D	209	ARG	N-CA-C	5.46	125.74	111.00
3	D	226	PRO	N-CA-CB	5.40	109.78	103.30
3	N	380	GLU	N-CA-C	-5.40	96.42	111.00
3	D	21	TRP	CA-CB-CG	5.40	123.95	113.70
3	N	248	PRO	N-CA-CB	5.40	109.78	103.30
3	D	248	PRO	N-CA-CB	5.36	109.73	103.30
3	D	839	LEU	CA-CB-CG	5.35	127.61	115.30
1	K	127	LEU	CA-CB-CG	5.33	127.55	115.30
2	M	207	LEU	CA-CB-CG	5.29	127.46	115.30
4	O	31	LEU	CA-CB-CG	5.27	127.41	115.30
3	N	208	PRO	CA-N-CD	-5.24	104.16	111.50
3	D	60	CYS	CA-CB-SG	5.19	123.35	114.00
3	D	380	GLU	N-CA-C	-5.19	97.00	111.00
2	M	244	PRO	CA-N-CD	-5.18	104.25	111.50
2	C	243	ARG	C-N-CD	-5.16	109.25	120.60
2	M	114	PHE	CB-CG-CD2	-5.16	117.19	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	LEU	CA-CB-CG	5.15	127.14	115.30
3	N	238	PRO	N-CA-CB	5.14	109.47	103.30
3	D	80	VAL	CA-C-N	-5.13	105.90	117.20
3	D	1389	LEU	CA-CB-CG	5.13	127.09	115.30
2	C	1097	LEU	CA-CB-CG	5.11	127.05	115.30
2	M	729	LEU	N-CA-C	5.10	124.77	111.00
4	E	51	LEU	CA-CB-CG	5.08	126.99	115.30
3	N	423	ASP	N-CA-C	5.07	124.70	111.00
2	C	207	LEU	CA-CB-CG	5.06	126.93	115.30
3	D	1312	LEU	CA-CB-CG	5.03	126.86	115.30
3	D	1207	TYR	CA-CB-CG	5.03	122.95	113.40
3	N	813	LEU	CA-CB-CG	5.02	126.84	115.30
2	C	728	HIS	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	231	0
1	B	1806	0	1861	211	0
1	K	1806	0	1861	199	0
1	L	1806	0	1861	202	0
2	C	8829	0	8933	1201	0
2	M	8829	0	8933	1179	0
3	D	10797	0	10873	1404	0
3	N	10797	0	10873	1285	0
4	E	769	0	775	92	0
4	O	769	0	775	99	0
5	F	2771	0	2844	340	0
5	P	2771	0	2844	315	0
6	A	31	0	0	0	0
6	B	23	0	0	0	0
6	C	81	0	0	0	0
6	D	137	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	10	0	0	0	0
6	F	31	0	0	0	0
6	K	21	0	0	0	0
6	L	25	0	0	0	0
6	M	69	0	0	0	0
6	N	108	0	0	0	0
6	O	6	0	0	0	0
6	P	20	0	0	0	0
7	C	61	0	61	3	0
7	M	61	0	61	3	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	A	253	0	0	49	0
9	B	307	0	0	49	0
9	C	1000	0	0	202	0
9	D	1418	0	0	282	0
9	E	112	0	0	22	0
9	F	456	0	0	98	0
9	K	213	0	0	34	0
9	L	237	0	0	58	0
9	M	998	0	0	255	0
9	N	1357	0	0	240	0
9	O	117	0	0	26	0
9	P	377	0	0	75	0
All	All	61089	0	54416	6365	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

All (6365) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.08	1.12
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.27	1.11
3:N:1045:MET:HG2	3:N:1073:SER:HA	1.35	1.08
2:C:630:ARG:HH21	2:C:705:ILE:HG22	1.18	1.07
3:N:52:PRO:HB2	3:N:80:VAL:HG13	1.34	1.06
3:D:197:SER:HB3	3:D:203:ALA:HB3	1.38	1.05
2:C:110:GLU:HG2	2:C:369:PRO:HB3	1.41	1.03
2:M:952:LEU:HD12	2:M:969:GLN:HE22	1.16	1.03
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.40	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:150:PRO:HA	2:M:158:TYR:HB3	1.42	1.02
3:D:796:ARG:HH11	3:D:861:GLN:HB2	1.22	1.01
2:M:169:GLY:HA2	2:M:263:ASP:HB3	1.40	1.01
3:D:422:ALA:HB3	3:D:427:VAL:HG22	1.42	1.01
2:C:150:PRO:HA	2:C:158:TYR:HB3	1.39	1.00
3:N:197:SER:HB3	3:N:203:ALA:HB3	1.42	1.00
3:N:898:GLU:HB2	3:N:921:ARG:HH22	1.27	1.00
3:N:1033:GLN:HE21	3:N:1036:ARG:HH11	1.10	1.00
3:D:1045:MET:HG2	3:D:1073:SER:HA	1.40	0.99
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.44	0.99
3:N:1476:THR:HG23	4:O:21:VAL:HG22	1.43	0.99
3:N:1205:TYR:HD2	3:N:1215:VAL:HG21	1.27	0.99
2:C:305:PRO:HB3	2:C:308:ARG:HH21	1.29	0.98
3:D:906:GLN:HB3	3:D:911:LEU:HD11	1.44	0.98
3:N:928:ALA:HA	3:N:931:LEU:HD12	1.42	0.98
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.41	0.98
3:D:1095:THR:HG23	3:D:1230:GLY:HA3	1.44	0.98
4:E:41:GLU:O	4:E:45:ARG:HG2	1.64	0.98
2:M:1114:GLY:H	2:M:1115:LEU:HD12	1.27	0.98
3:D:462:GLN:HA	3:D:513:ILE:HD13	1.47	0.97
3:D:1481:VAL:HG11	4:E:18:ARG:HA	1.45	0.97
3:N:1262:LEU:HD21	3:N:1351:GLU:HG3	1.46	0.97
3:N:9:ARG:HH12	3:N:506:GLY:HA2	1.27	0.97
2:M:404:LEU:HA	2:M:407:LYS:HD3	1.47	0.96
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.48	0.96
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.46	0.96
3:N:1101:VAL:HG21	3:N:1424:VAL:HG22	1.44	0.96
5:F:166:LEU:HB3	5:F:170:HIS:HB2	1.45	0.95
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.30	0.94
1:K:24:VAL:HG22	1:K:196:THR:HB	1.50	0.94
1:B:152:PRO:HD2	1:B:155:LYS:HD3	1.45	0.94
1:L:152:PRO:HD2	1:L:155:LYS:HD3	1.50	0.94
1:B:206:THR:HG22	1:B:209:GLU:HB2	1.50	0.93
3:N:422:ALA:HB3	3:N:427:VAL:HG22	1.50	0.93
2:C:232:GLU:HA	2:C:235:LEU:HD12	1.48	0.93
2:C:773:LEU:HB2	5:F:373:LYS:HB3	1.48	0.93
3:D:1066:THR:HG22	3:D:1069:GLU:HB2	1.51	0.93
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.50	0.93
3:D:572:ARG:HH21	5:F:83:GLN:HE21	1.17	0.93
2:C:41:ASN:HD22	2:C:41:ASN:H	0.96	0.93
2:C:979:THR:HG23	2:C:981:GLU:H	1.34	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:VAL:HG12	1:B:124:ASN:HD22	1.34	0.92
2:M:34:VAL:HB	2:M:38:LYS:HG3	1.52	0.92
5:P:361:LEU:HG	5:P:408:LEU:HD21	1.52	0.92
2:M:409:ARG:HA	2:M:454:SER:HA	1.50	0.92
3:N:704:ARG:HD2	3:N:705:ALA:H	1.35	0.92
2:M:857:ASP:HB2	2:M:978:ARG:HG2	1.48	0.91
2:M:1081:VAL:HG21	2:M:1111:ILE:HG22	1.49	0.91
5:P:88:ILE:HD13	5:P:193:ARG:HB2	1.50	0.91
2:M:197:LEU:HD13	2:M:207:LEU:HD11	1.52	0.91
2:M:724:ARG:HG3	2:M:740:GLU:HA	1.50	0.91
3:N:637:LEU:HD21	3:N:642:CYS:HA	1.50	0.91
2:C:135:VAL:HG11	2:C:407:LYS:HA	1.51	0.91
3:N:136:ASP:HB3	3:N:137:PRO:HD3	1.52	0.91
3:D:928:ALA:HA	3:D:931:LEU:HD12	1.53	0.91
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.53	0.90
1:B:57:TYR:HB3	1:B:141:GLU:HG3	1.53	0.90
2:M:1111:ILE:HD12	2:M:1112:PHE:H	1.36	0.90
2:M:979:THR:HG23	2:M:981:GLU:H	1.37	0.90
3:N:699:VAL:H	3:N:756:GLN:NE2	1.69	0.89
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.55	0.89
2:C:1008:ARG:HH21	2:C:1028:GLY:HA2	1.37	0.89
2:C:64:LEU:HD22	2:C:359:MET:HG3	1.53	0.89
2:C:328:LEU:HD13	2:C:433:THR:HB	1.52	0.89
3:D:1160:LEU:HD11	3:D:1174:LEU:HD21	1.55	0.89
2:C:689:VAL:HB	2:C:870:ILE:HG13	1.53	0.89
5:F:76:SER:O	5:F:80:PRO:HD2	1.73	0.89
3:D:191:LEU:HD12	3:D:211:VAL:HG21	1.52	0.89
3:D:133:ILE:HG21	3:D:454:ALA:HB1	1.53	0.89
5:F:160:ASP:HA	5:F:163:LEU:HD12	1.53	0.89
3:N:210:ARG:HH11	3:N:398:ALA:HB3	1.38	0.89
3:D:1209:LEU:HB3	3:D:1211:MET:HG2	1.54	0.88
3:N:616:GLN:HE22	3:N:619:LEU:HD12	1.34	0.88
2:C:1114:GLY:H	2:C:1115:LEU:HD12	1.38	0.88
2:M:1018:GLN:HE21	2:M:1063:ARG:HH22	1.18	0.88
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.53	0.88
3:N:1380:GLU:HB3	3:N:1418:LYS:HG3	1.52	0.88
2:C:358:ARG:HH22	2:C:374:ASN:HB3	1.38	0.88
3:D:1096:ARG:HH11	3:D:1096:ARG:HB2	1.37	0.88
2:M:146:VAL:HG22	2:M:162:ILE:HA	1.55	0.88
2:M:115:LEU:HD22	2:M:373:VAL:HG11	1.55	0.88
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:HB2	1:A:192:LEU:HD11	1.55	0.87
2:C:579:VAL:HB	2:C:890:LEU:HD22	1.57	0.87
3:N:565:ILE:H	3:N:565:ILE:HD12	1.39	0.87
5:P:394:ARG:HA	5:P:397:ILE:HD12	1.55	0.87
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.54	0.87
2:C:1096:ALA:O	3:D:13:ALA:HB2	1.74	0.87
1:A:63:HIS:HB3	2:C:746:GLY:HA2	1.57	0.87
1:K:186:LEU:HB2	1:K:192:LEU:HD11	1.55	0.86
2:C:433:THR:HG21	2:C:488:ALA:HB1	1.54	0.86
3:D:1310:ARG:HD3	3:D:1310:ARG:H	1.40	0.86
5:P:133:ALA:HB2	5:P:142:ARG:HH21	1.37	0.86
3:D:87:ARG:HB3	3:D:523:ASP:HB2	1.54	0.86
2:M:289:THR:HG22	2:M:290:LEU:HD23	1.56	0.86
2:C:692:GLU:HG2	2:C:696:LYS:HE3	1.57	0.86
3:D:572:ARG:HH21	5:F:83:GLN:NE2	1.73	0.86
3:N:119:SER:HB2	3:N:123:LEU:HB2	1.55	0.86
2:M:605:LYS:HB2	2:M:610:ARG:HH12	1.39	0.85
2:C:479:VAL:HG21	2:C:503:LEU:HD11	1.57	0.85
5:F:394:ARG:HA	5:F:397:ILE:HD12	1.57	0.85
3:N:1485:GLN:HE21	4:O:80:VAL:H	1.21	0.85
3:D:82:LYS:H	3:D:82:LYS:HE3	1.42	0.85
5:P:321:ILE:HD11	5:P:329:TYR:HB2	1.58	0.85
1:L:56:VAL:HG13	1:L:142:VAL:HG12	1.58	0.85
2:C:41:ASN:N	2:C:41:ASN:HD22	1.73	0.85
2:M:332:ARG:HH21	2:M:464:LEU:HD11	1.41	0.85
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.57	0.85
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.58	0.85
1:L:124:ASN:HD22	1:L:127:LEU:HD22	1.41	0.85
1:L:32:PHE:HB2	9:L:3706:HOH:O	1.76	0.85
2:C:860:HIS:HB2	9:C:9638:HOH:O	1.76	0.84
3:N:1057:VAL:HG13	3:N:1069:GLU:HB3	1.59	0.84
5:F:125:ASP:HA	5:F:128:ARG:NH1	1.92	0.84
2:M:1054:THR:HG22	2:M:1059:ASP:HB2	1.60	0.84
5:F:268:ILE:HA	5:F:271:LEU:HD12	1.58	0.84
3:N:566:ILE:HD11	5:P:192:LEU:HD21	1.59	0.84
2:C:49:ARG:HH11	2:C:49:ARG:HB2	1.40	0.84
3:N:145:VAL:HG22	3:N:146:PRO:HD2	1.60	0.84
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.60	0.84
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.58	0.84
2:C:146:VAL:HG22	2:C:162:ILE:HA	1.59	0.83
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.60	0.83
1:K:100:LEU:HB2	1:K:115:LEU:HD11	1.59	0.83
3:N:796:ARG:HD3	3:N:861:GLN:HB2	1.60	0.83
2:C:186:VAL:HG23	2:C:187:ASN:H	1.43	0.83
3:D:721:VAL:HG21	3:D:727:GLN:HE21	1.44	0.83
3:N:1160:LEU:HD11	3:N:1174:LEU:HD21	1.59	0.83
3:D:86:ARG:O	3:D:522:PRO:HD2	1.79	0.83
3:D:561:GLY:HA3	5:F:184:ARG:HH22	1.42	0.83
2:M:670:GLN:O	2:M:672:VAL:HG12	1.78	0.83
2:M:966:LEU:HD11	2:M:986:PRO:HG2	1.58	0.83
2:C:176:VAL:HG12	2:C:182:VAL:HG13	1.60	0.83
1:L:87:VAL:HG21	1:L:144:VAL:HG11	1.61	0.83
2:C:329:GLY:HA3	2:C:489:THR:HG23	1.61	0.82
1:K:117:VAL:HB	1:K:120:VAL:HG12	1.59	0.82
2:M:693:GLU:HG3	9:M:9861:HOH:O	1.78	0.82
2:C:115:LEU:HD22	2:C:373:VAL:HG11	1.61	0.82
3:D:493:ARG:HH22	3:D:1389:LEU:HG	1.42	0.82
3:D:560:GLN:HG2	5:F:218:GLN:HE22	1.44	0.82
3:D:1215:VAL:HG11	9:D:9876:HOH:O	1.79	0.82
3:N:152:LEU:HD23	3:N:152:LEU:H	1.44	0.82
5:P:166:LEU:HB3	5:P:170:HIS:HB2	1.61	0.82
3:N:53:ILE:HG23	3:N:54:LYS:H	1.44	0.82
4:E:67:GLU:HB2	4:E:73:LEU:HD11	1.61	0.82
5:F:205:ARG:HD2	5:F:251:ILE:HD13	1.62	0.82
3:D:422:ALA:H	3:D:427:VAL:HG11	1.45	0.81
5:F:88:ILE:HD13	5:F:193:ARG:HB2	1.60	0.81
2:M:1005:MET:HB2	3:N:648:MET:HE1	1.61	0.81
2:M:834:GLN:HA	9:M:2100:HOH:O	1.80	0.81
4:O:51:LEU:HG	4:O:53:GLY:H	1.46	0.81
3:D:1209:LEU:HD22	3:D:1211:MET:SD	2.21	0.81
3:D:101:HIS:HD1	3:D:103:TRP:HB2	1.45	0.81
3:N:18:ILE:HG23	3:N:518:PRO:HG3	1.62	0.81
3:N:806:PHE:CE1	3:N:813:LEU:HB3	2.16	0.81
3:N:558:LEU:HD13	5:P:145:PRO:HB3	1.62	0.81
2:M:507:ARG:HB2	2:M:507:ARG:HH11	1.46	0.81
3:N:542:ASP:O	3:N:546:ARG:HG2	1.81	0.81
3:N:186:VAL:HG21	3:N:213:VAL:HB	1.63	0.81
3:N:148:GLU:HB3	3:N:151:GLN:HB2	1.60	0.80
1:L:84:GLU:HB3	1:L:127:LEU:HD21	1.63	0.80
2:M:18:LEU:HB2	2:M:590:ASP:HB3	1.62	0.80
1:A:14:ARG:HH21	1:A:22:GLU:HB3	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:PRO:HB3	1:B:192:LEU:HD22	1.62	0.80
2:C:886:LEU:HG	3:D:951:ILE:HG13	1.63	0.80
3:N:1097:LYS:HA	9:N:9580:HOH:O	1.81	0.80
5:F:291:ILE:HG21	5:F:304:VAL:HG11	1.63	0.80
3:D:1066:THR:HG23	3:D:1069:GLU:H	1.47	0.80
3:N:1480:PHE:HD2	3:N:1481:VAL:HG22	1.46	0.80
2:C:724:ARG:HG3	2:C:741:GLY:H	1.46	0.80
5:F:123:ASP:HB2	5:F:126:LEU:HD13	1.63	0.80
5:P:406:ARG:HA	5:P:409:LYS:HG2	1.64	0.80
2:C:671:ASN:HD22	2:C:671:ASN:N	1.78	0.80
3:D:720:LEU:H	3:D:720:LEU:HD12	1.46	0.80
3:D:978:TYR:HA	9:D:9941:HOH:O	1.80	0.80
2:M:704:HIS:HB2	2:M:831:ARG:HE	1.46	0.80
2:C:650:ARG:HG3	2:C:653:ASP:HB2	1.63	0.80
2:M:312:ALA:HB1	2:M:318:PRO:HG2	1.64	0.80
3:N:119:SER:HB2	3:N:123:LEU:H	1.47	0.80
2:M:1015:LEU:HA	5:P:335:ASP:HB2	1.63	0.80
2:C:630:ARG:NH2	2:C:705:ILE:HG22	1.97	0.79
2:C:768:THR:HB	2:C:771:GLU:HB3	1.64	0.79
3:N:536:ALA:HA	5:P:315:VAL:H	1.45	0.79
1:A:152:PRO:HA	9:C:9876:HOH:O	1.82	0.79
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.63	0.79
2:M:1095:LEU:HD23	3:N:582:LEU:HD22	1.62	0.79
2:M:362:GLY:HA3	2:M:367:LEU:HD23	1.64	0.79
2:M:578:VAL:HG23	2:M:579:VAL:HG12	1.63	0.79
3:D:1040:GLY:O	3:D:1060:SER:HB3	1.82	0.79
3:N:422:ALA:H	3:N:427:VAL:HG11	1.46	0.79
5:P:76:SER:O	5:P:80:PRO:HD2	1.82	0.79
3:N:771:SER:HB2	3:N:778:LEU:HD13	1.64	0.79
1:A:95:GLN:HA	1:A:146:ARG:HH12	1.47	0.79
3:N:1352:ILE:O	3:N:1355:VAL:HG23	1.81	0.79
5:F:156:VAL:HA	5:F:159:ILE:HD12	1.63	0.79
3:N:1137:ARG:HA	3:N:1140:ILE:HD12	1.65	0.79
3:N:1223:ILE:H	3:N:1223:ILE:HD12	1.47	0.79
3:N:572:ARG:HH22	5:P:83:GLN:HG3	1.48	0.79
2:C:1013:TYR:HB3	9:C:2163:HOH:O	1.82	0.78
2:C:578:VAL:HG11	2:C:991:GLN:HB3	1.65	0.78
3:D:1127:GLU:HG3	3:D:1133:ARG:HH12	1.47	0.78
3:N:658:LEU:HD21	3:N:674:ARG:HG3	1.64	0.78
1:A:42:ARG:NH1	2:C:857:ASP:HB3	1.93	0.78
3:D:806:PHE:CE1	3:D:813:LEU:HB3	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:361:LEU:HD23	5:F:362:SER:H	1.46	0.78
2:M:606:VAL:HG22	2:M:645:VAL:HG13	1.65	0.78
3:D:1467:ILE:HG22	9:D:9901:HOH:O	1.83	0.78
3:D:800:LYS:HE3	3:D:830:ALA:HB3	1.63	0.78
1:L:185:ARG:HA	9:L:4234:HOH:O	1.83	0.78
3:D:1130:ARG:HB2	3:D:1130:ARG:HH11	1.46	0.78
1:L:13:VAL:HG11	1:L:208:LEU:HD11	1.66	0.78
2:M:140:ILE:HG23	2:M:333:ILE:HG13	1.66	0.78
2:M:176:VAL:HG12	2:M:182:VAL:HG13	1.65	0.78
3:N:428:LYS:HE3	3:N:434:ARG:HH12	1.47	0.78
3:N:535:PHE:HB3	5:P:314:PRO:HB3	1.64	0.78
3:D:493:ARG:NH1	3:D:1390:LEU:HB2	1.98	0.78
3:N:704:ARG:HG3	3:N:736:PHE:HB3	1.66	0.78
3:N:1144:LEU:HD12	3:N:1171:VAL:HG13	1.64	0.78
2:C:882:LEU:HD23	3:D:951:ILE:HG12	1.65	0.78
3:D:65:ARG:HG3	3:D:66:GLN:H	1.49	0.78
2:M:610:ARG:HB2	9:M:2445:HOH:O	1.83	0.78
3:D:871:LYS:HE3	3:D:873:LEU:HD21	1.64	0.78
3:N:52:PRO:HG3	3:N:78:VAL:HG22	1.64	0.78
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.65	0.78
1:L:45:LEU:HD21	1:L:177:VAL:HG22	1.65	0.78
2:M:83:CYS:HA	2:M:88:LEU:HB3	1.66	0.78
3:N:1040:GLY:O	3:N:1060:SER:HB3	1.82	0.77
3:N:1124:GLN:HE21	3:N:1133:ARG:HD3	1.48	0.77
3:D:756:GLN:HE21	3:D:760:ARG:HD2	1.47	0.77
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.67	0.77
1:L:103:ALA:HB1	1:L:107:LYS:HE3	1.66	0.77
3:D:1311:LEU:HA	9:D:9899:HOH:O	1.85	0.77
3:N:644:LEU:HD12	3:N:645:PRO:HD2	1.67	0.77
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.66	0.77
3:D:478:LEU:HD22	3:D:1388:ARG:CZ	2.15	0.77
3:D:73:CYS:HB3	3:D:76:CYS:O	1.84	0.77
2:C:292:ARG:HH11	2:C:299:LYS:HD3	1.49	0.77
3:N:86:ARG:O	3:N:522:PRO:HD2	1.85	0.77
3:N:58:CYS:HA	3:N:78:VAL:HG11	1.66	0.77
3:D:1147:ARG:HB2	3:D:1166:LEU:HD21	1.64	0.77
1:L:63:HIS:HB2	9:L:6262:HOH:O	1.84	0.77
3:N:907:GLU:HB3	9:N:2356:HOH:O	1.83	0.77
5:P:409:LYS:HB2	9:P:3891:HOH:O	1.85	0.77
3:D:1166:LEU:HD12	3:D:1171:VAL:HG22	1.67	0.77
3:D:41:ARG:HD3	3:D:42:ASP:H	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1406:ARG:HG3	3:N:1412:LYS:HG3	1.65	0.77
3:D:1194:CYS:HB2	9:D:9616:HOH:O	1.85	0.77
5:P:142:ARG:NH1	5:P:142:ARG:HB3	1.99	0.77
2:C:873:PRO:HG2	3:D:947:ILE:HD12	1.67	0.76
3:D:1262:LEU:HD21	3:D:1351:GLU:HG3	1.66	0.76
2:M:438:ILE:HD11	2:M:467:ILE:HD12	1.65	0.76
3:N:898:GLU:HB2	3:N:921:ARG:NH2	2.01	0.76
2:C:157:ARG:HD2	2:C:314:THR:HG22	1.68	0.76
2:C:41:ASN:H	2:C:41:ASN:ND2	1.77	0.76
3:D:116:LEU:HD23	3:D:468:LEU:HD11	1.68	0.76
5:F:117:SER:HA	9:F:9677:HOH:O	1.85	0.76
2:M:274:ARG:HD2	2:M:285:LEU:HB3	1.65	0.76
2:M:904:PRO:HD2	2:M:908:GLY:HA2	1.67	0.76
1:A:27:PRO:HG2	1:A:186:LEU:HD22	1.66	0.76
1:B:99:LEU:HD21	1:B:122:ILE:HD11	1.67	0.76
3:D:127:LEU:HD11	3:D:461:ILE:HD11	1.65	0.76
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.66	0.76
2:M:614:ARG:HG3	2:M:620:LEU:HD12	1.66	0.76
3:N:124:GLU:HB2	9:N:9606:HOH:O	1.83	0.76
3:N:105:VAL:HG21	3:N:128:TYR:HE2	1.49	0.76
3:D:1462:LEU:HD22	3:D:1473:PRO:HD2	1.67	0.76
3:D:633:VAL:HG22	3:D:635:PRO:HD3	1.66	0.76
3:D:1209:LEU:HD21	4:E:16:LYS:NZ	2.01	0.76
5:P:358:LEU:HD21	5:P:370:LYS:HZ2	1.49	0.76
2:M:511:GLU:O	2:M:526:PRO:HD3	1.86	0.76
3:N:1481:VAL:HG11	4:O:18:ARG:HA	1.68	0.76
3:D:148:GLU:HB3	3:D:151:GLN:HE21	1.50	0.76
3:D:1466:VAL:HG23	3:D:1472:ILE:HD11	1.68	0.76
2:M:100:LEU:HD21	2:M:368:THR:HA	1.68	0.76
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.68	0.76
3:N:1438:ALA:O	3:N:1443:THR:HG22	1.84	0.76
3:D:1273:VAL:HG22	3:D:1326:THR:OG1	1.84	0.75
3:D:1438:ALA:O	3:D:1443:THR:HG22	1.86	0.75
2:M:603:VAL:HG21	2:M:643:VAL:HG11	1.66	0.75
2:C:1090:LYS:HE2	2:C:1112:PHE:HE1	1.51	0.75
4:E:84:ARG:HG3	9:E:9600:HOH:O	1.86	0.75
3:N:141:ILE:HD13	3:N:450:TYR:HB2	1.67	0.75
3:D:793:THR:HG22	3:D:879:ARG:HA	1.68	0.75
1:B:176:ARG:HH22	3:D:884:ARG:HD3	1.52	0.75
2:C:83:CYS:HA	2:C:88:LEU:HB3	1.68	0.75
3:N:1120:VAL:HG23	3:N:1186:VAL:HB	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:260:ILE:HG23	5:P:264:MET:HB2	1.68	0.75
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.68	0.75
2:C:943:VAL:HG23	2:C:985:GLY:H	1.50	0.75
3:N:133:ILE:HG21	3:N:454:ALA:HB1	1.68	0.75
3:D:543:LEU:HA	3:D:546:ARG:HG3	1.67	0.75
3:N:907:GLU:HB2	9:N:2764:HOH:O	1.86	0.75
3:D:186:VAL:HG21	3:D:213:VAL:HB	1.69	0.75
5:F:112:ALA:HA	5:F:173:TYR:HD2	1.50	0.75
2:M:134:ARG:HH21	2:M:393:GLN:HA	1.50	0.75
3:N:899:LEU:HD12	3:N:900:ILE:HG23	1.69	0.75
2:C:603:VAL:HG21	2:C:643:VAL:HG11	1.68	0.75
3:D:119:SER:HB2	3:D:123:LEU:H	1.50	0.75
3:D:890:VAL:HG13	3:D:926:LYS:NZ	2.01	0.75
3:N:1281:VAL:HG21	3:N:1313:VAL:HG21	1.69	0.75
2:C:329:GLY:N	2:C:488:ALA:HB3	2.01	0.74
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.70	0.74
3:D:704:ARG:HD3	3:D:738:ALA:HB2	1.67	0.74
4:E:30:LEU:O	4:E:35:PHE:HA	1.88	0.74
5:F:310:ILE:HB	9:F:9734:HOH:O	1.87	0.74
5:F:396:ARG:HG2	9:F:9581:HOH:O	1.86	0.74
2:M:675:ALA:HA	2:M:989:VAL:HG12	1.69	0.74
3:N:1418:LYS:HG2	9:N:9876:HOH:O	1.86	0.74
3:D:493:ARG:HE	3:D:1388:ARG:HB3	1.51	0.74
2:M:1018:GLN:NE2	2:M:1063:ARG:HH22	1.86	0.74
3:N:1412:LYS:O	3:N:1414:PRO:HD3	1.87	0.74
5:P:164:LYS:HA	5:P:171:LYS:HE2	1.67	0.74
2:C:129:ILE:HD13	2:C:134:ARG:HB2	1.69	0.74
2:C:672:VAL:HG23	2:C:868:ASP:HB2	1.68	0.74
3:D:1213:ARG:H	3:D:1213:ARG:HE	1.32	0.74
3:D:1455:LYS:HD3	3:D:1456:LYS:N	2.02	0.74
1:L:161:ARG:HB2	9:L:6438:HOH:O	1.86	0.74
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.52	0.74
3:N:1036:ARG:HH21	3:N:1042:ARG:HA	1.52	0.74
2:C:110:GLU:H	2:C:368:THR:HG21	1.52	0.74
3:D:834:THR:HG22	3:D:838:ARG:HD2	1.70	0.74
2:M:691:SER:HB2	2:M:858:MET:SD	2.27	0.74
2:M:554:ASP:HB2	2:M:880:MET:HB2	1.68	0.74
3:N:1166:LEU:HD23	3:N:1166:LEU:H	1.51	0.74
3:N:194:GLY:H	3:N:206:ARG:HA	1.52	0.74
2:C:1091:GLU:HG2	3:D:606:ILE:HG21	1.68	0.74
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.50	0.74
1:L:156:HIS:CE1	1:L:166:PRO:HB3	2.22	0.74
5:P:131:VAL:HG13	5:P:178:ARG:HG2	1.70	0.74
2:C:930:LYS:HA	9:C:9664:HOH:O	1.87	0.74
3:N:679:ARG:HH12	3:N:681:ARG:HD2	1.52	0.74
3:N:907:GLU:HA	9:N:9764:HOH:O	1.87	0.74
5:P:133:ALA:HB2	5:P:142:ARG:NH2	2.03	0.74
3:N:1312:LEU:HB2	9:N:2666:HOH:O	1.85	0.74
3:N:192:ALA:O	3:N:195:VAL:HG23	1.88	0.74
2:C:54:ILE:HD11	2:C:356:ARG:HG2	1.69	0.73
5:F:260:ILE:HG23	5:F:264:MET:HB2	1.70	0.73
2:M:396:ASP:HA	2:M:633:GLN:HE22	1.53	0.73
1:K:42:ARG:HH12	2:M:857:ASP:HB3	1.51	0.73
5:P:266:GLU:HA	5:P:269:ASN:HD22	1.53	0.73
2:M:194:VAL:HA	2:M:197:LEU:HD12	1.68	0.73
5:P:142:ARG:HH11	5:P:142:ARG:HB3	1.54	0.73
2:C:493:ARG:HB3	9:C:9820:HOH:O	1.87	0.73
3:D:996:TRP:HA	3:D:999:THR:HG22	1.68	0.73
1:K:133:GLU:HG2	1:K:134:GLU:N	2.03	0.73
2:C:197:LEU:HA	2:C:200:LEU:HD12	1.71	0.73
3:D:1047:LYS:HE3	3:D:1051:GLU:HB2	1.71	0.73
3:N:984:THR:HG22	3:N:987:GLU:HG3	1.70	0.73
1:A:95:GLN:HA	1:A:146:ARG:NH1	2.03	0.73
2:C:670:GLN:O	2:C:672:VAL:HG12	1.88	0.73
3:D:152:LEU:HD23	3:D:152:LEU:H	1.50	0.73
3:D:838:ARG:HA	9:D:9946:HOH:O	1.89	0.73
5:F:125:ASP:HA	5:F:128:ARG:HH12	1.54	0.73
1:K:226:SER:O	1:K:228:PRO:HD3	1.88	0.73
2:M:95:TYR:CD2	2:M:114:PHE:HB3	2.23	0.73
3:N:422:ALA:HB1	5:P:178:ARG:HH12	1.54	0.73
1:B:101:LEU:HB3	9:B:9759:HOH:O	1.88	0.73
3:N:877:PRO:O	3:N:880:ILE:HG22	1.88	0.73
1:B:41:ARG:HG3	1:B:177:VAL:HG21	1.71	0.73
3:D:1144:LEU:HB3	3:D:1166:LEU:HD11	1.71	0.73
3:D:98:PRO:HB3	9:D:9932:HOH:O	1.89	0.73
5:F:108:GLU:HG3	5:F:176:ILE:HG21	1.71	0.73
1:L:175:ARG:O	3:N:851:LEU:HD21	1.88	0.73
3:N:984:THR:HG22	3:N:987:GLU:H	1.54	0.73
1:K:67:THR:H	2:M:627:ARG:NH2	1.86	0.73
2:M:139:GLN:HE21	2:M:334:ARG:HH11	1.35	0.73
2:M:773:LEU:O	2:M:777:ILE:HG13	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1033:GLN:NE2	3:N:1036:ARG:HH11	1.86	0.73
3:N:1379:VAL:HA	3:N:1420:LEU:HB3	1.70	0.73
5:P:85:LEU:HD13	5:P:193:ARG:HH11	1.54	0.73
3:D:1076:GLY:O	3:D:1079:LYS:HG3	1.89	0.72
3:D:1381:VAL:HB	3:D:1389:LEU:O	1.88	0.72
2:C:876:VAL:HG11	3:D:949:ILE:HG21	1.71	0.72
1:L:15:THR:HG21	9:L:6217:HOH:O	1.89	0.72
2:M:683:ASN:HA	2:M:687:ALA:HB3	1.71	0.72
9:M:9588:HOH:O	3:N:1071:PHE:HZ	1.72	0.72
3:N:607:LEU:HA	3:N:613:ARG:HB2	1.69	0.72
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.71	0.72
3:D:6:ARG:HG3	3:D:7:LYS:HG3	1.69	0.72
1:K:87:VAL:HG21	1:K:144:VAL:HG11	1.70	0.72
2:M:626:ARG:NH1	2:M:637:LEU:HD12	2.04	0.72
2:M:650:ARG:H	2:M:650:ARG:HD2	1.52	0.72
1:A:54:THR:HG22	1:A:158:ILE:HG13	1.71	0.72
3:D:906:GLN:HB3	3:D:911:LEU:CD1	2.20	0.72
2:M:141:HIS:HB3	2:M:418:LEU:HD23	1.69	0.72
2:M:436:GLY:HA2	2:M:538:GLN:O	1.89	0.72
2:M:768:THR:HB	2:M:771:GLU:HB3	1.70	0.72
3:N:1103:HIS:CD2	3:N:1463:LYS:H	2.07	0.72
1:L:58:ILE:HB	1:L:61:VAL:HB	1.72	0.72
2:M:329:GLY:HA3	2:M:489:THR:HG23	1.69	0.72
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.70	0.72
2:M:952:LEU:HD12	2:M:969:GLN:NE2	2.00	0.72
3:N:1156:LEU:HB3	9:N:2055:HOH:O	1.89	0.72
3:N:666:ILE:H	3:N:666:ILE:HD12	1.51	0.72
2:C:260:LEU:HB2	2:C:291:ALA:HB1	1.71	0.72
2:C:580:MET:HB3	2:C:584:GLU:CD	2.10	0.72
2:M:92:ALA:HB1	9:M:9636:HOH:O	1.89	0.72
3:N:570:GLU:HB2	5:P:214:GLN:HE21	1.55	0.72
3:N:906:GLN:HB3	3:N:911:LEU:HD11	1.70	0.72
1:K:9:PRO:HB2	1:L:224:TYR:HB3	1.71	0.72
2:M:938:LYS:HB3	2:M:939:ARG:HH21	1.53	0.72
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.71	0.72
3:D:135:LEU:HD13	3:D:147:VAL:HG23	1.70	0.72
1:A:97:VAL:HG23	9:A:9564:HOH:O	1.89	0.72
2:C:521:PRO:HB2	3:D:1055:VAL:HB	1.72	0.72
3:D:1191:PRO:HA	9:D:9616:HOH:O	1.90	0.72
3:D:1350:GLU:HG3	9:D:2523:HOH:O	1.90	0.72
3:D:961:LYS:HE2	3:D:962:GLN:HE22	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:129:ILE:HD13	2:M:134:ARG:HB2	1.71	0.72
2:M:721:ARG:HH21	2:M:783:ARG:HH21	1.37	0.72
2:M:1096:ALA:O	3:N:13:ALA:HB2	1.90	0.72
9:M:9642:HOH:O	3:N:651:GLU:HG3	1.90	0.72
1:B:199:ILE:HD11	1:B:211:LEU:HD13	1.71	0.72
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.71	0.72
2:C:478:VAL:HA	2:C:506:ASN:O	1.90	0.72
5:P:248:ASN:HA	5:P:251:ILE:HD12	1.71	0.72
3:N:951:ILE:HG23	3:N:1062:ARG:HE	1.55	0.71
2:C:137:VAL:HG23	2:C:391:LEU:HG	1.71	0.71
2:C:193:LEU:HB2	9:C:9631:HOH:O	1.90	0.71
2:C:36:PRO:HG2	2:C:70:GLU:HB3	1.69	0.71
2:C:96:ALA:HB2	9:C:9657:HOH:O	1.90	0.71
3:D:194:GLY:H	3:D:206:ARG:HA	1.53	0.71
3:N:187:LYS:HE2	3:N:213:VAL:HG12	1.72	0.71
2:C:145:GLY:H	2:C:163:ILE:HG23	1.56	0.71
2:C:274:ARG:HD2	2:C:285:LEU:HB3	1.72	0.71
2:M:16:PRO:HB3	2:M:460:ARG:HH22	1.55	0.71
3:N:1342:GLU:CD	3:N:1342:GLU:H	1.94	0.71
3:N:770:LEU:HD23	9:N:9909:HOH:O	1.90	0.71
5:P:97:GLU:HA	9:P:5302:HOH:O	1.89	0.71
2:C:557:ARG:CZ	2:C:879:ARG:HD3	2.20	0.71
3:D:1217:ILE:HD13	3:D:1480:PHE:HE2	1.55	0.71
3:D:1468:LEU:HD22	3:D:1470:ARG:HB2	1.73	0.71
3:D:420:VAL:HG23	9:D:2502:HOH:O	1.90	0.71
2:M:583:LEU:O	2:M:587:VAL:HG23	1.89	0.71
2:M:724:ARG:HG3	2:M:741:GLY:H	1.56	0.71
3:N:100:ALA:HA	9:N:9662:HOH:O	1.90	0.71
3:N:850:LEU:H	3:N:850:LEU:HD12	1.55	0.71
5:P:151:LEU:HD13	5:P:154:LYS:HB3	1.73	0.71
5:P:132:ARG:HE	5:P:184:ARG:HH12	1.38	0.71
3:D:1341:PRO:HA	3:D:1344:VAL:HG23	1.72	0.71
5:F:120:THR:HB	9:F:9677:HOH:O	1.90	0.71
2:M:244:PRO:HD2	2:M:245:GLY:H	1.56	0.71
1:A:11:PHE:HB2	9:A:9807:HOH:O	1.90	0.71
2:C:39:ARG:HE	2:C:39:ARG:HA	1.55	0.71
2:C:1085:PHE:HD2	3:D:1468:LEU:HA	1.55	0.71
1:K:156:HIS:HD2	1:K:157:GLY:H	1.39	0.71
2:M:676:ILE:HG22	2:M:988:VAL:HG13	1.73	0.71
2:C:626:ARG:H	2:C:639:GLN:NE2	1.88	0.71
3:D:1349:VAL:HG11	9:D:9931:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASN:HA	9:A:9646:HOH:O	1.90	0.71
3:N:207:PHE:HB3	3:N:208:PRO:HD2	1.71	0.71
2:C:313:LEU:HA	2:C:321:GLU:HG3	1.72	0.71
3:D:187:LYS:HE2	3:D:213:VAL:HG12	1.72	0.71
2:C:101:ILE:HG23	2:C:107:LEU:HD22	1.71	0.70
4:E:26:ARG:HH12	4:E:30:LEU:HD13	1.55	0.70
2:M:650:ARG:HB3	9:M:2078:HOH:O	1.91	0.70
3:N:120:ALA:HB1	9:N:9675:HOH:O	1.91	0.70
3:N:808:THR:HB	3:N:809:PRO:HD3	1.73	0.70
2:C:108:ILE:HB	2:C:368:THR:OG1	1.90	0.70
3:D:564:GLU:HA	3:D:567:ILE:HD12	1.73	0.70
3:D:667:ALA:HB2	3:D:676:MET:HE2	1.73	0.70
3:D:820:GLU:HB2	3:D:836:VAL:HG11	1.73	0.70
5:F:205:ARG:HD2	5:F:251:ILE:HG21	1.72	0.70
5:F:371:LEU:HD22	5:F:375:LEU:HD22	1.72	0.70
1:K:2:LEU:HD21	9:K:5231:HOH:O	1.90	0.70
3:N:117:ASP:HB2	3:N:495:ARG:NH2	2.05	0.70
5:P:395:GLU:O	5:P:399:GLN:HB2	1.91	0.70
2:C:505:GLY:HA3	9:C:9723:HOH:O	1.89	0.70
2:C:671:ASN:H	2:C:671:ASN:HD22	1.37	0.70
2:C:732:ALA:HA	2:C:735:ARG:CZ	2.21	0.70
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.73	0.70
2:M:232:GLU:HA	2:M:235:LEU:HD12	1.73	0.70
2:M:348:LEU:HD22	9:M:2250:HOH:O	1.90	0.70
3:N:1292:VAL:HG12	9:N:9607:HOH:O	1.89	0.70
3:N:209:ARG:HH22	3:N:397:LYS:HG3	1.55	0.70
2:C:244:PRO:HD2	2:C:245:GLY:H	1.55	0.70
2:C:701:THR:HG22	2:C:832:LYS:HA	1.72	0.70
3:D:150:ARG:HH11	3:D:150:ARG:HG3	1.56	0.70
3:D:177:ALA:HB1	3:D:199:LEU:HD22	1.74	0.70
3:D:445:ARG:HB2	3:D:445:ARG:HH11	1.56	0.70
3:N:116:LEU:HD11	3:N:465:LEU:HG	1.73	0.70
3:N:483:HIS:HB2	3:N:484:PRO:HD3	1.74	0.70
9:M:9956:HOH:O	3:N:724:GLN:HB3	1.90	0.70
2:C:676:ILE:HG23	3:D:948:THR:HB	1.72	0.70
3:D:1412:LYS:HG2	3:D:1414:PRO:HG3	1.72	0.70
1:L:59:GLU:HG3	1:L:139:ASN:ND2	2.06	0.70
2:M:648:ARG:H	2:M:648:ARG:HE	1.40	0.70
3:N:699:VAL:HG12	3:N:717:GLN:HA	1.72	0.70
2:C:683:ASN:HA	2:C:687:ALA:HB3	1.73	0.70
3:D:1262:LEU:HD23	3:D:1352:ILE:HG13	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1342:GLU:H	3:D:1342:GLU:CD	1.94	0.70
3:D:427:VAL:CG2	3:D:435:VAL:HB	2.22	0.70
3:D:478:LEU:HD21	3:D:500:ARG:NH2	2.05	0.70
2:M:139:GLN:HE22	2:M:415:PRO:HG2	1.57	0.70
1:A:127:LEU:HD12	1:A:128:HIS:N	2.06	0.70
2:C:861:LEU:HG	2:C:862:PRO:HD2	1.73	0.70
4:E:29:GLN:HB2	4:E:33:HIS:NE2	2.06	0.70
5:F:244:ARG:HG2	9:F:9669:HOH:O	1.92	0.70
2:M:905:ILE:HD12	2:M:905:ILE:H	1.57	0.70
2:M:1056:LYS:O	3:N:624:ASP:HB2	1.91	0.70
1:A:177:VAL:O	2:C:864:GLY:HA3	1.91	0.70
3:D:1277:ILE:HD12	3:D:1301:LYS:HB2	1.72	0.70
4:E:47:LYS:HA	9:E:9537:HOH:O	1.91	0.70
1:A:14:ARG:HH22	1:A:24:VAL:HG23	1.56	0.70
3:D:215:TYR:O	3:D:389:GLU:HB2	1.92	0.70
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.72	0.70
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.72	0.70
2:M:1098:ASP:HB2	3:N:21:TRP:HZ2	1.57	0.70
2:C:1111:ILE:HG13	2:C:1112:PHE:H	1.57	0.70
1:L:160:ASP:HB2	9:L:6438:HOH:O	1.92	0.70
1:L:78:ILE:HA	9:L:3720:HOH:O	1.90	0.70
2:M:1109:VAL:HG11	3:N:5:VAL:HG13	1.74	0.70
2:M:786:LYS:HA	9:M:9574:HOH:O	1.91	0.70
5:P:291:ILE:HG23	5:P:304:VAL:HG21	1.72	0.70
5:P:375:LEU:HB2	9:P:4033:HOH:O	1.91	0.70
2:C:66:LEU:HD13	2:C:372:LEU:HD23	1.73	0.69
3:D:637:LEU:HD21	3:D:642:CYS:HA	1.74	0.69
1:K:101:LEU:HD22	1:K:102:LYS:N	2.07	0.69
2:M:721:ARG:HH22	2:M:785:VAL:HG21	1.57	0.69
2:M:987:ILE:HG12	3:N:948:THR:HG21	1.74	0.69
3:N:1045:MET:CG	3:N:1073:SER:HA	2.19	0.69
3:D:445:ARG:HB2	3:D:445:ARG:NH1	2.07	0.69
2:M:1007:ALA:HB2	3:N:648:MET:HG3	1.73	0.69
2:M:256:TYR:CE1	2:M:293:PHE:HB2	2.27	0.69
2:M:27:ARG:HA	9:M:9713:HOH:O	1.92	0.69
3:N:507:ASN:HB2	9:N:9681:HOH:O	1.90	0.69
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.74	0.69
3:D:422:ALA:HB3	3:D:427:VAL:CG2	2.20	0.69
3:D:436:GLU:HB2	3:D:445:ARG:HB3	1.74	0.69
3:N:55:ASP:HA	3:N:82:LYS:HG3	1.74	0.69
3:N:761:ILE:HG21	9:O:3658:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:163:LEU:HD13	5:P:174:LEU:HD21	1.74	0.69
1:B:164:ALA:HA	9:B:9786:HOH:O	1.92	0.69
2:C:504:GLU:OE2	2:C:509:ALA:HB2	1.91	0.69
3:D:1412:LYS:O	3:D:1414:PRO:HD3	1.93	0.69
3:D:397:LYS:NZ	3:D:399:ARG:HH21	1.91	0.69
3:D:161:LEU:HD23	3:D:449:SER:HB3	1.73	0.69
1:K:34:VAL:HB	1:L:42:ARG:NH2	2.08	0.69
3:N:1115:THR:HG21	3:N:1151:ARG:HH21	1.57	0.69
3:N:1290:LEU:HD23	3:N:1291:SER:H	1.55	0.69
2:C:405:ARG:HD2	2:C:442:GLU:OE1	1.93	0.69
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.74	0.69
3:D:1491:THR:O	3:D:1495:ILE:HD13	1.93	0.69
3:D:544:TYR:O	3:D:548:ILE:HG12	1.92	0.69
3:D:804:LEU:HB2	3:D:830:ALA:O	1.92	0.69
5:F:93:LEU:HG	5:F:190:ALA:CB	2.23	0.69
2:M:244:PRO:HD3	9:M:2128:HOH:O	1.93	0.69
2:M:432:ARG:HG2	9:N:9826:HOH:O	1.92	0.69
3:N:1277:ILE:HD12	3:N:1301:LYS:HB2	1.72	0.69
3:D:477:LEU:HD22	3:D:492:ALA:HB1	1.73	0.69
3:D:639:LEU:N	3:D:639:LEU:HD12	2.07	0.69
1:K:222:LEU:HD11	1:L:218:LEU:HD23	1.74	0.69
1:L:54:THR:HB	9:L:6404:HOH:O	1.92	0.69
2:M:479:VAL:HG21	2:M:503:LEU:HD11	1.74	0.69
3:N:699:VAL:H	3:N:756:GLN:HE22	1.41	0.69
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.75	0.69
3:D:519:VAL:HA	3:D:544:TYR:OH	1.93	0.69
1:L:54:THR:HA	9:L:4010:HOH:O	1.93	0.69
2:M:405:ARG:HH21	2:M:566:THR:HG21	1.57	0.69
1:A:135:GLY:HA2	9:A:9673:HOH:O	1.92	0.69
3:D:1307:LYS:HD3	3:D:1307:LYS:H	1.55	0.69
3:D:1404:ASN:ND2	3:D:1408:ILE:HD12	2.07	0.69
3:D:153:LEU:HD12	3:D:154:THR:N	2.07	0.69
3:D:192:ALA:O	3:D:195:VAL:HG23	1.93	0.69
3:D:586:ARG:HD3	9:D:9830:HOH:O	1.92	0.69
2:M:672:VAL:HG23	2:M:868:ASP:HB2	1.75	0.69
3:N:1135:ARG:HH22	3:N:1350:GLU:HG2	1.57	0.69
1:A:14:ARG:NH2	1:A:24:VAL:HG23	2.08	0.69
5:F:144:ILE:HB	5:F:145:PRO:HD3	1.75	0.69
2:M:455:LEU:HD12	2:M:459:ALA:HB3	1.73	0.69
1:A:156:HIS:HD2	1:A:157:GLY:H	1.39	0.69
2:C:113:VAL:HG11	2:C:373:VAL:HB	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:671:ASN:ND2	2:C:671:ASN:H	1.91	0.69
2:C:724:ARG:HD2	2:C:740:GLU:HA	1.75	0.69
3:D:1209:LEU:HD21	4:E:16:LYS:HZ2	1.56	0.69
2:M:1090:LYS:HE3	3:N:88:TYR:O	1.93	0.69
2:M:630:ARG:HD3	2:M:705:ILE:HD12	1.75	0.69
3:N:138:LYS:HA	9:N:2186:HOH:O	1.92	0.69
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.58	0.69
2:C:1008:ARG:HD3	9:D:9977:HOH:O	1.93	0.69
3:D:1087:ARG:HG2	3:D:1234:THR:HA	1.74	0.69
3:D:131:LYS:HG3	3:D:568:ARG:HG2	1.75	0.69
1:K:27:PRO:HG2	1:K:186:LEU:HD22	1.73	0.69
2:M:186:VAL:HG23	2:M:187:ASN:H	1.57	0.69
3:N:559:ALA:HA	9:P:5830:HOH:O	1.92	0.69
3:D:208:PRO:HB2	3:D:395:VAL:HG22	1.74	0.68
1:K:34:VAL:HB	1:L:42:ARG:HH21	1.58	0.68
1:L:97:VAL:HG11	1:L:120:VAL:HG21	1.73	0.68
2:M:478:VAL:HG13	2:M:506:ASN:HB3	1.75	0.68
3:N:1465:ASN:HB3	9:N:9577:HOH:O	1.92	0.68
9:M:9737:HOH:O	5:P:331:ASP:HA	1.93	0.68
5:P:85:LEU:HA	5:P:88:ILE:HD12	1.75	0.68
3:D:1194:CYS:HB3	3:D:1373:ARG:NH2	2.08	0.68
3:D:28:LYS:HB2	3:D:41:ARG:HD2	1.73	0.68
3:D:562:ALA:HB1	3:D:567:ILE:HD11	1.74	0.68
1:L:116:PRO:HB3	9:L:6809:HOH:O	1.91	0.68
2:M:1013:TYR:HE1	2:M:1020:PRO:HG3	1.58	0.68
2:M:263:ASP:HB2	2:M:264:PRO:HD3	1.75	0.68
2:M:313:LEU:HD23	2:M:314:THR:HG23	1.74	0.68
3:N:1115:THR:CG2	3:N:1151:ARG:HH21	2.06	0.68
2:M:772:ARG:HD2	5:P:373:LYS:HD2	1.75	0.68
2:C:1055:LEU:HD21	2:C:1079:PRO:HG3	1.73	0.68
2:C:755:LEU:HD21	2:C:792:VAL:HG22	1.76	0.68
3:D:663:GLU:HA	9:D:2859:HOH:O	1.92	0.68
3:D:880:ILE:HG12	9:D:9915:HOH:O	1.93	0.68
2:M:769:PRO:HG2	9:P:5537:HOH:O	1.94	0.68
3:N:1112:CYS:HB2	3:N:1195:GLN:NE2	2.08	0.68
2:C:1115:LEU:HD23	3:D:85:VAL:HG13	1.76	0.68
2:C:207:LEU:HD23	2:C:211:LEU:HD22	1.76	0.68
3:D:1462:LEU:HG	9:D:9709:HOH:O	1.94	0.68
2:M:948:GLU:HG2	2:M:953:VAL:HG23	1.75	0.68
2:C:151:ASP:HB2	2:C:157:ARG:O	1.94	0.68
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1350:GLU:O	3:D:1354:LYS:HG2	1.94	0.68
2:M:1049:LEU:HG	2:M:1053:LEU:HD11	1.76	0.68
2:M:759:THR:HB	2:M:785:VAL:HG21	1.75	0.68
3:N:1209:LEU:HD23	3:N:1210:SER:N	2.09	0.68
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.09	0.68
3:D:704:ARG:NH1	3:D:738:ALA:HA	2.08	0.68
3:D:796:ARG:NH1	3:D:861:GLN:HB2	2.03	0.68
5:F:163:LEU:HB3	5:F:174:LEU:HG	1.74	0.68
5:F:85:LEU:HA	5:F:88:ILE:HD12	1.75	0.68
3:N:1381:VAL:HB	3:N:1389:LEU:O	1.92	0.68
3:N:779:ALA:HB2	9:N:9921:HOH:O	1.93	0.68
5:P:304:VAL:HG23	9:P:4374:HOH:O	1.92	0.68
3:D:662:GLU:HB2	9:D:9835:HOH:O	1.93	0.68
2:M:1025:ALA:HA	9:M:2101:HOH:O	1.92	0.68
2:M:722:ILE:HG21	2:M:821:GLU:OE2	1.94	0.68
3:N:402:PRO:HG2	3:N:444:VAL:HG11	1.75	0.68
3:N:441:ARG:HA	9:N:2108:HOH:O	1.94	0.68
1:B:73:GLU:HB3	1:B:77:GLU:CG	2.23	0.68
2:C:139:GLN:HB3	2:C:334:ARG:HD2	1.76	0.68
2:C:42:VAL:HG12	2:C:43:GLY:H	1.59	0.68
2:C:673:LEU:HD11	9:C:9804:HOH:O	1.92	0.68
2:C:678:PRO:O	3:D:943:THR:HA	1.93	0.68
2:C:94:LEU:HD11	9:C:9657:HOH:O	1.93	0.68
3:D:1465:ASN:HD21	3:D:1470:ARG:HH11	1.41	0.68
3:D:531:ASP:C	3:D:533:GLY:H	1.97	0.68
2:M:139:GLN:HG3	2:M:140:ILE:H	1.58	0.68
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.29	0.68
3:N:775:GLY:HA2	9:N:2387:HOH:O	1.94	0.68
5:P:247:ILE:HG22	5:P:251:ILE:HD11	1.76	0.68
2:C:200:LEU:HB2	9:C:9623:HOH:O	1.94	0.68
3:D:1407:LEU:HD22	9:D:9895:HOH:O	1.94	0.68
3:D:493:ARG:HG2	3:D:493:ARG:HH11	1.58	0.68
2:M:319:GLY:HA2	9:M:9629:HOH:O	1.93	0.68
2:M:478:VAL:HA	2:M:506:ASN:O	1.94	0.68
1:B:58:ILE:HD13	1:B:140:MET:HB3	1.74	0.68
2:C:1005:MET:CE	3:D:648:MET:HB2	2.24	0.68
2:C:696:LYS:HB2	9:C:9985:HOH:O	1.93	0.68
5:F:191:ASN:HA	5:F:194:LEU:HD23	1.75	0.68
3:N:119:SER:CB	3:N:123:LEU:HB2	2.24	0.68
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.75	0.67
2:C:1066:ALA:O	2:C:1070:ILE:HG13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:LEU:HD12	2:C:288:ARG:HD2	1.77	0.67
2:C:461:VAL:HG13	2:C:465:GLY:HA2	1.75	0.67
2:C:54:ILE:HB	9:C:9559:HOH:O	1.93	0.67
3:D:30:GLU:HB3	3:D:40:GLU:HB3	1.76	0.67
2:M:516:ARG:NE	3:N:1068:LEU:HD13	2.08	0.67
2:M:68:PHE:HE1	2:M:96:ALA:HB1	1.57	0.67
2:M:775:ARG:HD2	9:M:9624:HOH:O	1.93	0.67
2:C:114:PHE:HD1	2:C:114:PHE:H	1.40	0.67
3:D:1221:VAL:HB	9:D:9733:HOH:O	1.94	0.67
3:D:6:ARG:HH11	3:D:6:ARG:HB2	1.58	0.67
5:F:198:ILE:HD13	9:F:9669:HOH:O	1.94	0.67
2:M:690:ILE:HG23	2:M:852:ILE:HA	1.75	0.67
2:M:724:ARG:HH21	2:M:734:LEU:HB3	1.58	0.67
3:N:101:HIS:ND1	3:N:103:TRP:HB2	2.08	0.67
3:N:1095:THR:O	3:N:1099:VAL:HG23	1.95	0.67
2:C:393:GLN:HB2	2:C:406:HIS:CE1	2.29	0.67
3:D:153:LEU:CD1	3:D:157:GLU:HB2	2.24	0.67
3:D:97:THR:HG21	3:D:571:LYS:HD3	1.75	0.67
1:K:58:ILE:HB	1:K:61:VAL:HB	1.77	0.67
2:M:129:ILE:HG12	2:M:386:PHE:HB3	1.77	0.67
2:M:943:VAL:HG23	2:M:985:GLY:H	1.58	0.67
3:N:119:SER:H	3:N:123:LEU:HD13	1.60	0.67
3:N:1272:ALA:HA	3:N:1326:THR:HB	1.76	0.67
3:N:568:ARG:HB2	9:N:2150:HOH:O	1.93	0.67
4:O:30:LEU:O	4:O:35:PHE:HA	1.94	0.67
1:B:89:PHE:HB3	1:B:94:LEU:HD13	1.77	0.67
2:C:15:LEU:HD12	2:C:15:LEU:H	1.60	0.67
2:C:666:LEU:HD23	2:C:668:LEU:HD11	1.75	0.67
2:C:926:PHE:O	2:C:930:LYS:HG3	1.94	0.67
3:D:1109:GLU:HG2	3:D:1201:CYS:HA	1.76	0.67
3:D:1490:LYS:HG2	9:D:2182:HOH:O	1.93	0.67
2:C:1090:LYS:HE2	2:C:1112:PHE:CE1	2.30	0.67
2:C:597:ALA:HB2	2:C:655:LEU:HD21	1.76	0.67
2:C:89:THR:HG21	2:C:383:ARG:HH21	1.58	0.67
3:D:1130:ARG:NH1	3:D:1130:ARG:HB2	2.08	0.67
3:D:539:ASP:OD2	5:F:318:GLU:HB2	1.95	0.67
1:L:156:HIS:ND1	1:L:158:ILE:HG12	2.10	0.67
3:N:570:GLU:HB2	5:P:214:GLN:NE2	2.10	0.67
1:B:132:LEU:HG	1:B:136:GLY:HA3	1.76	0.67
2:C:479:VAL:CG2	2:C:503:LEU:HD11	2.25	0.67
2:C:80:GLN:HG2	2:C:90:TYR:CE2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:260:LEU:HG	2:M:261:ILE:HG13	1.76	0.67
3:N:502:PHE:CE1	3:N:509:PRO:HB3	2.30	0.67
3:N:658:LEU:HA	3:N:661:MET:HE3	1.76	0.67
2:M:1115:LEU:HB3	3:N:85:VAL:HG12	1.77	0.67
5:P:78:SER:HB2	5:P:82:ARG:CZ	2.25	0.67
2:C:25:SER:HB2	2:C:335:THR:HB	1.77	0.67
2:C:546:LEU:HD21	2:C:587:VAL:HG21	1.76	0.67
3:D:1112:CYS:HB2	3:D:1195:GLN:OE1	1.95	0.67
3:D:1310:ARG:NE	3:D:1327:ARG:HB3	2.09	0.67
5:F:196:VAL:HG22	5:F:213:ILE:HD13	1.76	0.67
1:K:61:VAL:HA	9:K:3779:HOH:O	1.95	0.67
1:L:121:GLU:HG3	9:L:4026:HOH:O	1.94	0.67
3:N:122:GLU:HB3	9:N:9714:HOH:O	1.94	0.67
3:N:12:LEU:HD23	3:N:13:ALA:H	1.59	0.67
1:A:161:ARG:HB2	1:A:161:ARG:NH1	2.10	0.67
2:C:1101:THR:HB	3:D:5:VAL:HG13	1.75	0.67
2:C:111:ASP:HA	9:C:9753:HOH:O	1.95	0.67
2:C:399:ASN:N	2:C:399:ASN:HD22	1.93	0.67
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.74	0.67
3:D:1462:LEU:HD22	3:D:1472:ILE:HG23	1.76	0.67
2:M:361:MET:HE2	9:M:2467:HOH:O	1.95	0.67
3:N:603:LEU:O	3:N:606:ILE:HB	1.94	0.67
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.75	0.67
1:K:89:PHE:HD1	1:K:120:VAL:HG23	1.60	0.67
2:M:36:PRO:HA	9:M:9625:HOH:O	1.94	0.67
2:M:723:THR:HG23	2:M:725:ASP:HB2	1.77	0.67
2:M:89:THR:O	2:M:91:GLN:HG3	1.95	0.67
3:N:737:ASN:HA	9:N:9578:HOH:O	1.94	0.67
5:P:144:ILE:HB	5:P:145:PRO:HD3	1.76	0.67
5:P:163:LEU:HB3	5:P:174:LEU:HG	1.77	0.67
2:C:1085:PHE:CD2	3:D:1468:LEU:HA	2.30	0.67
2:C:956:GLY:HA2	9:C:9651:HOH:O	1.95	0.67
3:D:493:ARG:NE	3:D:1388:ARG:HB3	2.10	0.67
1:L:59:GLU:HG3	1:L:139:ASN:HD22	1.60	0.67
3:N:1296:SER:HB3	9:N:9620:HOH:O	1.95	0.67
2:C:174:LEU:HA	9:C:9698:HOH:O	1.94	0.66
3:D:1143:GLY:HA2	9:D:9658:HOH:O	1.95	0.66
3:D:478:LEU:HD22	3:D:1388:ARG:NH2	2.10	0.66
3:D:213:VAL:HG21	9:D:2607:HOH:O	1.95	0.66
5:F:366:ALA:HB3	5:F:367:MET:HE2	1.77	0.66
2:M:512:ARG:HB3	2:M:523:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:396:VAL:HG21	3:N:447:VAL:HB	1.75	0.66
3:N:630:VAL:HA	3:N:744:GLN:HG2	1.75	0.66
1:A:101:LEU:HG	1:A:114:PHE:HA	1.78	0.66
1:A:59:GLU:CD	1:A:139:ASN:HD21	1.98	0.66
2:C:54:ILE:HG21	9:C:2001:HOH:O	1.96	0.66
2:C:605:LYS:HD3	2:C:610:ARG:NH1	2.11	0.66
5:F:113:ILE:HA	5:F:116:LEU:HD12	1.76	0.66
5:F:213:ILE:HG22	5:F:217:ASN:HD21	1.60	0.66
2:M:165:LEU:O	2:M:265:ARG:HB2	1.95	0.66
2:M:422:ARG:HB3	9:M:2451:HOH:O	1.95	0.66
9:L:5825:HOH:O	3:N:884:ARG:HG3	1.95	0.66
2:C:640:ARG:NH1	2:C:642:ARG:HH22	1.92	0.66
2:C:710:ILE:HB	2:C:790:LEU:HD13	1.77	0.66
4:E:60:ALA:O	4:E:63:TRP:HB2	1.96	0.66
2:M:569:VAL:HG12	2:M:996:LYS:O	1.95	0.66
2:M:669:GLY:HA3	2:M:995:MET:HA	1.77	0.66
3:N:1205:TYR:CD2	3:N:1215:VAL:HG21	2.20	0.66
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.76	0.66
5:P:366:ALA:HB3	5:P:367:MET:HE2	1.77	0.66
1:A:9:PRO:HD2	1:B:224:TYR:CZ	2.29	0.66
2:C:1067:TYR:CG	5:F:341:PRO:HB3	2.31	0.66
2:C:110:GLU:HG2	2:C:369:PRO:CB	2.21	0.66
3:D:210:ARG:CZ	3:D:398:ALA:HB3	2.25	0.66
3:D:400:VAL:HG21	3:D:441:ARG:NH1	2.11	0.66
2:M:350:ARG:HD3	2:M:353:ARG:NH2	2.10	0.66
2:M:636:ALA:HB2	2:M:703:ILE:HG22	1.75	0.66
3:N:1156:LEU:HD21	3:N:1177:ALA:HA	1.78	0.66
3:N:17:LYS:HD2	9:N:9847:HOH:O	1.94	0.66
3:N:191:LEU:HD12	3:N:211:VAL:HG21	1.77	0.66
1:A:10:VAL:HG12	1:A:12:THR:HG22	1.76	0.66
2:C:4:LYS:HB2	9:C:2452:HOH:O	1.94	0.66
2:C:405:ARG:HH12	2:C:563:ASN:ND2	1.93	0.66
2:C:717:LEU:HD21	9:C:9888:HOH:O	1.95	0.66
3:D:921:ARG:HD3	9:D:2819:HOH:O	1.95	0.66
1:K:94:LEU:HD21	1:K:119:ASP:HB3	1.78	0.66
2:M:1009:SER:HB2	3:N:651:GLU:O	1.94	0.66
2:M:18:LEU:HD23	2:M:404:LEU:HD21	1.78	0.66
2:M:736:ASP:O	2:M:744:ARG:HG2	1.95	0.66
2:M:860:HIS:NE2	2:M:975:TYR:HB2	2.11	0.66
3:N:1273:VAL:HG22	3:N:1326:THR:OG1	1.96	0.66
3:N:1481:VAL:HG13	4:O:18:ARG:HE	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:987:ILE:HG23	3:N:948:THR:HG21	1.78	0.66
5:P:269:ASN:O	5:P:273:ARG:HG3	1.96	0.66
1:A:145:ASP:HB3	9:A:9589:HOH:O	1.96	0.66
1:A:36:LEU:O	1:A:39:PRO:HD2	1.95	0.66
1:B:215:VAL:HA	9:B:9636:HOH:O	1.95	0.66
1:B:85:LEU:HD12	1:B:124:ASN:HB3	1.76	0.66
2:C:71:TYR:H	2:C:71:TYR:HD2	1.43	0.66
3:D:551:ASN:O	3:D:555:LYS:HG3	1.94	0.66
1:K:161:ARG:NH1	1:K:161:ARG:HB2	2.11	0.66
2:M:350:ARG:HD3	2:M:353:ARG:HH22	1.60	0.66
1:B:27:PRO:HG2	1:B:186:LEU:HD12	1.78	0.66
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.78	0.66
2:C:236:ILE:HG13	9:C:9661:HOH:O	1.94	0.66
2:C:355:VAL:CG2	2:C:372:LEU:HG	2.25	0.66
2:C:498:GLN:NE2	3:D:1068:LEU:HD12	2.11	0.66
3:D:1120:VAL:HB	3:D:1144:LEU:HD21	1.77	0.66
2:M:276:LYS:HD3	9:M:9595:HOH:O	1.95	0.66
2:M:890:LEU:HA	2:M:914:ILE:HD13	1.76	0.66
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.78	0.66
2:C:332:ARG:HE	2:C:464:LEU:HD11	1.60	0.66
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.77	0.66
5:F:136:LEU:HD11	9:F:9637:HOH:O	1.95	0.66
2:M:1114:GLY:N	2:M:1115:LEU:HD12	2.06	0.66
5:P:222:ARG:HH12	5:P:246:ALA:HB2	1.60	0.66
5:P:323:ASP:HB3	5:P:325:LYS:HE2	1.77	0.66
2:C:1090:LYS:HE3	3:D:88:TYR:O	1.96	0.66
5:F:369:LEU:HD23	9:F:9551:HOH:O	1.95	0.66
5:F:79:ASP:HB3	5:F:80:PRO:HD3	1.78	0.66
1:K:224:TYR:HB3	1:L:9:PRO:HB2	1.77	0.66
2:M:1025:ALA:HB3	9:M:2395:HOH:O	1.96	0.66
2:M:36:PRO:HG2	2:M:70:GLU:HB3	1.77	0.66
2:M:44:ILE:HG22	9:M:9965:HOH:O	1.96	0.66
2:M:674:VAL:HG23	2:M:869:VAL:O	1.96	0.66
3:N:1262:LEU:CD2	3:N:1351:GLU:HG3	2.25	0.66
5:P:112:ALA:HA	5:P:173:TYR:HD2	1.60	0.66
1:B:156:HIS:ND1	1:B:158:ILE:HG12	2.10	0.66
1:L:124:ASN:ND2	1:L:127:LEU:HD22	2.09	0.66
3:N:397:LYS:HE2	3:N:399:ARG:HE	1.61	0.66
1:A:8:ALA:HB1	1:B:224:TYR:CE1	2.31	0.65
2:C:92:ALA:HB1	9:C:9614:HOH:O	1.94	0.65
3:D:1243:THR:OG1	3:D:1253:THR:HB	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1252:ILE:H	3:D:1252:ILE:HD12	1.61	0.65
3:D:1279:GLY:O	3:D:1318:TYR:HA	1.97	0.65
2:M:292:ARG:HB2	2:M:299:LYS:HE2	1.78	0.65
3:N:146:PRO:HG2	9:N:9732:HOH:O	1.95	0.65
3:N:629:SER:OG	3:N:726:ILE:HG13	1.96	0.65
2:C:948:GLU:HG3	2:C:955:PRO:HG3	1.79	0.65
3:D:1354:LYS:HD3	9:D:2563:HOH:O	1.95	0.65
3:D:397:LYS:HE2	3:D:399:ARG:HE	1.61	0.65
5:F:317:LEU:O	5:F:329:TYR:HB3	1.96	0.65
2:M:22:GLN:NE2	2:M:336:VAL:HG21	2.12	0.65
2:M:810:ASP:HB3	2:M:813:VAL:HG22	1.78	0.65
3:N:427:VAL:CG2	3:N:435:VAL:HB	2.26	0.65
2:C:1015:LEU:HA	9:C:9582:HOH:O	1.97	0.65
2:C:166:PRO:HA	9:C:9900:HOH:O	1.95	0.65
3:D:172:PRO:HD2	3:D:389:GLU:O	1.96	0.65
5:F:198:ILE:HA	9:F:9906:HOH:O	1.96	0.65
5:F:401:GLU:O	5:F:405:LEU:HB2	1.97	0.65
1:K:36:LEU:O	1:K:39:PRO:HD2	1.97	0.65
1:L:62:LEU:HD12	9:L:3756:HOH:O	1.95	0.65
3:N:73:CYS:HB3	3:N:76:CYS:O	1.95	0.65
3:N:754:PHE:HZ	4:O:21:VAL:HG13	1.60	0.65
3:N:875:THR:HG21	3:N:902:LEU:HD13	1.79	0.65
1:B:178:ALA:HA	9:B:9711:HOH:O	1.97	0.65
2:C:409:ARG:HD2	9:C:9854:HOH:O	1.96	0.65
2:C:328:LEU:HD22	2:C:433:THR:HG22	1.78	0.65
2:C:480:THR:HG22	2:C:482:GLU:H	1.61	0.65
2:C:534:VAL:H	2:C:538:GLN:HE22	1.42	0.65
2:C:651:LYS:HA	9:C:9597:HOH:O	1.97	0.65
3:D:396:VAL:HG21	3:D:447:VAL:HB	1.77	0.65
3:D:810:GLU:O	3:D:813:LEU:HG	1.95	0.65
5:F:213:ILE:HG22	5:F:217:ASN:ND2	2.11	0.65
9:D:2501:HOH:O	5:F:315:VAL:HB	1.95	0.65
5:F:393:THR:HG22	5:F:394:ARG:H	1.61	0.65
5:F:92:PRO:HB2	9:F:9705:HOH:O	1.97	0.65
2:M:936:VAL:HA	9:M:2535:HOH:O	1.94	0.65
3:N:1267:ARG:HH11	3:N:1267:ARG:HB2	1.62	0.65
3:D:119:SER:OG	3:D:123:LEU:HD13	1.96	0.65
5:F:321:ILE:HB	5:F:327:SER:OG	1.97	0.65
5:F:395:GLU:O	5:F:399:GLN:HB2	1.96	0.65
2:M:410:ILE:HD11	2:M:455:LEU:HB3	1.77	0.65
3:N:681:ARG:HD3	9:N:2105:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1008:ARG:HE	2:C:1028:GLY:C	2.00	0.65
2:C:197:LEU:HD22	2:C:202:TYR:HD2	1.61	0.65
3:D:964:LEU:HD22	3:D:1058:ARG:HH11	1.60	0.65
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.78	0.65
5:F:260:ILE:HD11	5:F:310:ILE:HG22	1.76	0.65
2:M:1050:GLN:HG2	2:M:1079:PRO:HG2	1.78	0.65
2:M:397:GLU:HA	2:M:403:SER:HB2	1.79	0.65
2:M:462:ASP:HA	9:M:9945:HOH:O	1.97	0.65
3:N:795:VAL:HG11	3:N:863:VAL:HG13	1.79	0.65
3:D:141:ILE:HG21	3:D:161:LEU:HD21	1.79	0.65
2:M:150:PRO:CA	2:M:158:TYR:HB3	2.24	0.65
2:M:16:PRO:HG2	2:M:460:ARG:HH12	1.61	0.65
3:N:804:LEU:HD11	9:N:2794:HOH:O	1.97	0.65
2:C:588:VAL:HB	9:C:9652:HOH:O	1.97	0.65
2:C:65:VAL:HG11	9:C:9671:HOH:O	1.97	0.65
3:N:799:LYS:HA	9:N:2865:HOH:O	1.97	0.65
5:P:291:ILE:HG21	5:P:304:VAL:HG11	1.76	0.65
3:D:520:LEU:HD23	3:D:540:LEU:HD22	1.77	0.65
2:M:918:LEU:HD23	2:M:968:LEU:HA	1.77	0.65
3:N:1059:SER:OG	3:N:1065:LEU:HD22	1.97	0.65
3:N:1243:THR:OG1	3:N:1253:THR:HB	1.96	0.65
9:N:9710:HOH:O	5:P:222:ARG:HA	1.97	0.65
1:B:58:ILE:HB	1:B:61:VAL:HB	1.77	0.65
2:C:729:LEU:HD21	5:F:419:ARG:HH12	1.62	0.65
3:D:1166:LEU:HD23	3:D:1166:LEU:H	1.62	0.65
5:F:405:LEU:HD21	9:F:9615:HOH:O	1.97	0.65
2:M:182:VAL:HG12	2:M:193:LEU:HD13	1.79	0.65
2:M:605:LYS:CB	2:M:610:ARG:HH12	2.10	0.65
3:N:434:ARG:HB2	3:N:447:VAL:HG13	1.78	0.65
5:P:303:ARG:HB3	9:P:4374:HOH:O	1.96	0.65
1:A:198:ARG:HG3	9:A:9618:HOH:O	1.96	0.64
1:B:94:LEU:HD21	1:B:119:ASP:HB2	1.80	0.64
2:C:612:VAL:HG22	2:C:622:GLU:HA	1.77	0.64
3:D:528:VAL:O	3:D:535:PHE:HA	1.97	0.64
5:F:274:THR:HA	9:F:9616:HOH:O	1.98	0.64
1:L:205:VAL:HG11	9:L:3729:HOH:O	1.96	0.64
1:L:95:GLN:HA	1:L:146:ARG:HD2	1.78	0.64
2:M:578:VAL:HG11	2:M:991:GLN:HB3	1.79	0.64
4:O:41:GLU:O	4:O:45:ARG:HG2	1.97	0.64
4:O:60:ALA:O	4:O:63:TRP:HB2	1.97	0.64
2:C:276:LYS:HB3	9:C:2071:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:664:GLY:HA2	9:C:9904:HOH:O	1.97	0.64
5:F:273:ARG:HA	5:F:276:ARG:HD2	1.79	0.64
1:L:95:GLN:H	1:L:95:GLN:HE21	1.44	0.64
2:M:437:ARG:CZ	2:M:488:ALA:HA	2.27	0.64
3:N:1383:ASP:HB2	3:N:1416:ALA:HB3	1.80	0.64
3:N:14:SER:H	3:N:17:LYS:NZ	1.96	0.64
3:N:6:ARG:HH11	3:N:6:ARG:HB3	1.62	0.64
3:N:628:ARG:HD3	3:N:744:GLN:NE2	2.11	0.64
2:C:150:PRO:CA	2:C:158:TYR:HB3	2.22	0.64
2:C:162:ILE:O	2:C:164:PRO:HD3	1.97	0.64
2:C:1085:PHE:CE2	3:D:1468:LEU:HG	2.32	0.64
3:D:402:PRO:HG2	3:D:444:VAL:HG11	1.79	0.64
3:N:715:ALA:O	3:N:764:LEU:HD12	1.96	0.64
1:A:58:ILE:HG22	9:A:9790:HOH:O	1.96	0.64
2:C:690:ILE:HG23	2:C:852:ILE:HG23	1.80	0.64
3:D:704:ARG:HE	3:D:705:ALA:H	1.45	0.64
2:C:983:ILE:HG23	3:D:944:THR:O	1.98	0.64
5:F:111:GLU:O	5:F:115:LYS:HG2	1.96	0.64
2:M:1016:ILE:HG12	9:M:9737:HOH:O	1.96	0.64
2:M:758:ARG:HB3	2:M:788:THR:O	1.97	0.64
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.79	0.64
3:N:422:ALA:H	3:N:427:VAL:CG1	2.10	0.64
3:N:428:LYS:HE3	3:N:434:ARG:NH1	2.13	0.64
3:N:810:GLU:O	3:N:813:LEU:HG	1.98	0.64
1:A:156:HIS:CD2	1:A:157:GLY:H	2.14	0.64
2:C:34:VAL:HB	2:C:38:LYS:HG3	1.78	0.64
3:D:119:SER:H	3:D:123:LEU:HD22	1.62	0.64
3:D:210:ARG:HH11	3:D:210:ARG:HB3	1.62	0.64
1:L:22:GLU:HG2	1:L:198:ARG:HG2	1.80	0.64
2:M:739:GLU:HB3	9:M:9693:HOH:O	1.97	0.64
3:N:106:LYS:HD2	9:N:9666:HOH:O	1.97	0.64
3:N:119:SER:HB2	3:N:123:LEU:N	2.12	0.64
3:N:1314:LYS:HE2	3:N:1317:ASP:OD2	1.97	0.64
3:N:564:GLU:HA	3:N:567:ILE:HD12	1.78	0.64
3:N:898:GLU:CB	3:N:921:ARG:HH22	2.07	0.64
1:B:140:MET:HB2	9:B:9655:HOH:O	1.96	0.64
3:D:911:LEU:O	3:D:915:VAL:HG23	1.98	0.64
3:D:952:ASP:HA	3:D:1062:ARG:HH21	1.63	0.64
1:K:67:THR:H	2:M:627:ARG:HH21	1.44	0.64
2:M:276:LYS:HB3	9:M:9589:HOH:O	1.96	0.64
2:M:697:ARG:HD3	9:M:9861:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1079:LYS:HG3	9:N:2729:HOH:O	1.98	0.64
3:N:770:LEU:HD12	3:N:1210:SER:O	1.97	0.64
1:B:101:LEU:HG	1:B:114:PHE:HA	1.80	0.64
2:C:299:LYS:HB2	9:C:2062:HOH:O	1.98	0.64
3:D:423:ASP:HB2	5:F:178:ARG:HD2	1.78	0.64
4:E:54:LEU:O	4:E:54:LEU:HD23	1.98	0.64
1:L:123:MET:C	1:L:125:PRO:HD3	2.18	0.64
5:P:260:ILE:HD11	5:P:310:ILE:HG22	1.78	0.64
1:A:222:LEU:HD12	1:B:215:VAL:HB	1.78	0.64
1:A:8:ALA:HB1	1:B:224:TYR:HE1	1.62	0.64
2:C:244:PRO:HG2	2:C:246:ASP:OD2	1.98	0.64
2:C:627:ARG:HG2	9:C:9654:HOH:O	1.96	0.64
2:C:676:ILE:CG2	2:C:988:VAL:HG22	2.28	0.64
3:D:1304:LYS:HA	9:D:2309:HOH:O	1.97	0.64
3:D:529:GLN:HE22	3:D:533:GLY:HA2	1.62	0.64
2:M:218:VAL:HA	2:M:221:LEU:HD23	1.77	0.64
5:P:336:GLU:HG2	9:P:4181:HOH:O	1.97	0.64
1:B:27:PRO:O	1:B:28:LEU:HD23	1.98	0.64
2:C:21:ILE:HD12	2:C:21:ILE:H	1.61	0.64
3:D:1410:GLU:HA	9:D:9586:HOH:O	1.96	0.64
3:D:961:LYS:HE2	3:D:962:GLN:NE2	2.13	0.64
2:M:251:ASP:HB3	2:M:252:LYS:HD2	1.80	0.64
2:M:726:ILE:HG22	9:M:9724:HOH:O	1.97	0.64
3:N:1061:PHE:HA	9:N:9777:HOH:O	1.96	0.64
3:N:1279:GLY:O	3:N:1318:TYR:HA	1.98	0.64
3:N:502:PHE:HZ	3:N:512:MET:HE2	1.62	0.64
2:C:367:LEU:HD22	2:C:371:LYS:HG2	1.80	0.64
2:C:376:ARG:HB3	2:C:377:PRO:HD3	1.80	0.64
3:D:127:LEU:HD21	3:D:461:ILE:HD11	1.79	0.64
3:D:543:LEU:HD22	3:D:580:ALA:HB1	1.80	0.64
3:D:561:GLY:HA3	5:F:184:ARG:NH2	2.13	0.64
1:K:123:MET:C	1:K:125:PRO:HD3	2.17	0.64
2:M:264:PRO:HB3	2:M:289:THR:HG21	1.79	0.64
3:N:535:PHE:O	5:P:315:VAL:N	2.30	0.64
5:P:361:LEU:HD22	5:P:366:ALA:HB2	1.80	0.64
1:B:47:SER:O	1:B:49:PRO:N	2.31	0.63
2:C:328:LEU:HB2	2:C:488:ALA:HB2	1.79	0.63
2:C:347:GLY:HA2	2:C:350:ARG:HD2	1.79	0.63
3:D:178:LEU:HD21	9:D:9605:HOH:O	1.98	0.63
3:D:393:ILE:H	3:D:393:ILE:HD12	1.62	0.63
3:D:535:PHE:HB2	9:D:9783:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:608:SER:HB3	3:D:1443:THR:OG1	1.99	0.63
1:L:110:LYS:HG3	9:L:5854:HOH:O	1.98	0.63
1:L:137:ARG:NH1	1:L:137:ARG:HB3	2.13	0.63
1:L:38:ASN:HB3	1:L:39:PRO:HD3	1.79	0.63
2:M:93:PRO:HG3	2:M:117:HIS:HE1	1.63	0.63
3:N:1389:LEU:HD12	3:N:1390:LEU:H	1.63	0.63
3:N:800:LYS:HE3	3:N:830:ALA:HB3	1.80	0.63
3:N:834:THR:HB	3:N:838:ARG:HB3	1.81	0.63
2:C:732:ALA:HB3	9:C:9819:HOH:O	1.98	0.63
2:C:971:LYS:HA	2:C:988:VAL:HA	1.80	0.63
3:D:209:ARG:HD2	3:D:210:ARG:HD3	1.81	0.63
3:D:369:ALA:HB3	9:D:9708:HOH:O	1.98	0.63
5:F:321:ILE:HD11	5:F:329:TYR:HB2	1.80	0.63
3:N:1102:THR:HG22	3:N:1222:GLY:HA2	1.79	0.63
3:N:1252:ILE:HG13	9:N:9664:HOH:O	1.96	0.63
2:M:1090:LYS:HZ2	3:N:90:MET:HG2	1.63	0.63
5:P:122:LEU:HA	9:P:4507:HOH:O	1.98	0.63
1:B:132:LEU:HD21	1:B:136:GLY:O	1.98	0.63
2:C:1008:ARG:HE	2:C:1028:GLY:CA	2.11	0.63
2:C:71:TYR:HB2	9:C:9570:HOH:O	1.97	0.63
3:D:12:LEU:HD13	3:D:511:TRP:HB2	1.79	0.63
2:M:180:GLY:HA2	9:M:2207:HOH:O	1.97	0.63
2:M:97:ARG:HG3	9:M:2023:HOH:O	1.98	0.63
3:N:134:VAL:HG12	3:N:152:LEU:HB3	1.81	0.63
2:C:144:PRO:HA	2:C:163:ILE:HG12	1.78	0.63
2:C:32:ALA:HB2	2:C:73:LEU:HD21	1.81	0.63
2:C:610:ARG:HD3	9:C:9851:HOH:O	1.99	0.63
2:C:625:LEU:HD11	2:C:641:PRO:HG3	1.79	0.63
2:C:606:VAL:HG22	2:C:645:VAL:HG13	1.79	0.63
3:D:1082:ALA:O	3:D:1086:LEU:HD13	1.98	0.63
3:D:672:ALA:HB2	9:F:9781:HOH:O	1.97	0.63
3:D:85:VAL:O	3:D:89:ARG:HD2	1.98	0.63
3:D:996:TRP:HE3	3:D:999:THR:HG21	1.64	0.63
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	1.79	0.63
2:M:157:ARG:HA	2:M:157:ARG:CZ	2.27	0.63
2:M:557:ARG:CZ	2:M:879:ARG:HD3	2.27	0.63
3:N:95:LEU:HD21	3:N:574:LEU:HD11	1.79	0.63
2:C:267:TYR:H	2:C:267:TYR:HD2	1.47	0.63
3:D:1141:GLU:HG2	3:D:1168:MET:CE	2.29	0.63
3:D:787:LEU:HD21	3:D:947:ILE:HD11	1.81	0.63
3:D:850:LEU:HD12	3:D:850:LEU:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1090:LYS:HE2	2:M:1112:PHE:CE1	2.34	0.63
2:M:191:PHE:HZ	2:M:196:LEU:HB2	1.63	0.63
2:M:367:LEU:HB3	2:M:371:LYS:HG2	1.80	0.63
2:M:549:PHE:CD2	2:M:886:LEU:HB3	2.33	0.63
3:N:1134:LEU:HB3	9:N:2295:HOH:O	1.98	0.63
3:N:206:ARG:O	3:N:206:ARG:HD3	1.98	0.63
2:C:264:PRO:HB3	2:C:289:THR:HG21	1.81	0.63
2:C:47:ALA:HB1	2:C:345:ARG:HB3	1.81	0.63
2:C:625:LEU:HB3	2:C:639:GLN:HB2	1.79	0.63
3:D:1102:THR:HG22	3:D:1222:GLY:HA2	1.81	0.63
2:C:1020:PRO:O	3:D:622:ARG:HD2	1.98	0.63
2:M:145:GLY:HA3	9:M:9589:HOH:O	1.99	0.63
2:M:199:VAL:HG13	2:M:235:LEU:HG	1.81	0.63
2:M:585:GLU:HG2	2:M:589:ARG:HH12	1.63	0.63
2:M:610:ARG:HB3	9:M:2240:HOH:O	1.97	0.63
2:M:739:GLU:HG3	9:M:9586:HOH:O	1.98	0.63
2:M:944:LEU:HD11	2:M:963:LEU:HD21	1.79	0.63
3:N:1123:PHE:CE2	3:N:1184:GLN:HA	2.33	0.63
3:N:1475:GLY:O	3:N:1478:SER:HB3	1.97	0.63
3:N:723:GLY:HA3	9:N:9617:HOH:O	1.99	0.63
5:P:167:PRO:HB2	5:P:169:GLU:OE2	1.99	0.63
5:P:185:GLN:HA	5:P:188:ILE:HD12	1.81	0.63
1:A:173:PRO:HA	1:A:202:ASP:OD2	1.98	0.63
2:C:437:ARG:HA	2:C:467:ILE:HG21	1.79	0.63
2:C:726:ILE:HG22	9:C:2208:HOH:O	1.98	0.63
2:C:722:ILE:HG23	2:C:805:ARG:NH2	2.14	0.63
2:C:987:ILE:HG23	3:D:948:THR:CG2	2.28	0.63
2:C:993:PHE:HE1	2:C:995:MET:HG2	1.63	0.63
3:D:1192:LEU:HD22	3:D:1345:GLU:HG2	1.81	0.63
3:D:1258:ARG:CZ	3:D:1262:LEU:HD11	2.28	0.63
3:D:1258:ARG:NH2	3:D:1262:LEU:HD11	2.13	0.63
3:D:1274:ILE:HD11	3:D:1334:GLN:HE21	1.64	0.63
3:D:1379:VAL:HA	3:D:1420:LEU:HB2	1.78	0.63
3:D:9:ARG:HA	3:D:1434:TRP:CH2	2.34	0.63
3:D:546:ARG:NH2	3:D:550:ARG:HH22	1.97	0.63
3:D:32:ILE:O	5:F:258:ILE:HG23	1.98	0.63
2:M:728:HIS:CE1	2:M:775:ARG:HH12	2.17	0.63
2:M:1085:PHE:CD2	3:N:1468:LEU:HA	2.34	0.63
3:N:982:PHE:HB3	9:N:9805:HOH:O	1.99	0.63
1:B:59:GLU:HG3	1:B:139:ASN:ND2	2.13	0.63
3:D:1087:ARG:HB3	3:D:1234:THR:HG23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:98:THR:HG22	9:K:3875:HOH:O	1.98	0.63
2:M:944:LEU:HD21	2:M:963:LEU:HD22	1.79	0.63
3:N:961:LYS:HG2	9:N:9802:HOH:O	1.98	0.63
1:A:107:LYS:HD3	9:A:9680:HOH:O	1.99	0.63
1:K:117:VAL:HB	1:K:120:VAL:CG1	2.27	0.63
1:L:206:THR:HG22	1:L:209:GLU:H	1.64	0.63
2:M:1090:LYS:HZ2	3:N:90:MET:CG	2.11	0.63
3:N:972:LEU:O	3:N:976:GLN:HG3	1.99	0.63
1:B:14:ARG:HG2	9:B:9546:HOH:O	1.99	0.62
2:C:673:LEU:HD22	2:C:867:VAL:HA	1.81	0.62
3:D:704:ARG:NE	3:D:705:ALA:H	1.97	0.62
9:D:2389:HOH:O	5:F:134:LYS:HD2	1.99	0.62
5:F:279:GLN:HA	9:F:9783:HOH:O	1.97	0.62
3:N:208:PRO:HB2	3:N:395:VAL:HG13	1.80	0.62
3:N:767:HIS:NE2	4:O:6:ILE:HD13	2.14	0.62
1:A:42:ARG:HH21	1:B:34:VAL:HB	1.64	0.62
2:C:595:LEU:O	2:C:655:LEU:HG	1.99	0.62
3:D:1205:TYR:CD2	3:D:1215:VAL:HG21	2.34	0.62
2:M:328:LEU:HD13	2:M:433:THR:HB	1.80	0.62
3:N:610:LYS:HG2	3:N:611:GLN:HG2	1.80	0.62
3:N:705:ALA:HB3	3:N:706:PRO:HD3	1.81	0.62
5:P:364:ARG:HD3	9:P:3916:HOH:O	1.98	0.62
5:P:404:ALA:HB3	9:P:4808:HOH:O	1.99	0.62
3:D:537:THR:C	5:F:317:LEU:HB2	2.19	0.62
3:D:996:TRP:CE3	3:D:999:THR:HG21	2.33	0.62
4:E:58:PRO:HA	9:E:9569:HOH:O	1.99	0.62
2:M:799:ILE:HD13	2:M:799:ILE:N	2.15	0.62
3:N:1314:LYS:HD3	3:N:1314:LYS:H	1.64	0.62
3:N:161:LEU:HD22	3:N:452:ILE:HG21	1.80	0.62
2:C:1034:GLU:HA	2:C:1037:VAL:HG23	1.81	0.62
2:C:208:ALA:O	2:C:218:VAL:HG21	1.99	0.62
3:D:1261:GLU:OE1	3:D:1268:PRO:HA	1.99	0.62
3:D:656:PHE:HB3	3:D:694:VAL:HG11	1.81	0.62
3:D:65:ARG:HB3	9:D:2111:HOH:O	1.99	0.62
3:D:84:ILE:O	3:D:87:ARG:HG3	2.00	0.62
2:M:771:GLU:O	2:M:775:ARG:HG2	1.98	0.62
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.81	0.62
3:N:996:TRP:NE1	3:N:1056:PRO:HG3	2.13	0.62
3:N:1175:ILE:O	3:N:1179:GLU:HG3	1.99	0.62
3:N:441:ARG:O	3:N:443:VAL:HG23	1.99	0.62
3:N:661:MET:HE3	3:N:673:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:5620:HOH:O	3:N:813:LEU:HD11	1.99	0.62
5:P:128:ARG:HG3	9:P:5446:HOH:O	1.99	0.62
5:P:367:MET:HG3	9:P:6021:HOH:O	1.98	0.62
1:A:20:TYR:HD2	1:A:21:GLY:H	1.48	0.62
1:B:158:ILE:HD13	9:B:9554:HOH:O	1.99	0.62
1:B:214:ALA:HA	1:B:217:ILE:HD12	1.80	0.62
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.82	0.62
2:C:697:ARG:HG2	9:C:9985:HOH:O	1.99	0.62
3:D:422:ALA:H	3:D:427:VAL:CG1	2.12	0.62
3:D:562:ALA:HB1	3:D:567:ILE:CD1	2.29	0.62
3:D:864:VAL:HG23	3:D:877:PRO:HD3	1.82	0.62
1:K:222:LEU:HD12	1:L:215:VAL:HB	1.80	0.62
2:M:709:GLU:HG3	2:M:824:ARG:HG3	1.80	0.62
2:M:876:VAL:HA	9:M:9833:HOH:O	1.97	0.62
3:N:112:ILE:HD13	3:N:461:ILE:HG21	1.82	0.62
3:N:573:MET:SD	5:P:210:LEU:HD13	2.40	0.62
1:A:110:LYS:HB2	1:A:112:ARG:HD3	1.80	0.62
1:A:150:TYR:HE2	1:A:152:PRO:HG3	1.65	0.62
2:C:884:GLN:HG3	2:C:885:ILE:N	2.13	0.62
3:D:1126:ASP:HB2	9:D:2250:HOH:O	2.00	0.62
3:D:211:VAL:HG22	3:D:393:ILE:HG23	1.81	0.62
3:D:477:LEU:HD23	9:D:9637:HOH:O	1.99	0.62
3:D:560:GLN:HG3	5:F:221:ILE:HG21	1.81	0.62
5:F:255:ALA:HB3	9:F:9577:HOH:O	1.98	0.62
5:F:336:GLU:HG2	5:F:337:HIS:HD2	1.64	0.62
1:L:226:SER:O	1:L:228:PRO:HD3	1.99	0.62
2:M:139:GLN:NE2	2:M:418:LEU:HD13	2.15	0.62
2:M:913:GLU:HG3	9:M:2025:HOH:O	2.00	0.62
3:N:1123:PHE:HE2	3:N:1184:GLN:HA	1.65	0.62
3:N:1109:GLU:HG2	3:N:1201:CYS:HA	1.80	0.62
3:N:928:ALA:CA	3:N:931:LEU:HD12	2.25	0.62
2:C:369:PRO:HG2	2:C:370:ALA:H	1.65	0.62
2:C:49:ARG:NH1	2:C:49:ARG:HB2	2.13	0.62
3:D:1266:ARG:O	3:D:1268:PRO:HD3	2.00	0.62
3:D:401:TYR:CE2	3:D:415:VAL:HG13	2.35	0.62
3:D:637:LEU:HD12	3:D:641:GLN:OE1	1.99	0.62
3:D:658:LEU:HD11	3:D:674:ARG:NH1	2.12	0.62
4:E:39:VAL:HB	9:E:9616:HOH:O	1.98	0.62
5:F:268:ILE:HG22	9:F:9636:HOH:O	1.99	0.62
5:F:352:GLU:O	5:F:356:LYS:HG3	1.99	0.62
5:F:406:ARG:HG2	9:F:9822:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:572:ARG:NH2	5:F:83:GLN:HE21	1.92	0.62
1:K:102:LYS:HG2	9:K:3628:HOH:O	1.98	0.62
1:L:110:LYS:HB2	1:L:110:LYS:HZ2	1.64	0.62
2:M:144:PRO:HA	2:M:163:ILE:HG12	1.81	0.62
3:N:776:GLU:OE1	3:N:912:LYS:HD3	1.99	0.62
4:O:31:LEU:HD23	4:O:35:PHE:CE1	2.35	0.62
5:P:132:ARG:HG3	9:P:4300:HOH:O	1.99	0.62
5:P:416:ARG:CZ	5:P:419:ARG:HB2	2.29	0.62
3:D:808:THR:HB	3:D:809:PRO:HD3	1.82	0.62
3:D:89:ARG:HA	9:D:9588:HOH:O	1.99	0.62
5:F:225:GLU:HG3	5:F:226:LYS:HG3	1.81	0.62
2:M:432:ARG:HD2	2:M:519:GLY:HA3	1.80	0.62
2:M:698:ASP:HA	9:M:9660:HOH:O	1.99	0.62
3:N:1462:LEU:HD22	3:N:1472:ILE:HG23	1.82	0.62
3:N:45:PHE:HD1	3:N:86:ARG:HH22	1.48	0.62
2:C:420:ARG:HD2	2:C:420:ARG:H	1.65	0.62
2:C:511:GLU:O	2:C:526:PRO:HD3	1.99	0.62
2:C:627:ARG:HG3	2:C:628:PHE:H	1.65	0.62
2:C:630:ARG:HH22	2:C:707:ARG:HB2	1.65	0.62
3:D:1217:ILE:HD13	3:D:1480:PHE:CE2	2.34	0.62
3:D:658:LEU:HD11	3:D:674:ARG:HH11	1.65	0.62
3:D:9:ARG:HA	3:D:1434:TRP:HH2	1.63	0.62
5:F:163:LEU:HD22	5:F:174:LEU:HG	1.81	0.62
5:F:215:GLU:HG2	9:F:9685:HOH:O	1.99	0.62
1:L:150:TYR:CE2	3:N:857:ILE:HG13	2.35	0.62
2:M:611:ILE:HD11	2:M:641:PRO:HG3	1.82	0.62
3:N:422:ALA:HB3	3:N:427:VAL:CG2	2.28	0.62
3:N:824:ASN:HB2	9:N:9584:HOH:O	1.99	0.62
5:P:132:ARG:NE	5:P:184:ARG:HH12	1.98	0.62
5:P:351:SER:O	5:P:355:GLU:HB2	2.00	0.62
2:C:254:VAL:HG13	2:C:258:TYR:HE1	1.65	0.62
2:C:773:LEU:HB2	5:F:373:LYS:CB	2.26	0.62
2:C:798:GLY:H	2:C:827:VAL:HG11	1.65	0.62
3:D:1153:VAL:HG12	3:D:1155:VAL:HG23	1.81	0.62
3:D:1236:LEU:HA	3:D:1359:GLN:OE1	2.00	0.62
4:E:48:MET:HB2	4:E:54:LEU:HD12	1.81	0.62
2:M:1092:LEU:HD22	2:M:1099:VAL:HG22	1.81	0.62
2:M:455:LEU:CD1	2:M:459:ALA:HB3	2.30	0.62
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.81	0.62
3:N:843:PHE:CE1	3:N:864:VAL:HG11	2.35	0.62
1:B:223:THR:HG21	9:B:9702:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1018:GLN:HA	9:C:2163:HOH:O	2.00	0.61
2:C:397:GLU:HA	2:C:403:SER:HB3	1.81	0.61
2:M:207:LEU:HD13	2:M:221:LEU:HD13	1.82	0.61
2:M:769:PRO:HD2	9:M:9955:HOH:O	1.99	0.61
3:N:1485:GLN:HE21	4:O:80:VAL:N	1.94	0.61
3:N:14:SER:H	3:N:17:LYS:HZ2	1.48	0.61
3:N:584:ASN:ND2	3:N:590:PRO:HD2	2.15	0.61
3:N:863:VAL:HG23	9:N:9576:HOH:O	2.00	0.61
3:N:907:GLU:HG2	3:N:908:LYS:N	2.14	0.61
5:P:207:LEU:HB3	5:P:212:LEU:HG	1.82	0.61
5:P:358:LEU:HD21	5:P:370:LYS:NZ	2.15	0.61
1:B:101:LEU:HB2	1:B:114:PHE:CD2	2.35	0.61
1:B:39:PRO:O	1:B:43:ILE:HG12	1.99	0.61
2:C:198:ARG:NH1	2:C:231:PRO:HG3	2.14	0.61
2:C:290:LEU:HA	9:C:9607:HOH:O	2.00	0.61
2:C:798:GLY:HA2	9:C:9552:HOH:O	2.00	0.61
3:D:1057:VAL:HG13	3:D:1069:GLU:HB3	1.82	0.61
3:D:805:GLU:HA	9:D:2416:HOH:O	1.99	0.61
3:D:87:ARG:HB3	3:D:523:ASP:CB	2.30	0.61
3:D:899:LEU:HD12	3:D:900:ILE:HG23	1.82	0.61
3:D:908:LYS:HG2	9:D:2314:HOH:O	1.99	0.61
5:F:315:VAL:HG11	9:F:9826:HOH:O	1.99	0.61
2:M:349:ALA:HB3	9:M:2321:HOH:O	1.99	0.61
3:N:494:LYS:HA	3:N:497:GLU:OE1	2.00	0.61
3:D:542:ASP:O	3:D:546:ARG:HG2	2.00	0.61
4:E:33:HIS:CD2	4:E:89:MET:HG2	2.35	0.61
5:F:214:GLN:HA	5:F:217:ASN:HD22	1.66	0.61
2:M:603:VAL:HG21	2:M:643:VAL:CG1	2.30	0.61
2:M:671:ASN:HD21	2:M:993:PHE:HD2	1.48	0.61
2:M:755:LEU:HD11	2:M:792:VAL:HG22	1.82	0.61
2:M:816:LYS:HB2	2:M:819:VAL:HG21	1.82	0.61
3:N:15:PRO:HA	3:N:18:ILE:HG12	1.82	0.61
1:A:28:LEU:HD23	9:A:9575:HOH:O	1.99	0.61
2:C:715:THR:HG22	2:C:717:LEU:HG	1.83	0.61
3:D:1334:GLN:HA	9:D:2080:HOH:O	1.99	0.61
3:D:1495:ILE:HG13	9:E:9600:HOH:O	2.01	0.61
3:D:964:LEU:HD22	3:D:1058:ARG:NH1	2.15	0.61
3:N:1105:ILE:HD11	3:N:1374:GLN:NE2	2.14	0.61
3:N:209:ARG:NH1	3:N:397:LYS:HB2	2.16	0.61
3:N:400:VAL:HG11	3:N:441:ARG:NH1	2.15	0.61
2:C:189:ARG:HG2	9:C:2128:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:908:LYS:CB	3:D:1027:GLY:HA3	2.24	0.61
3:D:1394:VAL:HB	3:D:1397:LYS:HD2	1.83	0.61
2:C:1103:ASP:OD1	3:D:3:LYS:HG3	1.99	0.61
3:D:963:TYR:CD2	3:D:1002:LYS:HB3	2.35	0.61
3:N:214:GLU:HB2	3:N:390:PRO:HD2	1.82	0.61
3:N:513:ILE:HG23	9:N:9680:HOH:O	2.00	0.61
1:B:36:LEU:O	1:B:39:PRO:HD2	2.00	0.61
1:B:50:GLY:HA2	9:B:9692:HOH:O	1.99	0.61
3:D:1336:LEU:HA	3:D:1344:VAL:HG22	1.81	0.61
3:D:728:LEU:HD12	9:D:9655:HOH:O	1.99	0.61
4:E:61:GLU:O	4:E:65:MET:HG3	2.00	0.61
5:F:335:ASP:OD1	5:F:338:LEU:HB2	2.00	0.61
1:K:58:ILE:HD12	1:K:138:LEU:HD11	1.81	0.61
1:K:62:LEU:H	1:K:62:LEU:HD12	1.66	0.61
2:M:1086:ARG:HB3	2:M:1112:PHE:HE2	1.63	0.61
2:M:160:ALA:HB2	2:M:310:LEU:HD13	1.81	0.61
2:M:958:THR:HG23	2:M:961:GLU:HG2	1.82	0.61
3:N:153:LEU:HD11	3:N:158:TYR:N	2.15	0.61
3:N:178:LEU:HG	3:N:200:ASP:H	1.64	0.61
3:N:699:VAL:CG1	3:N:717:GLN:HE21	2.14	0.61
3:N:950:GLY:H	3:N:953:ASP:HB2	1.64	0.61
2:C:132:ALA:HA	9:C:2298:HOH:O	2.01	0.61
2:C:554:ASP:OD2	2:C:556:ASN:HB3	2.01	0.61
2:C:774:LEU:HA	2:C:777:ILE:HD12	1.82	0.61
2:C:579:VAL:HB	2:C:890:LEU:CD2	2.29	0.61
3:D:1063:GLU:HB3	9:D:2628:HOH:O	2.00	0.61
3:D:126:VAL:HG12	3:D:132:TYR:HB2	1.81	0.61
3:D:1380:GLU:HB2	3:D:1420:LEU:HD23	1.82	0.61
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.65	0.61
3:N:1465:ASN:HD21	3:N:1470:ARG:HD3	1.64	0.61
3:N:396:VAL:HG22	9:N:9723:HOH:O	1.99	0.61
3:N:490:ALA:HA	9:N:9651:HOH:O	2.01	0.61
3:N:551:ASN:O	3:N:555:LYS:HG3	2.01	0.61
4:O:51:LEU:HD12	4:O:52:GLU:H	1.66	0.61
2:C:742:VAL:HG21	9:C:9745:HOH:O	2.00	0.61
2:C:758:ARG:HB3	2:C:788:THR:O	2.00	0.61
3:D:1109:GLU:OE1	3:D:1201:CYS:HB2	2.00	0.61
3:D:530:VAL:HB	3:D:534:ARG:HB2	1.82	0.61
5:F:278:LEU:O	5:F:282:LEU:HG	2.01	0.61
2:M:370:ALA:HB1	9:P:6741:HOH:O	2.00	0.61
2:M:565:GLN:HA	2:M:995:MET:HE1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1004:THR:HG21	9:N:2721:HOH:O	2.00	0.61
5:P:133:ALA:CB	5:P:142:ARG:HH21	2.12	0.61
5:P:151:LEU:HB2	5:P:155:THR:OG1	2.00	0.61
5:P:403:LYS:NZ	5:P:403:LYS:HA	2.15	0.61
1:B:68:ILE:HD12	1:B:71:VAL:HG21	1.82	0.61
2:C:199:VAL:HG22	2:C:235:LEU:HG	1.83	0.61
2:C:332:ARG:HB2	2:C:466:PHE:HE1	1.66	0.61
2:C:572:ILE:HD13	9:C:9934:HOH:O	2.00	0.61
2:C:83:CYS:HA	2:C:88:LEU:HD23	1.82	0.61
2:C:861:LEU:HD23	2:C:863:ASP:H	1.66	0.61
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.36	0.61
3:D:851:LEU:HB2	9:D:2266:HOH:O	2.01	0.61
4:E:48:MET:CB	4:E:54:LEU:HB2	2.30	0.61
3:N:1150:ALA:HA	9:N:2289:HOH:O	2.01	0.61
3:N:1259:VAL:HG22	3:N:1355:VAL:HG21	1.83	0.61
3:N:374:GLU:HA	9:N:9796:HOH:O	2.01	0.61
3:N:474:GLU:O	3:N:478:LEU:HG	1.99	0.61
2:M:873:PRO:HB3	3:N:949:ILE:HD13	1.81	0.61
5:P:363:GLU:HA	5:P:367:MET:HG2	1.81	0.61
2:C:110:GLU:HB2	2:C:368:THR:HB	1.82	0.61
2:C:816:LYS:HE2	2:C:819:VAL:HG21	1.83	0.61
3:D:1084:THR:HG23	9:D:9917:HOH:O	2.00	0.61
4:E:26:ARG:HA	4:E:29:GLN:OE1	2.00	0.61
3:D:1495:ILE:HG12	4:E:80:VAL:HG11	1.82	0.61
5:F:196:VAL:HG13	5:F:213:ILE:HD11	1.83	0.61
5:F:274:THR:O	5:F:278:LEU:HG	2.01	0.61
1:K:181:VAL:HG11	9:K:4850:HOH:O	2.01	0.61
2:M:1034:GLU:HA	2:M:1037:VAL:HG23	1.82	0.61
2:M:264:PRO:HD2	9:M:9627:HOH:O	2.00	0.61
3:N:1350:GLU:O	3:N:1354:LYS:HG2	2.00	0.61
2:M:1046:ALA:HB1	3:N:1471:LEU:HD11	1.83	0.61
3:N:807:ALA:HB3	9:N:9993:HOH:O	2.00	0.61
3:N:906:GLN:HB3	3:N:911:LEU:CD1	2.30	0.61
3:N:984:THR:H	3:N:987:GLU:CD	2.03	0.61
3:D:1066:THR:CG2	3:D:1069:GLU:HB2	2.29	0.60
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	1.83	0.60
3:D:1271:LYS:HG2	9:D:9620:HOH:O	2.00	0.60
3:D:961:LYS:HG2	3:D:962:GLN:OE1	2.01	0.60
5:F:393:THR:HG21	9:F:9713:HOH:O	2.01	0.60
5:F:80:PRO:HA	5:F:83:GLN:HB2	1.83	0.60
1:K:85:LEU:HD12	1:K:124:ASN:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:290:LEU:HB3	2:M:302:VAL:CG1	2.31	0.60
2:M:627:ARG:HA	9:M:9736:HOH:O	2.01	0.60
2:C:393:GLN:HB2	2:C:406:HIS:HE1	1.66	0.60
3:D:139:GLY:O	3:D:147:VAL:HB	2.01	0.60
3:D:818:ARG:HB2	9:D:2824:HOH:O	2.00	0.60
2:M:396:ASP:HB2	2:M:406:HIS:CD2	2.36	0.60
2:M:428:ARG:HG2	2:M:451:LEU:HG	1.83	0.60
3:N:1058:ARG:HH11	3:N:1058:ARG:HG3	1.65	0.60
3:N:1159:ARG:HD3	9:N:2291:HOH:O	2.01	0.60
3:N:148:GLU:HA	9:N:2003:HOH:O	2.00	0.60
1:A:19:GLU:HB2	9:A:9772:HOH:O	2.01	0.60
1:B:152:PRO:HG2	9:B:9720:HOH:O	2.01	0.60
1:B:2:LEU:HD12	1:B:3:ASP:N	2.16	0.60
2:C:610:ARG:HB2	9:C:9615:HOH:O	2.01	0.60
2:C:798:GLY:H	2:C:827:VAL:CG1	2.14	0.60
3:D:546:ARG:O	3:D:550:ARG:HG2	2.00	0.60
4:E:25:LYS:HA	4:E:28:GLN:HE21	1.66	0.60
5:F:248:ASN:HA	5:F:251:ILE:HD12	1.83	0.60
1:L:143:ARG:HD2	1:L:160:ASP:OD1	2.00	0.60
2:M:1054:THR:CG2	2:M:1079:PRO:HB3	2.19	0.60
2:M:159:ILE:HD11	9:M:9954:HOH:O	2.01	0.60
2:M:162:ILE:O	2:M:164:PRO:HD3	2.01	0.60
2:M:513:VAL:HB	9:M:2021:HOH:O	1.99	0.60
3:N:488:ARG:HB3	3:N:488:ARG:NH1	2.17	0.60
3:N:730:PRO:HA	3:N:733:CYS:SG	2.42	0.60
5:P:87:GLU:O	5:P:91:VAL:HG23	2.00	0.60
1:B:97:VAL:HG11	1:B:120:VAL:HG21	1.83	0.60
2:C:1056:LYS:HE3	3:D:751:LEU:HD11	1.83	0.60
3:D:996:TRP:CD2	3:D:1056:PRO:HG2	2.37	0.60
3:D:1141:GLU:HG2	3:D:1168:MET:HE2	1.82	0.60
3:D:156:GLU:CD	3:D:156:GLU:H	2.03	0.60
1:K:53:VAL:HG13	1:K:142:VAL:HG23	1.84	0.60
2:M:1002:GLU:HG2	9:N:9803:HOH:O	2.01	0.60
2:M:39:ARG:NE	2:M:39:ARG:HA	2.17	0.60
2:M:464:LEU:HG	9:M:9933:HOH:O	2.02	0.60
2:M:69:LEU:HB2	2:M:97:ARG:HB2	1.83	0.60
2:M:774:LEU:HA	2:M:777:ILE:HD12	1.83	0.60
2:M:859:PRO:O	2:M:867:VAL:HG22	2.02	0.60
2:M:897:LEU:HD21	2:M:920:GLN:NE2	2.17	0.60
3:N:1149:LEU:HD12	3:N:1161:GLU:O	2.01	0.60
3:N:1314:LYS:HD3	3:N:1314:LYS:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:61:GLY:HA3	3:N:64:LYS:HE3	1.84	0.60
2:M:1042:ALA:HB3	3:N:710:ARG:HB3	1.82	0.60
5:P:151:LEU:HD22	5:P:153:PRO:HD2	1.82	0.60
1:A:101:LEU:HD21	1:A:113:ASP:HB3	1.82	0.60
2:C:1067:TYR:O	2:C:1071:ILE:HG12	2.02	0.60
2:C:408:ARG:NH1	2:C:542:VAL:HG23	2.16	0.60
2:C:732:ALA:O	2:C:735:ARG:HG3	2.02	0.60
2:C:9:ILE:HD12	2:C:9:ILE:O	2.02	0.60
3:D:98:PRO:HG3	3:D:515:GLU:HB3	1.83	0.60
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.83	0.60
4:E:92:ILE:HD12	9:E:9526:HOH:O	2.00	0.60
1:L:106:PRO:HD3	9:L:4025:HOH:O	2.00	0.60
2:M:371:LYS:HA	9:M:9635:HOH:O	2.00	0.60
2:M:676:ILE:CG2	2:M:988:VAL:HG13	2.32	0.60
3:N:422:ALA:HB1	5:P:178:ARG:NH1	2.17	0.60
5:P:280:GLN:OE1	5:P:281:GLU:HB2	2.01	0.60
1:A:131:THR:HG22	9:A:9698:HOH:O	2.00	0.60
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.84	0.60
1:B:133:GLU:HG2	9:B:9517:HOH:O	2.02	0.60
2:C:405:ARG:HD3	2:C:543:ASN:OD1	2.01	0.60
2:C:672:VAL:CG2	2:C:868:ASP:HB2	2.31	0.60
2:C:72:ARG:HG2	9:C:2099:HOH:O	2.01	0.60
3:D:396:VAL:HG23	9:D:9780:HOH:O	2.00	0.60
3:D:448:GLU:HB2	9:D:2438:HOH:O	2.00	0.60
4:E:25:LYS:HA	4:E:28:GLN:NE2	2.17	0.60
5:F:87:GLU:O	5:F:91:VAL:HG23	2.02	0.60
2:M:752:GLY:H	2:M:792:VAL:HB	1.66	0.60
3:N:140:ALA:HA	9:N:2102:HOH:O	2.00	0.60
3:N:468:LEU:HB3	9:N:9852:HOH:O	2.02	0.60
3:N:838:ARG:HD3	3:N:874:GLU:HB3	1.83	0.60
3:N:895:VAL:HG23	9:N:2424:HOH:O	2.00	0.60
2:C:1056:LYS:HB3	3:D:624:ASP:H	1.66	0.60
2:C:110:GLU:OE2	2:C:369:PRO:HD3	2.02	0.60
2:C:669:GLY:HA3	2:C:995:MET:HA	1.82	0.60
3:D:964:LEU:HD13	3:D:1058:ARG:NH1	2.16	0.60
3:D:1124:GLN:NE2	3:D:1135:ARG:HA	2.17	0.60
3:D:135:LEU:CD1	3:D:147:VAL:HG23	2.32	0.60
1:K:138:LEU:HB2	9:K:4454:HOH:O	2.01	0.60
2:M:142:ARG:HA	9:M:2057:HOH:O	2.00	0.60
2:M:413:LEU:H	2:M:413:LEU:HD12	1.67	0.60
2:M:630:ARG:HH21	2:M:706:GLU:HA	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1146:GLY:HA3	3:N:1207:TYR:HB2	1.83	0.60
2:M:1071:ILE:O	3:N:659:LYS:HB2	2.02	0.60
3:N:75:ARG:HB2	9:N:9667:HOH:O	2.01	0.60
5:P:102:LEU:O	5:P:106:VAL:HG23	2.02	0.60
1:B:226:SER:O	1:B:228:PRO:HD3	2.02	0.60
2:C:269:LEU:HG	2:C:285:LEU:HD21	1.82	0.60
2:C:338:GLU:HA	2:C:341:THR:HG22	1.83	0.60
3:D:1357:ARG:HG3	9:D:2129:HOH:O	2.01	0.60
3:D:1382:THR:HA	3:D:1389:LEU:HD13	1.83	0.60
3:D:153:LEU:HD12	3:D:154:THR:H	1.65	0.60
3:D:171:LEU:HD22	3:D:390:PRO:HG3	1.82	0.60
3:D:890:VAL:HG22	3:D:926:LYS:HE2	1.84	0.60
1:K:193:ASP:HA	2:M:938:LYS:NZ	2.17	0.60
2:M:166:PRO:HD3	2:M:265:ARG:HG3	1.84	0.60
2:M:288:ARG:HB3	9:M:9790:HOH:O	2.00	0.60
2:M:716:LYS:HD3	9:M:9645:HOH:O	2.02	0.60
3:N:423:ASP:OD1	5:P:174:LEU:HD13	2.01	0.60
1:B:132:LEU:HD22	9:B:9527:HOH:O	2.01	0.60
1:B:150:TYR:CD2	3:D:857:ILE:HG13	2.37	0.60
1:B:212:ASN:O	1:B:215:VAL:HG22	2.02	0.60
2:C:776:SER:HB3	9:F:9725:HOH:O	2.02	0.60
3:D:1380:GLU:HG3	3:D:1381:VAL:N	2.17	0.60
3:D:204:LEU:HD22	9:D:9905:HOH:O	2.00	0.60
3:D:572:ARG:HH12	5:F:79:ASP:CG	2.05	0.60
3:D:566:ILE:HG23	5:F:214:GLN:OE1	2.01	0.60
1:L:88:ARG:HH11	1:L:88:ARG:HG2	1.67	0.60
2:M:151:ASP:HB2	2:M:157:ARG:O	2.01	0.60
2:M:197:LEU:HB3	2:M:202:TYR:HB2	1.83	0.60
2:M:203:ASP:OD1	2:M:205:GLU:HG3	2.02	0.60
2:M:208:ALA:O	2:M:218:VAL:HG21	2.01	0.60
2:M:207:LEU:HD22	2:M:221:LEU:HD22	1.84	0.60
2:M:308:ARG:HD2	9:M:9801:HOH:O	2.00	0.60
2:M:498:GLN:O	2:M:501:THR:HG23	2.01	0.60
2:M:704:HIS:CB	2:M:831:ARG:HE	2.12	0.60
3:N:1220:ALA:HB1	3:N:1223:ILE:HD13	1.84	0.60
3:N:211:VAL:HG13	3:N:393:ILE:HA	1.83	0.60
9:N:2863:HOH:O	4:O:92:ILE:HD13	2.01	0.60
5:P:96:LEU:HD12	5:P:97:GLU:OE2	2.01	0.60
1:B:206:THR:CG2	1:B:209:GLU:H	2.14	0.60
2:C:575:GLN:HB2	2:C:670:GLN:HG2	1.84	0.60
3:D:1354:LYS:HB3	9:D:2873:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.84	0.60
3:D:117:ASP:HB2	3:D:495:ARG:NH2	2.17	0.60
3:D:58:CYS:SG	3:D:59:ALA:N	2.75	0.60
3:D:957:PRO:HG3	3:D:1010:ASN:HD22	1.66	0.60
5:F:261:PRO:O	5:F:265:VAL:HG23	2.01	0.60
5:F:416:ARG:HB3	9:F:9549:HOH:O	2.00	0.60
1:K:88:ARG:HD2	1:K:121:GLU:HG2	1.84	0.60
1:K:18:ARG:O	1:K:207:PRO:HD3	2.02	0.60
2:M:166:PRO:HB2	9:M:9850:HOH:O	2.02	0.60
2:M:183:SER:HB3	2:M:190:LYS:HD3	1.83	0.60
2:M:23:VAL:HG13	9:M:2537:HOH:O	2.02	0.60
2:M:378:LEU:HB2	9:M:9803:HOH:O	2.02	0.60
2:M:855:VAL:HG23	9:M:9763:HOH:O	2.01	0.60
2:M:971:LYS:HA	2:M:988:VAL:HA	1.84	0.60
3:N:500:ARG:HH12	3:N:1387:SER:HA	1.67	0.60
3:N:434:ARG:HB2	3:N:447:VAL:CG1	2.32	0.60
3:N:584:ASN:HD21	3:N:590:PRO:HB2	1.67	0.60
3:N:769:LEU:HA	9:N:9921:HOH:O	2.02	0.60
2:C:29:ALA:HB2	2:C:337:GLY:CA	2.32	0.59
2:C:129:ILE:CG1	2:C:386:PHE:HB3	2.31	0.59
3:D:483:HIS:ND1	3:D:483:HIS:N	2.50	0.59
3:D:671:LYS:HG3	5:F:422:LEU:HA	1.84	0.59
5:F:126:LEU:HA	9:F:9910:HOH:O	2.01	0.59
5:F:402:ASN:O	5:F:406:ARG:HG3	2.01	0.59
2:M:191:PHE:CE2	2:M:195:LEU:HB3	2.37	0.59
2:M:233:GLU:OE1	2:M:237:ARG:HD3	2.02	0.59
2:M:244:PRO:HG2	2:M:246:ASP:OD2	2.02	0.59
3:N:1245:GLY:HA2	9:N:2088:HOH:O	2.01	0.59
3:N:510:GLU:O	3:N:513:ILE:HD12	2.02	0.59
3:N:679:ARG:HB2	3:N:682:ASP:OD2	2.01	0.59
5:P:393:THR:HG22	5:P:394:ARG:H	1.67	0.59
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.37	0.59
1:B:5:LYS:O	1:B:8:ALA:HB2	2.02	0.59
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.83	0.59
2:C:395:LYS:HE3	2:C:407:LYS:HD2	1.84	0.59
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.84	0.59
3:D:1096:ARG:CB	3:D:1096:ARG:HH11	2.12	0.59
3:D:1312:LEU:HB3	9:D:9676:HOH:O	2.01	0.59
3:D:170:PRO:HG3	9:D:2967:HOH:O	2.01	0.59
3:D:818:ARG:HB3	9:D:9738:HOH:O	2.02	0.59
5:F:351:SER:O	5:F:355:GLU:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5:LYS:O	1:L:8:ALA:HB2	2.01	0.59
2:M:1040:LEU:HD21	2:M:1048:THR:HG22	1.85	0.59
2:M:545:ASN:O	2:M:581:THR:HG21	2.02	0.59
3:N:1327:ARG:HB2	9:N:2252:HOH:O	2.01	0.59
3:N:1106:VAL:HG21	3:N:1474:ALA:HB2	1.82	0.59
3:N:625:TYR:O	3:N:749:VAL:HG23	2.02	0.59
1:A:5:LYS:O	1:A:8:ALA:HB2	2.01	0.59
2:C:148:PHE:HB3	9:C:9945:HOH:O	2.02	0.59
2:C:405:ARG:HH12	2:C:563:ASN:HD22	1.50	0.59
3:D:1087:ARG:HA	3:D:1090:ASP:HB2	1.82	0.59
3:D:1107:VAL:HG12	3:D:1217:ILE:HA	1.85	0.59
3:D:1156:LEU:HB3	9:D:2264:HOH:O	2.02	0.59
3:D:1206:GLY:HA3	3:D:1366:LYS:NZ	2.17	0.59
9:D:9632:HOH:O	4:E:7:ASP:HB2	2.02	0.59
5:F:198:ILE:HG21	9:F:9669:HOH:O	2.02	0.59
2:M:1018:GLN:HG3	2:M:1060:ILE:HD11	1.84	0.59
2:M:89:THR:HA	2:M:129:ILE:O	2.03	0.59
3:N:535:PHE:HA	9:N:2026:HOH:O	2.01	0.59
2:C:157:ARG:HD3	2:C:158:TYR:H	1.68	0.59
2:C:172:ILE:H	2:C:172:ILE:HD12	1.68	0.59
2:C:625:LEU:HD13	2:C:639:GLN:O	2.02	0.59
2:C:881:ASN:HD22	2:C:881:ASN:H	1.50	0.59
2:C:897:LEU:HG	2:C:920:GLN:NE2	2.16	0.59
3:D:119:SER:CB	3:D:123:LEU:HB2	2.33	0.59
1:K:57:TYR:CE2	1:K:59:GLU:HA	2.37	0.59
2:M:874:LEU:CD1	3:N:783:ARG:HB2	2.32	0.59
2:M:944:LEU:HD11	2:M:963:LEU:CD2	2.32	0.59
3:N:404:GLU:HB3	3:N:414:ARG:NE	2.17	0.59
3:N:513:ILE:HA	9:N:9680:HOH:O	2.02	0.59
1:A:123:MET:O	1:A:125:PRO:HD3	2.02	0.59
1:A:20:TYR:HD2	1:A:21:GLY:N	2.01	0.59
1:A:58:ILE:HB	1:A:61:VAL:HB	1.84	0.59
2:C:171:TRP:HB2	9:C:2032:HOH:O	2.02	0.59
2:C:897:LEU:HB3	2:C:899:GLN:HE21	1.66	0.59
3:D:1180:ALA:HB2	9:D:9936:HOH:O	2.01	0.59
5:F:187:LEU:HD23	5:F:191:ASN:ND2	2.18	0.59
1:L:171:PHE:O	1:L:173:PRO:HD3	2.01	0.59
2:M:299:LYS:HB3	9:M:9701:HOH:O	2.01	0.59
3:N:170:PRO:HB3	9:N:2454:HOH:O	2.03	0.59
3:N:764:LEU:HB3	3:N:767:HIS:CD2	2.38	0.59
1:A:181:VAL:O	2:C:937:ASP:HA	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:902:ILE:O	2:C:904:PRO:HD3	2.02	0.59
3:D:1257:PRO:HA	9:D:9962:HOH:O	2.03	0.59
3:D:424:GLY:HA2	3:D:436:GLU:HA	1.85	0.59
3:D:525:ARG:HA	3:D:538:SER:HB3	1.84	0.59
1:K:91:ASN:O	1:K:94:LEU:HD12	2.01	0.59
2:M:1113:GLU:HB3	9:M:9896:HOH:O	2.01	0.59
3:N:1472:ILE:HA	9:N:9577:HOH:O	2.02	0.59
3:N:135:LEU:HD13	3:N:147:VAL:HG23	1.85	0.59
5:P:371:LEU:HD23	9:P:4033:HOH:O	2.01	0.59
1:B:143:ARG:HD2	1:B:158:ILE:HG21	1.84	0.59
1:B:59:GLU:HG2	1:B:139:ASN:O	2.02	0.59
2:C:1016:ILE:HD12	3:D:526:PRO:HG2	1.85	0.59
3:D:161:LEU:HD22	3:D:452:ILE:HG21	1.83	0.59
5:F:153:PRO:HG2	5:F:154:LYS:HE2	1.84	0.59
5:F:108:GLU:HG3	5:F:176:ILE:CG2	2.33	0.59
1:L:36:LEU:O	1:L:39:PRO:HD2	2.03	0.59
3:N:1198:TYR:OH	3:N:1397:LYS:HE2	2.02	0.59
3:N:1466:VAL:HG23	3:N:1472:ILE:HD11	1.85	0.59
3:N:592:THR:HA	9:N:9695:HOH:O	2.02	0.59
2:M:1043:TYR:CE1	3:N:710:ARG:HB2	2.37	0.59
1:B:140:MET:HG2	9:B:9759:HOH:O	2.01	0.59
2:C:431:HIS:CD2	2:C:433:THR:H	2.20	0.59
2:C:694:LEU:HD11	2:C:868:ASP:HB3	1.85	0.59
2:C:846:LYS:HD3	3:D:741:ASP:HB2	1.84	0.59
5:F:247:ILE:HG22	5:F:251:ILE:HD11	1.85	0.59
5:F:287:THR:HG23	5:F:289:GLU:HB2	1.84	0.59
3:N:421:LEU:HD12	3:N:435:VAL:HG11	1.84	0.59
3:N:462:GLN:HG3	3:N:513:ILE:HD13	1.85	0.59
3:N:85:VAL:HB	3:N:89:ARG:CZ	2.33	0.59
4:O:54:LEU:HG	4:O:58:PRO:HD2	1.84	0.59
2:C:529:VAL:HG11	9:C:9866:HOH:O	2.03	0.59
2:C:976:ASP:CB	2:C:979:THR:HG22	2.33	0.59
3:D:1083:ASP:HB3	3:D:1087:ARG:HH21	1.66	0.59
3:D:1106:VAL:HA	9:D:9733:HOH:O	2.02	0.59
3:D:119:SER:HB2	3:D:123:LEU:N	2.17	0.59
3:D:1488:ASP:HB3	9:E:9588:HOH:O	2.02	0.59
5:F:77:THR:O	5:F:81:VAL:HG23	2.03	0.59
3:N:1209:LEU:HD23	3:N:1210:SER:H	1.67	0.59
3:N:1104:GLU:HA	3:N:1461:GLY:HA2	1.85	0.59
1:A:9:PRO:HB3	1:A:25:LEU:HD21	1.84	0.59
2:C:11:GLU:HG2	2:C:537:LYS:HZ1	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:572:ILE:HG21	9:C:9934:HOH:O	2.03	0.59
2:C:701:THR:HG21	9:C:9689:HOH:O	2.02	0.59
3:D:1129:THR:HG23	3:D:1130:ARG:H	1.68	0.59
4:E:50:THR:HG22	9:E:9512:HOH:O	2.03	0.59
1:K:102:LYS:HG3	1:K:139:ASN:HB2	1.84	0.59
2:M:35:PRO:HD2	2:M:38:LYS:HG3	1.85	0.59
2:M:328:LEU:HD11	2:M:434:HIS:HD2	1.68	0.59
2:M:474:VAL:HG11	2:M:529:VAL:HG12	1.85	0.59
2:M:517:ARG:HH11	2:M:522:VAL:HG11	1.68	0.59
3:N:1066:THR:HG23	3:N:1069:GLU:H	1.67	0.59
4:O:51:LEU:HD21	9:O:5430:HOH:O	2.02	0.59
3:N:563:PRO:HG3	5:P:188:ILE:HG21	1.85	0.59
2:C:1118:LYS:HB2	9:C:2203:HOH:O	2.01	0.58
2:C:354:GLY:HA2	9:C:2531:HOH:O	2.01	0.58
3:D:1013:GLU:HB2	9:D:9981:HOH:O	2.02	0.58
3:D:1251:ASP:O	3:D:1270:ALA:HB3	2.03	0.58
3:D:500:ARG:HG3	9:D:9596:HOH:O	2.02	0.58
4:E:45:ARG:O	4:E:47:LYS:HE3	2.02	0.58
5:F:203:THR:HG22	9:F:9554:HOH:O	2.02	0.58
1:K:100:LEU:HG	9:K:3875:HOH:O	2.03	0.58
1:K:112:ARG:HB3	1:K:112:ARG:HH11	1.67	0.58
1:K:156:HIS:CD2	1:K:157:GLY:H	2.21	0.58
1:K:38:ASN:HB3	1:K:39:PRO:HD3	1.84	0.58
2:M:513:VAL:HG13	9:M:9802:HOH:O	2.03	0.58
2:M:51:THR:HG21	9:M:2462:HOH:O	2.03	0.58
2:M:571:LEU:HD21	2:M:700:TYR:CD2	2.38	0.58
3:N:52:PRO:CG	3:N:78:VAL:HG13	2.33	0.58
3:N:863:VAL:HA	9:N:9691:HOH:O	2.02	0.58
3:N:998:GLU:HG2	9:N:9800:HOH:O	2.02	0.58
4:O:62:THR:HA	4:O:65:MET:HE2	1.84	0.58
1:A:226:SER:O	1:A:228:PRO:HD3	2.02	0.58
1:B:76:VAL:HG11	9:B:9646:HOH:O	2.03	0.58
2:C:470:PRO:HG2	2:C:538:GLN:OE1	2.02	0.58
3:D:1107:VAL:HG21	9:D:9876:HOH:O	2.02	0.58
3:D:380:GLU:O	3:D:382:GLU:N	2.36	0.58
3:D:550:ARG:HA	9:D:9736:HOH:O	2.03	0.58
5:F:138:SER:O	5:F:141:VAL:HG12	2.03	0.58
1:K:32:PHE:HB2	9:K:4770:HOH:O	2.04	0.58
2:M:260:LEU:HB2	2:M:291:ALA:HB1	1.85	0.58
2:M:860:HIS:CD2	2:M:975:TYR:HB2	2.38	0.58
3:N:1004:THR:O	3:N:1007:VAL:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:728:LEU:HD22	3:N:745:MET:SD	2.43	0.58
2:C:113:VAL:O	2:C:115:LEU:HD23	2.03	0.58
2:C:182:VAL:HG21	9:C:9561:HOH:O	2.02	0.58
2:C:525:SER:OG	2:C:527:GLU:HG3	2.03	0.58
2:C:601:GLY:O	2:C:648:ARG:HA	2.03	0.58
3:D:1399:ASP:O	3:D:1403:LEU:HB2	2.03	0.58
3:D:104:PHE:CD2	3:D:1448:THR:HG23	2.39	0.58
3:N:493:ARG:HH22	3:N:1388:ARG:HB3	1.68	0.58
3:N:1472:ILE:HD13	9:N:9577:HOH:O	2.03	0.58
3:N:644:LEU:HD12	3:N:645:PRO:CD	2.33	0.58
3:N:799:LYS:H	3:N:826:PRO:HG2	1.68	0.58
3:N:860:LEU:HB2	3:N:861:GLN:NE2	2.19	0.58
5:P:128:ARG:CZ	5:P:128:ARG:HB2	2.33	0.58
3:N:573:MET:HE3	5:P:210:LEU:HD22	1.84	0.58
5:P:392:VAL:HG21	9:P:3916:HOH:O	2.04	0.58
1:A:158:ILE:HG21	9:A:9755:HOH:O	2.03	0.58
1:A:191:ASP:O	1:A:192:LEU:HD23	2.04	0.58
2:C:486:MET:HE3	2:C:491:GLU:HA	1.85	0.58
1:A:72:LYS:HA	2:C:608:GLY:N	2.18	0.58
3:D:145:VAL:HB	9:D:9617:HOH:O	2.03	0.58
2:C:1085:PHE:HE2	3:D:1468:LEU:HG	1.67	0.58
4:E:87:LYS:O	4:E:91:ARG:HG3	2.03	0.58
1:K:95:GLN:HG2	9:K:3707:HOH:O	2.02	0.58
2:M:479:VAL:CG2	2:M:503:LEU:HD11	2.33	0.58
2:M:772:ARG:HG3	2:M:773:LEU:N	2.18	0.58
2:M:87:ASP:HA	9:M:9630:HOH:O	2.03	0.58
3:N:165:LYS:HB3	3:N:395:VAL:HG11	1.84	0.58
3:N:141:ILE:HG12	3:N:449:SER:HA	1.85	0.58
3:N:729:HIS:HE1	3:N:731:LEU:HG	1.68	0.58
5:P:321:ILE:HB	5:P:327:SER:OG	2.03	0.58
2:C:1021:LEU:HD13	5:F:331:ASP:O	2.04	0.58
2:C:276:LYS:O	2:C:280:LYS:HB2	2.03	0.58
3:D:834:THR:HB	3:D:838:ARG:HB3	1.84	0.58
2:M:998:TYR:CZ	2:M:1000:MET:HA	2.38	0.58
2:M:460:ARG:HB3	2:M:460:ARG:NH1	2.19	0.58
2:M:948:GLU:OE1	2:M:955:PRO:HA	2.04	0.58
2:M:998:TYR:OH	2:M:1000:MET:HA	2.03	0.58
3:N:1128:VAL:HG11	9:N:2608:HOH:O	2.02	0.58
5:P:185:GLN:O	5:P:189:GLU:HG3	2.04	0.58
2:C:261:ILE:HD11	9:C:9806:HOH:O	2.02	0.58
2:C:805:ARG:HD3	9:C:2549:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1377:LYS:HG3	3:D:1394:VAL:HG13	1.86	0.58
3:D:428:LYS:HG2	9:D:2371:HOH:O	2.02	0.58
3:D:659:LYS:HD3	3:D:659:LYS:O	2.03	0.58
3:D:907:GLU:O	3:D:911:LEU:HD13	2.03	0.58
2:M:420:ARG:HD2	2:M:420:ARG:H	1.68	0.58
2:M:816:LYS:HE2	2:M:819:VAL:HG21	1.84	0.58
3:N:150:ARG:HD3	9:N:9837:HOH:O	2.04	0.58
3:N:385:VAL:HA	9:P:4715:HOH:O	2.03	0.58
3:N:424:GLY:HA2	3:N:436:GLU:HA	1.85	0.58
3:N:953:ASP:HB3	9:N:9719:HOH:O	2.01	0.58
4:O:10:PHE:HE2	4:O:16:LYS:HG3	1.68	0.58
2:C:305:PRO:HB3	2:C:308:ARG:NH2	2.08	0.58
2:C:993:PHE:CE1	2:C:995:MET:HG2	2.38	0.58
3:D:1121:PRO:HB3	9:D:2672:HOH:O	2.02	0.58
3:D:1448:THR:O	3:D:1452:ILE:HD13	2.03	0.58
3:D:1468:LEU:HD23	3:D:1468:LEU:O	2.03	0.58
2:C:1091:GLU:OE1	3:D:613:ARG:HG2	2.03	0.58
5:F:93:LEU:HG	5:F:190:ALA:HB1	1.86	0.58
1:K:74:ASP:OD1	1:K:76:VAL:HG23	2.03	0.58
1:L:2:LEU:HD13	1:L:3:ASP:OD1	2.04	0.58
2:M:15:LEU:HD22	2:M:583:LEU:HD21	1.84	0.58
3:N:863:VAL:HG11	9:N:2870:HOH:O	2.03	0.58
1:L:77:GLU:HB2	3:N:872:ARG:NH2	2.18	0.58
5:P:201:LYS:HB2	9:P:6229:HOH:O	2.03	0.58
1:B:7:LYS:HD3	9:B:9540:HOH:O	2.02	0.58
3:D:101:HIS:ND1	3:D:103:TRP:HB2	2.17	0.58
3:D:1066:THR:CG2	3:D:1069:GLU:H	2.15	0.58
3:D:589:ALA:HB2	9:D:2639:HOH:O	2.03	0.58
1:K:99:LEU:HB3	1:K:114:PHE:HD2	1.67	0.58
2:M:769:PRO:HB2	9:M:9652:HOH:O	2.03	0.58
3:N:1036:ARG:NH2	3:N:1042:ARG:HA	2.17	0.58
3:N:1124:GLN:N	3:N:1133:ARG:O	2.37	0.58
3:N:1376:MET:HB3	9:N:2499:HOH:O	2.04	0.58
3:N:1459:LEU:HD13	3:N:1465:ASN:ND2	2.19	0.58
3:N:152:LEU:HD23	3:N:152:LEU:N	2.17	0.58
3:N:658:LEU:HD23	3:N:673:ALA:HB3	1.86	0.58
4:O:10:PHE:CE2	4:O:16:LYS:HG3	2.39	0.58
5:P:361:LEU:HD21	5:P:404:ALA:HB1	1.83	0.58
2:C:195:LEU:HD12	2:C:234:ALA:HB1	1.86	0.58
3:D:537:THR:O	5:F:317:LEU:HB2	2.03	0.58
3:D:633:VAL:HB	3:D:740:PHE:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:817:GLU:O	3:D:821:VAL:HG23	2.04	0.58
5:F:126:LEU:HB3	9:F:9770:HOH:O	2.02	0.58
1:K:20:TYR:HD2	1:K:21:GLY:H	1.52	0.58
1:L:164:ALA:HA	9:L:4389:HOH:O	2.03	0.58
2:M:1000:MET:O	2:M:1003:ASP:HB3	2.04	0.58
2:M:49:ARG:HH11	2:M:49:ARG:HB2	1.69	0.58
2:M:571:LEU:HG	2:M:701:THR:H	1.69	0.58
2:M:897:LEU:HD21	2:M:920:GLN:HE21	1.68	0.58
3:N:1000:THR:O	3:N:1003:VAL:HG22	2.04	0.58
3:N:183:GLU:HA	3:N:186:VAL:HG12	1.84	0.58
3:N:423:ASP:HB3	5:P:175:HIS:HA	1.84	0.58
3:N:890:VAL:HG11	3:N:922:LEU:HD13	1.86	0.58
4:O:48:MET:N	4:O:54:LEU:HB2	2.19	0.58
5:P:401:GLU:O	5:P:405:LEU:HB2	2.03	0.58
1:B:14:ARG:HD2	9:B:9699:HOH:O	2.04	0.58
1:B:27:PRO:HG2	1:B:186:LEU:CD1	2.34	0.58
2:C:203:ASP:HA	9:C:2206:HOH:O	2.01	0.58
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.03	0.58
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.86	0.58
3:D:1264:GLU:OE1	3:D:1425:THR:HB	2.03	0.58
3:D:86:ARG:HH11	3:D:86:ARG:HG2	1.68	0.58
5:F:264:MET:O	5:F:267:THR:HB	2.04	0.58
2:M:1115:LEU:HD12	2:M:1115:LEU:N	2.19	0.58
2:M:169:GLY:HA3	9:M:2243:HOH:O	2.04	0.58
3:N:116:LEU:HD23	3:N:468:LEU:HD11	1.84	0.58
3:N:1263:PHE:HA	3:N:1375:MET:HE1	1.85	0.58
3:N:211:VAL:HG22	3:N:393:ILE:HG23	1.86	0.58
3:N:30:GLU:HG3	3:N:41:ARG:HG2	1.86	0.58
2:C:538:GLN:HB2	9:C:9681:HOH:O	2.03	0.57
2:C:897:LEU:HG	2:C:920:GLN:HE21	1.68	0.57
1:A:31:GLY:HA2	2:C:939:ARG:HH22	1.68	0.57
3:D:1111:ASP:HB2	9:D:2820:HOH:O	2.03	0.57
3:D:1130:ARG:HG3	9:D:9602:HOH:O	2.02	0.57
3:D:1389:LEU:HD22	9:D:2920:HOH:O	2.03	0.57
5:F:87:GLU:HG3	9:F:9969:HOH:O	2.03	0.57
2:M:579:VAL:HG11	2:M:887:GLU:HG3	1.85	0.57
2:M:73:LEU:HB3	2:M:94:LEU:HB2	1.86	0.57
2:M:973:VAL:O	2:M:974:LEU:HD12	2.03	0.57
3:N:509:PRO:HG2	9:N:9632:HOH:O	2.03	0.57
3:N:462:GLN:HA	3:N:513:ILE:HD13	1.85	0.57
9:L:3698:HOH:O	3:N:842:VAL:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1115:LEU:HD12	2:C:1115:LEU:N	2.19	0.57
2:C:268:ASP:HB3	2:C:272:ALA:HB2	1.86	0.57
2:C:682:TYR:HE2	9:D:2879:HOH:O	1.85	0.57
3:D:1288:GLU:OE1	3:D:1289:LYS:HE3	2.04	0.57
2:C:886:LEU:CG	3:D:951:ILE:HG13	2.34	0.57
3:D:992:ILE:O	3:D:995:LEU:HB3	2.04	0.57
5:F:220:LEU:O	5:F:224:VAL:HG23	2.04	0.57
2:M:853:LEU:HD23	2:M:858:MET:HB3	1.84	0.57
2:M:861:LEU:HD21	2:M:925:TYR:CE2	2.39	0.57
2:M:1049:LEU:HD23	3:N:1472:ILE:HG13	1.86	0.57
1:A:123:MET:C	1:A:125:PRO:HD3	2.24	0.57
1:A:143:ARG:HD2	1:A:145:ASP:OD1	2.04	0.57
1:B:73:GLU:HB3	1:B:77:GLU:HG3	1.86	0.57
2:C:328:LEU:HD11	2:C:434:HIS:HD2	1.68	0.57
1:A:178:ALA:CB	2:C:864:GLY:H	2.16	0.57
2:C:676:ILE:HG21	2:C:988:VAL:HG22	1.85	0.57
3:D:1000:THR:O	3:D:1003:VAL:HG22	2.03	0.57
3:D:1003:VAL:HG21	3:D:1041:LEU:HD23	1.87	0.57
3:D:1333:HIS:ND1	3:D:1421:LEU:HD23	2.18	0.57
3:D:1425:THR:HG23	3:D:1426:LYS:N	2.18	0.57
3:D:434:ARG:HB2	3:D:447:VAL:HG13	1.85	0.57
3:D:929:ARG:HH11	3:D:929:ARG:HG3	1.69	0.57
5:F:154:LYS:O	5:F:158:GLU:HG3	2.04	0.57
1:K:133:GLU:HG2	1:K:134:GLU:H	1.68	0.57
1:K:13:VAL:HG12	1:K:15:THR:HG22	1.86	0.57
1:K:5:LYS:O	1:K:8:ALA:HB2	2.04	0.57
2:M:573:ARG:HG3	2:M:698:ASP:O	2.04	0.57
2:M:707:ARG:HH12	2:M:709:GLU:HB2	1.69	0.57
3:N:1109:GLU:HG2	3:N:1202:GLN:H	1.68	0.57
3:N:132:TYR:HA	9:N:9655:HOH:O	2.04	0.57
3:N:1478:SER:OG	3:N:1480:PHE:HB3	2.04	0.57
4:O:31:LEU:HD21	4:O:60:ALA:HB2	1.85	0.57
5:P:131:VAL:HG12	5:P:181:GLU:HG3	1.87	0.57
5:P:350:LEU:HA	5:P:422:LEU:HD13	1.86	0.57
5:P:75:ILE:HB	9:P:3733:HOH:O	2.02	0.57
1:A:191:ASP:HB3	9:A:9741:HOH:O	2.04	0.57
2:C:362:GLY:HA3	2:C:367:LEU:HD22	1.84	0.57
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.84	0.57
3:D:1223:ILE:HD12	3:D:1223:ILE:H	1.69	0.57
3:D:1409:ALA:HB3	9:D:9722:HOH:O	2.05	0.57
3:D:32:ILE:HG22	5:F:258:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:466:LYS:HE3	9:D:2265:HOH:O	2.03	0.57
3:D:969:ARG:O	3:D:972:LEU:HB3	2.04	0.57
3:D:970:LYS:HB2	3:D:970:LYS:NZ	2.19	0.57
1:L:30:ARG:NH2	2:M:854:PRO:HG3	2.19	0.57
2:M:144:PRO:HB3	9:M:2335:HOH:O	2.03	0.57
2:M:428:ARG:HE	2:M:451:LEU:HD21	1.69	0.57
2:M:598:GLU:O	2:M:651:LYS:HG3	2.04	0.57
3:N:1033:GLN:HE21	3:N:1036:ARG:HD3	1.68	0.57
3:N:1494:ALA:HB2	9:N:2863:HOH:O	2.03	0.57
3:N:196:VAL:HG13	3:N:202:VAL:CG1	2.34	0.57
3:N:369:ALA:HB2	9:N:9972:HOH:O	2.04	0.57
9:M:9643:HOH:O	3:N:647:ARG:HG2	2.04	0.57
3:N:679:ARG:HH22	3:N:681:ARG:HE	1.51	0.57
3:N:87:ARG:HB3	3:N:523:ASP:HB2	1.86	0.57
5:P:291:ILE:O	5:P:295:MET:HB2	2.04	0.57
5:P:358:LEU:CG	5:P:370:LYS:HG3	2.34	0.57
1:A:11:PHE:CD1	1:B:225:PHE:HA	2.39	0.57
2:C:1060:ILE:HG23	2:C:1061:GLU:N	2.19	0.57
2:C:175:GLU:HB3	2:C:183:SER:OG	2.03	0.57
2:C:910:LYS:HB2	2:C:913:GLU:OE1	2.04	0.57
3:D:1418:LYS:HB3	9:D:2451:HOH:O	2.03	0.57
3:D:207:PHE:CB	3:D:208:PRO:HD2	2.35	0.57
3:D:805:GLU:OE1	3:D:809:PRO:HD2	2.04	0.57
2:M:3:ILE:HG12	9:M:9707:HOH:O	2.05	0.57
2:M:430:VAL:HG11	9:N:2751:HOH:O	2.04	0.57
3:N:540:LEU:HA	3:N:543:LEU:HD12	1.86	0.57
3:N:707:THR:HG21	3:N:713:ILE:HD12	1.87	0.57
5:P:130:VAL:HG21	5:P:159:ILE:HG21	1.87	0.57
1:A:89:PHE:CZ	1:A:146:ARG:HB2	2.39	0.57
2:C:209:ARG:HB3	9:C:2024:HOH:O	2.03	0.57
2:C:599:GLU:HG2	2:C:600:ASP:N	2.19	0.57
2:C:874:LEU:O	3:D:1029:ARG:HD2	2.04	0.57
3:D:1088:THR:HA	9:D:2611:HOH:O	2.05	0.57
3:D:1132:LEU:HD21	9:D:9739:HOH:O	2.04	0.57
3:D:195:VAL:HG13	9:D:2497:HOH:O	2.04	0.57
2:M:861:LEU:HD23	2:M:862:PRO:HD2	1.86	0.57
3:N:1314:LYS:HG2	9:N:9784:HOH:O	2.04	0.57
3:N:774:SER:HB3	3:N:1362:LYS:O	2.05	0.57
3:N:1432:LYS:HD2	3:N:1433:SER:H	1.70	0.57
5:P:262:VAL:HG12	5:P:266:GLU:OE2	2.05	0.57
5:P:356:LYS:HB3	9:P:6439:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:95:THR:HB	5:P:96:LEU:HD23	1.86	0.57
1:A:207:PRO:HB2	9:A:9571:HOH:O	2.05	0.57
1:B:117:VAL:HB	9:B:9771:HOH:O	2.05	0.57
1:B:123:MET:C	1:B:125:PRO:HD3	2.24	0.57
1:B:156:HIS:CE1	1:B:166:PRO:HB3	2.39	0.57
1:B:176:ARG:HD2	1:B:200:TRP:CE3	2.40	0.57
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.85	0.57
2:C:535:SER:O	2:C:538:GLN:HG2	2.03	0.57
2:C:626:ARG:HB2	2:C:639:GLN:HE21	1.69	0.57
2:C:644:VAL:HG22	2:C:647:GLN:OE1	2.04	0.57
3:D:1235:GLN:C	3:D:1359:GLN:HE22	2.07	0.57
3:D:1307:LYS:CD	3:D:1307:LYS:H	2.16	0.57
3:D:15:PRO:HA	3:D:18:ILE:HG12	1.86	0.57
3:D:486:ARG:HA	3:D:489:ARG:HG2	1.87	0.57
3:D:704:ARG:HB2	3:D:736:PHE:HD2	1.70	0.57
5:F:82:ARG:HG2	5:F:86:HIS:NE2	2.19	0.57
1:L:132:LEU:HG	1:L:136:GLY:HA3	1.85	0.57
1:L:41:ARG:CZ	1:L:177:VAL:HG23	2.34	0.57
2:M:31:GLN:HB3	2:M:71:TYR:OH	2.04	0.57
2:M:589:ARG:HB2	2:M:589:ARG:HH11	1.68	0.57
2:M:537:LYS:HG3	2:M:905:ILE:HD11	1.87	0.57
2:M:916:GLU:HA	9:M:9951:HOH:O	2.04	0.57
2:M:957:LYS:HG2	9:M:9918:HOH:O	2.03	0.57
3:N:1353:GLN:HB3	3:N:1357:ARG:NE	2.19	0.57
3:N:117:ASP:HB2	3:N:495:ARG:CZ	2.35	0.57
3:N:699:VAL:HG11	3:N:717:GLN:HE21	1.70	0.57
4:O:88:GLU:HA	4:O:91:ARG:HD2	1.86	0.57
1:A:57:TYR:CE2	1:A:161:ARG:HD2	2.40	0.57
1:B:220:GLU:HG2	9:B:9739:HOH:O	2.04	0.57
2:C:571:LEU:HG	9:C:2194:HOH:O	2.05	0.57
2:C:739:GLU:HG3	9:C:2340:HOH:O	2.05	0.57
3:D:491:LYS:HG3	9:D:9968:HOH:O	2.05	0.57
3:D:64:LYS:HD3	5:F:376:ILE:O	2.04	0.57
3:D:965:GLU:HA	3:D:968:ASP:OD2	2.04	0.57
3:D:96:ALA:HB3	9:D:2030:HOH:O	2.04	0.57
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.39	0.57
1:K:162:ILE:HD13	9:M:9894:HOH:O	2.03	0.57
2:M:1000:MET:HB3	2:M:1002:GLU:HG3	1.86	0.57
2:M:285:LEU:HG	2:M:287:GLY:O	2.05	0.57
2:M:393:GLN:HB3	7:M:8002:RBT:H25	1.87	0.57
3:N:209:ARG:NH2	3:N:397:LYS:HG3	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:380:GLU:O	3:N:382:GLU:N	2.37	0.57
3:N:480:GLU:OE2	3:N:484:PRO:HG2	2.04	0.57
3:N:536:ALA:HA	5:P:315:VAL:O	2.04	0.57
1:B:87:VAL:HG21	1:B:144:VAL:HG11	1.86	0.57
2:C:1042:ALA:HB3	3:D:710:ARG:HB3	1.86	0.57
2:C:1055:LEU:CD2	2:C:1079:PRO:HG3	2.35	0.57
2:C:113:VAL:HG13	9:C:9695:HOH:O	2.04	0.57
2:C:239:PHE:HE1	2:C:250:ARG:HB3	1.69	0.57
2:C:358:ARG:NH2	2:C:374:ASN:HB3	2.14	0.57
2:C:329:GLY:H	2:C:488:ALA:HB3	1.68	0.57
2:C:430:VAL:CG1	3:D:1075:HIS:HA	2.35	0.57
3:D:1104:GLU:HA	3:D:1461:GLY:HA2	1.86	0.57
3:D:776:GLU:HB3	3:D:912:LYS:HE2	1.87	0.57
3:D:913:ASP:HB3	9:D:9764:HOH:O	2.04	0.57
5:F:286:PRO:HD3	9:F:9783:HOH:O	2.04	0.57
1:L:115:LEU:O	1:L:115:LEU:HD12	2.04	0.57
1:L:18:ARG:O	1:L:207:PRO:HD3	2.05	0.57
2:M:352:ALA:HA	2:M:355:VAL:HG12	1.87	0.57
2:M:569:VAL:HG11	2:M:996:LYS:NZ	2.19	0.57
2:M:630:ARG:HA	2:M:705:ILE:CD1	2.35	0.57
3:N:1019:PRO:HB2	9:N:9719:HOH:O	2.04	0.57
1:L:65:PHE:CD1	3:N:813:LEU:HD22	2.39	0.57
9:N:2624:HOH:O	5:P:140:ARG:HB2	2.05	0.57
1:A:206:THR:CG2	1:A:209:GLU:H	2.17	0.57
2:C:436:GLY:HA3	2:C:469:THR:OG1	2.04	0.57
2:C:553:ASP:OD1	2:C:843:HIS:ND1	2.38	0.57
2:C:918:LEU:HB3	2:C:968:LEU:HD23	1.87	0.57
3:D:1147:ARG:O	3:D:1165:TYR:HA	2.05	0.57
2:M:1017:THR:HG23	9:M:9737:HOH:O	2.05	0.57
2:M:601:GLY:O	2:M:648:ARG:HA	2.05	0.57
2:M:602:GLU:HB3	9:M:2158:HOH:O	2.04	0.57
3:N:1063:GLU:HG3	3:N:1064:GLY:H	1.70	0.57
3:N:1417:TRP:HA	9:N:9876:HOH:O	2.04	0.57
3:N:510:GLU:HG3	9:N:9632:HOH:O	2.05	0.57
4:O:21:VAL:HG12	9:O:4298:HOH:O	2.03	0.57
5:P:138:SER:O	5:P:141:VAL:HG12	2.04	0.57
5:P:262:VAL:HG23	9:P:3903:HOH:O	2.04	0.57
2:C:289:THR:HG22	2:C:290:LEU:H	1.69	0.56
2:C:516:ARG:HG3	3:D:1068:LEU:HD13	1.87	0.56
3:D:393:ILE:HG22	9:D:9647:HOH:O	2.03	0.56
3:D:565:ILE:HB	5:F:84:TYR:CD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:969:ARG:HG3	3:D:970:LYS:N	2.20	0.56
5:F:291:ILE:O	5:F:295:MET:HB2	2.05	0.56
1:K:61:VAL:HG21	1:K:68:ILE:HD11	1.87	0.56
1:L:80:LEU:HG	3:N:844:ALA:HB2	1.86	0.56
2:M:571:LEU:HD21	2:M:700:TYR:HA	1.87	0.56
2:M:719:PRO:HB2	9:M:9649:HOH:O	2.04	0.56
2:M:755:LEU:HB2	2:M:790:LEU:HG	1.87	0.56
3:N:486:ARG:O	3:N:486:ARG:HD3	2.05	0.56
3:N:693:GLU:HA	4:O:48:MET:HE1	1.86	0.56
3:N:807:ALA:HB2	3:N:833:GLU:OE1	2.04	0.56
3:N:987:GLU:HA	9:N:9775:HOH:O	2.05	0.56
5:P:132:ARG:HE	5:P:184:ARG:NH1	2.03	0.56
5:P:385:GLU:O	5:P:397:ILE:HD13	2.04	0.56
1:A:205:VAL:HG23	1:A:206:THR:N	2.20	0.56
2:C:147:TYR:HE2	2:C:280:LYS:HZ3	1.53	0.56
2:C:462:ASP:CB	2:C:468:ARG:HD2	2.35	0.56
2:C:605:LYS:HD2	2:C:612:VAL:CG2	2.35	0.56
3:D:955:VAL:HB	3:D:1011:PHE:HE1	1.68	0.56
3:D:102:ILE:HG13	9:D:9670:HOH:O	2.05	0.56
3:D:1320:GLU:H	3:D:1323:GLN:NE2	2.02	0.56
3:D:1389:LEU:HG	3:D:1390:LEU:H	1.70	0.56
3:D:1422:MET:HB2	3:D:1426:LYS:HD3	1.86	0.56
3:D:1462:LEU:HB3	3:D:1472:ILE:HD12	1.87	0.56
3:D:207:PHE:HB3	3:D:208:PRO:HD2	1.86	0.56
4:E:48:MET:N	4:E:54:LEU:HB2	2.20	0.56
4:E:33:HIS:HD2	4:E:89:MET:HE2	1.70	0.56
1:L:100:LEU:HB3	9:L:3994:HOH:O	2.06	0.56
3:N:1321:ALA:HB3	9:N:9918:HOH:O	2.04	0.56
3:N:136:ASP:CB	3:N:137:PRO:HD3	2.32	0.56
3:N:142:LEU:HD13	9:N:2845:HOH:O	2.05	0.56
3:N:197:SER:HB2	3:N:205:TYR:CZ	2.40	0.56
3:N:552:ASN:O	3:N:556:LYS:HD3	2.05	0.56
3:N:633:VAL:HG22	3:N:635:PRO:HD3	1.86	0.56
3:N:844:ALA:O	3:N:867:ARG:HB3	2.04	0.56
3:N:945:SER:OG	3:N:947:ILE:HG23	2.05	0.56
1:A:9:PRO:HD2	1:B:224:TYR:CE1	2.39	0.56
2:C:412:ALA:CB	2:C:451:LEU:HB3	2.35	0.56
3:D:825:ALA:HB1	9:D:2139:HOH:O	2.05	0.56
3:D:924:MET:O	3:D:927:THR:HB	2.05	0.56
2:M:1097:LEU:HD22	2:M:1097:LEU:H	1.70	0.56
2:M:198:ARG:HH21	2:M:203:ASP:HB3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:428:ARG:NE	2:M:451:LEU:HD21	2.20	0.56
3:N:1145:TYR:CE2	3:N:1168:MET:HB2	2.40	0.56
3:N:911:LEU:HG	9:N:9875:HOH:O	2.05	0.56
1:A:74:ASP:OD1	1:A:77:GLU:HB2	2.04	0.56
1:B:124:ASN:HA	9:B:9553:HOH:O	2.03	0.56
1:B:57:TYR:HB3	1:B:141:GLU:CG	2.32	0.56
2:C:773:LEU:O	2:C:777:ILE:HG13	2.04	0.56
3:D:1234:THR:HG21	9:D:2202:HOH:O	2.05	0.56
3:D:49:ILE:HB	3:D:50:PHE:CD1	2.40	0.56
3:D:644:LEU:HD12	3:D:645:PRO:CD	2.36	0.56
3:D:72:VAL:HG12	9:D:2118:HOH:O	2.05	0.56
3:D:921:ARG:HA	9:D:2819:HOH:O	2.03	0.56
5:F:109:GLY:O	5:F:113:ILE:HG13	2.05	0.56
5:F:149:GLU:HA	5:F:149:GLU:OE1	2.05	0.56
1:K:125:PRO:HD2	9:K:3778:HOH:O	2.04	0.56
1:L:101:LEU:HB2	1:L:114:PHE:CD2	2.41	0.56
2:M:206:THR:HA	9:M:2520:HOH:O	2.06	0.56
2:M:51:THR:HB	2:M:348:LEU:HD23	1.86	0.56
3:N:178:LEU:HD21	9:N:9629:HOH:O	2.05	0.56
3:N:645:PRO:HG3	3:N:725:SER:O	2.04	0.56
4:O:66:LYS:HD2	9:O:5393:HOH:O	2.06	0.56
5:P:166:LEU:O	5:P:171:LYS:HB2	2.05	0.56
5:P:361:LEU:HD13	5:P:366:ALA:HB1	1.86	0.56
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.88	0.56
2:C:89:THR:HA	2:C:129:ILE:O	2.06	0.56
3:D:1127:GLU:HG3	3:D:1133:ARG:NH1	2.17	0.56
3:D:469:ASP:HB2	9:D:2079:HOH:O	2.04	0.56
5:F:101:GLU:HG2	9:F:9941:HOH:O	2.06	0.56
5:F:136:LEU:HD12	5:F:137:GLY:N	2.20	0.56
5:F:404:ALA:HB3	9:F:9597:HOH:O	2.04	0.56
1:L:102:LYS:HG3	1:L:139:ASN:HB2	1.87	0.56
1:L:228:PRO:O	1:L:229:GLN:HG3	2.06	0.56
2:M:532:MET:HG3	2:M:533:ASP:N	2.21	0.56
2:M:860:HIS:HE2	2:M:975:TYR:HB2	1.68	0.56
3:N:119:SER:H	3:N:123:LEU:HB2	1.71	0.56
3:N:197:SER:CB	3:N:203:ALA:HB3	2.28	0.56
3:N:171:LEU:HB2	3:N:390:PRO:HA	1.86	0.56
3:N:397:LYS:NZ	3:N:399:ARG:HH21	2.03	0.56
3:N:493:ARG:O	3:N:497:GLU:HG3	2.06	0.56
3:N:59:ALA:HB3	9:N:2262:HOH:O	2.04	0.56
5:P:163:LEU:HB3	5:P:174:LEU:CG	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.41	0.56
1:B:205:VAL:HG11	9:B:9687:HOH:O	2.05	0.56
2:C:209:ARG:O	2:C:213:ALA:HB2	2.05	0.56
2:C:220:GLY:HA3	9:C:9659:HOH:O	2.06	0.56
3:D:134:VAL:HG12	3:D:152:LEU:HB3	1.87	0.56
3:D:704:ARG:HB2	3:D:736:PHE:CD2	2.41	0.56
3:D:708:LEU:O	3:D:1227:GLN:HG2	2.05	0.56
3:D:58:CYS:HA	3:D:78:VAL:HG11	1.88	0.56
3:D:813:LEU:O	3:D:817:GLU:HB2	2.05	0.56
5:F:102:LEU:HD12	5:F:187:LEU:HG	1.86	0.56
1:L:49:PRO:HD2	9:L:3855:HOH:O	2.05	0.56
2:M:252:LYS:NZ	2:M:296:GLY:HA3	2.21	0.56
2:M:629:TYR:HB2	2:M:637:LEU:HG	1.87	0.56
2:M:409:ARG:HH22	7:M:8002:RBT:H18	1.69	0.56
2:M:913:GLU:O	2:M:916:GLU:HB3	2.05	0.56
3:N:104:PHE:CD2	3:N:1448:THR:HG23	2.41	0.56
4:O:48:MET:CB	4:O:54:LEU:HB2	2.36	0.56
5:P:102:LEU:HD13	5:P:187:LEU:HG	1.86	0.56
5:P:291:ILE:CG2	5:P:304:VAL:HG21	2.36	0.56
1:B:206:THR:HG23	1:B:209:GLU:H	1.71	0.56
2:C:433:THR:HG21	2:C:488:ALA:CB	2.30	0.56
2:C:704:HIS:CG	2:C:831:ARG:HH21	2.22	0.56
3:D:10:ILE:HG13	3:D:1434:TRP:CZ2	2.41	0.56
3:D:1205:TYR:HE1	3:D:1221:VAL:HG13	1.70	0.56
3:D:1277:ILE:CD1	3:D:1301:LYS:HB2	2.35	0.56
3:D:148:GLU:CB	3:D:151:GLN:HE21	2.19	0.56
3:D:493:ARG:HH12	3:D:1390:LEU:HB2	1.69	0.56
3:D:754:PHE:HZ	4:E:21:VAL:HG13	1.69	0.56
1:L:101:LEU:HG	1:L:114:PHE:HA	1.87	0.56
2:M:169:GLY:HA2	2:M:263:ASP:CB	2.26	0.56
2:M:208:ALA:HB1	2:M:218:VAL:HG13	1.87	0.56
2:M:346:VAL:HA	9:M:2321:HOH:O	2.06	0.56
2:M:100:LEU:HG	2:M:368:THR:HG23	1.86	0.56
2:M:66:LEU:HD23	9:M:2181:HOH:O	2.04	0.56
2:M:807:ARG:NH1	2:M:807:ARG:HB2	2.20	0.56
3:N:1342:GLU:HG2	9:N:2451:HOH:O	2.05	0.56
3:N:1364:HIS:ND1	3:N:1366:LYS:HB2	2.21	0.56
3:N:9:ARG:NH1	3:N:506:GLY:HA2	2.09	0.56
3:N:65:ARG:HG3	3:N:66:GLN:H	1.70	0.56
1:A:35:THR:HG21	1:B:43:ILE:HD11	1.88	0.56
1:K:42:ARG:HG2	1:K:42:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:201:THR:HB	9:L:3796:HOH:O	2.06	0.56
1:L:212:ASN:O	1:L:215:VAL:HG22	2.05	0.56
2:M:24:GLU:HB3	9:M:9804:HOH:O	2.04	0.56
2:M:290:LEU:HB3	2:M:302:VAL:HG11	1.86	0.56
2:M:34:VAL:HB	2:M:38:LYS:CG	2.32	0.56
2:M:405:ARG:HD2	2:M:442:GLU:CD	2.26	0.56
3:N:1011:PHE:HB3	3:N:1021:TYR:CD1	2.41	0.56
3:N:12:LEU:HD11	3:N:512:MET:HG2	1.88	0.56
4:O:18:ARG:HH22	4:O:77:GLU:HG2	1.71	0.56
1:A:206:THR:HG22	1:A:209:GLU:H	1.69	0.56
1:A:209:GLU:O	1:A:213:GLN:HG3	2.05	0.56
1:B:38:ASN:OD1	2:C:979:THR:HA	2.06	0.56
3:D:141:ILE:CG2	3:D:161:LEU:HD21	2.36	0.56
3:D:424:GLY:HA2	3:D:435:VAL:O	2.05	0.56
3:D:68:PHE:HA	3:D:71:LYS:NZ	2.21	0.56
5:F:403:LYS:HA	5:F:403:LYS:NZ	2.21	0.56
1:K:157:GLY:HA3	9:K:5169:HOH:O	2.06	0.56
1:L:143:ARG:HH11	1:L:158:ILE:HG23	1.71	0.56
2:M:178:PRO:HA	9:M:9615:HOH:O	2.05	0.56
2:M:195:LEU:HD12	2:M:234:ALA:HB1	1.86	0.56
2:M:254:VAL:HG11	9:M:2051:HOH:O	2.04	0.56
2:M:329:GLY:N	2:M:488:ALA:HB3	2.21	0.56
2:M:926:PHE:O	2:M:930:LYS:HG3	2.06	0.56
1:K:193:ASP:HA	2:M:938:LYS:HZ2	1.70	0.56
3:N:1124:GLN:HG2	3:N:1133:ARG:HG2	1.87	0.56
3:N:1287:GLU:HA	9:N:2127:HOH:O	2.06	0.56
3:N:96:ALA:H	3:N:551:ASN:HD21	1.53	0.56
5:P:416:ARG:NH1	5:P:419:ARG:HB2	2.21	0.56
1:B:112:ARG:HH12	1:B:126:ASP:HA	1.71	0.56
2:C:1088:LEU:HB2	9:D:9563:HOH:O	2.04	0.56
2:C:715:THR:CG2	2:C:717:LEU:HG	2.35	0.56
3:D:1155:VAL:HG11	3:D:1183:ILE:HD11	1.88	0.56
3:D:1102:THR:HG22	3:D:1222:GLY:CA	2.36	0.56
3:D:1280:VAL:HG23	3:D:1295:GLU:O	2.05	0.56
3:D:136:ASP:HB3	3:D:137:PRO:CD	2.23	0.56
3:D:711:LEU:HD12	3:D:778:LEU:HD23	1.87	0.56
2:M:282:GLY:HA2	2:M:308:ARG:NH2	2.20	0.56
2:M:461:VAL:HG13	2:M:465:GLY:HA2	1.87	0.56
2:M:964:LYS:O	2:M:968:LEU:HD23	2.04	0.56
3:N:112:ILE:HG13	3:N:124:GLU:OE2	2.06	0.56
3:N:1271:LYS:HG2	3:N:1272:ALA:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1402:ALA:HB2	3:N:1415:VAL:CG2	2.35	0.56
3:N:1465:ASN:ND2	3:N:1470:ARG:HD3	2.21	0.56
3:N:631:ILE:HG12	3:N:743:ASP:O	2.06	0.56
5:P:152:ASP:HB2	5:P:153:PRO:HD3	1.87	0.56
2:C:1109:VAL:HG22	3:D:3:LYS:HG3	1.88	0.56
2:C:378:LEU:O	2:C:382:ILE:HG13	2.06	0.56
2:C:532:MET:HG3	2:C:533:ASP:N	2.21	0.56
2:C:583:LEU:O	2:C:587:VAL:HG23	2.05	0.56
3:D:103:TRP:HD1	9:D:9830:HOH:O	1.88	0.56
3:D:1333:HIS:O	3:D:1336:LEU:HB3	2.06	0.56
3:D:1367:HIS:O	3:D:1371:VAL:HG23	2.05	0.56
3:D:534:ARG:HD3	9:D:9954:HOH:O	2.06	0.56
3:D:711:LEU:CD1	3:D:778:LEU:HD23	2.36	0.56
2:C:949:LYS:HD2	3:D:796:ARG:HH21	1.70	0.56
3:D:866:VAL:HG13	9:D:9991:HOH:O	2.04	0.56
5:F:277:GLN:HG3	9:F:9616:HOH:O	2.06	0.56
1:L:58:ILE:HD12	1:L:138:LEU:HD11	1.86	0.56
2:M:244:PRO:HB2	9:M:2065:HOH:O	2.05	0.56
2:M:557:ARG:NH1	2:M:879:ARG:HD3	2.21	0.56
3:N:153:LEU:HD23	9:N:9640:HOH:O	2.06	0.56
3:N:18:ILE:HG23	3:N:518:PRO:CG	2.33	0.56
3:N:545:ARG:HD3	9:N:2016:HOH:O	2.06	0.56
2:M:1007:ALA:HB2	3:N:648:MET:CE	2.36	0.56
4:O:17:TYR:CD2	4:O:17:TYR:N	2.72	0.56
5:P:358:LEU:HD11	5:P:370:LYS:HE3	1.87	0.56
1:A:224:TYR:CD2	1:B:9:PRO:HG2	2.41	0.55
2:C:959:PRO:O	2:C:963:LEU:HD23	2.06	0.55
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.86	0.55
3:D:1061:PHE:HA	9:D:9657:HOH:O	2.06	0.55
3:D:109:PRO:HD3	9:D:9737:HOH:O	2.05	0.55
3:D:1299:PHE:HB2	9:D:9590:HOH:O	2.05	0.55
3:D:1364:HIS:NE2	3:D:1366:LYS:HE3	2.21	0.55
3:D:181:ASP:O	3:D:185:VAL:HG23	2.06	0.55
9:C:9810:HOH:O	3:D:943:THR:HG21	2.06	0.55
3:D:963:TYR:CE2	3:D:1002:LYS:HB3	2.41	0.55
5:F:141:VAL:HA	9:F:9945:HOH:O	2.06	0.55
1:K:28:LEU:HD23	9:L:5369:HOH:O	2.07	0.55
1:K:9:PRO:HB3	1:K:25:LEU:HD21	1.88	0.55
1:L:33:GLY:O	1:L:195:LEU:HD22	2.06	0.55
2:M:223:ASP:OD1	2:M:224:GLU:HG2	2.07	0.55
2:M:256:TYR:HE1	2:M:293:PHE:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:418:LEU:HB3	9:M:9836:HOH:O	2.06	0.55
2:M:455:LEU:HD12	2:M:456:ALA:O	2.05	0.55
2:M:643:VAL:HG13	2:M:647:GLN:CD	2.26	0.55
2:M:71:TYR:H	2:M:71:TYR:HD2	1.54	0.55
2:M:852:ILE:HG12	9:M:2100:HOH:O	2.06	0.55
3:N:637:LEU:HD11	3:N:641:GLN:C	2.27	0.55
3:N:704:ARG:HD2	3:N:705:ALA:N	2.14	0.55
3:N:99:ALA:HA	3:N:575:GLN:HE22	1.71	0.55
5:P:128:ARG:HG2	9:P:4300:HOH:O	2.04	0.55
5:P:156:VAL:HB	9:P:5172:HOH:O	2.05	0.55
5:P:404:ALA:O	5:P:408:LEU:HD23	2.06	0.55
1:A:141:GLU:HG3	9:A:9639:HOH:O	2.07	0.55
1:A:198:ARG:HH21	2:C:932:GLU:HG2	1.71	0.55
3:D:1496:GLU:OE1	3:D:1500:LYS:HE3	2.06	0.55
3:D:178:LEU:HD12	3:D:200:ASP:HB2	1.89	0.55
3:D:187:LYS:CE	3:D:213:VAL:HG12	2.37	0.55
3:D:475:LYS:HA	3:D:478:LEU:HG	1.87	0.55
3:D:93:ILE:HG12	3:D:548:ILE:HD12	1.88	0.55
5:F:147:LEU:HD22	9:F:9955:HOH:O	2.05	0.55
2:M:1016:ILE:HG23	3:N:526:PRO:HG2	1.88	0.55
2:M:209:ARG:O	2:M:213:ALA:HB2	2.06	0.55
2:M:142:ARG:NH1	2:M:325:ILE:HG12	2.21	0.55
2:M:460:ARG:HG3	9:M:9945:HOH:O	2.06	0.55
2:M:495:THR:H	2:M:530:GLU:CD	2.09	0.55
2:M:671:ASN:ND2	2:M:993:PHE:HB2	2.21	0.55
3:N:1066:THR:CG2	3:N:1069:GLU:H	2.19	0.55
3:N:1428:ALA:O	3:N:1431:THR:HG23	2.05	0.55
3:N:397:LYS:HD3	9:N:2726:HOH:O	2.06	0.55
3:N:843:PHE:HE1	3:N:864:VAL:HG11	1.70	0.55
3:N:983:LEU:HA	3:N:987:GLU:OE2	2.06	0.55
5:P:113:ILE:HG23	5:P:127:ILE:CG2	2.36	0.55
5:P:291:ILE:HG13	9:P:4835:HOH:O	2.07	0.55
5:P:85:LEU:HB3	9:P:4001:HOH:O	2.06	0.55
1:A:117:VAL:HB	1:A:120:VAL:HG12	1.87	0.55
1:A:149:GLY:O	1:A:171:PHE:HB2	2.06	0.55
2:C:437:ARG:O	2:C:467:ILE:HD13	2.07	0.55
2:C:41:ASN:O	2:C:46:ALA:HB2	2.07	0.55
3:D:214:GLU:HB2	3:D:390:PRO:HD2	1.87	0.55
3:D:462:GLN:NE2	3:D:513:ILE:HB	2.22	0.55
3:D:844:ALA:O	3:D:867:ARG:HB3	2.05	0.55
1:L:27:PRO:O	1:L:28:LEU:HD23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:29:GLU:N	9:L:3706:HOH:O	2.39	0.55
2:M:267:TYR:CD1	2:M:272:ALA:HB1	2.41	0.55
2:M:660:ALA:HB1	2:M:667:ALA:O	2.05	0.55
2:M:676:ILE:O	2:M:676:ILE:HG23	2.06	0.55
2:M:880:MET:HE2	9:M:2314:HOH:O	2.06	0.55
2:M:976:ASP:CB	2:M:979:THR:HG22	2.37	0.55
2:M:577:PRO:HG3	2:M:993:PHE:CE2	2.42	0.55
3:N:1051:GLU:HG2	9:N:9879:HOH:O	2.06	0.55
3:N:1102:THR:HG22	3:N:1222:GLY:CA	2.36	0.55
5:P:299:TRP:HE3	9:P:4374:HOH:O	1.90	0.55
1:A:88:ARG:HD3	9:A:9724:HOH:O	2.06	0.55
2:C:50:GLU:HA	2:C:266:ARG:HH11	1.71	0.55
2:C:516:ARG:HD3	2:C:521:PRO:HA	1.87	0.55
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.42	0.55
2:C:69:LEU:HB2	2:C:97:ARG:HB2	1.87	0.55
3:D:1432:LYS:HZ1	3:D:1460:ILE:HG13	1.71	0.55
3:D:493:ARG:HH22	3:D:1389:LEU:CG	2.17	0.55
3:D:493:ARG:HG2	3:D:493:ARG:NH1	2.20	0.55
3:D:631:ILE:HG12	3:D:743:ASP:O	2.07	0.55
3:D:957:PRO:HG2	3:D:1007:VAL:HA	1.88	0.55
4:E:13:VAL:HG12	4:E:75:PHE:CE1	2.42	0.55
1:L:143:ARG:NH1	1:L:158:ILE:HD12	2.22	0.55
2:M:798:GLY:H	2:M:827:VAL:CG1	2.20	0.55
3:N:61:GLY:CA	3:N:64:LYS:HE3	2.35	0.55
3:N:756:GLN:O	3:N:760:ARG:HG2	2.06	0.55
3:N:984:THR:HG23	3:N:986:ARG:H	1.71	0.55
2:C:208:ALA:HA	2:C:218:VAL:HG22	1.89	0.55
2:C:199:VAL:HG13	2:C:235:LEU:CD2	2.36	0.55
2:C:413:LEU:HD21	2:C:448:ASN:HD21	1.72	0.55
2:C:569:VAL:HG23	2:C:635:THR:HG22	1.87	0.55
3:D:1196:THR:HG23	9:D:9568:HOH:O	2.06	0.55
3:D:36:THR:C	3:D:38:LYS:H	2.10	0.55
3:D:592:THR:N	3:D:600:LEU:HD21	2.21	0.55
3:D:603:LEU:O	3:D:606:ILE:HB	2.07	0.55
3:D:634:GLY:O	3:D:637:LEU:HB3	2.05	0.55
3:D:654:LYS:HD3	3:D:674:ARG:HH22	1.70	0.55
3:D:692:GLU:HG2	3:D:720:LEU:HD13	1.89	0.55
3:D:940:THR:O	3:D:943:THR:HG23	2.06	0.55
1:K:107:LYS:HE2	9:K:4981:HOH:O	2.07	0.55
9:K:6366:HOH:O	1:L:219:ARG:HD2	2.07	0.55
2:M:269:LEU:HD12	2:M:288:ARG:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.89	0.55
3:N:58:CYS:SG	3:N:59:ALA:N	2.79	0.55
3:N:634:GLY:O	3:N:637:LEU:HB3	2.07	0.55
3:N:679:ARG:NH1	3:N:681:ARG:HD2	2.22	0.55
2:M:984:GLU:OE1	3:N:945:SER:HA	2.06	0.55
5:P:139:ALA:HA	5:P:142:ARG:HG3	1.88	0.55
5:P:220:LEU:O	5:P:224:VAL:HG23	2.05	0.55
1:A:122:ILE:HB	9:A:9608:HOH:O	2.07	0.55
2:C:134:ARG:HH21	2:C:394:PHE:N	2.03	0.55
2:C:692:GLU:HG2	2:C:696:LYS:CE	2.33	0.55
2:C:769:PRO:HB3	9:F:9661:HOH:O	2.07	0.55
3:D:119:SER:H	3:D:123:LEU:HB2	1.71	0.55
3:D:591:VAL:HG12	3:D:592:THR:O	2.06	0.55
3:D:829:VAL:HG21	9:D:9902:HOH:O	2.07	0.55
3:D:957:PRO:HB3	3:D:959:GLU:OE1	2.05	0.55
1:K:41:ARG:O	1:K:45:LEU:HD12	2.05	0.55
2:M:167:LYS:HD2	2:M:168:ARG:HE	1.72	0.55
2:M:343:GLN:HG2	2:M:385:PHE:HB2	1.89	0.55
2:M:395:LYS:HE2	2:M:397:GLU:OE1	2.06	0.55
2:M:430:VAL:HG13	2:M:430:VAL:O	2.06	0.55
3:N:1047:LYS:HB3	3:N:1048:PRO:CD	2.36	0.55
3:N:105:VAL:HG21	3:N:128:TYR:CE2	2.38	0.55
3:N:1377:LYS:HA	9:N:9789:HOH:O	2.06	0.55
3:N:216:VAL:HG13	9:N:2148:HOH:O	2.06	0.55
3:N:907:GLU:O	3:N:911:LEU:HD13	2.06	0.55
4:O:84:ARG:CZ	4:O:84:ARG:HB2	2.37	0.55
1:A:85:LEU:HA	1:A:124:ASN:HD22	1.71	0.55
2:C:139:GLN:HB3	2:C:334:ARG:CD	2.36	0.55
2:C:437:ARG:NH2	2:C:469:THR:HG22	2.22	0.55
2:C:877:PRO:HG2	3:D:1023:MET:SD	2.46	0.55
3:D:1144:LEU:HA	3:D:1147:ARG:HG3	1.87	0.55
3:D:379:ALA:HB3	9:D:2344:HOH:O	2.05	0.55
2:M:11:GLU:HG2	9:M:9823:HOH:O	2.06	0.55
2:M:404:LEU:HA	2:M:407:LYS:CD	2.31	0.55
2:M:625:LEU:HD22	2:M:639:GLN:HB2	1.89	0.55
3:N:1194:CYS:HB3	3:N:1373:ARG:NH2	2.22	0.55
3:N:1472:ILE:HG22	3:N:1474:ALA:H	1.72	0.55
3:N:15:PRO:HG3	9:N:9590:HOH:O	2.07	0.55
3:N:86:ARG:HG2	3:N:523:ASP:OD1	2.07	0.55
2:M:1043:TYR:HA	3:N:710:ARG:HH21	1.70	0.55
3:N:814:ALA:HB3	9:N:9595:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:160:ASP:HA	5:P:163:LEU:HD12	1.88	0.55
2:C:1008:ARG:HE	2:C:1029:GLY:N	2.05	0.55
2:C:1008:ARG:NH2	2:C:1028:GLY:HA2	2.16	0.55
2:C:502:PRO:HG2	9:C:2171:HOH:O	2.07	0.55
2:C:72:ARG:HG3	2:C:72:ARG:HH11	1.71	0.55
2:C:80:GLN:HG2	2:C:90:TYR:HE2	1.72	0.55
3:D:119:SER:N	3:D:123:LEU:HB2	2.22	0.55
3:D:645:PRO:HG3	3:D:725:SER:O	2.06	0.55
3:D:704:ARG:HH11	3:D:738:ALA:HA	1.71	0.55
1:L:92:PRO:HD3	9:L:4614:HOH:O	2.05	0.55
2:M:200:LEU:HD13	2:M:300:ASP:CG	2.27	0.55
2:M:208:ALA:HA	2:M:218:VAL:HG22	1.88	0.55
2:M:41:ASN:O	2:M:46:ALA:HB2	2.06	0.55
2:M:56:GLU:HB2	2:M:64:LEU:HD23	1.89	0.55
2:M:584:GLU:O	2:M:588:VAL:HG13	2.06	0.55
3:N:1036:ARG:HH21	3:N:1042:ARG:CA	2.20	0.55
3:N:1118:ILE:CG2	3:N:1346:ARG:HH12	2.19	0.55
3:N:1434:TRP:CZ3	3:N:1457:ASP:HB2	2.41	0.55
1:A:125:PRO:HA	9:A:9608:HOH:O	2.06	0.55
1:B:26:GLU:HG2	1:B:27:PRO:HA	1.88	0.55
2:C:1001:VAL:HG23	9:C:2003:HOH:O	2.06	0.55
2:C:1058:ASP:OD2	2:C:1083:GLU:HB2	2.07	0.55
2:C:208:ALA:HB1	2:C:218:VAL:HG13	1.89	0.55
2:C:455:LEU:H	2:C:455:LEU:HD23	1.72	0.55
3:D:434:ARG:HB2	3:D:447:VAL:HG22	1.89	0.55
3:D:56:TYR:CE2	3:D:66:GLN:HA	2.42	0.55
3:D:570:GLU:HB2	5:F:214:GLN:NE2	2.22	0.55
4:E:26:ARG:NH1	4:E:30:LEU:HD13	2.21	0.55
5:F:163:LEU:HB3	5:F:174:LEU:CG	2.37	0.55
2:M:1008:ARG:HH21	2:M:1029:GLY:H	1.55	0.55
2:M:604:ALA:HB3	2:M:612:VAL:O	2.07	0.55
3:N:1147:ARG:O	3:N:1165:TYR:HA	2.07	0.55
3:N:481:MET:HB3	3:N:1388:ARG:HH21	1.71	0.55
4:O:33:HIS:CG	4:O:89:MET:HG2	2.42	0.55
5:P:192:LEU:O	5:P:196:VAL:HG23	2.07	0.55
1:A:138:LEU:HG	9:A:9590:HOH:O	2.07	0.55
1:B:14:ARG:HH22	1:B:24:VAL:HG21	1.72	0.55
2:C:10:ARG:HA	2:C:10:ARG:NE	2.21	0.55
2:C:234:ALA:HB3	9:C:2169:HOH:O	2.05	0.55
2:C:335:THR:HG21	9:C:9892:HOH:O	2.06	0.55
2:C:578:VAL:HA	2:C:900:ARG:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:838:LYS:HD2	2:C:846:LYS:NZ	2.21	0.55
3:D:1455:LYS:C	3:D:1455:LYS:HD3	2.28	0.55
3:D:491:LYS:HD3	3:D:492:ALA:N	2.22	0.55
3:D:570:GLU:OE2	5:F:214:GLN:HG3	2.05	0.55
5:F:166:LEU:O	5:F:171:LYS:HB2	2.06	0.55
2:M:1054:THR:HG22	2:M:1059:ASP:CB	2.33	0.55
3:N:1384:PRO:HD2	9:N:2419:HOH:O	2.06	0.55
3:D:633:VAL:C	3:D:635:PRO:HD3	2.28	0.54
2:M:367:LEU:HD23	2:M:371:LYS:HZ2	1.71	0.54
2:M:724:ARG:HG3	2:M:741:GLY:N	2.21	0.54
3:N:1353:GLN:HE21	3:N:1357:ARG:HE	1.54	0.54
3:N:1462:LEU:HD22	3:N:1472:ILE:CG2	2.37	0.54
9:M:9708:HOH:O	3:N:1472:ILE:HG21	2.07	0.54
3:N:427:VAL:HG21	3:N:435:VAL:HB	1.88	0.54
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.42	0.54
1:B:184:THR:O	1:B:192:LEU:HB2	2.07	0.54
2:C:100:LEU:HD12	2:C:101:ILE:O	2.07	0.54
2:C:115:LEU:HD22	2:C:373:VAL:CG1	2.34	0.54
2:C:11:GLU:HG2	2:C:537:LYS:NZ	2.21	0.54
2:C:162:ILE:HD12	2:C:172:ILE:HB	1.89	0.54
2:C:200:LEU:HD13	2:C:300:ASP:CG	2.28	0.54
2:C:294:GLU:HB2	9:C:2414:HOH:O	2.06	0.54
2:C:355:VAL:HG21	9:C:9583:HOH:O	2.07	0.54
2:C:332:ARG:NE	2:C:464:LEU:HD11	2.20	0.54
2:C:722:ILE:CD1	2:C:823:VAL:HG21	2.37	0.54
2:C:904:PRO:HA	9:C:9895:HOH:O	2.07	0.54
3:D:956:ILE:HG12	3:D:1039:CYS:O	2.06	0.54
3:D:1068:LEU:HD23	3:D:1072:ILE:HG12	1.88	0.54
3:D:1204:CYS:HB3	9:D:9616:HOH:O	2.07	0.54
3:D:397:LYS:HZ3	3:D:399:ARG:HH21	1.54	0.54
3:D:417:PRO:HD2	9:D:2246:HOH:O	2.07	0.54
3:D:525:ARG:HA	3:D:538:SER:CB	2.37	0.54
3:D:599:PRO:HB2	9:D:2237:HOH:O	2.07	0.54
3:D:865:THR:HG23	3:D:874:GLU:HG2	1.89	0.54
3:D:895:VAL:O	3:D:899:LEU:HG	2.07	0.54
4:E:54:LEU:HG	4:E:58:PRO:CG	2.37	0.54
5:F:195:VAL:HG22	5:F:243:ILE:HD13	1.88	0.54
1:K:91:ASN:H	1:K:94:LEU:HD12	1.72	0.54
2:M:218:VAL:O	2:M:221:LEU:HG	2.08	0.54
2:M:50:GLU:HA	2:M:266:ARG:NH1	2.21	0.54
2:M:572:ILE:HD11	2:M:698:ASP:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:937:ASP:HB3	2:M:940:GLU:H	1.72	0.54
3:N:1087:ARG:HA	3:N:1090:ASP:HB2	1.87	0.54
3:N:516:ALA:O	3:N:518:PRO:HD3	2.07	0.54
1:B:65:PHE:CD1	3:D:813:LEU:HD22	2.42	0.54
2:C:101:ILE:HG23	2:C:107:LEU:CD2	2.36	0.54
2:C:136:ILE:CG2	2:C:336:VAL:HG13	2.37	0.54
2:C:433:THR:CG2	2:C:488:ALA:HB1	2.32	0.54
2:C:598:GLU:O	2:C:651:LYS:HG3	2.07	0.54
2:C:666:LEU:CD2	2:C:668:LEU:HD11	2.36	0.54
2:C:70:GLU:HB3	9:C:9739:HOH:O	2.06	0.54
2:C:498:GLN:CD	3:D:1068:LEU:HD12	2.27	0.54
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.42	0.54
3:D:1405:GLU:HA	9:D:9722:HOH:O	2.05	0.54
3:D:145:VAL:HG11	9:D:9838:HOH:O	2.07	0.54
3:D:1459:LEU:HB2	3:D:1470:ARG:HH12	1.73	0.54
3:D:183:GLU:HA	3:D:186:VAL:HG12	1.89	0.54
3:D:186:VAL:HG11	3:D:213:VAL:HB	1.89	0.54
3:D:984:THR:HG22	3:D:987:GLU:H	1.71	0.54
3:D:996:TRP:CG	3:D:1056:PRO:HG2	2.42	0.54
3:D:998:GLU:HA	9:D:2134:HOH:O	2.07	0.54
5:F:92:PRO:HG3	9:F:9899:HOH:O	2.06	0.54
1:K:124:ASN:OD1	1:K:127:LEU:HB3	2.07	0.54
1:K:149:GLY:O	1:K:171:PHE:HB2	2.06	0.54
2:M:1049:LEU:O	2:M:1053:LEU:HG	2.07	0.54
2:M:875:GLY:HA2	9:M:9982:HOH:O	2.08	0.54
3:N:1045:MET:HB3	3:N:1072:ILE:HG22	1.89	0.54
3:N:199:LEU:HD21	9:N:2547:HOH:O	2.07	0.54
4:O:47:LYS:HA	4:O:54:LEU:HB3	1.89	0.54
1:A:23:PHE:CD1	1:A:211:LEU:HD23	2.43	0.54
1:A:86:VAL:HG13	1:A:124:ASN:HB2	1.90	0.54
2:C:197:LEU:HB3	2:C:202:TYR:HB2	1.88	0.54
2:C:352:ALA:HB2	9:C:2449:HOH:O	2.08	0.54
2:C:360:LEU:HD12	9:C:9932:HOH:O	2.06	0.54
2:C:604:ALA:HB3	2:C:612:VAL:O	2.07	0.54
2:C:676:ILE:O	2:C:676:ILE:HG23	2.08	0.54
2:C:724:ARG:O	2:C:734:LEU:HD11	2.08	0.54
3:D:126:VAL:O	3:D:132:TYR:HD1	1.91	0.54
3:D:128:TYR:CE1	3:D:461:ILE:HG13	2.43	0.54
3:D:1385:GLY:HA2	9:D:2643:HOH:O	2.07	0.54
3:D:1381:VAL:HG23	3:D:1391:GLU:O	2.08	0.54
3:D:1460:ILE:HB	9:D:2209:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5:LYS:HE2	9:L:5741:HOH:O	2.08	0.54
2:M:172:ILE:H	2:M:172:ILE:HD12	1.72	0.54
2:M:276:LYS:O	2:M:280:LYS:HB2	2.07	0.54
2:M:904:PRO:HG3	9:M:9570:HOH:O	2.06	0.54
3:N:1289:LYS:HD3	9:N:9605:HOH:O	2.07	0.54
3:N:430:ASP:HB3	9:N:9974:HOH:O	2.07	0.54
3:N:861:GLN:H	3:N:861:GLN:CD	2.11	0.54
1:A:18:ARG:O	1:A:207:PRO:HD3	2.06	0.54
2:C:135:VAL:CG1	2:C:407:LYS:HA	2.33	0.54
3:D:130:SER:HB3	3:D:132:TYR:CE1	2.43	0.54
3:D:660:LYS:HG2	3:D:694:VAL:HG22	1.89	0.54
2:C:885:ILE:HD12	3:D:949:ILE:HB	1.90	0.54
5:F:123:ASP:H	5:F:126:LEU:HD22	1.72	0.54
2:M:1111:ILE:HD12	2:M:1112:PHE:N	2.15	0.54
2:M:213:ALA:HB1	9:M:2130:HOH:O	2.07	0.54
2:M:622:GLU:HG3	9:M:2445:HOH:O	2.07	0.54
2:M:738:ASP:HB3	2:M:744:ARG:HB3	1.89	0.54
3:N:36:THR:C	3:N:38:LYS:H	2.10	0.54
3:N:602:SER:O	3:N:606:ILE:HG12	2.07	0.54
4:O:33:HIS:CD2	4:O:89:MET:HG2	2.42	0.54
5:P:273:ARG:HD3	9:P:6834:HOH:O	2.07	0.54
1:B:154:GLU:HB2	9:B:9819:HOH:O	2.07	0.54
2:C:204:GLN:NE2	2:C:222:MET:HA	2.22	0.54
2:C:724:ARG:NE	2:C:737:LEU:O	2.40	0.54
3:D:10:ILE:HG13	3:D:1434:TRP:CE2	2.43	0.54
3:D:1122:LEU:HD23	3:D:1178:ALA:HB2	1.89	0.54
3:D:1206:GLY:HA3	3:D:1366:LYS:HZ3	1.73	0.54
3:D:147:VAL:HG22	9:D:9643:HOH:O	2.07	0.54
3:D:169:TYR:N	3:D:170:PRO:HD2	2.23	0.54
3:D:474:GLU:O	3:D:478:LEU:HG	2.08	0.54
3:D:560:GLN:HG2	5:F:218:GLN:NE2	2.19	0.54
3:D:826:PRO:HB3	3:D:828:LYS:NZ	2.23	0.54
3:D:842:VAL:HG13	9:D:9694:HOH:O	2.08	0.54
5:F:412:GLU:HG3	5:F:418:LEU:HD22	1.90	0.54
5:F:79:ASP:HB3	5:F:80:PRO:CD	2.37	0.54
1:K:110:LYS:CB	1:K:112:ARG:HD3	2.36	0.54
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.37	0.54
2:M:1000:MET:SD	2:M:1001:VAL:HG22	2.47	0.54
2:M:1005:MET:HE1	3:N:645:PRO:HB2	1.88	0.54
2:M:164:PRO:HB2	9:M:2243:HOH:O	2.07	0.54
2:M:708:TYR:HD1	2:M:708:TYR:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:133:ILE:HG22	3:N:455:ARG:N	2.22	0.54
3:N:1495:ILE:HG23	9:N:2275:HOH:O	2.07	0.54
3:N:491:LYS:HG3	9:N:9735:HOH:O	2.07	0.54
2:C:859:PRO:O	2:C:867:VAL:HG22	2.07	0.54
2:C:884:GLN:HG3	2:C:885:ILE:HD13	1.90	0.54
3:D:139:GLY:H	3:D:147:VAL:HG21	1.71	0.54
3:D:70:GLY:H	3:D:71:LYS:HE3	1.71	0.54
3:D:761:ILE:HD13	4:E:20:THR:HA	1.90	0.54
5:F:132:ARG:O	5:F:136:LEU:HG	2.07	0.54
1:K:80:LEU:HB3	9:K:5934:HOH:O	2.06	0.54
2:M:1014:SER:HB3	2:M:1017:THR:O	2.07	0.54
2:M:318:PRO:HD3	9:M:2029:HOH:O	2.06	0.54
2:M:22:GLN:CD	2:M:336:VAL:HG21	2.28	0.54
3:N:1425:THR:HG23	3:N:1426:LYS:N	2.23	0.54
3:N:770:LEU:HD11	3:N:919:PHE:CE2	2.42	0.54
5:P:274:THR:O	5:P:278:LEU:HG	2.07	0.54
3:D:1249:ALA:HA	9:D:2205:HOH:O	2.06	0.54
3:D:703:ASN:ND2	3:D:704:ARG:H	2.05	0.54
9:C:9869:HOH:O	5:F:378:GLY:HA2	2.07	0.54
2:M:145:GLY:O	2:M:163:ILE:HG23	2.08	0.54
2:M:282:GLY:HA3	9:M:2102:HOH:O	2.08	0.54
3:N:1018:ASN:HB3	3:N:1021:TYR:HB3	1.89	0.54
3:N:850:LEU:O	3:N:853:VAL:HB	2.07	0.54
4:O:29:GLN:HB2	4:O:33:HIS:CD2	2.43	0.54
5:P:318:GLU:HB2	9:P:6126:HOH:O	2.08	0.54
1:A:28:LEU:HD13	1:A:32:PHE:HB3	1.90	0.54
1:B:18:ARG:O	1:B:207:PRO:HD3	2.08	0.54
2:C:292:ARG:HB2	2:C:299:LYS:HE2	1.90	0.54
2:C:290:LEU:HB3	2:C:302:VAL:HG11	1.90	0.54
2:C:5:ARG:HB3	2:C:902:ILE:HB	1.90	0.54
2:C:64:LEU:CD1	2:C:100:LEU:HD13	2.38	0.54
2:C:774:LEU:HG	2:C:775:ARG:NH1	2.21	0.54
2:C:889:HIS:CD2	2:C:970:GLY:HA3	2.43	0.54
3:D:1047:LYS:HG2	3:D:1053:PHE:CE2	2.43	0.54
3:D:1269:LYS:HB3	9:D:2172:HOH:O	2.07	0.54
1:K:58:ILE:HG21	1:K:68:ILE:HD11	1.90	0.54
1:K:91:ASN:HB3	9:K:3958:HOH:O	2.08	0.54
2:M:182:VAL:CG1	2:M:193:LEU:HD13	2.38	0.54
2:M:621:VAL:HG22	9:M:9943:HOH:O	2.07	0.54
2:M:640:ARG:HD3	2:M:642:ARG:NH2	2.23	0.54
3:N:1220:ALA:HB1	3:N:1223:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1404:ASN:HD22	3:N:1408:ILE:HD12	1.72	0.54
3:N:1420:LEU:HD12	3:N:1421:LEU:N	2.22	0.54
3:N:512:MET:CE	3:N:1452:ILE:HD11	2.38	0.54
3:N:139:GLY:O	3:N:147:VAL:HB	2.07	0.54
3:N:553:ARG:HD2	3:N:570:GLU:OE2	2.08	0.54
2:M:1109:VAL:HG11	3:N:5:VAL:HG22	1.90	0.54
5:P:415:THR:O	5:P:417:LYS:HG3	2.08	0.54
2:C:690:ILE:HG22	2:C:852:ILE:HA	1.89	0.54
3:D:1109:GLU:CD	3:D:1202:GLN:H	2.11	0.54
3:D:613:ARG:HG3	9:D:9563:HOH:O	2.08	0.54
5:F:100:VAL:HG12	5:F:104:ARG:HH21	1.72	0.54
1:L:132:LEU:HD21	1:L:136:GLY:O	2.08	0.54
1:L:81:ASN:HB2	9:L:3720:HOH:O	2.08	0.54
2:M:52:PHE:CG	2:M:68:PHE:HB2	2.43	0.54
2:M:729:LEU:HB3	9:M:2363:HOH:O	2.08	0.54
5:P:132:ARG:O	5:P:136:LEU:HG	2.08	0.54
1:B:57:TYR:CE2	1:B:161:ARG:HG2	2.43	0.53
2:C:66:LEU:HD13	2:C:372:LEU:CD2	2.37	0.53
2:C:426:ASP:OD1	2:C:427:VAL:HG23	2.07	0.53
2:C:586:ARG:HG2	9:C:9765:HOH:O	2.07	0.53
2:C:747:ALA:HA	9:C:9611:HOH:O	2.07	0.53
2:C:798:GLY:HA3	2:C:828:ALA:O	2.08	0.53
3:D:1269:LYS:HD2	9:D:9761:HOH:O	2.08	0.53
3:D:1103:HIS:CD2	3:D:1463:LYS:H	2.26	0.53
3:D:191:LEU:HB3	3:D:195:VAL:HG21	1.90	0.53
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.89	0.53
9:B:9647:HOH:O	3:D:842:VAL:HB	2.08	0.53
5:F:325:LYS:HB3	9:F:9864:HOH:O	2.07	0.53
5:F:363:GLU:HA	5:F:367:MET:HG2	1.90	0.53
2:M:173:ASP:O	2:M:184:MET:HA	2.08	0.53
2:M:433:THR:HG21	2:M:488:ALA:HB1	1.90	0.53
2:M:328:LEU:HD22	2:M:433:THR:HG22	1.90	0.53
2:M:693:GLU:OE1	2:M:696:LYS:HD2	2.08	0.53
3:N:1034:GLN:HA	3:N:1037:GLN:HE21	1.72	0.53
3:N:119:SER:N	3:N:123:LEU:HB2	2.23	0.53
3:N:1432:LYS:CD	3:N:1433:SER:H	2.22	0.53
3:N:787:LEU:HD11	3:N:947:ILE:HG12	1.89	0.53
3:N:868:TYR:HB3	9:N:2374:HOH:O	2.07	0.53
5:P:100:VAL:CG1	5:P:104:ARG:HH21	2.21	0.53
5:P:399:GLN:HA	9:P:5295:HOH:O	2.09	0.53
1:B:211:LEU:O	1:B:215:VAL:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:115:LEU:HA	2:C:375:SER:HB3	1.89	0.53
2:C:444:PRO:HG2	2:C:452:ILE:CD1	2.38	0.53
2:C:583:LEU:HG	2:C:586:ARG:HB2	1.89	0.53
2:C:660:ALA:HB1	2:C:667:ALA:O	2.07	0.53
3:D:1168:MET:HE1	3:D:1171:VAL:HB	1.90	0.53
3:D:117:ASP:HA	9:D:9715:HOH:O	2.07	0.53
3:D:1246:VAL:HG23	9:D:2655:HOH:O	2.08	0.53
2:C:1095:LEU:HD23	3:D:582:LEU:CD2	2.38	0.53
3:D:650:LEU:HD13	3:D:688:TRP:HZ3	1.73	0.53
3:D:916:TYR:HE2	3:D:920:LEU:HD13	1.73	0.53
3:D:957:PRO:CG	3:D:1007:VAL:HA	2.38	0.53
2:M:137:VAL:HG22	2:M:391:LEU:O	2.07	0.53
2:M:332:ARG:NH2	2:M:464:LEU:HD11	2.17	0.53
2:M:47:ALA:HB1	9:M:2250:HOH:O	2.07	0.53
3:N:243:ALA:HA	9:N:2678:HOH:O	2.07	0.53
3:N:52:PRO:HB2	3:N:80:VAL:CG1	2.24	0.53
3:N:958:GLU:HG2	9:N:2414:HOH:O	2.09	0.53
1:A:86:VAL:CG1	1:A:124:ASN:HB2	2.38	0.53
2:C:118:ILE:H	2:C:118:ILE:HD12	1.73	0.53
2:C:637:LEU:HB3	9:C:2008:HOH:O	2.09	0.53
2:C:983:ILE:HG21	2:C:987:ILE:CD1	2.36	0.53
3:D:178:LEU:HD11	9:D:2125:HOH:O	2.08	0.53
3:D:413:ASP:OD1	3:D:421:LEU:HD22	2.08	0.53
3:D:553:ARG:HH12	5:F:211:ASP:HA	1.73	0.53
3:D:601:ARG:NE	3:D:606:ILE:HD13	2.23	0.53
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.89	0.53
3:D:875:THR:HB	9:D:9915:HOH:O	2.07	0.53
2:M:147:TYR:HB3	2:M:323:ASP:OD2	2.07	0.53
2:M:351:LEU:HD12	9:M:9797:HOH:O	2.09	0.53
2:M:779:GLY:HA3	9:M:9697:HOH:O	2.09	0.53
2:M:862:PRO:HA	2:M:975:TYR:CE1	2.43	0.53
3:N:1101:VAL:HG22	3:N:1428:ALA:HB2	1.90	0.53
3:N:661:MET:CE	3:N:673:ALA:HB1	2.39	0.53
3:N:781:PRO:HG2	3:N:911:LEU:HD23	1.89	0.53
3:N:920:LEU:HD21	9:N:9647:HOH:O	2.07	0.53
5:P:396:ARG:HH11	5:P:399:GLN:NE2	2.06	0.53
2:C:224:GLU:HG3	9:C:9602:HOH:O	2.06	0.53
3:D:561:GLY:HA3	5:F:184:ARG:HH12	1.74	0.53
3:D:65:ARG:HA	9:D:9875:HOH:O	2.09	0.53
3:D:699:VAL:HB	3:D:716:PHE:O	2.08	0.53
5:F:126:LEU:O	5:F:130:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:GLU:HG3	1:L:201:THR:O	2.08	0.53
3:N:1114:THR:HG23	3:N:1114:THR:O	2.09	0.53
3:N:1114:THR:CG2	3:N:1195:GLN:HB3	2.38	0.53
3:N:4:GLU:HG2	9:N:2118:HOH:O	2.07	0.53
3:N:656:PHE:HB3	3:N:694:VAL:HG11	1.89	0.53
3:N:822:ALA:HB3	9:N:9584:HOH:O	2.06	0.53
5:P:119:ILE:HG22	9:P:6420:HOH:O	2.09	0.53
9:M:9851:HOH:O	5:P:373:LYS:HB3	2.08	0.53
1:A:156:HIS:CD2	1:A:157:GLY:N	2.76	0.53
1:A:184:THR:HG23	1:A:192:LEU:HD12	1.91	0.53
1:A:211:LEU:O	1:A:215:VAL:HG13	2.08	0.53
2:C:1081:VAL:HB	2:C:1086:ARG:HE	1.74	0.53
2:C:1115:LEU:H	2:C:1115:LEU:HD12	1.74	0.53
3:D:1445:HIS:HB2	9:D:9607:HOH:O	2.07	0.53
3:D:652:LEU:HB3	3:D:653:PHE:HD1	1.72	0.53
3:D:668:PRO:HD2	3:D:672:ALA:CB	2.39	0.53
5:F:82:ARG:HB3	9:F:9818:HOH:O	2.09	0.53
2:M:1085:PHE:O	2:M:1089:VAL:HG23	2.09	0.53
2:M:134:ARG:HH21	2:M:393:GLN:CA	2.20	0.53
2:M:19:THR:HG22	2:M:22:GLN:HB2	1.89	0.53
3:N:191:LEU:HD22	3:N:195:VAL:HG21	1.91	0.53
3:N:137:PRO:HD2	3:N:453:ASP:CB	2.38	0.53
3:N:639:LEU:HB2	9:N:9843:HOH:O	2.07	0.53
5:P:163:LEU:HB3	5:P:174:LEU:CD1	2.38	0.53
1:A:81:ASN:O	1:A:84:GLU:HB2	2.08	0.53
2:C:1030:GLN:HE22	3:D:628:ARG:HH21	1.55	0.53
2:C:1085:PHE:HE1	2:C:1111:ILE:HD13	1.72	0.53
2:C:271:GLU:HG2	9:C:2393:HOH:O	2.08	0.53
2:C:193:LEU:HD23	2:C:307:LEU:HD13	1.90	0.53
2:C:505:GLY:N	9:C:9917:HOH:O	2.42	0.53
3:D:1131:SER:HB3	9:D:2678:HOH:O	2.07	0.53
3:D:122:GLU:O	3:D:126:VAL:HG23	2.09	0.53
3:D:1377:LYS:O	3:D:1395:LEU:N	2.37	0.53
3:D:1393:GLN:HB2	3:D:1398:TRP:CZ2	2.43	0.53
3:D:150:ARG:HG3	3:D:150:ARG:NH1	2.23	0.53
3:D:400:VAL:HG21	3:D:441:ARG:HH11	1.72	0.53
1:K:89:PHE:CB	1:K:94:LEU:HD13	2.38	0.53
2:M:198:ARG:NH2	2:M:203:ASP:HB3	2.24	0.53
2:M:605:LYS:HD3	2:M:610:ARG:NH2	2.23	0.53
3:N:957:PRO:HG3	3:N:1007:VAL:HA	1.91	0.53
3:N:1337:GLU:OE1	3:N:1337:GLU:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:545:ARG:CZ	5:P:257:THR:HA	2.37	0.53
1:L:65:PHE:HD1	3:N:813:LEU:HD13	1.73	0.53
1:B:101:LEU:HD22	9:B:9576:HOH:O	2.09	0.53
1:B:99:LEU:HG	1:B:114:PHE:CD2	2.44	0.53
2:C:1097:LEU:HD22	2:C:1097:LEU:H	1.73	0.53
2:C:831:ARG:HG2	2:C:831:ARG:HH11	1.74	0.53
3:D:1236:LEU:HD23	3:D:1359:GLN:NE2	2.24	0.53
3:D:1258:ARG:HG2	3:D:1355:VAL:HG21	1.90	0.53
3:D:102:ILE:HD12	3:D:579:ASP:CG	2.29	0.53
3:D:678:GLU:HG3	3:D:679:ARG:HG3	1.90	0.53
1:K:103:ALA:HB1	1:K:107:LYS:HD3	1.91	0.53
1:K:212:ASN:O	1:K:215:VAL:HG22	2.08	0.53
1:K:78:ILE:HA	1:K:81:ASN:ND2	2.24	0.53
2:M:11:GLU:HA	9:M:2470:HOH:O	2.09	0.53
2:M:346:VAL:O	2:M:350:ARG:HG2	2.09	0.53
2:M:841:ASN:HD22	2:M:841:ASN:C	2.10	0.53
3:N:1063:GLU:HG3	3:N:1064:GLY:N	2.23	0.53
3:N:397:LYS:CE	3:N:399:ARG:HE	2.22	0.53
3:N:480:GLU:O	3:N:484:PRO:HD2	2.09	0.53
4:O:37:ASN:HA	4:O:93:TYR:CE2	2.43	0.53
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.43	0.53
2:C:160:ALA:O	2:C:173:ASP:HA	2.09	0.53
2:C:176:VAL:C	2:C:178:PRO:HD3	2.28	0.53
2:C:237:ARG:HG2	9:C:2366:HOH:O	2.08	0.53
2:C:292:ARG:HD2	2:C:299:LYS:HE2	1.91	0.53
2:C:535:SER:H	2:C:538:GLN:NE2	2.07	0.53
2:C:924:VAL:HA	9:C:2430:HOH:O	2.09	0.53
2:C:862:PRO:HG3	2:C:975:TYR:HE1	1.72	0.53
3:D:1083:ASP:HB3	3:D:1087:ARG:NH2	2.24	0.53
3:D:1383:ASP:HB3	3:D:1416:ALA:H	1.73	0.53
3:D:422:ALA:HA	9:D:2456:HOH:O	2.08	0.53
3:D:466:LYS:HD3	9:D:2238:HOH:O	2.09	0.53
3:D:563:PRO:HG2	3:D:566:ILE:HD12	1.89	0.53
3:D:97:THR:CG2	3:D:571:LYS:HD3	2.37	0.53
3:D:616:GLN:OE1	3:D:619:LEU:HB3	2.09	0.53
3:D:667:ALA:HB2	3:D:676:MET:CE	2.38	0.53
3:D:68:PHE:HA	3:D:71:LYS:HZ2	1.74	0.53
3:D:762:GLN:NE2	4:E:20:THR:HG21	2.24	0.53
5:F:361:LEU:HD23	5:F:362:SER:N	2.20	0.53
1:L:101:LEU:HD11	1:L:113:ASP:HB2	1.91	0.53
1:L:186:LEU:O	1:L:186:LEU:HD23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1043:TYR:HA	3:N:710:ARG:NH2	2.24	0.53
2:M:639:GLN:HG2	9:M:9781:HOH:O	2.08	0.53
2:M:68:PHE:HZ	2:M:71:TYR:HB3	1.73	0.53
2:M:798:GLY:H	2:M:827:VAL:HG11	1.74	0.53
3:N:1304:LYS:HB3	9:N:9605:HOH:O	2.09	0.53
3:N:424:GLY:HA3	9:N:9639:HOH:O	2.09	0.53
4:O:87:LYS:HE2	4:O:91:ARG:NH2	2.23	0.53
5:P:109:GLY:O	5:P:113:ILE:HG13	2.09	0.53
5:P:351:SER:HA	9:P:5760:HOH:O	2.09	0.53
2:C:1083:GLU:OE1	2:C:1086:ARG:HD2	2.09	0.53
2:C:333:ILE:O	2:C:465:GLY:HA3	2.08	0.53
3:D:1136:LYS:HA	9:D:2241:HOH:O	2.09	0.53
3:D:1233:GLY:HA2	3:D:1236:LEU:HG	1.90	0.53
3:D:30:GLU:HB3	3:D:40:GLU:CB	2.39	0.53
3:D:209:ARG:HH21	3:D:397:LYS:HG3	1.72	0.53
3:D:817:GLU:HG2	3:D:840:LYS:NZ	2.24	0.53
1:K:156:HIS:CD2	1:K:157:GLY:N	2.77	0.53
2:M:250:ARG:HB2	9:M:2343:HOH:O	2.08	0.53
2:M:376:ARG:HB3	2:M:377:PRO:HD3	1.91	0.53
2:M:584:GLU:CD	2:M:584:GLU:H	2.11	0.53
2:M:694:LEU:HD11	2:M:868:ASP:HB3	1.91	0.53
3:N:210:ARG:NH1	3:N:398:ALA:HB3	2.18	0.53
5:P:302:LYS:HG3	5:P:303:ARG:N	2.24	0.53
5:P:328:PHE:O	5:P:331:ASP:N	2.34	0.53
5:P:392:VAL:HG22	9:P:5988:HOH:O	2.09	0.53
5:P:404:ALA:HA	9:P:5252:HOH:O	2.09	0.53
5:P:417:LYS:HD3	9:P:6175:HOH:O	2.09	0.53
1:B:73:GLU:HB3	1:B:77:GLU:HG2	1.91	0.53
2:C:1056:LYS:HE3	3:D:751:LEU:CD1	2.39	0.53
2:C:313:LEU:CA	2:C:321:GLU:HG3	2.37	0.53
2:C:325:ILE:HG22	9:C:9742:HOH:O	2.08	0.53
5:F:117:SER:OG	5:F:124:PRO:HG3	2.09	0.53
5:F:187:LEU:HD23	5:F:191:ASN:HD21	1.74	0.53
2:M:168:ARG:HB2	9:M:9850:HOH:O	2.09	0.53
2:M:405:ARG:HH22	2:M:563:ASN:HD21	1.56	0.53
2:M:723:THR:CG2	2:M:725:ASP:HB2	2.38	0.53
2:M:757:GLY:HA2	2:M:789:SER:HB3	1.91	0.53
3:N:1144:LEU:HA	3:N:1147:ARG:HG3	1.92	0.53
3:N:1236:LEU:HD11	3:N:1356:TYR:CE1	2.44	0.53
3:N:1323:GLN:HA	9:N:9758:HOH:O	2.09	0.53
3:N:1492:LEU:HB3	3:N:1493:LYS:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:969:ARG:O	3:N:972:LEU:HB3	2.08	0.53
5:P:269:ASN:HB3	5:P:273:ARG:HH21	1.73	0.53
1:A:86:VAL:HG21	1:A:202:ASP:O	2.08	0.52
2:C:267:TYR:HE2	9:C:9988:HOH:O	1.92	0.52
2:C:567:GLN:HB2	2:C:997:LEU:CD2	2.39	0.52
2:C:630:ARG:HG2	9:C:2367:HOH:O	2.09	0.52
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.73	0.52
3:D:1357:ARG:NH1	9:D:2523:HOH:O	2.42	0.52
3:D:480:GLU:O	3:D:484:PRO:HD2	2.08	0.52
3:D:809:PRO:O	3:D:812:ALA:HB3	2.08	0.52
1:K:39:PRO:O	1:K:43:ILE:HG12	2.09	0.52
1:L:63:HIS:HB3	9:L:5868:HOH:O	2.09	0.52
2:M:708:TYR:N	2:M:708:TYR:CD1	2.77	0.52
3:N:1087:ARG:HG3	3:N:1238:MET:HB2	1.90	0.52
3:N:1136:LYS:O	3:N:1140:ILE:HG13	2.10	0.52
3:N:1435:LEU:HG	3:N:1467:ILE:HD12	1.90	0.52
3:N:183:GLU:O	3:N:186:VAL:HG12	2.09	0.52
3:N:804:LEU:HB2	3:N:830:ALA:O	2.09	0.52
5:P:365:GLU:OE1	5:P:400:ILE:HD12	2.09	0.52
1:B:131:THR:HG22	9:B:9666:HOH:O	2.08	0.52
2:C:815:LEU:HD23	9:C:9551:HOH:O	2.07	0.52
2:C:878:SER:HB3	3:D:1029:ARG:HD3	1.91	0.52
3:D:1182:GLU:HG2	9:D:2146:HOH:O	2.09	0.52
3:D:1148:VAL:HG21	3:D:1203:LYS:HA	1.91	0.52
3:D:494:LYS:HD2	9:D:2781:HOH:O	2.09	0.52
3:D:972:LEU:O	3:D:976:GLN:HG3	2.10	0.52
5:F:398:ARG:HB2	9:F:9753:HOH:O	2.09	0.52
1:K:63:HIS:HD2	1:K:65:PHE:H	1.56	0.52
2:M:220:GLY:HA3	9:M:9600:HOH:O	2.08	0.52
2:M:507:ARG:HG3	9:M:9704:HOH:O	2.08	0.52
2:M:976:ASP:OD1	2:M:978:ARG:HG3	2.10	0.52
3:N:1148:VAL:HG21	3:N:1203:LYS:HA	1.91	0.52
3:N:1459:LEU:HA	3:N:1464:GLU:OE1	2.09	0.52
3:N:181:ASP:O	3:N:185:VAL:HG23	2.09	0.52
3:N:436:GLU:HB2	3:N:445:ARG:HB2	1.91	0.52
3:N:699:VAL:HG21	3:N:760:ARG:HB3	1.92	0.52
5:P:78:SER:HB2	5:P:82:ARG:NH1	2.24	0.52
1:A:181:VAL:HG12	9:A:9562:HOH:O	2.09	0.52
1:B:185:ARG:HG3	1:B:190:THR:HG23	1.90	0.52
2:C:557:ARG:NH1	2:C:879:ARG:HG2	2.24	0.52
2:C:569:VAL:HG12	2:C:996:LYS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:777:ILE:HD13	9:C:9807:HOH:O	2.08	0.52
2:C:552:HIS:CD2	2:C:886:LEU:HD12	2.44	0.52
2:C:946:ARG:HD2	2:C:984:GLU:HB3	1.91	0.52
3:D:1465:ASN:HD21	3:D:1470:ARG:NH1	2.07	0.52
3:D:164:GLY:HA2	9:D:9578:HOH:O	2.09	0.52
3:D:179:VAL:HG13	3:D:389:GLU:HG3	1.90	0.52
3:D:477:LEU:HD13	3:D:492:ALA:O	2.10	0.52
5:F:119:ILE:HD13	5:F:170:HIS:ND1	2.24	0.52
1:K:18:ARG:HG3	9:K:3636:HOH:O	2.09	0.52
1:L:185:ARG:HG3	1:L:190:THR:HG22	1.91	0.52
2:M:269:LEU:HD12	2:M:288:ARG:H	1.72	0.52
2:M:315:ALA:HB2	9:M:2290:HOH:O	2.09	0.52
2:M:369:PRO:HD3	9:M:9686:HOH:O	2.09	0.52
2:M:513:VAL:HG22	9:M:2542:HOH:O	2.10	0.52
2:M:724:ARG:HG3	2:M:740:GLU:CA	2.31	0.52
3:N:12:LEU:HB2	9:N:9681:HOH:O	2.08	0.52
3:N:1394:VAL:HB	3:N:1397:LYS:HD2	1.90	0.52
3:N:1423:GLY:HA2	9:N:9678:HOH:O	2.07	0.52
3:N:1495:ILE:HG12	4:O:80:VAL:HG11	1.91	0.52
3:N:1485:GLN:NE2	4:O:80:VAL:H	1.99	0.52
1:B:84:GLU:HG2	1:B:127:LEU:HD11	1.92	0.52
2:C:1014:SER:OG	5:F:331:ASP:HA	2.10	0.52
2:C:12:VAL:HG13	2:C:13:ILE:HG12	1.91	0.52
2:C:431:HIS:H	2:C:434:HIS:CE1	2.27	0.52
2:C:607:ASP:HB3	2:C:610:ARG:H	1.75	0.52
2:C:838:LYS:HG3	2:C:997:LEU:HB2	1.91	0.52
3:D:116:LEU:HB3	3:D:118:LEU:HD21	1.91	0.52
3:D:607:LEU:HA	3:D:613:ARG:HB2	1.92	0.52
3:D:704:ARG:HH11	3:D:738:ALA:CB	2.22	0.52
3:D:728:LEU:HD22	3:D:745:MET:SD	2.49	0.52
3:D:806:PHE:CZ	3:D:813:LEU:HB3	2.44	0.52
4:E:13:VAL:HG11	4:E:19:LEU:HB2	1.90	0.52
1:K:110:LYS:HB2	1:K:112:ARG:HD3	1.91	0.52
1:L:206:THR:CG2	1:L:209:GLU:H	2.22	0.52
2:M:209:ARG:HD2	9:M:2006:HOH:O	2.09	0.52
2:M:790:LEU:HD12	2:M:791:ARG:N	2.25	0.52
3:N:1066:THR:HG22	3:N:1069:GLU:HB2	1.91	0.52
3:N:185:VAL:CG1	3:N:191:LEU:HD21	2.39	0.52
4:O:58:PRO:HB2	9:O:3710:HOH:O	2.08	0.52
5:P:342:VAL:HG23	5:P:343:ASP:OD1	2.10	0.52
1:B:101:LEU:HD21	1:B:113:ASP:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:PHE:HB2	9:B:9547:HOH:O	2.08	0.52
2:C:186:VAL:HG23	2:C:187:ASN:N	2.18	0.52
2:C:415:PRO:HA	9:C:9744:HOH:O	2.10	0.52
2:C:458:TYR:HB3	2:C:470:PRO:HG3	1.92	0.52
2:C:551:GLU:HB3	2:C:906:PHE:HD2	1.74	0.52
2:C:937:ASP:HB2	2:C:940:GLU:H	1.74	0.52
3:D:112:ILE:HG13	3:D:124:GLU:OE2	2.10	0.52
3:D:48:ARG:HB2	9:D:2881:HOH:O	2.08	0.52
5:F:81:VAL:HG12	5:F:85:LEU:HD12	1.92	0.52
1:K:182:GLU:O	1:K:194:LYS:HB3	2.08	0.52
1:K:32:PHE:CE2	1:L:43:ILE:HD13	2.45	0.52
2:M:495:THR:HB	2:M:530:GLU:HG3	1.91	0.52
2:M:630:ARG:HD2	2:M:631:SER:O	2.09	0.52
2:M:690:ILE:HA	9:M:2014:HOH:O	2.09	0.52
2:M:841:ASN:HD21	2:M:845:ASN:H	1.58	0.52
3:N:13:ALA:HA	3:N:17:LYS:NZ	2.24	0.52
3:N:660:LYS:HD2	3:N:663:GLU:OE2	2.09	0.52
3:N:776:GLU:HG3	9:N:2316:HOH:O	2.08	0.52
3:N:795:VAL:CG1	3:N:863:VAL:HG13	2.38	0.52
1:A:198:ARG:HB2	1:A:200:TRP:CH2	2.44	0.52
1:B:178:ALA:O	1:B:197:LEU:HD12	2.09	0.52
2:C:22:GLN:O	2:C:121:MET:HE1	2.10	0.52
2:C:205:GLU:O	2:C:209:ARG:HD2	2.08	0.52
2:C:413:LEU:HD12	2:C:413:LEU:H	1.74	0.52
2:C:541:SER:HB2	9:C:9852:HOH:O	2.09	0.52
2:C:735:ARG:HH11	2:C:735:ARG:HG2	1.74	0.52
2:C:727:PRO:HG2	2:C:785:VAL:HG12	1.90	0.52
2:C:858:MET:SD	2:C:867:VAL:HG23	2.50	0.52
3:D:1272:ALA:CA	3:D:1326:THR:HB	2.39	0.52
3:D:165:LYS:HB3	3:D:395:VAL:HG11	1.91	0.52
3:D:18:ILE:HD12	3:D:518:PRO:CG	2.39	0.52
3:D:211:VAL:HG13	3:D:393:ILE:HA	1.90	0.52
3:D:65:ARG:HD2	9:D:9875:HOH:O	2.09	0.52
5:F:385:GLU:O	5:F:397:ILE:HD13	2.10	0.52
1:L:22:GLU:OE2	1:L:198:ARG:HD3	2.09	0.52
2:M:722:ILE:O	2:M:722:ILE:HG23	2.08	0.52
2:M:759:THR:HB	2:M:785:VAL:CG2	2.40	0.52
3:N:104:PHE:CE2	3:N:1448:THR:HG23	2.44	0.52
3:N:213:VAL:HG22	3:N:214:GLU:H	1.74	0.52
5:P:358:LEU:HG	5:P:370:LYS:HG3	1.92	0.52
1:A:63:HIS:HB3	2:C:746:GLY:CA	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASN:OD1	1:A:92:PRO:HD2	2.10	0.52
1:B:92:PRO:HA	1:B:146:ARG:NH1	2.25	0.52
2:C:101:ILE:HG21	9:C:2533:HOH:O	2.09	0.52
2:C:1084:SER:HA	9:D:9711:HOH:O	2.09	0.52
2:C:111:ASP:HB3	2:C:112:GLU:OE2	2.09	0.52
2:C:333:ILE:CD1	2:C:467:ILE:HG13	2.39	0.52
2:C:405:ARG:O	2:C:408:ARG:HG3	2.08	0.52
2:C:742:VAL:HG23	9:C:2308:HOH:O	2.09	0.52
2:C:91:GLN:HE21	2:C:119:PRO:HD3	1.75	0.52
3:D:434:ARG:HB2	3:D:447:VAL:CG1	2.40	0.52
3:D:642:CYS:SG	3:D:716:PHE:HB2	2.50	0.52
4:E:13:VAL:HG23	9:E:9514:HOH:O	2.08	0.52
1:K:68:ILE:HD13	1:K:138:LEU:HD21	1.91	0.52
1:L:57:TYR:HA	9:L:4389:HOH:O	2.09	0.52
2:M:145:GLY:H	2:M:163:ILE:HG12	1.73	0.52
2:M:196:LEU:O	2:M:199:VAL:HB	2.10	0.52
2:M:64:LEU:HA	9:M:9659:HOH:O	2.10	0.52
3:N:1253:THR:OG1	3:N:1258:ARG:HD3	2.10	0.52
3:N:493:ARG:NH2	3:N:1388:ARG:HB3	2.24	0.52
3:N:428:LYS:CE	3:N:434:ARG:HH12	2.20	0.52
3:N:574:LEU:O	3:N:578:VAL:HG23	2.10	0.52
3:N:642:CYS:SG	3:N:716:PHE:HB2	2.50	0.52
3:N:729:HIS:CE1	3:N:731:LEU:HG	2.44	0.52
4:O:47:LYS:N	4:O:54:LEU:HD22	2.25	0.52
4:O:95:GLY:HA3	9:O:3795:HOH:O	2.10	0.52
1:A:110:LYS:HG3	9:A:9565:HOH:O	2.09	0.52
2:C:412:ALA:HB2	2:C:451:LEU:HB3	1.92	0.52
2:C:507:ARG:N	9:C:9917:HOH:O	2.30	0.52
2:C:585:GLU:O	2:C:588:VAL:HG22	2.10	0.52
1:A:72:LYS:HA	2:C:608:GLY:CA	2.39	0.52
2:C:724:ARG:NH1	2:C:734:LEU:HD23	2.24	0.52
2:C:78:PHE:HB2	2:C:88:LEU:HD21	1.91	0.52
2:C:808:ARG:H	2:C:808:ARG:HD2	1.74	0.52
2:C:432:ARG:HH12	3:D:1047:LYS:CD	2.23	0.52
3:D:633:VAL:HG22	3:D:635:PRO:CD	2.37	0.52
1:L:30:ARG:HH11	1:L:30:ARG:HG2	1.75	0.52
2:M:243:ARG:HD2	2:M:243:ARG:O	2.09	0.52
2:M:328:LEU:CD2	2:M:437:ARG:HD3	2.40	0.52
2:M:497:ALA:HA	2:M:515:ALA:HA	1.91	0.52
2:M:808:ARG:HA	9:M:2211:HOH:O	2.08	0.52
2:M:561:GLY:HA3	2:M:842:ARG:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:172:PRO:HD2	3:N:389:GLU:O	2.09	0.52
3:N:583:ASP:OD2	3:N:604:THR:HG21	2.09	0.52
3:N:704:ARG:NH2	3:N:737:ASN:O	2.43	0.52
3:N:706:PRO:HA	9:N:2317:HOH:O	2.10	0.52
4:O:70:THR:HG21	4:O:72:ARG:CZ	2.40	0.52
5:P:93:LEU:HG	5:P:190:ALA:CB	2.40	0.52
2:C:251:ASP:HB3	2:C:252:LYS:HD2	1.92	0.52
2:C:352:ALA:O	2:C:356:ARG:HG3	2.10	0.52
2:C:464:LEU:O	2:C:466:PHE:N	2.43	0.52
2:C:748:GLU:HB3	9:C:2077:HOH:O	2.09	0.52
2:C:393:GLN:HB3	7:C:8001:RBT:O9	2.10	0.52
2:C:861:LEU:HD23	2:C:863:ASP:N	2.24	0.52
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.10	0.52
3:D:786:ILE:HD12	3:D:1028:ALA:HA	1.92	0.52
3:D:1432:LYS:CG	3:D:1433:SER:H	2.23	0.52
3:D:476:GLU:HG2	9:D:9637:HOH:O	2.10	0.52
3:D:523:ASP:O	3:D:526:PRO:HG3	2.09	0.52
3:D:799:LYS:H	3:D:826:PRO:HG2	1.74	0.52
5:F:120:THR:CG2	5:F:122:LEU:HD13	2.39	0.52
2:M:160:ALA:O	2:M:173:ASP:HA	2.10	0.52
2:M:200:LEU:HD13	2:M:300:ASP:OD2	2.10	0.52
2:M:643:VAL:HG13	2:M:647:GLN:OE1	2.10	0.52
2:M:52:PHE:HE1	2:M:66:LEU:HG	1.75	0.52
3:N:1197:ARG:HD2	3:N:1198:TYR:CE1	2.45	0.52
3:N:185:VAL:HG12	3:N:191:LEU:HD21	1.91	0.52
3:N:671:LYS:HA	3:N:674:ARG:HD3	1.90	0.52
3:N:678:GLU:HA	9:N:9708:HOH:O	2.10	0.52
3:N:875:THR:HG23	9:N:9855:HOH:O	2.09	0.52
2:C:863:ASP:O	2:C:865:THR:N	2.43	0.52
2:C:432:ARG:HH12	3:D:1047:LYS:HD3	1.75	0.52
3:D:1302:GLU:HG3	9:D:9705:HOH:O	2.09	0.52
3:D:1412:LYS:HA	9:D:9952:HOH:O	2.08	0.52
1:B:65:PHE:HE1	3:D:806:PHE:HZ	1.57	0.52
3:D:81:THR:O	3:D:82:LYS:O	2.28	0.52
3:D:928:ALA:HB2	9:D:9640:HOH:O	2.10	0.52
1:K:150:TYR:CE1	2:M:696:LYS:HA	2.44	0.52
1:K:218:LEU:O	1:K:222:LEU:HD23	2.10	0.52
1:K:20:TYR:CD2	1:K:21:GLY:N	2.78	0.52
2:M:134:ARG:N	9:M:9669:HOH:O	2.42	0.52
2:M:194:VAL:HG13	2:M:197:LEU:HD12	1.91	0.52
2:M:16:PRO:CB	2:M:460:ARG:HH22	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:54:ILE:HB	9:M:9580:HOH:O	2.09	0.52
2:M:705:ILE:HB	9:M:2015:HOH:O	2.10	0.52
2:M:842:ARG:HD3	9:M:9622:HOH:O	2.08	0.52
3:N:127:LEU:HB3	3:N:132:TYR:O	2.10	0.52
3:N:9:ARG:HA	3:N:1455:LYS:O	2.10	0.52
2:C:101:ILE:HG22	2:C:102:HIS:N	2.25	0.51
2:C:109:LYS:HE2	9:C:9753:HOH:O	2.09	0.51
2:C:720:GLU:HA	2:C:759:THR:O	2.10	0.51
2:C:770:GLU:HG2	9:C:2045:HOH:O	2.09	0.51
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.92	0.51
3:D:849:ALA:HB2	9:D:9991:HOH:O	2.10	0.51
5:F:312:GLN:HA	9:F:9731:HOH:O	2.09	0.51
1:L:192:LEU:HD12	9:L:4234:HOH:O	2.10	0.51
1:L:57:TYR:CZ	1:L:161:ARG:HG2	2.45	0.51
2:M:249:LYS:HG3	9:M:2241:HOH:O	2.10	0.51
2:M:69:LEU:HD23	9:M:2238:HOH:O	2.09	0.51
2:M:742:VAL:HG12	2:M:743:VAL:N	2.25	0.51
3:N:1277:ILE:CD1	3:N:1301:LYS:HB2	2.39	0.51
3:N:1379:VAL:HG11	3:N:1395:LEU:HD23	1.92	0.51
3:N:1491:THR:O	3:N:1495:ILE:HD13	2.09	0.51
3:N:529:GLN:HA	9:N:2026:HOH:O	2.10	0.51
3:N:800:LYS:HG2	3:N:829:VAL:HG12	1.92	0.51
4:O:84:ARG:HB2	4:O:84:ARG:NH1	2.25	0.51
1:A:41:ARG:O	1:A:45:LEU:HD12	2.09	0.51
2:C:297:GLU:HG2	9:C:2227:HOH:O	2.11	0.51
2:C:327:HIS:CE1	2:C:489:THR:HA	2.46	0.51
2:C:497:ALA:HA	2:C:515:ALA:HA	1.92	0.51
2:C:588:VAL:HG12	2:C:666:LEU:HD12	1.92	0.51
2:C:674:VAL:HG11	2:C:992:MET:HB3	1.92	0.51
3:D:1151:ARG:HD3	9:D:9868:HOH:O	2.10	0.51
3:D:1412:LYS:HB2	9:D:2083:HOH:O	2.10	0.51
3:D:1434:TRP:CZ3	3:D:1457:ASP:HB2	2.45	0.51
3:D:1498:ALA:HB1	9:D:2558:HOH:O	2.10	0.51
3:D:210:ARG:HG3	3:D:398:ALA:H	1.75	0.51
3:D:395:VAL:HG23	9:D:9647:HOH:O	2.09	0.51
3:D:133:ILE:HG23	3:D:456:MET:SD	2.51	0.51
3:D:513:ILE:HG22	9:D:9932:HOH:O	2.10	0.51
3:D:539:ASP:CG	5:F:318:GLU:HB2	2.31	0.51
2:M:405:ARG:HH22	2:M:563:ASN:ND2	2.06	0.51
2:M:625:LEU:HD13	2:M:639:GLN:O	2.10	0.51
3:N:1165:TYR:HE2	3:N:1206:GLY:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:512:MET:HE2	3:N:1452:ILE:HD11	1.92	0.51
3:N:115:LEU:HD22	3:N:502:PHE:HE1	1.75	0.51
3:N:53:ILE:HG23	3:N:54:LYS:N	2.20	0.51
3:N:572:ARG:HH11	5:P:80:PRO:HG3	1.75	0.51
3:N:917:GLN:HA	3:N:917:GLN:NE2	2.25	0.51
2:C:728:HIS:HB3	9:C:9568:HOH:O	2.10	0.51
2:C:945:ARG:HG2	2:C:946:ARG:N	2.24	0.51
3:D:1352:ILE:CG2	3:D:1368:ILE:HD13	2.40	0.51
3:D:1382:THR:HG22	9:D:2107:HOH:O	2.11	0.51
3:D:1396:GLU:HA	3:D:1399:ASP:OD2	2.09	0.51
3:D:179:VAL:O	3:D:183:GLU:HB2	2.10	0.51
3:D:404:GLU:HB3	3:D:414:ARG:HD3	1.92	0.51
3:D:63:TYR:HB3	3:D:68:PHE:CE1	2.45	0.51
3:D:795:VAL:HG11	3:D:863:VAL:HG13	1.91	0.51
3:D:947:ILE:O	3:D:947:ILE:HD12	2.10	0.51
4:E:54:LEU:HA	4:E:58:PRO:HG2	1.93	0.51
5:F:365:GLU:CD	5:F:397:ILE:HA	2.31	0.51
1:K:189:ARG:HD2	1:K:191:ASP:OD1	2.09	0.51
1:L:112:ARG:HB3	1:L:112:ARG:NH1	2.25	0.51
2:M:428:ARG:CZ	2:M:451:LEU:HD11	2.41	0.51
2:M:473:ARG:HD2	2:M:475:VAL:HG22	1.91	0.51
2:M:724:ARG:CG	2:M:740:GLU:HA	2.32	0.51
2:M:958:THR:HA	9:M:9663:HOH:O	2.09	0.51
2:M:944:LEU:HD21	2:M:963:LEU:CD2	2.39	0.51
3:N:1147:ARG:O	3:N:1166:LEU:HD23	2.09	0.51
3:N:80:VAL:HG12	3:N:81:THR:O	2.11	0.51
3:N:984:THR:HB	3:N:987:GLU:OE1	2.09	0.51
2:C:352:ALA:HA	2:C:355:VAL:CG1	2.40	0.51
2:C:39:ARG:HA	2:C:39:ARG:NE	2.25	0.51
2:C:557:ARG:HB2	9:C:9575:HOH:O	2.11	0.51
2:C:876:VAL:HB	2:C:877:PRO:HD3	1.93	0.51
2:C:918:LEU:HD23	2:C:967:PHE:O	2.11	0.51
2:C:932:GLU:HB3	9:C:2388:HOH:O	2.10	0.51
3:D:125:GLN:HB2	9:D:2691:HOH:O	2.11	0.51
3:D:1377:LYS:HE2	3:D:1394:VAL:HG22	1.92	0.51
3:D:149:LYS:HA	9:D:9643:HOH:O	2.10	0.51
3:D:477:LEU:HD22	3:D:492:ALA:CB	2.39	0.51
3:D:502:PHE:CE1	3:D:509:PRO:HB3	2.45	0.51
3:D:62:LYS:HG3	9:D:2590:HOH:O	2.10	0.51
4:E:33:HIS:HB2	4:E:37:ASN:ND2	2.25	0.51
1:K:123:MET:O	1:K:125:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1051:GLU:HG2	2:M:1056:LYS:HD2	1.91	0.51
2:M:211:LEU:HD11	2:M:308:ARG:HA	1.93	0.51
2:M:140:ILE:HA	2:M:332:ARG:O	2.11	0.51
2:M:520:GLU:HB2	9:M:2193:HOH:O	2.10	0.51
3:N:1189:ARG:HD3	9:N:2289:HOH:O	2.09	0.51
3:N:1213:ARG:HB2	3:N:1214:PRO:CD	2.40	0.51
3:N:1311:LEU:H	3:N:1311:LEU:HD23	1.74	0.51
3:N:168:THR:HB	3:N:393:ILE:HD12	1.91	0.51
1:B:54:THR:HB	1:B:143:ARG:HD3	1.93	0.51
2:C:230:ARG:HB3	9:C:9986:HOH:O	2.10	0.51
2:C:334:ARG:HH12	2:C:415:PRO:HG2	1.76	0.51
2:C:383:ARG:HB2	2:C:383:ARG:NH1	2.26	0.51
2:C:470:PRO:HB3	2:C:485:TYR:CZ	2.46	0.51
2:C:625:LEU:CD1	2:C:641:PRO:HG3	2.40	0.51
2:C:703:ILE:HD11	2:C:830:LYS:HG2	1.93	0.51
3:D:1156:LEU:HD11	3:D:1176:LYS:HD2	1.91	0.51
3:D:1418:LYS:HG3	9:D:2791:HOH:O	2.10	0.51
3:D:196:VAL:HG13	3:D:202:VAL:CG1	2.41	0.51
3:D:37:LEU:HD13	3:D:535:PHE:HZ	1.76	0.51
3:D:693:GLU:HA	9:D:2933:HOH:O	2.10	0.51
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	1.91	0.51
2:M:1054:THR:HG21	2:M:1079:PRO:CB	2.19	0.51
2:M:1090:LYS:HG2	2:M:1112:PHE:CZ	2.45	0.51
2:M:380:ALA:HA	2:M:383:ARG:HG2	1.93	0.51
2:M:882:LEU:HD11	3:N:1038:LEU:HD23	1.92	0.51
3:N:1412:LYS:HG2	3:N:1414:PRO:HG3	1.92	0.51
3:N:514:LEU:HD23	9:N:9590:HOH:O	2.09	0.51
2:C:150:PRO:HB2	9:C:9683:HOH:O	2.10	0.51
2:C:971:LYS:HB3	2:C:987:ILE:C	2.30	0.51
3:D:112:ILE:HG12	3:D:128:TYR:OH	2.10	0.51
3:D:1148:VAL:HG13	3:D:1163:GLY:O	2.11	0.51
3:D:583:ASP:OD2	3:D:604:THR:HG21	2.11	0.51
4:E:26:ARG:O	4:E:29:GLN:HG2	2.10	0.51
5:F:273:ARG:O	5:F:276:ARG:HB2	2.10	0.51
2:C:1010:THR:HG21	5:F:341:PRO:HB2	1.93	0.51
1:L:116:PRO:HD2	9:L:4491:HOH:O	2.10	0.51
1:L:94:LEU:HD21	1:L:119:ASP:HB2	1.93	0.51
2:M:1066:ALA:O	2:M:1070:ILE:HG13	2.10	0.51
2:M:1098:ASP:HB2	3:N:21:TRP:CZ2	2.41	0.51
2:M:216:GLU:HA	9:M:9842:HOH:O	2.09	0.51
2:M:250:ARG:HB3	9:M:9639:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:367:LEU:O	2:M:371:LYS:HB3	2.11	0.51
2:M:563:ASN:HB2	9:M:9967:HOH:O	2.09	0.51
2:M:751:PRO:HA	2:M:792:VAL:HB	1.92	0.51
3:N:1391:GLU:HG2	3:N:1393:GLN:HG3	1.90	0.51
3:N:52:PRO:HD2	3:N:79:GLU:O	2.11	0.51
3:N:787:LEU:O	3:N:787:LEU:HD12	2.10	0.51
5:P:264:MET:O	5:P:267:THR:HB	2.11	0.51
1:B:81:ASN:O	1:B:84:GLU:HB3	2.10	0.51
2:C:1097:LEU:HD21	3:D:103:TRP:CZ3	2.46	0.51
2:C:30:LEU:HD12	2:C:30:LEU:O	2.11	0.51
2:C:139:GLN:OE1	2:C:415:PRO:HD3	2.11	0.51
2:C:561:GLY:HA3	2:C:842:ARG:O	2.10	0.51
2:C:716:LYS:HE2	9:F:9964:HOH:O	2.10	0.51
2:C:946:ARG:CD	2:C:984:GLU:HB3	2.41	0.51
3:D:955:VAL:HG21	3:D:1015:TYR:CE2	2.45	0.51
3:D:1047:LYS:HB2	3:D:1051:GLU:OE2	2.10	0.51
3:D:417:PRO:HB2	9:D:2401:HOH:O	2.10	0.51
3:D:675:ARG:O	3:D:678:GLU:HG2	2.10	0.51
3:D:795:VAL:HG23	3:D:879:ARG:HH12	1.76	0.51
3:D:804:LEU:HD23	3:D:804:LEU:H	1.76	0.51
5:F:141:VAL:HG23	9:F:9945:HOH:O	2.09	0.51
5:F:235:PHE:HA	9:F:9866:HOH:O	2.10	0.51
2:M:1086:ARG:HD3	2:M:1112:PHE:HD2	1.75	0.51
2:M:185:LYS:HD3	2:M:190:LYS:HG2	1.92	0.51
2:M:902:ILE:O	2:M:904:PRO:HD3	2.11	0.51
3:N:1281:VAL:HG21	3:N:1313:VAL:CG2	2.38	0.51
3:N:1493:LYS:O	3:N:1497:GLU:HG2	2.10	0.51
3:N:183:GLU:HA	3:N:186:VAL:CG1	2.41	0.51
3:N:426:LYS:HD2	3:N:428:LYS:NZ	2.25	0.51
3:N:57:GLU:HG2	3:N:58:CYS:O	2.11	0.51
3:N:787:LEU:HD21	3:N:947:ILE:CD1	2.40	0.51
5:P:287:THR:C	5:P:289:GLU:H	2.14	0.51
2:C:91:GLN:HG2	2:C:119:PRO:HG3	1.93	0.51
2:C:682:TYR:HB3	2:C:689:VAL:HG22	1.92	0.51
2:C:724:ARG:HB2	2:C:740:GLU:HG3	1.92	0.51
2:C:690:ILE:HD13	2:C:833:LEU:HD21	1.93	0.51
2:C:976:ASP:HB2	2:C:979:THR:HG22	1.93	0.51
3:D:817:GLU:HG3	3:D:839:LEU:HD22	1.92	0.51
4:E:47:LYS:HA	4:E:54:LEU:HB3	1.93	0.51
4:E:73:LEU:HD12	4:E:73:LEU:H	1.76	0.51
5:F:419:ARG:O	5:F:421:PHE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:189:ARG:HG2	2:M:189:ARG:HH11	1.75	0.51
3:N:144:GLY:HA2	9:N:2845:HOH:O	2.11	0.51
3:N:706:PRO:HD2	9:N:9656:HOH:O	2.09	0.51
3:N:790:TYR:CE1	3:N:1022:VAL:HG13	2.46	0.51
1:A:6:LEU:HD11	9:A:9781:HOH:O	2.10	0.51
1:A:83:LYS:HD3	9:C:9668:HOH:O	2.11	0.51
1:B:57:TYR:HB2	9:B:9571:HOH:O	2.11	0.51
2:C:1005:MET:HE1	3:D:648:MET:HB2	1.90	0.51
3:D:1087:ARG:HD3	9:D:9927:HOH:O	2.11	0.51
3:D:1211:MET:SD	3:D:1213:ARG:HD2	2.51	0.51
3:D:1278:ASP:HB2	3:D:1318:TYR:HE1	1.76	0.51
3:D:526:PRO:O	3:D:537:THR:HA	2.11	0.51
3:D:584:ASN:OD1	3:D:590:PRO:HD2	2.11	0.51
3:D:809:PRO:HB2	3:D:812:ALA:HB2	1.92	0.51
3:D:1476:THR:HG23	4:E:21:VAL:HG22	1.92	0.51
5:F:218:GLN:HA	5:F:221:ILE:HD12	1.93	0.51
5:F:299:TRP:CE3	5:F:303:ARG:HD3	2.45	0.51
5:F:88:ILE:HG22	9:F:9899:HOH:O	2.10	0.51
1:K:122:ILE:HD12	9:K:4058:HOH:O	2.11	0.51
1:L:65:PHE:HB2	9:L:3775:HOH:O	2.11	0.51
2:M:1101:THR:O	2:M:1102:LEU:HD23	2.10	0.51
2:M:242:LEU:HD23	9:M:2128:HOH:O	2.10	0.51
2:M:328:LEU:HD23	2:M:437:ARG:HD3	1.93	0.51
2:M:442:GLU:HG2	2:M:454:SER:OG	2.11	0.51
2:M:510:ALA:HB3	2:M:513:VAL:HG23	1.91	0.51
2:M:804:VAL:HG21	9:M:2269:HOH:O	2.10	0.51
2:M:80:GLN:O	2:M:83:CYS:HB2	2.11	0.51
2:M:939:ARG:HD3	2:M:982:PRO:HD3	1.92	0.51
3:N:171:LEU:HD22	3:N:390:PRO:HG3	1.92	0.51
3:N:379:ALA:HB2	9:N:2174:HOH:O	2.11	0.51
3:N:129:PHE:C	3:N:568:ARG:HH21	2.13	0.51
3:N:637:LEU:HD11	3:N:642:CYS:N	2.26	0.51
1:A:24:VAL:HG13	1:A:196:THR:HG22	1.93	0.51
2:C:207:LEU:HD22	2:C:221:LEU:HD22	1.93	0.51
2:C:29:ALA:HB2	2:C:337:GLY:HA3	1.93	0.51
2:C:328:LEU:HD11	2:C:434:HIS:CD2	2.46	0.51
2:C:602:GLU:HA	2:C:647:GLN:O	2.11	0.51
3:D:1057:VAL:HA	3:D:1069:GLU:CD	2.31	0.51
3:D:1310:ARG:CZ	3:D:1327:ARG:HB3	2.41	0.51
3:D:153:LEU:HD11	3:D:158:TYR:N	2.26	0.51
3:D:42:ASP:O	3:D:43:GLY:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:702:LEU:HD21	9:D:9734:HOH:O	2.11	0.51
5:F:306:GLU:O	5:F:310:ILE:HG13	2.11	0.51
1:K:124:ASN:HA	9:K:5696:HOH:O	2.10	0.51
1:L:26:GLU:HB3	1:L:194:LYS:HG3	1.93	0.51
1:L:216:GLU:HB2	9:L:4064:HOH:O	2.11	0.51
2:M:551:GLU:OE1	2:M:906:PHE:HA	2.11	0.51
2:M:697:ARG:HB2	9:M:2289:HOH:O	2.10	0.51
2:M:93:PRO:HA	9:M:2449:HOH:O	2.11	0.51
3:N:105:VAL:HG13	3:N:124:GLU:OE1	2.10	0.51
3:N:1493:LYS:HD3	3:N:1496:GLU:OE2	2.10	0.51
3:N:768:ASN:HD22	3:N:768:ASN:N	2.08	0.51
5:P:156:VAL:HA	5:P:159:ILE:HD12	1.93	0.51
5:P:280:GLN:HB2	9:P:4160:HOH:O	2.11	0.51
1:B:133:GLU:HG3	1:B:134:GLU:N	2.26	0.50
1:B:81:ASN:HB3	9:B:9545:HOH:O	2.11	0.50
2:C:437:ARG:CZ	2:C:469:THR:HG22	2.41	0.50
2:C:56:GLU:HG2	2:C:64:LEU:HD23	1.91	0.50
2:C:713:ARG:HH12	2:C:818:GLY:HA3	1.75	0.50
3:D:1003:VAL:HG21	3:D:1041:LEU:CD2	2.41	0.50
3:D:104:PHE:CE2	3:D:1448:THR:HG23	2.46	0.50
3:D:1304:LYS:HB3	9:D:9963:HOH:O	2.10	0.50
3:D:1432:LYS:HG3	3:D:1433:SER:H	1.75	0.50
3:D:1432:LYS:NZ	3:D:1460:ILE:HG13	2.25	0.50
3:D:191:LEU:HG	9:D:2144:HOH:O	2.11	0.50
3:D:213:VAL:HG23	3:D:391:ALA:HA	1.92	0.50
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.22	0.50
5:F:247:ILE:O	5:F:251:ILE:HG13	2.11	0.50
2:M:208:ALA:HA	2:M:221:LEU:HD21	1.92	0.50
2:M:326:ASP:HB2	2:M:431:HIS:ND1	2.26	0.50
2:M:437:ARG:NH2	2:M:488:ALA:HA	2.25	0.50
2:M:629:TYR:HE1	9:M:9647:HOH:O	1.93	0.50
3:N:1128:VAL:HG21	9:N:2608:HOH:O	2.11	0.50
3:N:1149:LEU:HD22	9:N:9815:HOH:O	2.11	0.50
3:N:1310:ARG:HD2	3:N:1327:ARG:HD2	1.91	0.50
3:N:1404:ASN:ND2	3:N:1408:ILE:HD12	2.26	0.50
3:N:1478:SER:O	3:N:1482:ARG:HG3	2.11	0.50
3:N:554:LEU:HD21	3:N:571:LYS:HG3	1.92	0.50
3:N:693:GLU:HA	4:O:48:MET:CE	2.41	0.50
1:A:72:LYS:HB3	1:A:131:THR:OG1	2.10	0.50
1:A:227:ASN:H	1:A:227:ASN:ND2	2.09	0.50
1:B:1:MET:HB2	9:B:9722:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:708:TYR:CE2	2:C:793:PRO:HD2	2.45	0.50
2:C:954:THR:OG1	2:C:957:LYS:HG3	2.11	0.50
3:D:400:VAL:HG12	3:D:401:TYR:HD1	1.77	0.50
3:D:693:GLU:HG3	9:D:2933:HOH:O	2.11	0.50
3:D:630:VAL:O	3:D:726:ILE:HG13	2.10	0.50
2:C:889:HIS:HE1	3:D:951:ILE:H	1.57	0.50
4:E:73:LEU:HD12	9:E:9555:HOH:O	2.11	0.50
5:F:363:GLU:HA	5:F:367:MET:CE	2.41	0.50
2:M:148:PHE:HZ	2:M:281:LEU:HD13	1.77	0.50
2:M:486:MET:HE3	2:M:491:GLU:HA	1.92	0.50
2:M:54:ILE:HG23	2:M:54:ILE:O	2.11	0.50
2:M:678:PRO:HD2	9:N:9608:HOH:O	2.12	0.50
2:M:861:LEU:HD22	2:M:863:ASP:OD1	2.11	0.50
3:N:119:SER:OG	3:N:123:LEU:HD12	2.11	0.50
3:N:523:ASP:O	3:N:526:PRO:HG3	2.12	0.50
3:N:562:ALA:HB1	3:N:567:ILE:CD1	2.41	0.50
5:P:74:LYS:HE3	9:P:3589:HOH:O	2.11	0.50
1:A:49:PRO:HB3	1:A:148:VAL:HG22	1.92	0.50
1:A:89:PHE:HZ	1:A:146:ARG:HB2	1.75	0.50
2:C:243:ARG:O	2:C:243:ARG:HD2	2.11	0.50
2:C:517:ARG:NH1	2:C:522:VAL:HG11	2.26	0.50
2:C:601:GLY:HA2	2:C:616:GLU:HG2	1.93	0.50
2:C:678:PRO:HG3	3:D:947:ILE:HD11	1.94	0.50
3:D:1478:SER:O	3:D:1482:ARG:HG3	2.10	0.50
3:D:530:VAL:HA	9:D:9858:HOH:O	2.11	0.50
3:D:602:SER:O	3:D:606:ILE:HG12	2.11	0.50
3:D:774:SER:C	3:D:776:GLU:H	2.14	0.50
3:D:790:TYR:HA	9:D:9833:HOH:O	2.10	0.50
3:D:817:GLU:OE1	3:D:839:LEU:HD21	2.11	0.50
1:B:176:ARG:NH2	3:D:884:ARG:HD3	2.23	0.50
3:D:790:TYR:CZ	3:D:905:PRO:HB2	2.47	0.50
3:D:787:LEU:HD21	3:D:947:ILE:CD1	2.41	0.50
5:F:112:ALA:HA	5:F:173:TYR:CD2	2.39	0.50
5:F:267:THR:O	5:F:271:LEU:HG	2.10	0.50
2:M:21:ILE:HD12	2:M:21:ILE:H	1.75	0.50
2:M:61:LYS:NZ	2:M:102:HIS:HE1	2.09	0.50
2:M:925:TYR:C	2:M:925:TYR:CD1	2.85	0.50
3:N:1128:VAL:HG22	9:N:9896:HOH:O	2.12	0.50
3:N:10:ILE:HD11	3:N:1434:TRP:NE1	2.26	0.50
3:N:1473:PRO:HD3	9:N:9577:HOH:O	2.11	0.50
3:N:139:GLY:H	3:N:147:VAL:HG21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:32:ILE:HG12	3:N:38:LYS:O	2.11	0.50
3:N:502:PHE:CZ	3:N:509:PRO:HB3	2.47	0.50
3:N:601:ARG:HH22	3:N:612:GLY:HA2	1.77	0.50
3:N:809:PRO:HB2	3:N:812:ALA:HB2	1.93	0.50
5:P:119:ILE:HD13	5:P:170:HIS:CG	2.46	0.50
5:P:323:ASP:O	5:P:325:LYS:N	2.44	0.50
1:A:9:PRO:HB3	1:A:25:LEU:CG	2.42	0.50
2:C:6:PHE:CE2	2:C:913:GLU:HB3	2.46	0.50
3:D:783:ARG:HH21	3:D:1029:ARG:CZ	2.24	0.50
3:D:1068:LEU:HD23	3:D:1068:LEU:O	2.11	0.50
3:D:154:THR:CG2	3:D:156:GLU:HG2	2.41	0.50
3:D:183:GLU:O	3:D:186:VAL:HG12	2.12	0.50
2:C:1052:MET:HG3	3:D:623:VAL:CG2	2.41	0.50
2:C:1042:ALA:CB	3:D:710:ARG:HB3	2.41	0.50
5:F:154:LYS:HE3	9:F:9774:HOH:O	2.10	0.50
5:F:209:PHE:CE2	5:F:213:ILE:HD11	2.47	0.50
1:K:162:ILE:HG13	1:K:163:ASN:ND2	2.27	0.50
1:K:184:THR:O	1:K:192:LEU:HB2	2.11	0.50
1:L:156:HIS:HE1	1:L:166:PRO:HB3	1.75	0.50
2:M:206:THR:HG21	9:M:2430:HOH:O	2.10	0.50
2:M:896:PHE:O	2:M:924:VAL:HG11	2.11	0.50
2:M:984:GLU:O	3:N:946:GLY:HA3	2.11	0.50
3:N:1007:VAL:HG23	3:N:1008:PHE:N	2.26	0.50
3:N:1264:GLU:OE2	3:N:1424:VAL:HG12	2.11	0.50
3:N:148:GLU:CB	3:N:151:GLN:HB2	2.37	0.50
3:N:455:ARG:HG2	3:N:455:ARG:HH11	1.76	0.50
3:N:972:LEU:HD13	9:N:2106:HOH:O	2.11	0.50
5:P:88:ILE:CD1	5:P:193:ARG:HB2	2.35	0.50
1:B:26:GLU:HG2	1:B:27:PRO:CA	2.42	0.50
1:A:221:HIS:HB3	1:B:36:LEU:HD21	1.92	0.50
2:C:313:LEU:HD12	2:C:313:LEU:O	2.12	0.50
2:C:496:ILE:HD12	2:C:496:ILE:H	1.77	0.50
2:C:517:ARG:HH11	2:C:522:VAL:HG11	1.76	0.50
3:D:1139:ASP:HB3	3:D:1357:ARG:NH2	2.27	0.50
3:D:1214:PRO:HB2	9:D:2041:HOH:O	2.10	0.50
3:D:1379:VAL:HG11	3:D:1395:LEU:HD23	1.93	0.50
3:D:397:LYS:CE	3:D:399:ARG:HE	2.24	0.50
3:D:704:ARG:HH11	3:D:738:ALA:CA	2.24	0.50
9:B:9819:HOH:O	3:D:840:LYS:HD2	2.12	0.50
5:F:262:VAL:HG23	9:F:9657:HOH:O	2.11	0.50
1:K:187:GLY:HA3	9:K:4787:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:115:LEU:HD11	9:L:3925:HOH:O	2.12	0.50
2:M:1016:ILE:HD13	2:M:1016:ILE:H	1.74	0.50
2:M:407:LYS:HD2	9:M:9923:HOH:O	2.12	0.50
2:M:473:ARG:HG2	2:M:473:ARG:HH11	1.76	0.50
2:M:546:LEU:HB3	9:M:9622:HOH:O	2.10	0.50
2:M:772:ARG:HB2	2:M:772:ARG:HH11	1.77	0.50
3:N:628:ARG:HD3	3:N:744:GLN:HE22	1.75	0.50
5:P:222:ARG:NH1	5:P:246:ALA:HB2	2.26	0.50
5:P:350:LEU:HD23	5:P:351:SER:N	2.27	0.50
1:A:57:TYR:CD2	1:A:161:ARG:HD2	2.46	0.50
2:C:1000:MET:HB2	2:C:1002:GLU:HG3	1.93	0.50
2:C:670:GLN:HE22	2:C:699:PHE:CA	2.25	0.50
2:C:722:ILE:HG22	2:C:820:ARG:NH2	2.27	0.50
3:D:1392:GLY:HA3	9:D:9721:HOH:O	2.11	0.50
3:D:60:CYS:HB3	9:D:9808:HOH:O	2.12	0.50
3:D:625:TYR:O	3:D:749:VAL:HG23	2.11	0.50
5:F:407:LYS:HB3	9:F:9858:HOH:O	2.11	0.50
1:K:102:LYS:HG3	1:K:139:ASN:CB	2.42	0.50
2:M:1018:GLN:CG	2:M:1060:ILE:HD11	2.42	0.50
2:M:197:LEU:HD22	2:M:202:TYR:HD2	1.77	0.50
2:M:139:GLN:O	2:M:333:ILE:HA	2.11	0.50
2:M:464:LEU:O	2:M:466:PHE:N	2.45	0.50
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.94	0.50
2:M:520:GLU:HB2	9:M:2526:HOH:O	2.11	0.50
2:M:589:ARG:HD3	2:M:596:TYR:CE2	2.47	0.50
3:N:1290:LEU:CD2	3:N:1291:SER:H	2.23	0.50
3:N:131:LYS:O	3:N:133:ILE:HD13	2.12	0.50
3:N:1422:MET:HE2	9:N:9889:HOH:O	2.11	0.50
3:N:424:GLY:HA2	3:N:435:VAL:O	2.11	0.50
3:N:820:GLU:HA	3:N:825:ALA:O	2.12	0.50
3:N:820:GLU:HB2	3:N:836:VAL:HG11	1.94	0.50
5:P:133:ALA:HB3	9:P:5172:HOH:O	2.11	0.50
9:N:9682:HOH:O	5:P:87:GLU:HG3	2.10	0.50
1:A:102:LYS:HE2	1:A:139:ASN:HB2	1.94	0.50
1:B:1:MET:HG3	9:B:9588:HOH:O	2.11	0.50
1:B:41:ARG:HG3	1:B:177:VAL:CG2	2.38	0.50
2:C:1025:ALA:HA	9:C:9555:HOH:O	2.10	0.50
2:C:346:VAL:O	2:C:350:ARG:HG3	2.12	0.50
2:C:456:ALA:HB1	2:C:538:GLN:O	2.12	0.50
2:C:703:ILE:HD11	9:C:9934:HOH:O	2.10	0.50
3:D:106:LYS:HE3	9:D:2691:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1147:ARG:O	3:D:1166:LEU:HD23	2.12	0.50
3:D:116:LEU:O	3:D:118:LEU:HG	2.12	0.50
3:D:1274:ILE:HD11	3:D:1334:GLN:NE2	2.26	0.50
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.11	0.50
5:F:305:GLU:O	5:F:309:LYS:HG3	2.11	0.50
1:K:54:THR:HG22	1:K:158:ILE:HG13	1.93	0.50
1:K:89:PHE:HB3	1:K:94:LEU:HD13	1.93	0.50
2:M:290:LEU:H	2:M:290:LEU:HD23	1.77	0.50
2:M:313:LEU:CD2	2:M:314:THR:HG23	2.41	0.50
2:M:602:GLU:HA	2:M:647:GLN:O	2.12	0.50
2:M:551:GLU:HA	2:M:906:PHE:CE2	2.47	0.50
3:N:386:HIS:HA	9:N:9796:HOH:O	2.11	0.50
3:N:600:LEU:HD12	3:N:600:LEU:H	1.75	0.50
3:N:637:LEU:HD11	3:N:641:GLN:HB2	1.92	0.50
1:L:150:TYR:HE2	3:N:857:ILE:HG13	1.76	0.50
4:O:90:GLU:HA	9:O:4303:HOH:O	2.11	0.50
5:P:110:MET:HE1	9:P:6261:HOH:O	2.11	0.50
5:P:122:LEU:HD12	9:P:4507:HOH:O	2.10	0.50
1:B:23:PHE:CD2	1:B:211:LEU:HD22	2.47	0.50
2:C:265:ARG:HB3	2:C:267:TYR:CE2	2.46	0.50
2:C:25:SER:CB	2:C:335:THR:HB	2.41	0.50
2:C:572:ILE:HG13	9:C:2021:HOH:O	2.12	0.50
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.26	0.50
2:C:724:ARG:CD	2:C:740:GLU:HA	2.42	0.50
2:C:675:ALA:CA	2:C:989:VAL:HG12	2.35	0.50
3:D:952:ASP:HA	3:D:1062:ARG:NH2	2.26	0.50
3:D:1458:GLU:HB3	9:D:2112:HOH:O	2.12	0.50
3:D:150:ARG:HD2	9:D:2177:HOH:O	2.10	0.50
3:D:631:ILE:O	3:D:632:VAL:HG23	2.11	0.50
3:D:637:LEU:HD11	3:D:642:CYS:N	2.26	0.50
4:E:43:GLU:CD	4:E:43:GLU:H	2.14	0.50
5:F:287:THR:C	5:F:289:GLU:H	2.14	0.50
5:F:295:MET:HE2	5:F:295:MET:HA	1.93	0.50
5:F:369:LEU:HD11	5:F:401:GLU:HB2	1.93	0.50
1:L:101:LEU:HD21	1:L:113:ASP:HB3	1.93	0.50
1:L:143:ARG:HD2	1:L:160:ASP:CG	2.32	0.50
2:M:103:LYS:HA	2:M:103:LYS:NZ	2.27	0.50
2:M:18:LEU:HD22	2:M:590:ASP:HB2	1.94	0.50
2:M:45:GLN:HA	9:M:9965:HOH:O	2.12	0.50
2:M:601:GLY:HA2	2:M:616:GLU:HG2	1.93	0.50
3:N:103:TRP:CH2	3:N:1447:LEU:HD23	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1145:TYR:HE2	3:N:1168:MET:HB2	1.76	0.50
3:N:1173:LEU:HA	9:N:2439:HOH:O	2.12	0.50
3:N:1240:THR:O	3:N:1257:PRO:HB3	2.12	0.50
3:N:123:LEU:HD21	3:N:152:LEU:HD22	1.94	0.50
3:N:683:ILE:HB	9:N:9759:HOH:O	2.11	0.50
4:O:87:LYS:HE2	4:O:91:ARG:CZ	2.42	0.50
1:B:26:GLU:HG3	1:B:184:THR:HG21	1.94	0.50
2:C:1090:LYS:HG2	2:C:1112:PHE:CZ	2.47	0.50
2:C:333:ILE:HD13	2:C:467:ILE:HG13	1.92	0.50
2:C:73:LEU:HB3	2:C:94:LEU:HD13	1.93	0.50
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.12	0.50
3:D:1168:MET:CE	3:D:1171:VAL:HB	2.42	0.50
3:D:1468:LEU:HD13	3:D:1470:ARG:HD3	1.93	0.50
3:D:141:ILE:HD13	3:D:449:SER:OG	2.12	0.50
3:D:87:ARG:CB	3:D:523:ASP:HB2	2.35	0.50
1:K:41:ARG:HH11	1:K:177:VAL:HB	1.77	0.50
1:L:108:GLU:HB2	9:L:4517:HOH:O	2.10	0.50
2:M:248:PRO:HB2	9:M:2239:HOH:O	2.12	0.50
2:M:357:GLU:O	2:M:360:LEU:HG	2.12	0.50
2:M:724:ARG:CG	2:M:741:GLY:H	2.24	0.50
2:M:552:HIS:CD2	2:M:886:LEU:HD12	2.47	0.50
3:N:169:TYR:N	3:N:170:PRO:CD	2.75	0.50
3:N:42:ASP:O	3:N:43:GLY:O	2.29	0.50
3:N:576:GLU:O	3:N:579:ASP:HB2	2.12	0.50
5:P:317:LEU:O	5:P:329:TYR:HB3	2.11	0.50
1:A:168:ASP:HB3	9:C:9876:HOH:O	2.11	0.49
1:A:24:VAL:HG22	1:A:196:THR:HB	1.94	0.49
1:A:212:ASN:O	1:A:215:VAL:HG22	2.11	0.49
1:B:208:LEU:HB2	9:B:9610:HOH:O	2.12	0.49
1:B:13:VAL:HG13	1:B:23:PHE:CD1	2.47	0.49
2:C:1008:ARG:NH1	2:C:1011:GLY:HA3	2.27	0.49
2:C:515:ALA:C	2:C:516:ARG:HG2	2.32	0.49
2:C:603:VAL:HG12	9:C:9913:HOH:O	2.12	0.49
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	1.94	0.49
3:D:474:GLU:HG3	3:D:500:ARG:HE	1.77	0.49
3:D:669:ASN:O	3:D:672:ALA:HB3	2.11	0.49
3:D:984:THR:HG23	3:D:986:ARG:H	1.77	0.49
4:E:40:LEU:O	4:E:40:LEU:HD22	2.12	0.49
1:L:105:GLY:HA2	9:L:4025:HOH:O	2.12	0.49
1:L:206:THR:HG22	1:L:209:GLU:HG3	1.94	0.49
2:M:1023:GLY:HA2	9:M:2349:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:244:PRO:CD	2:M:245:GLY:H	2.24	0.49
2:M:358:ARG:HB3	2:M:371:LYS:O	2.12	0.49
2:M:721:ARG:NH2	2:M:785:VAL:HG21	2.25	0.49
2:M:979:THR:HG21	9:M:2061:HOH:O	2.10	0.49
3:N:999:THR:O	3:N:1002:LYS:HB2	2.12	0.49
3:N:953:ASP:OD1	3:N:1019:PRO:HG2	2.12	0.49
3:N:1045:MET:HG2	3:N:1073:SER:CA	2.23	0.49
3:N:1273:VAL:O	3:N:1325:LEU:HB2	2.12	0.49
3:N:679:ARG:HH22	3:N:681:ARG:NE	2.10	0.49
3:N:754:PHE:HE2	3:N:1476:THR:HG21	1.77	0.49
3:N:81:THR:O	3:N:82:LYS:C	2.50	0.49
4:O:43:GLU:H	4:O:43:GLU:CD	2.15	0.49
4:O:54:LEU:HA	4:O:58:PRO:HG2	1.94	0.49
4:O:74:VAL:HG12	4:O:79:LEU:HD21	1.94	0.49
2:M:1021:LEU:HD21	5:P:332:PHE:HA	1.93	0.49
1:B:132:LEU:HD13	1:B:138:LEU:HD13	1.94	0.49
1:B:184:THR:HG23	1:B:192:LEU:HB3	1.94	0.49
1:B:227:ASN:HD22	1:B:227:ASN:N	2.09	0.49
2:C:473:ARG:HD2	2:C:475:VAL:HG23	1.94	0.49
2:C:599:GLU:HG2	2:C:600:ASP:H	1.77	0.49
1:A:72:LYS:O	2:C:608:GLY:HA3	2.12	0.49
2:C:64:LEU:HD22	2:C:359:MET:CG	2.33	0.49
2:C:882:LEU:HD21	3:D:951:ILE:HA	1.94	0.49
3:D:1004:THR:HG22	9:D:9570:HOH:O	2.11	0.49
3:D:481:MET:HB2	9:D:2197:HOH:O	2.12	0.49
3:D:86:ARG:HG3	3:D:86:ARG:O	2.12	0.49
3:D:959:GLU:CD	3:D:959:GLU:H	2.15	0.49
5:F:411:HIS:HA	5:F:414:ARG:HG3	1.93	0.49
2:M:387:SER:OG	2:M:388:ARG:HD3	2.12	0.49
2:M:52:PHE:CE1	2:M:66:LEU:HG	2.47	0.49
2:M:549:PHE:CE2	2:M:886:LEU:HB3	2.48	0.49
3:N:996:TRP:O	3:N:1000:THR:HG22	2.12	0.49
3:N:1003:VAL:O	3:N:1006:ALA:HB3	2.11	0.49
3:N:115:LEU:HD22	3:N:502:PHE:CE1	2.47	0.49
3:N:528:VAL:HG13	9:P:4960:HOH:O	2.11	0.49
3:N:655:PRO:HA	3:N:658:LEU:HD12	1.94	0.49
2:M:1115:LEU:HD23	3:N:85:VAL:N	2.26	0.49
1:A:150:TYR:CD1	2:C:696:LYS:HD3	2.47	0.49
2:C:140:ILE:CD1	2:C:412:ALA:HA	2.42	0.49
2:C:500:ASN:HB3	9:C:2232:HOH:O	2.12	0.49
3:D:1045:MET:HB2	9:D:9822:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1192:LEU:HG	3:D:1369:GLU:HG2	1.94	0.49
3:D:1262:LEU:HD23	3:D:1352:ILE:CG1	2.40	0.49
3:D:131:LYS:HE2	3:D:568:ARG:CB	2.43	0.49
3:D:584:ASN:ND2	3:D:590:PRO:HD2	2.27	0.49
3:D:872:ARG:HB3	9:D:9663:HOH:O	2.12	0.49
4:E:17:TYR:N	4:E:17:TYR:HD2	2.11	0.49
5:F:152:ASP:HB2	5:F:153:PRO:HD3	1.95	0.49
2:M:292:ARG:HD2	2:M:299:LYS:HG2	1.95	0.49
2:M:418:LEU:HD12	2:M:418:LEU:N	2.27	0.49
2:M:525:SER:OG	2:M:528:GLU:HG3	2.11	0.49
2:M:975:TYR:HA	2:M:982:PRO:HA	1.93	0.49
3:N:1031:ASN:HB3	3:N:1034:GLN:CD	2.32	0.49
3:N:1191:PRO:HB3	3:N:1370:ILE:HD13	1.94	0.49
3:N:1266:ARG:O	3:N:1268:PRO:HD3	2.12	0.49
3:N:185:VAL:HG22	9:N:2294:HOH:O	2.12	0.49
3:N:421:LEU:HD11	3:N:437:VAL:HG22	1.93	0.49
3:N:550:ARG:HD2	3:N:573:MET:HB3	1.95	0.49
3:N:584:ASN:CG	3:N:590:PRO:HD2	2.32	0.49
3:N:637:LEU:CD1	3:N:641:GLN:HB2	2.43	0.49
3:N:864:VAL:HG12	3:N:865:THR:H	1.77	0.49
2:M:772:ARG:CD	5:P:373:LYS:HD2	2.42	0.49
5:P:79:ASP:HB3	5:P:80:PRO:CD	2.42	0.49
1:A:76:VAL:HA	1:A:79:ILE:HG12	1.94	0.49
2:C:274:ARG:O	2:C:274:ARG:HG2	2.12	0.49
2:C:942:GLU:HG3	9:D:2549:HOH:O	2.11	0.49
2:C:676:ILE:HG22	2:C:988:VAL:HG22	1.93	0.49
3:D:1037:GLN:CD	3:D:1042:ARG:HB3	2.32	0.49
3:D:1330:ILE:HB	3:D:1347:TYR:CZ	2.46	0.49
3:D:10:ILE:HD13	3:D:1447:LEU:HG	1.94	0.49
3:D:397:LYS:HG3	9:D:9821:HOH:O	2.12	0.49
3:D:57:GLU:HG2	3:D:58:CYS:N	2.27	0.49
3:D:804:LEU:HD23	9:D:2035:HOH:O	2.11	0.49
5:F:151:LEU:HB2	5:F:155:THR:H	1.78	0.49
5:F:192:LEU:O	5:F:192:LEU:HD23	2.11	0.49
5:F:215:GLU:N	9:F:9685:HOH:O	2.44	0.49
5:F:234:LYS:HD3	5:F:236:SER:HB3	1.93	0.49
1:L:101:LEU:HD12	1:L:114:PHE:CD1	2.47	0.49
1:K:9:PRO:HD2	1:L:224:TYR:CD1	2.48	0.49
2:M:228:ALA:HB2	9:M:9769:HOH:O	2.12	0.49
2:M:257:VAL:HG12	2:M:263:ASP:OD1	2.13	0.49
3:N:1333:HIS:O	3:N:1336:LEU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:462:GLN:CG	3:N:513:ILE:HD13	2.43	0.49
3:N:555:LYS:HB3	9:N:9736:HOH:O	2.11	0.49
5:P:299:TRP:CZ3	5:P:303:ARG:HG2	2.48	0.49
5:P:337:HIS:H	5:P:337:HIS:CD2	2.28	0.49
1:A:2:LEU:HD23	9:A:9587:HOH:O	2.12	0.49
2:C:1045:ALA:HB1	2:C:1048:THR:HB	1.95	0.49
2:C:140:ILE:HD11	2:C:412:ALA:HA	1.93	0.49
2:C:34:VAL:CB	2:C:38:LYS:HG3	2.42	0.49
2:C:34:VAL:CG1	2:C:38:LYS:HG3	2.42	0.49
2:C:498:GLN:O	2:C:501:THR:HG23	2.11	0.49
2:C:56:GLU:HB3	9:C:9885:HOH:O	2.12	0.49
3:D:1240:THR:O	3:D:1257:PRO:HB3	2.11	0.49
3:D:1285:GLU:H	3:D:1285:GLU:CD	2.15	0.49
3:D:639:LEU:CD1	3:D:640:HIS:H	2.25	0.49
3:D:6:ARG:NH1	3:D:6:ARG:HB2	2.27	0.49
3:D:744:GLN:HG3	9:D:2560:HOH:O	2.12	0.49
3:D:770:LEU:HB2	3:D:1210:SER:O	2.11	0.49
2:C:873:PRO:HG2	3:D:947:ILE:O	2.12	0.49
5:F:227:PHE:CZ	5:F:229:TYR:HA	2.48	0.49
9:D:9783:HOH:O	5:F:314:PRO:HA	2.12	0.49
5:F:333:ILE:HG13	9:F:9704:HOH:O	2.10	0.49
1:K:69:PRO:O	1:K:71:VAL:HG23	2.11	0.49
2:M:507:ARG:HH11	2:M:507:ARG:CB	2.22	0.49
2:M:61:LYS:HE2	9:M:9621:HOH:O	2.11	0.49
3:N:1034:GLN:O	3:N:1038:LEU:HD12	2.13	0.49
3:N:956:ILE:HG12	3:N:1039:CYS:O	2.12	0.49
3:N:1068:LEU:C	3:N:1070:TYR:H	2.14	0.49
3:N:1078:ARG:HH11	3:N:1078:ARG:HG3	1.76	0.49
3:N:1263:PHE:CE1	3:N:1352:ILE:HD13	2.47	0.49
3:N:1103:HIS:HD2	3:N:1463:LYS:H	1.58	0.49
3:N:696:HIS:HB3	9:N:2096:HOH:O	2.11	0.49
5:P:261:PRO:O	5:P:265:VAL:HG23	2.13	0.49
1:A:86:VAL:HG23	1:A:202:ASP:OD1	2.13	0.49
1:B:3:ASP:HB3	9:B:9533:HOH:O	2.13	0.49
2:C:137:VAL:O	2:C:391:LEU:HD21	2.13	0.49
2:C:198:ARG:HG2	9:C:2206:HOH:O	2.12	0.49
2:C:794:PRO:HD2	9:C:9555:HOH:O	2.12	0.49
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.42	0.49
3:D:150:ARG:NH1	3:D:464:LEU:HD22	2.27	0.49
3:D:28:LYS:HD2	3:D:552:ASN:HD21	1.77	0.49
3:D:795:VAL:HG23	3:D:879:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:404:ALA:O	5:F:408:LEU:HD23	2.13	0.49
1:K:91:ASN:CG	1:K:92:PRO:HD2	2.32	0.49
1:L:100:LEU:HB2	1:L:115:LEU:HD21	1.94	0.49
1:L:65:PHE:HD1	3:N:813:LEU:HD22	1.75	0.49
2:M:326:ASP:HA	2:M:331:ARG:HD3	1.93	0.49
2:M:580:MET:HB3	2:M:584:GLU:CD	2.33	0.49
2:M:605:LYS:HD3	2:M:610:ARG:HH22	1.76	0.49
2:M:625:LEU:O	2:M:627:ARG:N	2.44	0.49
2:M:637:LEU:HD23	2:M:637:LEU:N	2.28	0.49
2:M:736:ASP:HA	2:M:744:ARG:HD3	1.95	0.49
2:M:983:ILE:CG2	2:M:987:ILE:HD11	2.43	0.49
3:N:154:THR:HG23	3:N:157:GLU:H	1.76	0.49
3:N:202:VAL:O	3:N:204:LEU:HG	2.13	0.49
3:N:526:PRO:HB2	5:P:317:LEU:HD11	1.95	0.49
3:N:817:GLU:O	3:N:821:VAL:HG23	2.12	0.49
5:P:160:ASP:HB2	9:P:4635:HOH:O	2.11	0.49
5:P:371:LEU:HD22	5:P:375:LEU:HD22	1.94	0.49
1:A:14:ARG:HH21	1:A:22:GLU:CB	2.21	0.49
1:B:62:LEU:HD23	9:B:9681:HOH:O	2.12	0.49
2:C:232:GLU:CA	2:C:235:LEU:HD12	2.33	0.49
2:C:437:ARG:HG3	2:C:469:THR:HB	1.94	0.49
3:D:1050:GLY:HA2	9:D:9762:HOH:O	2.12	0.49
3:D:843:PHE:CD1	3:D:849:ALA:HA	2.48	0.49
3:D:905:PRO:HD3	9:D:2488:HOH:O	2.12	0.49
5:F:323:ASP:O	5:F:325:LYS:N	2.46	0.49
1:L:184:THR:O	1:L:192:LEU:HB2	2.12	0.49
2:M:1049:LEU:HD11	2:M:1053:LEU:HD21	1.93	0.49
2:M:191:PHE:CZ	2:M:196:LEU:HB2	2.44	0.49
2:M:720:GLU:HA	2:M:759:THR:O	2.13	0.49
2:M:833:LEU:HD12	2:M:834:GLN:H	1.77	0.49
3:N:1020:LEU:HB2	9:N:9719:HOH:O	2.11	0.49
3:N:1326:THR:HG22	3:N:1327:ARG:H	1.78	0.49
3:N:1459:LEU:HD13	3:N:1465:ASN:HD21	1.77	0.49
3:N:992:ILE:O	3:N:995:LEU:HB3	2.13	0.49
4:O:45:ARG:HB2	4:O:46:PRO:CD	2.43	0.49
5:P:195:VAL:HG12	5:P:213:ILE:HG23	1.94	0.49
1:A:184:THR:HG23	1:A:192:LEU:HB2	1.95	0.49
2:C:290:LEU:HB3	2:C:302:VAL:CG1	2.43	0.49
2:C:532:MET:HE3	9:C:9909:HOH:O	2.12	0.49
3:D:907:GLU:HG3	3:D:1026:SER:HA	1.94	0.49
3:D:1281:VAL:HG21	3:D:1313:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3:LYS:H	3:D:3:LYS:HD3	1.76	0.49
3:D:409:VAL:HG21	9:F:9706:HOH:O	2.11	0.49
3:D:421:LEU:HD12	3:D:435:VAL:HG11	1.94	0.49
3:D:584:ASN:HB2	3:D:602:SER:HB3	1.93	0.49
3:D:600:LEU:HB3	9:D:9656:HOH:O	2.13	0.49
4:E:22:VAL:HG21	4:E:75:PHE:CD1	2.48	0.49
1:K:91:ASN:OD1	1:K:92:PRO:HD2	2.13	0.49
2:M:100:LEU:HD21	2:M:368:THR:CA	2.42	0.49
2:M:1097:LEU:H	2:M:1097:LEU:CD2	2.25	0.49
2:M:1101:THR:HB	2:M:1109:VAL:HG12	1.95	0.49
2:M:863:ASP:O	2:M:865:THR:N	2.45	0.49
3:N:11:ALA:HB1	3:N:507:ASN:OD1	2.13	0.49
3:N:1205:TYR:O	3:N:1366:LYS:HD3	2.12	0.49
3:N:1280:VAL:HG23	3:N:1295:GLU:O	2.12	0.49
3:N:172:PRO:HB3	3:N:178:LEU:HB3	1.93	0.49
3:N:198:ARG:HD3	9:N:2083:HOH:O	2.12	0.49
3:N:524:LEU:C	3:N:526:PRO:HD3	2.33	0.49
3:N:563:PRO:O	3:N:567:ILE:HG13	2.12	0.49
3:N:703:ASN:ND2	3:N:704:ARG:H	2.10	0.49
2:M:1043:TYR:HE1	3:N:710:ARG:O	1.95	0.49
5:P:266:GLU:HA	9:P:6839:HOH:O	2.12	0.49
1:B:189:ARG:HG2	9:B:9767:HOH:O	2.13	0.49
2:C:1000:MET:HG3	9:C:2365:HOH:O	2.13	0.49
2:C:1016:ILE:CD1	3:D:526:PRO:HG2	2.43	0.49
2:C:1104:GLU:HB3	9:D:9955:HOH:O	2.12	0.49
2:C:16:PRO:HB3	2:C:460:ARG:HH22	1.77	0.49
2:C:235:LEU:HB2	9:C:9661:HOH:O	2.13	0.49
2:C:356:ARG:HA	9:C:9719:HOH:O	2.13	0.49
2:C:564:MET:SD	2:C:846:LYS:HG3	2.53	0.49
3:D:1036:ARG:HH21	3:D:1042:ARG:HA	1.77	0.49
3:D:1203:LYS:HG3	9:D:2820:HOH:O	2.12	0.49
3:D:1198:TYR:OH	3:D:1432:LYS:HG2	2.13	0.49
3:D:1472:ILE:HG22	3:D:1474:ALA:H	1.78	0.49
3:D:434:ARG:HB2	3:D:447:VAL:CG2	2.43	0.49
3:D:654:LYS:CB	3:D:655:PRO:HD3	2.41	0.49
3:D:827:ILE:O	3:D:837:GLY:HA3	2.13	0.49
4:E:17:TYR:N	4:E:17:TYR:CD2	2.80	0.49
5:F:256:ARG:HD2	9:F:9723:HOH:O	2.12	0.49
2:M:1016:ILE:HD13	2:M:1016:ILE:N	2.27	0.49
2:M:145:GLY:C	2:M:163:ILE:HG23	2.33	0.49
2:M:268:ASP:HB2	2:M:272:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:62:GLY:O	2:M:103:LYS:HG3	2.12	0.49
2:M:918:LEU:HD23	2:M:968:LEU:CA	2.42	0.49
3:N:103:TRP:HH2	3:N:1447:LEU:HD23	1.76	0.49
3:N:186:VAL:HG13	3:N:187:LYS:N	2.28	0.49
3:N:562:ALA:HB1	3:N:567:ILE:HD11	1.94	0.49
3:N:785:ILE:HG12	3:N:935:LYS:HA	1.95	0.49
1:A:54:THR:HG21	9:A:9616:HOH:O	2.13	0.49
1:B:165:ILE:HG12	9:B:9582:HOH:O	2.12	0.49
2:C:1004:LYS:HE3	2:C:1027:PHE:HE1	1.77	0.49
2:C:254:VAL:HG13	2:C:258:TYR:CE1	2.47	0.49
2:C:285:LEU:HD23	2:C:287:GLY:H	1.77	0.49
2:C:202:TYR:OH	2:C:304:LEU:HD22	2.12	0.49
2:C:537:LYS:HD2	2:C:537:LYS:H	1.77	0.49
2:C:889:HIS:CE1	3:D:951:ILE:H	2.31	0.49
3:D:168:THR:OG1	3:D:393:ILE:HB	2.13	0.49
3:D:171:LEU:HB2	3:D:390:PRO:HA	1.94	0.49
4:E:64:ALA:HA	4:E:67:GLU:CD	2.33	0.49
5:F:217:ASN:O	5:F:221:ILE:HG13	2.12	0.49
5:F:261:PRO:HA	9:F:9657:HOH:O	2.12	0.49
2:M:1016:ILE:HD11	5:P:330:GLY:O	2.13	0.49
2:M:188:LYS:HD2	9:M:2372:HOH:O	2.13	0.49
2:M:195:LEU:CD2	2:M:238:LEU:HG	2.43	0.49
2:M:140:ILE:HD11	2:M:412:ALA:HA	1.95	0.49
3:N:1068:LEU:C	3:N:1070:TYR:N	2.65	0.49
3:N:210:ARG:HD3	9:N:2267:HOH:O	2.13	0.49
3:N:715:ALA:HB3	3:N:764:LEU:HA	1.94	0.49
3:N:774:SER:C	3:N:776:GLU:H	2.16	0.49
1:A:178:ALA:HB2	2:C:864:GLY:H	1.77	0.48
1:A:23:PHE:HE1	1:A:208:LEU:HD13	1.77	0.48
1:A:86:VAL:HA	9:A:9642:HOH:O	2.12	0.48
2:C:1075:ASP:HB3	4:E:32:ARG:NH1	2.28	0.48
2:C:216:GLU:OE1	2:C:217:LEU:HG	2.13	0.48
2:C:265:ARG:N	9:C:9833:HOH:O	2.45	0.48
2:C:549:PHE:HB3	2:C:552:HIS:HD2	1.77	0.48
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.12	0.48
3:D:1149:LEU:HD12	3:D:1161:GLU:O	2.13	0.48
3:D:126:VAL:O	3:D:132:TYR:CD1	2.65	0.48
3:D:131:LYS:HD2	5:F:83:GLN:NE2	2.28	0.48
3:D:397:LYS:HZ1	3:D:399:ARG:HH21	1.60	0.48
3:D:41:ARG:HG2	9:D:9791:HOH:O	2.13	0.48
3:D:42:ASP:O	3:D:46:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:48:MET:HB3	4:E:54:LEU:HB2	1.93	0.48
5:F:151:LEU:HD21	9:F:9796:HOH:O	2.11	0.48
1:L:75:VAL:O	1:L:79:ILE:HG23	2.12	0.48
2:M:1008:ARG:NH2	2:M:1028:GLY:HA2	2.27	0.48
2:M:115:LEU:HA	2:M:375:SER:OG	2.13	0.48
2:M:141:HIS:HB2	9:M:2274:HOH:O	2.12	0.48
2:M:264:PRO:HB3	2:M:289:THR:CG2	2.43	0.48
2:M:139:GLN:NE2	2:M:415:PRO:HG2	2.26	0.48
2:M:612:VAL:HG22	2:M:622:GLU:HA	1.95	0.48
2:M:724:ARG:HG2	2:M:737:LEU:HD22	1.94	0.48
3:N:1129:THR:C	3:N:1130:ARG:HD2	2.33	0.48
3:N:1166:LEU:HD23	3:N:1166:LEU:N	2.22	0.48
3:N:1326:THR:HG22	3:N:1327:ARG:N	2.27	0.48
3:N:1480:PHE:CD2	3:N:1481:VAL:HG22	2.37	0.48
3:N:838:ARG:HB2	9:N:2421:HOH:O	2.12	0.48
5:P:338:LEU:HB2	9:P:5855:HOH:O	2.13	0.48
5:P:409:LYS:HE3	5:P:410:TYR:CD1	2.48	0.48
2:C:1034:GLU:HA	2:C:1037:VAL:CG2	2.42	0.48
2:C:473:ARG:HA	2:C:531:PHE:HD1	1.77	0.48
2:C:731:GLU:OE2	2:C:734:LEU:HB3	2.13	0.48
3:D:100:ALA:HB2	9:D:2526:HOH:O	2.13	0.48
3:D:427:VAL:HB	3:D:435:VAL:HB	1.95	0.48
3:D:521:PRO:O	3:D:525:ARG:HG2	2.13	0.48
3:D:661:MET:HE2	3:D:677:LEU:HD11	1.95	0.48
5:F:297:PRO:HD2	9:F:9885:HOH:O	2.12	0.48
2:C:1014:SER:HB2	5:F:331:ASP:O	2.13	0.48
1:K:90:LEU:HB3	9:K:6576:HOH:O	2.13	0.48
1:L:159:LYS:HE2	9:L:5625:HOH:O	2.13	0.48
1:L:55:SER:HB3	9:L:4758:HOH:O	2.13	0.48
2:M:331:ARG:NH1	2:M:427:VAL:HG13	2.27	0.48
2:M:822:VAL:HG21	2:M:824:ARG:NH2	2.28	0.48
2:M:564:MET:HG2	2:M:840:ALA:HB3	1.95	0.48
2:M:855:VAL:HG12	9:M:9776:HOH:O	2.12	0.48
3:N:1176:LYS:HA	3:N:1179:GLU:OE1	2.14	0.48
3:N:1243:THR:HG22	3:N:1244:GLY:H	1.77	0.48
3:N:1416:ALA:HA	9:N:9795:HOH:O	2.13	0.48
3:N:1475:GLY:HA2	4:O:17:TYR:CD1	2.48	0.48
3:N:452:ILE:HG23	3:N:452:ILE:O	2.14	0.48
3:N:704:ARG:HG3	3:N:736:PHE:CB	2.42	0.48
3:N:759:ALA:O	3:N:763:MET:HB3	2.13	0.48
3:N:788:GLY:O	3:N:792:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:820:GLU:HG2	3:N:825:ALA:O	2.13	0.48
3:N:860:LEU:HA	3:N:877:PRO:HB2	1.95	0.48
3:N:928:ALA:O	3:N:931:LEU:HB2	2.13	0.48
4:O:17:TYR:HD2	4:O:17:TYR:N	2.10	0.48
1:A:215:VAL:HB	1:B:222:LEU:HD23	1.94	0.48
2:C:133:ASP:HB2	2:C:395:LYS:HB2	1.94	0.48
2:C:267:TYR:CD1	2:C:272:ALA:HB1	2.48	0.48
2:C:41:ASN:N	2:C:41:ASN:ND2	2.44	0.48
2:C:486:MET:CE	2:C:491:GLU:HA	2.43	0.48
2:C:726:ILE:HG21	9:C:2381:HOH:O	2.14	0.48
2:C:818:GLY:HA2	9:F:9939:HOH:O	2.12	0.48
3:D:8:VAL:O	3:D:1434:TRP:HH2	1.96	0.48
3:D:183:GLU:OE1	3:D:216:VAL:HG21	2.13	0.48
3:D:235:ALA:HB3	9:D:9702:HOH:O	2.14	0.48
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.44	0.48
5:F:393:THR:O	5:F:397:ILE:HG13	2.13	0.48
1:K:128:HIS:HB2	9:K:5129:HOH:O	2.13	0.48
1:K:184:THR:O	1:K:192:LEU:HD12	2.14	0.48
2:M:141:HIS:O	2:M:332:ARG:N	2.44	0.48
2:M:175:GLU:HA	9:M:9821:HOH:O	2.12	0.48
2:M:198:ARG:HD2	2:M:228:ALA:O	2.13	0.48
2:M:952:LEU:HD22	2:M:952:LEU:N	2.27	0.48
3:N:1083:ASP:HB3	3:N:1087:ARG:HH11	1.78	0.48
3:N:1152:GLU:HG2	3:N:1160:LEU:O	2.12	0.48
3:N:135:LEU:HD21	3:N:138:LYS:C	2.34	0.48
5:P:292:ALA:HB1	5:P:299:TRP:O	2.13	0.48
5:P:397:ILE:HD11	9:P:3604:HOH:O	2.13	0.48
1:A:82:LEU:O	1:A:85:LEU:HB3	2.13	0.48
1:B:65:PHE:HE1	3:D:806:PHE:CZ	2.30	0.48
2:C:208:ALA:HA	2:C:221:LEU:HD21	1.95	0.48
2:C:285:LEU:HG	2:C:287:GLY:O	2.13	0.48
2:C:313:LEU:HB2	2:C:321:GLU:HG3	1.95	0.48
2:C:332:ARG:HG2	2:C:333:ILE:N	2.28	0.48
2:C:586:ARG:HD2	2:C:590:ASP:OD2	2.12	0.48
2:C:632:ASN:HB2	2:C:633:GLN:OE1	2.14	0.48
2:C:745:ILE:HG13	9:C:9560:HOH:O	2.13	0.48
2:C:754:ILE:HD13	2:C:791:ARG:CD	2.44	0.48
3:D:1119:SER:HA	3:D:1186:VAL:O	2.13	0.48
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.43	0.48
3:D:169:TYR:N	3:D:170:PRO:CD	2.76	0.48
3:D:221:ALA:HA	9:D:2023:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:720:LEU:CD1	3:D:720:LEU:H	2.21	0.48
3:D:850:LEU:O	3:D:853:VAL:HB	2.13	0.48
5:F:260:ILE:CG2	5:F:264:MET:HB2	2.42	0.48
5:F:303:ARG:HB2	9:F:9813:HOH:O	2.12	0.48
1:L:208:LEU:HD23	9:L:3621:HOH:O	2.14	0.48
2:M:184:MET:HE3	2:M:186:VAL:HG13	1.95	0.48
2:M:212:GLY:HA3	2:M:218:VAL:HG23	1.94	0.48
2:M:231:PRO:HB2	9:M:9582:HOH:O	2.12	0.48
2:M:403:SER:O	2:M:407:LYS:HG3	2.14	0.48
2:M:474:VAL:HG23	2:M:478:VAL:O	2.13	0.48
3:N:151:GLN:HB3	9:N:2161:HOH:O	2.13	0.48
3:N:471:GLU:O	3:N:475:LYS:HG3	2.13	0.48
3:N:639:LEU:HD11	3:N:928:ALA:HB1	1.94	0.48
3:N:683:ILE:HG23	3:N:687:VAL:HG21	1.95	0.48
3:N:999:THR:HA	3:N:1002:LYS:HD2	1.94	0.48
5:P:323:ASP:HB3	5:P:325:LYS:CE	2.43	0.48
1:A:198:ARG:C	1:A:199:ILE:HD12	2.33	0.48
1:B:124:ASN:OD1	1:B:127:LEU:HB2	2.14	0.48
2:C:1033:GLY:HA3	9:C:2546:HOH:O	2.14	0.48
2:C:158:TYR:HE1	2:C:313:LEU:HG	1.76	0.48
2:C:643:VAL:HB	9:C:9995:HOH:O	2.12	0.48
2:C:588:VAL:HG21	2:C:664:GLY:O	2.13	0.48
2:C:72:ARG:HG3	2:C:72:ARG:NH1	2.29	0.48
2:C:774:LEU:HG	2:C:775:ARG:HH11	1.78	0.48
2:C:842:ARG:NH2	2:C:887:GLU:OE1	2.47	0.48
3:D:197:SER:CB	3:D:203:ALA:HB3	2.26	0.48
3:D:890:VAL:HG13	3:D:926:LYS:HZ3	1.76	0.48
3:D:573:MET:CE	5:F:210:LEU:HB3	2.44	0.48
5:F:372:ARG:HB2	9:F:9662:HOH:O	2.13	0.48
1:K:127:LEU:HD11	1:K:129:ILE:HD13	1.94	0.48
1:K:102:LYS:HE2	1:K:139:ASN:ND2	2.28	0.48
2:M:479:VAL:HG22	2:M:508:ILE:HD13	1.94	0.48
2:M:484:VAL:HA	9:M:9640:HOH:O	2.14	0.48
2:M:598:GLU:HB3	9:M:9689:HOH:O	2.14	0.48
2:M:601:GLY:HA3	2:M:615:TYR:HA	1.94	0.48
2:M:722:ILE:HG13	2:M:757:GLY:O	2.12	0.48
2:M:833:LEU:HA	9:M:9723:HOH:O	2.12	0.48
3:N:1212:ALA:HB3	9:N:9663:HOH:O	2.13	0.48
3:N:126:VAL:O	3:N:132:TYR:HD1	1.95	0.48
3:N:1283:ILE:HG23	3:N:1290:LEU:HD21	1.94	0.48
3:N:1437:ALA:HA	3:N:1440:PHE:CE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:66:LYS:HE3	9:O:4365:HOH:O	2.12	0.48
5:P:406:ARG:CA	5:P:409:LYS:HG2	2.41	0.48
1:B:76:VAL:HA	1:B:79:ILE:HG12	1.96	0.48
2:C:383:ARG:HB2	2:C:383:ARG:CZ	2.44	0.48
2:C:625:LEU:O	2:C:627:ARG:N	2.47	0.48
2:C:64:LEU:HB2	2:C:359:MET:SD	2.52	0.48
3:D:117:ASP:HB2	3:D:495:ARG:CZ	2.43	0.48
3:D:1462:LEU:HD23	3:D:1462:LEU:N	2.29	0.48
3:D:820:GLU:HA	3:D:825:ALA:O	2.13	0.48
3:D:890:VAL:HG13	3:D:926:LYS:HZ1	1.76	0.48
2:C:876:VAL:CG2	3:D:949:ILE:HG13	2.43	0.48
4:E:50:THR:HB	9:E:9581:HOH:O	2.14	0.48
5:F:234:LYS:CD	5:F:236:SER:HB3	2.43	0.48
5:F:296:GLY:HA3	9:F:9885:HOH:O	2.13	0.48
5:F:81:VAL:O	5:F:85:LEU:HB2	2.13	0.48
1:K:181:VAL:HG12	2:M:938:LYS:HZ2	1.79	0.48
2:M:163:ILE:HB	2:M:171:TRP:CZ2	2.48	0.48
2:M:371:LYS:HB2	9:M:9605:HOH:O	2.12	0.48
2:M:580:MET:HB2	9:M:2487:HOH:O	2.14	0.48
2:M:732:ALA:O	2:M:735:ARG:HG3	2.13	0.48
2:M:910:LYS:HB3	2:M:912:PRO:HD2	1.96	0.48
2:M:98:LEU:HB2	9:M:9745:HOH:O	2.12	0.48
3:N:1034:GLN:O	3:N:1037:GLN:HG3	2.14	0.48
3:N:1310:ARG:HD3	9:N:2012:HOH:O	2.12	0.48
3:N:1118:ILE:HG21	3:N:1346:ARG:HH12	1.77	0.48
3:N:469:ASP:HA	9:N:2490:HOH:O	2.13	0.48
3:N:96:ALA:N	3:N:551:ASN:HD21	2.10	0.48
3:N:87:ARG:CB	3:N:523:ASP:HB2	2.43	0.48
4:O:52:GLU:HB3	4:O:55:PHE:CZ	2.49	0.48
5:P:335:ASP:HB3	9:P:5855:HOH:O	2.12	0.48
5:P:358:LEU:HD21	5:P:370:LYS:HG3	1.96	0.48
1:A:13:VAL:HG12	1:A:15:THR:HG22	1.95	0.48
2:C:101:ILE:HD12	2:C:107:LEU:HD13	1.95	0.48
2:C:1021:LEU:HG	2:C:1022:GLY:N	2.28	0.48
2:C:103:LYS:HG3	9:C:2004:HOH:O	2.12	0.48
2:C:212:GLY:C	2:C:215:GLY:H	2.17	0.48
2:C:218:VAL:HA	2:C:221:LEU:HD23	1.96	0.48
2:C:165:LEU:O	2:C:265:ARG:HD2	2.13	0.48
2:C:56:GLU:CG	2:C:64:LEU:HD23	2.44	0.48
2:C:85:GLU:HB3	2:C:86:LYS:HD2	1.94	0.48
3:D:1003:VAL:O	3:D:1007:VAL:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1261:GLU:HB2	9:D:2175:HOH:O	2.13	0.48
3:D:1269:LYS:HD3	9:D:2172:HOH:O	2.13	0.48
3:D:1379:VAL:HA	3:D:1420:LEU:CB	2.44	0.48
3:D:519:VAL:HG13	3:D:544:TYR:CE1	2.49	0.48
2:C:1005:MET:HE3	3:D:648:MET:HB2	1.93	0.48
3:D:690:ALA:O	3:D:694:VAL:HG23	2.13	0.48
3:D:811:GLU:HB3	9:D:2229:HOH:O	2.13	0.48
3:D:996:TRP:HA	3:D:999:THR:CG2	2.42	0.48
4:E:54:LEU:HD21	9:E:9513:HOH:O	2.12	0.48
5:F:408:LEU:HA	5:F:411:HIS:CE1	2.48	0.48
1:L:212:ASN:N	1:L:212:ASN:HD22	2.10	0.48
2:M:445:GLU:HG2	9:M:9869:HOH:O	2.14	0.48
2:M:79:PRO:HG2	2:M:82:GLU:HB2	1.96	0.48
2:M:873:PRO:O	2:M:876:VAL:HG23	2.13	0.48
3:N:1156:LEU:HD13	3:N:1176:LYS:HD2	1.96	0.48
3:N:1363:LEU:HD11	3:N:1368:ILE:HD11	1.95	0.48
3:N:115:LEU:CD1	3:N:499:VAL:HG22	2.44	0.48
5:P:287:THR:N	5:P:290:GLU:OE1	2.47	0.48
1:A:198:ARG:NH2	2:C:932:GLU:HG2	2.28	0.48
2:C:1076:VAL:HG23	3:D:752:SER:HA	1.94	0.48
2:C:717:LEU:HD22	9:C:9827:HOH:O	2.14	0.48
2:C:737:LEU:HD22	2:C:741:GLY:O	2.14	0.48
2:C:886:LEU:HG	3:D:951:ILE:CG1	2.41	0.48
3:D:1090:ASP:O	3:D:1093:TYR:N	2.47	0.48
3:D:1128:VAL:O	3:D:1129:THR:C	2.52	0.48
3:D:1192:LEU:HD22	3:D:1345:GLU:OE2	2.14	0.48
3:D:1311:LEU:HD23	3:D:1311:LEU:H	1.79	0.48
3:D:36:THR:O	3:D:38:LYS:N	2.47	0.48
3:D:422:ALA:O	3:D:427:VAL:HG21	2.14	0.48
5:F:128:ARG:O	5:F:132:ARG:HG2	2.14	0.48
5:F:171:LYS:HG3	5:F:175:HIS:CD2	2.48	0.48
5:F:312:GLN:HB2	9:F:9679:HOH:O	2.12	0.48
5:F:358:LEU:HD21	5:F:370:LYS:HE3	1.96	0.48
1:K:150:TYR:CE2	1:K:152:PRO:HG3	2.49	0.48
1:L:46:SER:O	1:L:148:VAL:HB	2.13	0.48
2:M:572:ILE:CG2	2:M:703:ILE:HD13	2.44	0.48
3:N:1197:ARG:HG3	9:N:9686:HOH:O	2.13	0.48
3:N:421:LEU:HD12	3:N:435:VAL:CG1	2.43	0.48
3:N:984:THR:HG21	9:N:9778:HOH:O	2.13	0.48
1:A:183:ASP:HB3	9:A:9739:HOH:O	2.13	0.48
1:A:19:GLU:O	1:A:200:TRP:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1063:ARG:O	2:C:1066:ALA:HB3	2.14	0.48
2:C:1068:GLU:HG2	9:C:2098:HOH:O	2.14	0.48
2:C:114:PHE:CD1	2:C:114:PHE:N	2.79	0.48
2:C:181:VAL:HG11	9:C:2375:HOH:O	2.13	0.48
2:C:358:ARG:HB3	2:C:371:LYS:O	2.14	0.48
2:C:776:SER:HA	2:C:780:GLU:HB3	1.96	0.48
2:C:897:LEU:HB3	2:C:899:GLN:NE2	2.28	0.48
2:C:915:LYS:O	2:C:968:LEU:HD22	2.14	0.48
2:C:943:VAL:HG11	2:C:973:VAL:HG22	1.96	0.48
3:D:957:PRO:HA	3:D:1010:ASN:ND2	2.29	0.48
3:D:1130:ARG:CB	3:D:1130:ARG:HH11	2.21	0.48
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	1.95	0.48
3:D:1399:ASP:HB3	9:D:2288:HOH:O	2.13	0.48
3:D:171:LEU:HD11	3:D:388:HIS:CB	2.43	0.48
3:D:521:PRO:C	3:D:525:ARG:HH11	2.17	0.48
3:D:692:GLU:HG3	9:D:2470:HOH:O	2.13	0.48
5:F:153:PRO:HG2	5:F:154:LYS:H	1.79	0.48
2:M:176:VAL:C	2:M:178:PRO:HD3	2.34	0.48
2:M:435:TYR:C	2:M:437:ARG:H	2.17	0.48
2:M:683:ASN:O	2:M:872:ASN:ND2	2.46	0.48
2:M:911:GLU:O	2:M:915:LYS:HG2	2.14	0.48
3:N:949:ILE:HD11	3:N:1023:MET:CE	2.44	0.48
9:M:9654:HOH:O	3:N:1038:LEU:HG	2.13	0.48
3:N:28:LYS:O	3:N:43:GLY:HA2	2.13	0.48
3:N:18:ILE:HD12	3:N:518:PRO:CD	2.44	0.48
3:N:47:GLU:OE1	3:N:52:PRO:HA	2.14	0.48
3:N:68:PHE:O	3:N:71:LYS:HG2	2.14	0.48
5:P:112:ALA:HA	5:P:173:TYR:CD2	2.47	0.48
3:N:535:PHE:CB	5:P:314:PRO:HB3	2.41	0.48
3:N:131:LYS:HE3	5:P:83:GLN:NE2	2.29	0.48
2:C:1054:THR:CG2	2:C:1059:ASP:HB2	2.44	0.48
2:C:212:GLY:HA3	2:C:218:VAL:HG23	1.95	0.48
2:C:724:ARG:HH12	2:C:734:LEU:HD23	1.79	0.48
2:C:975:TYR:HA	2:C:982:PRO:HA	1.95	0.48
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.13	0.48
3:D:1008:PHE:HZ	3:D:1032:PRO:HA	1.79	0.48
3:D:186:VAL:HA	9:D:2144:HOH:O	2.12	0.48
3:D:421:LEU:HD11	3:D:437:VAL:HG22	1.95	0.48
3:D:756:GLN:O	3:D:760:ARG:HG2	2.12	0.48
2:M:501:THR:HG22	9:M:9802:HOH:O	2.14	0.48
2:M:551:GLU:HG3	2:M:552:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:897:LEU:HB3	2:M:899:GLN:HG2	1.96	0.48
2:M:565:GLN:HG2	2:M:995:MET:HE2	1.96	0.48
3:N:1036:ARG:HH21	3:N:1043:GLY:H	1.62	0.48
3:N:1493:LYS:HA	3:N:1496:GLU:HG2	1.96	0.48
3:N:172:PRO:HB3	3:N:178:LEU:CB	2.44	0.48
3:N:413:ASP:OD1	3:N:421:LEU:HD22	2.14	0.48
3:N:434:ARG:HB2	3:N:447:VAL:HG22	1.95	0.48
3:N:699:VAL:HG12	3:N:717:GLN:HG3	1.96	0.48
3:N:882:PHE:O	3:N:886:VAL:HG23	2.14	0.48
5:P:193:ARG:HG2	9:P:6583:HOH:O	2.13	0.48
1:A:109:VAL:HG23	9:A:9621:HOH:O	2.13	0.47
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.94	0.47
2:C:1084:SER:O	2:C:1087:VAL:HG12	2.13	0.47
2:C:155:PRO:HD2	9:C:9771:HOH:O	2.14	0.47
2:C:318:PRO:HB3	9:C:9983:HOH:O	2.13	0.47
2:C:334:ARG:NH1	2:C:415:PRO:HG2	2.29	0.47
2:C:479:VAL:HG22	2:C:508:ILE:HD13	1.95	0.47
2:C:559:LEU:HD23	2:C:560:MET:N	2.29	0.47
2:C:640:ARG:HH11	2:C:642:ARG:HH22	1.60	0.47
2:C:729:LEU:HD21	5:F:419:ARG:NH1	2.28	0.47
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.79	0.47
3:D:205:TYR:HD2	9:D:2180:HOH:O	1.96	0.47
3:D:86:ARG:NH1	3:D:86:ARG:HG2	2.28	0.47
4:E:70:THR:HG22	4:E:72:ARG:HG3	1.96	0.47
5:F:358:LEU:CD2	5:F:370:LYS:HE3	2.44	0.47
5:F:93:LEU:HD22	5:F:98:GLU:HB3	1.94	0.47
2:M:274:ARG:O	2:M:274:ARG:HG2	2.14	0.47
2:M:357:GLU:HG2	9:M:2237:HOH:O	2.13	0.47
2:M:451:LEU:HD12	2:M:451:LEU:H	1.79	0.47
2:M:517:ARG:NH1	2:M:522:VAL:HG11	2.29	0.47
3:N:1187:PRO:O	3:N:1188:VAL:HG23	2.14	0.47
3:N:462:GLN:HA	3:N:513:ILE:CD1	2.43	0.47
3:N:50:PHE:HB3	3:N:522:PRO:HG2	1.96	0.47
3:N:12:LEU:HD22	3:N:511:TRP:CB	2.44	0.47
4:O:34:GLY:HA3	9:O:3795:HOH:O	2.13	0.47
5:P:208:SER:HB2	5:P:211:ASP:OD1	2.14	0.47
5:P:357:ALA:HA	9:P:6501:HOH:O	2.12	0.47
1:B:188:GLN:HG3	9:B:9555:HOH:O	2.14	0.47
1:A:219:ARG:HH22	1:B:223:THR:CG2	2.27	0.47
2:C:761:PHE:CD1	2:C:761:PHE:N	2.82	0.47
3:D:1033:GLN:NE2	3:D:1036:ARG:HH11	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1055:VAL:HG13	9:D:9682:HOH:O	2.15	0.47
3:D:1042:ARG:O	3:D:1057:VAL:HB	2.15	0.47
3:D:1264:GLU:OE2	3:D:1424:VAL:N	2.47	0.47
3:D:171:LEU:HD13	3:D:389:GLU:C	2.34	0.47
3:D:421:LEU:HD12	3:D:435:VAL:CG1	2.44	0.47
3:D:717:GLN:HG2	9:D:9975:HOH:O	2.14	0.47
3:D:928:ALA:O	3:D:931:LEU:HB2	2.14	0.47
4:E:87:LYS:HB2	9:E:9533:HOH:O	2.15	0.47
1:K:102:LYS:HE2	1:K:139:ASN:CG	2.34	0.47
1:K:9:PRO:HB3	1:K:25:LEU:CD2	2.44	0.47
2:M:1114:GLY:H	2:M:1115:LEU:CD1	2.13	0.47
2:M:170:PRO:HG2	2:M:258:TYR:CD2	2.49	0.47
2:M:672:VAL:HA	9:M:9988:HOH:O	2.14	0.47
2:M:909:ALA:C	2:M:910:LYS:HD2	2.34	0.47
3:N:1097:LYS:O	3:N:1101:VAL:HG23	2.14	0.47
3:N:127:LEU:HD12	3:N:128:TYR:N	2.29	0.47
3:N:135:LEU:CD1	3:N:147:VAL:HG23	2.43	0.47
3:N:177:ALA:HB1	3:N:199:LEU:HB3	1.95	0.47
3:N:396:VAL:HG23	9:N:2489:HOH:O	2.13	0.47
3:N:520:LEU:HD12	3:N:521:PRO:CD	2.36	0.47
2:M:1115:LEU:CB	3:N:85:VAL:HG12	2.43	0.47
5:P:141:VAL:HB	9:P:3900:HOH:O	2.14	0.47
2:C:137:VAL:HG11	9:C:9854:HOH:O	2.14	0.47
2:C:139:GLN:HE22	2:C:415:PRO:HD3	1.78	0.47
2:C:534:VAL:H	2:C:538:GLN:NE2	2.11	0.47
2:C:704:HIS:HB2	2:C:831:ARG:NE	2.29	0.47
2:C:926:PHE:CD2	2:C:930:LYS:HE2	2.50	0.47
3:D:1264:GLU:OE2	3:D:1424:VAL:HG12	2.14	0.47
3:D:191:LEU:HD22	3:D:195:VAL:HG21	1.96	0.47
3:D:30:GLU:N	9:D:9793:HOH:O	2.48	0.47
3:D:619:LEU:HD23	3:D:619:LEU:C	2.35	0.47
3:D:994:GLN:O	3:D:998:GLU:HG3	2.14	0.47
5:F:256:ARG:NE	5:F:260:ILE:HD12	2.28	0.47
1:L:184:THR:HG23	1:L:192:LEU:HB3	1.94	0.47
2:M:143:SER:HB3	2:M:332:ARG:HB2	1.96	0.47
2:M:206:THR:O	2:M:210:GLU:HG3	2.14	0.47
2:M:313:LEU:HD21	9:M:9818:HOH:O	2.14	0.47
2:M:48:PHE:HD2	9:M:9965:HOH:O	1.98	0.47
2:M:401:LEU:HD11	2:M:546:LEU:HD11	1.96	0.47
2:M:834:GLN:HG3	2:M:837:ASP:OD1	2.13	0.47
3:N:27:GLU:O	3:N:28:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:624:ASP:HB3	3:N:625:TYR:CD1	2.49	0.47
3:N:679:ARG:NH2	3:N:681:ARG:HE	2.12	0.47
3:N:827:ILE:HG22	9:N:9576:HOH:O	2.14	0.47
2:M:1115:LEU:HD21	3:N:84:ILE:HD12	1.96	0.47
4:O:33:HIS:HB3	9:O:4303:HOH:O	2.14	0.47
4:O:51:LEU:HG	4:O:53:GLY:N	2.23	0.47
5:P:323:ASP:C	5:P:325:LYS:H	2.18	0.47
1:A:54:THR:HG23	1:A:156:HIS:CE1	2.49	0.47
1:A:223:THR:HG21	9:A:9697:HOH:O	2.15	0.47
1:B:123:MET:O	1:B:125:PRO:HD3	2.15	0.47
1:B:182:GLU:O	1:B:194:LYS:HB3	2.14	0.47
2:C:1111:ILE:HG13	9:C:2143:HOH:O	2.14	0.47
2:C:173:ASP:O	2:C:184:MET:HA	2.14	0.47
2:C:517:ARG:NH1	2:C:524:VAL:HG23	2.30	0.47
2:C:405:ARG:NH2	2:C:566:THR:HG21	2.29	0.47
2:C:654:LEU:HD13	2:C:664:GLY:N	2.29	0.47
2:C:681:GLY:C	3:D:635:PRO:HG2	2.35	0.47
2:C:68:PHE:HE1	2:C:96:ALA:HB1	1.79	0.47
2:C:808:ARG:HH11	2:C:808:ARG:HG2	1.79	0.47
3:D:1104:GLU:O	3:D:1106:VAL:HG23	2.15	0.47
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.14	0.47
3:D:1476:THR:HA	9:E:9539:HOH:O	2.13	0.47
3:D:520:LEU:CD2	3:D:540:LEU:HD22	2.45	0.47
5:F:120:THR:HA	9:F:9593:HOH:O	2.15	0.47
5:F:141:VAL:O	5:F:145:PRO:HD2	2.14	0.47
5:F:392:VAL:HG22	9:F:9999:HOH:O	2.14	0.47
1:K:115:LEU:HD13	9:K:4988:HOH:O	2.14	0.47
1:K:224:TYR:CD2	1:L:9:PRO:HG2	2.49	0.47
1:K:25:LEU:C	1:K:25:LEU:HD23	2.35	0.47
2:M:1055:LEU:HD22	2:M:1066:ALA:HB2	1.97	0.47
2:M:1060:ILE:HG22	2:M:1061:GLU:N	2.30	0.47
2:M:218:VAL:HG22	2:M:221:LEU:CD2	2.43	0.47
2:M:380:ALA:HA	2:M:383:ARG:HD3	1.97	0.47
2:M:383:ARG:HG3	9:M:9841:HOH:O	2.13	0.47
2:M:380:ALA:O	2:M:384:GLU:HB2	2.13	0.47
2:M:413:LEU:HB3	9:M:2107:HOH:O	2.13	0.47
2:M:944:LEU:O	2:M:948:GLU:HG3	2.14	0.47
3:N:1192:LEU:HD21	3:N:1345:GLU:HB3	1.97	0.47
3:N:126:VAL:HG12	3:N:132:TYR:HB2	1.96	0.47
3:N:191:LEU:HB3	3:N:195:VAL:HG21	1.96	0.47
3:N:30:GLU:HB3	3:N:40:GLU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:571:LYS:NZ	3:N:571:LYS:HB2	2.29	0.47
3:N:957:PRO:CG	3:N:1007:VAL:HG12	2.45	0.47
4:O:42:PRO:HG3	9:O:4575:HOH:O	2.15	0.47
4:O:86:GLN:O	4:O:90:GLU:HG3	2.14	0.47
1:A:50:GLY:O	1:A:146:ARG:HA	2.14	0.47
1:A:20:TYR:CD2	1:A:21:GLY:N	2.82	0.47
2:C:1087:VAL:HG22	2:C:1091:GLU:OE2	2.14	0.47
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.95	0.47
2:C:19:THR:HG21	2:C:124:ASP:O	2.14	0.47
2:C:227:PHE:HD2	2:C:230:ARG:HH21	1.63	0.47
2:C:396:ASP:HB2	2:C:406:HIS:CD2	2.49	0.47
2:C:433:THR:O	2:C:433:THR:HG22	2.14	0.47
2:C:471:TYR:CD1	2:C:486:MET:HE1	2.50	0.47
2:C:555:ALA:HA	3:D:1070:TYR:OH	2.13	0.47
3:D:1232:PRO:HA	3:D:1235:GLN:OE1	2.14	0.47
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.14	0.47
3:D:1377:LYS:HD2	9:D:2614:HOH:O	2.14	0.47
3:D:36:THR:HB	3:D:38:LYS:HG3	1.96	0.47
3:D:427:VAL:HG21	3:D:435:VAL:HB	1.94	0.47
3:D:454:ALA:C	3:D:455:ARG:HD2	2.35	0.47
3:D:70:GLY:N	3:D:71:LYS:HE3	2.28	0.47
5:F:291:ILE:HG23	5:F:304:VAL:HG21	1.96	0.47
5:F:358:LEU:HD12	5:F:367:MET:HE1	1.95	0.47
1:L:67:THR:HB	9:L:5724:HOH:O	2.13	0.47
2:M:31:GLN:NE2	9:M:9625:HOH:O	2.47	0.47
2:M:626:ARG:CB	2:M:626:ARG:HH11	2.27	0.47
2:M:780:GLU:O	2:M:782:ALA:N	2.48	0.47
2:M:945:ARG:HG3	2:M:949:LYS:HE3	1.95	0.47
3:N:1123:PHE:HA	3:N:1135:ARG:H	1.79	0.47
3:N:1141:GLU:HG2	3:N:1168:MET:HE1	1.95	0.47
3:N:1324:PRO:HA	9:N:9625:HOH:O	2.15	0.47
3:N:134:VAL:HG21	9:N:9914:HOH:O	2.14	0.47
3:N:1413:THR:HG21	9:N:9838:HOH:O	2.14	0.47
3:N:470:LEU:HG	9:N:2490:HOH:O	2.12	0.47
3:N:669:ASN:O	3:N:672:ALA:HB3	2.13	0.47
4:O:33:HIS:HB2	4:O:37:ASN:ND2	2.29	0.47
3:N:563:PRO:HA	5:P:185:GLN:HG2	1.95	0.47
5:P:369:LEU:O	5:P:373:LYS:HB2	2.14	0.47
5:P:408:LEU:HD13	5:P:411:HIS:HE1	1.79	0.47
5:P:416:ARG:HB2	9:P:6288:HOH:O	2.15	0.47
1:A:162:ILE:HA	9:A:9677:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:THR:HG22	1:B:158:ILE:HG13	1.95	0.47
2:C:146:VAL:HG13	2:C:161:SER:O	2.14	0.47
2:C:158:TYR:CE1	2:C:313:LEU:HG	2.49	0.47
2:C:557:ARG:HG3	2:C:560:MET:SD	2.55	0.47
2:C:605:LYS:HD2	2:C:612:VAL:HG21	1.96	0.47
2:C:914:ILE:HG22	2:C:915:LYS:HE3	1.97	0.47
2:C:91:GLN:HB2	9:C:9756:HOH:O	2.14	0.47
2:C:969:GLN:HB3	9:D:2189:HOH:O	2.15	0.47
3:D:1147:ARG:NH1	3:D:1190:SER:HB2	2.29	0.47
3:D:1363:LEU:HD12	3:D:1364:HIS:O	2.14	0.47
3:D:216:VAL:HG11	9:D:2023:HOH:O	2.13	0.47
3:D:416:ALA:HB3	3:D:417:PRO:HD3	1.97	0.47
3:D:399:ARG:HB2	3:D:444:VAL:HG13	1.95	0.47
3:D:838:ARG:HH11	3:D:874:GLU:HB3	1.79	0.47
5:F:102:LEU:CD1	5:F:187:LEU:HG	2.45	0.47
5:F:135:ILE:O	5:F:135:ILE:HD13	2.15	0.47
1:L:103:ALA:HB1	1:L:107:LYS:CE	2.40	0.47
2:M:13:ILE:HB	9:M:9847:HOH:O	2.14	0.47
2:M:253:ALA:HB3	9:M:9639:HOH:O	2.15	0.47
2:M:863:ASP:OD1	2:M:865:THR:HG22	2.15	0.47
2:M:996:LYS:HD2	9:M:9723:HOH:O	2.14	0.47
3:N:957:PRO:HG2	3:N:1007:VAL:HG12	1.96	0.47
3:N:1128:VAL:HG13	9:N:9896:HOH:O	2.15	0.47
3:N:1143:GLY:HA2	3:N:1365:ASP:OD1	2.14	0.47
3:N:1262:LEU:HD11	3:N:1351:GLU:HG3	1.95	0.47
3:N:580:ALA:HA	3:N:584:ASN:OD1	2.14	0.47
3:N:750:PRO:HB2	3:N:756:GLN:OE1	2.14	0.47
3:N:827:ILE:O	3:N:837:GLY:HA3	2.14	0.47
2:M:1102:LEU:HD11	3:N:9:ARG:HB2	1.97	0.47
5:P:81:VAL:HG12	5:P:85:LEU:HG	1.95	0.47
1:A:18:ARG:NH2	1:A:88:ARG:NH2	2.62	0.47
2:C:794:PRO:HB2	2:C:1027:PHE:CZ	2.50	0.47
2:C:259:GLY:HA2	9:C:9711:HOH:O	2.13	0.47
2:C:603:VAL:HG22	2:C:613:VAL:HG12	1.96	0.47
2:C:723:THR:HG21	9:C:2057:HOH:O	2.15	0.47
2:C:80:GLN:O	2:C:83:CYS:HB2	2.14	0.47
3:D:108:VAL:HB	9:D:9737:HOH:O	2.15	0.47
3:D:196:VAL:HG13	3:D:202:VAL:HG13	1.96	0.47
3:D:33:ASN:HD21	3:D:35:ARG:CD	2.27	0.47
3:D:553:ARG:NH1	5:F:211:ASP:HA	2.30	0.47
3:D:973:GLN:HG2	9:D:2020:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:220:LEU:HB2	5:F:243:ILE:HD11	1.97	0.47
1:L:102:LYS:HE3	1:L:139:ASN:HB2	1.95	0.47
2:M:1013:TYR:OH	2:M:1063:ARG:HD2	2.15	0.47
2:M:420:ARG:CD	2:M:420:ARG:H	2.28	0.47
3:N:1023:MET:O	3:N:1028:ALA:HB3	2.15	0.47
3:N:130:SER:HB3	3:N:132:TYR:CE1	2.50	0.47
3:N:513:ILE:HA	9:N:9662:HOH:O	2.14	0.47
3:N:530:VAL:HG23	3:N:534:ARG:O	2.15	0.47
3:N:76:CYS:HB3	9:N:9734:HOH:O	2.13	0.47
3:N:809:PRO:O	3:N:812:ALA:HB3	2.15	0.47
5:P:147:LEU:HG	9:P:6001:HOH:O	2.15	0.47
5:P:93:LEU:HG	5:P:190:ALA:HB1	1.97	0.47
5:P:286:PRO:HA	9:P:6329:HOH:O	2.14	0.47
5:P:399:GLN:O	5:P:403:LYS:HB2	2.14	0.47
1:B:48:ILE:HG22	1:B:173:PRO:HD2	1.97	0.47
2:C:196:LEU:H	2:C:196:LEU:HD12	1.79	0.47
2:C:262:ALA:HB1	9:C:2112:HOH:O	2.15	0.47
2:C:31:GLN:HE21	2:C:31:GLN:HB3	1.60	0.47
2:C:431:HIS:CD2	2:C:433:THR:HG1	2.33	0.47
2:C:704:HIS:O	2:C:705:ILE:HG13	2.14	0.47
2:C:957:LYS:HE2	2:C:965:GLU:OE2	2.15	0.47
3:D:1302:GLU:OE2	3:D:1304:LYS:HG3	2.15	0.47
3:D:1369:GLU:O	3:D:1372:VAL:HG12	2.15	0.47
3:D:704:ARG:HG2	3:D:736:PHE:HB3	1.96	0.47
1:K:198:ARG:HB2	1:K:200:TRP:CZ3	2.50	0.47
1:L:190:THR:HA	9:L:4234:HOH:O	2.14	0.47
2:M:1037:VAL:O	2:M:1041:GLU:HG3	2.14	0.47
2:M:1090:LYS:HD2	3:N:90:MET:SD	2.55	0.47
2:M:150:PRO:HG3	2:M:158:TYR:HD2	1.80	0.47
2:M:169:GLY:CA	2:M:263:ASP:HB3	2.28	0.47
2:M:301:GLU:HG3	9:M:9587:HOH:O	2.15	0.47
2:M:302:VAL:O	2:M:306:THR:HG23	2.15	0.47
2:M:35:PRO:HD2	2:M:38:LYS:CG	2.45	0.47
2:M:49:ARG:NH1	2:M:49:ARG:HB2	2.29	0.47
2:M:971:LYS:HD2	2:M:986:PRO:HB2	1.96	0.47
3:N:1065:LEU:HB2	9:N:9777:HOH:O	2.13	0.47
3:N:1400:VAL:HG21	9:N:2015:HOH:O	2.13	0.47
3:N:208:PRO:HB2	3:N:395:VAL:HG22	1.96	0.47
3:N:443:VAL:HG12	3:N:445:ARG:HD2	1.96	0.47
2:M:1035:MET:HG2	3:N:707:THR:O	2.13	0.47
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:117:SER:OG	5:P:124:PRO:HG3	2.14	0.47
5:P:302:LYS:HA	9:P:3857:HOH:O	2.14	0.47
5:P:85:LEU:HD22	5:P:193:ARG:HD3	1.96	0.47
2:C:1060:ILE:HG23	2:C:1061:GLU:H	1.78	0.47
2:C:455:LEU:HD23	2:C:455:LEU:N	2.30	0.47
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.39	0.47
2:C:777:ILE:HG22	2:C:778:PHE:CD1	2.50	0.47
2:C:955:PRO:HD3	9:C:9862:HOH:O	2.15	0.47
2:C:554:ASP:HA	3:D:1061:PHE:CZ	2.49	0.47
3:D:404:GLU:HB3	3:D:414:ARG:CD	2.45	0.47
3:D:441:ARG:O	3:D:443:VAL:N	2.48	0.47
3:D:925:GLU:HG2	3:D:926:LYS:N	2.29	0.47
5:F:225:GLU:HB3	9:F:9625:HOH:O	2.14	0.47
1:L:150:TYR:CD2	3:N:857:ILE:HG13	2.50	0.47
2:M:248:PRO:HA	9:M:9909:HOH:O	2.14	0.47
2:M:333:ILE:HG22	2:M:465:GLY:CA	2.45	0.47
2:M:676:ILE:HG13	2:M:871:LEU:HB2	1.97	0.47
2:M:902:ILE:HG23	9:M:2487:HOH:O	2.15	0.47
3:N:1047:LYS:HA	3:N:1053:PHE:CE1	2.50	0.47
3:N:441:ARG:O	3:N:443:VAL:N	2.48	0.47
5:P:102:LEU:HD22	5:P:183:ALA:O	2.15	0.47
5:P:151:LEU:CD2	5:P:153:PRO:HD2	2.43	0.47
5:P:332:PHE:CD1	5:P:332:PHE:N	2.82	0.47
1:A:112:ARG:HB3	1:A:112:ARG:HH11	1.80	0.47
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.97	0.47
1:B:107:LYS:HD2	9:B:9570:HOH:O	2.14	0.47
1:B:94:LEU:HD11	1:B:119:ASP:HB2	1.97	0.47
1:B:2:LEU:HD12	1:B:3:ASP:HB2	1.97	0.47
2:C:1008:ARG:HH12	2:C:1011:GLY:HA3	1.80	0.47
2:C:1090:LYS:HG2	2:C:1112:PHE:HZ	1.80	0.47
2:C:409:ARG:HB3	9:C:9854:HOH:O	2.15	0.47
3:D:1393:GLN:HB2	9:D:9959:HOH:O	2.15	0.47
3:D:516:ALA:O	3:D:518:PRO:HD3	2.15	0.47
2:C:1005:MET:HB3	3:D:629:SER:HB2	1.96	0.47
5:F:226:LYS:HD2	5:F:242:TRP:CZ2	2.50	0.47
2:M:208:ALA:HB1	2:M:218:VAL:CG1	2.45	0.47
2:M:305:PRO:HB3	2:M:308:ARG:NH2	2.30	0.47
2:M:551:GLU:HA	2:M:906:PHE:CZ	2.50	0.47
2:M:56:GLU:HG2	2:M:64:LEU:HD23	1.97	0.47
2:M:675:ALA:HB3	2:M:870:ILE:HG23	1.97	0.47
2:M:688:ILE:HD12	2:M:688:ILE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:707:ARG:HH11	2:M:707:ARG:HG2	1.80	0.47
2:M:768:THR:O	2:M:772:ARG:HB3	2.15	0.47
2:M:959:PRO:HD3	9:M:9576:HOH:O	2.15	0.47
3:N:1283:ILE:N	3:N:1315:ASP:OD1	2.48	0.47
3:N:42:ASP:HA	3:N:46:ASP:OD1	2.14	0.47
4:O:48:MET:HB2	4:O:54:LEU:CD1	2.44	0.47
5:P:141:VAL:O	5:P:145:PRO:HD2	2.14	0.47
5:P:104:ARG:HG3	5:P:229:TYR:CZ	2.49	0.47
5:P:273:ARG:O	5:P:276:ARG:HB2	2.15	0.47
1:A:85:LEU:HA	1:A:124:ASN:ND2	2.30	0.47
1:A:33:GLY:O	1:A:195:LEU:HD22	2.14	0.47
2:C:1114:GLY:N	2:C:1115:LEU:HD12	2.19	0.47
2:C:521:PRO:HB2	3:D:1055:VAL:CB	2.44	0.47
2:C:816:LYS:HB2	2:C:819:VAL:HG21	1.96	0.47
2:C:874:LEU:HD12	3:D:784:ASP:OD2	2.15	0.47
3:D:1106:VAL:O	3:D:1108:ARG:HG2	2.14	0.47
3:D:1156:LEU:CD1	3:D:1176:LYS:HD2	2.45	0.47
3:D:1213:ARG:HB2	3:D:1214:PRO:CD	2.44	0.47
3:D:210:ARG:NH1	3:D:398:ALA:HB3	2.29	0.47
3:D:543:LEU:HD21	3:D:600:LEU:HD12	1.96	0.47
3:D:787:LEU:HD11	3:D:947:ILE:HG12	1.97	0.47
4:E:19:LEU:HD12	4:E:19:LEU:O	2.14	0.47
1:L:143:ARG:HD3	1:L:158:ILE:HG21	1.97	0.47
2:M:841:ASN:ND2	2:M:844:GLY:H	2.13	0.47
2:M:862:PRO:HA	2:M:975:TYR:HE1	1.78	0.47
3:N:1091:SER:HA	9:N:9674:HOH:O	2.14	0.47
3:N:205:TYR:CD1	3:N:393:ILE:HD11	2.49	0.47
3:N:34:TYR:OH	5:P:264:MET:HG3	2.15	0.47
3:N:462:GLN:O	3:N:466:LYS:HG3	2.14	0.47
3:N:965:GLU:HA	3:N:968:ASP:HB2	1.97	0.47
5:P:372:ARG:HB2	9:P:4888:HOH:O	2.15	0.47
1:A:2:LEU:HG	9:A:9752:HOH:O	2.14	0.46
1:A:3:ASP:O	1:A:7:LYS:HB2	2.15	0.46
2:C:1052:MET:HG3	3:D:623:VAL:HG22	1.96	0.46
2:C:148:PHE:HZ	2:C:281:LEU:HD22	1.79	0.46
2:C:208:ALA:HB1	2:C:218:VAL:CG1	2.44	0.46
2:C:820:ARG:HG3	9:C:2214:HOH:O	2.14	0.46
3:D:1283:ILE:N	3:D:1315:ASP:OD1	2.47	0.46
3:D:1331:ASP:N	9:D:9620:HOH:O	2.47	0.46
3:D:1475:GLY:N	9:D:9610:HOH:O	2.47	0.46
3:D:1491:THR:HG22	9:E:9526:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:131:LYS:HA	3:D:456:MET:HG3	1.97	0.46
3:D:701:LEU:O	3:D:747:VAL:HA	2.15	0.46
3:D:986:ARG:HB2	9:D:9937:HOH:O	2.13	0.46
4:E:92:ILE:HD11	9:E:9551:HOH:O	2.15	0.46
1:K:143:ARG:NH2	1:K:158:ILE:HG23	2.30	0.46
1:K:91:ASN:H	1:K:94:LEU:CD1	2.28	0.46
2:M:1018:GLN:CB	2:M:1060:ILE:HD11	2.45	0.46
2:M:101:ILE:HG22	2:M:102:HIS:N	2.29	0.46
2:M:794:PRO:HB2	2:M:1027:PHE:CZ	2.50	0.46
2:M:191:PHE:HE2	2:M:195:LEU:HB3	1.80	0.46
2:M:86:LYS:HE2	9:M:9638:HOH:O	2.15	0.46
2:M:95:TYR:HE1	9:M:2165:HOH:O	1.98	0.46
3:N:1109:GLU:HA	9:N:9614:HOH:O	2.15	0.46
3:N:1114:THR:HG22	3:N:1195:GLN:HB3	1.96	0.46
3:N:185:VAL:HG13	9:N:9598:HOH:O	2.15	0.46
5:P:365:GLU:CD	5:P:397:ILE:HA	2.35	0.46
1:B:109:VAL:HG21	1:B:138:LEU:HD11	1.97	0.46
1:B:158:ILE:HA	9:B:9554:HOH:O	2.16	0.46
2:C:398:THR:OG1	2:C:633:GLN:HG3	2.16	0.46
2:C:495:THR:HG21	2:C:524:VAL:HG21	1.96	0.46
1:A:67:THR:HG21	2:C:609:ASN:HD21	1.80	0.46
2:C:580:MET:O	2:C:902:ILE:HA	2.15	0.46
3:D:209:ARG:HD2	3:D:210:ARG:HG2	1.96	0.46
3:D:4:GLU:HB2	9:D:9686:HOH:O	2.15	0.46
4:E:26:ARG:HD2	4:E:29:GLN:OE1	2.15	0.46
5:F:84:TYR:O	5:F:88:ILE:HG13	2.15	0.46
1:K:94:LEU:HD11	1:K:119:ASP:OD1	2.14	0.46
1:K:58:ILE:HG21	1:K:68:ILE:CD1	2.45	0.46
2:M:1061:GLU:HB3	9:M:9973:HOH:O	2.14	0.46
2:M:160:ALA:HB3	2:M:174:LEU:HB2	1.97	0.46
2:M:176:VAL:O	2:M:178:PRO:HD3	2.14	0.46
2:M:139:GLN:HE22	2:M:418:LEU:HD13	1.80	0.46
2:M:492:ASP:HB3	2:M:518:LYS:CD	2.45	0.46
2:M:571:LEU:HD23	2:M:670:GLN:HG3	1.97	0.46
2:M:18:LEU:HD13	2:M:590:ASP:CG	2.35	0.46
2:M:695:LEU:HD21	2:M:833:LEU:O	2.15	0.46
3:N:1119:SER:HA	3:N:1186:VAL:O	2.14	0.46
3:N:1314:LYS:HZ1	3:N:1317:ASP:HB2	1.80	0.46
3:N:1353:GLN:HE21	3:N:1353:GLN:HB3	1.58	0.46
3:N:399:ARG:HB3	3:N:402:PRO:HG3	1.97	0.46
3:N:646:LYS:HA	3:N:720:LEU:CD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:656:PHE:HB3	3:N:694:VAL:CG1	2.44	0.46
4:O:26:ARG:NH1	4:O:29:GLN:NE2	2.63	0.46
1:A:205:VAL:CG2	1:A:206:THR:N	2.78	0.46
1:A:81:ASN:HA	1:A:84:GLU:OE1	2.16	0.46
1:A:9:PRO:HB3	1:A:25:LEU:CD2	2.46	0.46
1:B:99:LEU:HG	1:B:114:PHE:HB3	1.98	0.46
1:B:146:ARG:HG3	1:B:146:ARG:O	2.15	0.46
1:B:150:TYR:CE2	3:D:857:ILE:HG13	2.51	0.46
1:B:219:ARG:O	1:B:223:THR:HG23	2.15	0.46
2:C:405:ARG:HB3	9:C:9823:HOH:O	2.14	0.46
2:C:474:VAL:HG13	2:C:530:GLU:C	2.36	0.46
2:C:679:PHE:C	3:D:943:THR:HG22	2.35	0.46
3:D:907:GLU:HG2	9:D:2314:HOH:O	2.15	0.46
1:K:210:ALA:HA	1:K:213:GLN:NE2	2.30	0.46
2:M:143:SER:CB	2:M:332:ARG:HB2	2.46	0.46
2:M:444:PRO:HG3	7:M:8002:RBT:H302	1.96	0.46
2:M:510:ALA:HB1	9:M:9985:HOH:O	2.16	0.46
2:M:578:VAL:CG2	2:M:579:VAL:HG12	2.40	0.46
2:M:5:ARG:HB3	2:M:902:ILE:HB	1.96	0.46
2:M:838:LYS:HG3	2:M:997:LEU:HB2	1.98	0.46
3:N:1390:LEU:HB3	9:N:2303:HOH:O	2.14	0.46
2:M:1007:ALA:CB	3:N:648:MET:HG3	2.42	0.46
5:P:403:LYS:HA	5:P:403:LYS:HZ3	1.80	0.46
1:B:105:GLY:O	1:B:132:LEU:HD23	2.14	0.46
1:B:33:GLY:O	1:B:195:LEU:HD22	2.16	0.46
9:A:9751:HOH:O	1:B:219:ARG:HG3	2.15	0.46
2:C:557:ARG:NH2	2:C:879:ARG:HD3	2.30	0.46
2:C:589:ARG:HD3	2:C:596:TYR:CE2	2.50	0.46
3:D:1107:VAL:O	3:D:1218:GLY:N	2.46	0.46
3:D:1173:LEU:HD23	3:D:1174:LEU:HD23	1.98	0.46
3:D:1250:ALA:HB3	9:D:9761:HOH:O	2.15	0.46
3:D:137:PRO:HD2	3:D:453:ASP:CB	2.45	0.46
3:D:996:TRP:O	3:D:999:THR:HG22	2.14	0.46
4:E:72:ARG:HH11	4:E:72:ARG:HG2	1.81	0.46
3:D:553:ARG:HD3	5:F:214:GLN:HB3	1.96	0.46
5:F:303:ARG:HA	9:F:9749:HOH:O	2.15	0.46
5:F:420:ASP:HB2	9:F:9781:HOH:O	2.15	0.46
1:K:28:LEU:HA	9:L:5369:HOH:O	2.16	0.46
2:M:127:PHE:O	2:M:133:ASP:HA	2.15	0.46
2:M:212:GLY:C	2:M:215:GLY:H	2.19	0.46
2:M:510:ALA:HA	9:M:9562:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:626:ARG:HH12	2:M:637:LEU:HD12	1.76	0.46
2:M:741:GLY:HA3	9:M:9662:HOH:O	2.14	0.46
2:M:798:GLY:HA3	2:M:828:ALA:O	2.15	0.46
2:M:905:ILE:HG22	2:M:906:PHE:CD1	2.50	0.46
2:M:976:ASP:HB3	2:M:979:THR:HG22	1.96	0.46
3:N:112:ILE:O	3:N:116:LEU:HB2	2.16	0.46
3:N:1173:LEU:HD23	3:N:1174:LEU:HD23	1.98	0.46
3:N:1426:LYS:HA	3:N:1429:LEU:HB2	1.98	0.46
3:N:424:GLY:N	9:N:2715:HOH:O	2.47	0.46
3:N:785:ILE:HD12	3:N:785:ILE:H	1.79	0.46
3:N:957:PRO:CD	3:N:1007:VAL:HG12	2.45	0.46
4:O:51:LEU:HD12	4:O:52:GLU:N	2.30	0.46
4:O:48:MET:HB2	4:O:54:LEU:HD12	1.97	0.46
1:B:41:ARG:NH1	1:B:177:VAL:HG23	2.31	0.46
2:C:1111:ILE:HG13	2:C:1112:PHE:N	2.29	0.46
2:C:244:PRO:CD	2:C:245:GLY:H	2.22	0.46
2:C:399:ASN:HD21	2:C:402:SER:HB2	1.81	0.46
2:C:462:ASP:CG	2:C:463:GLU:H	2.19	0.46
2:C:630:ARG:HD3	9:C:9834:HOH:O	2.15	0.46
3:D:1254:GLN:OE1	3:D:1254:GLN:HA	2.16	0.46
3:D:1282:ARG:CZ	3:D:1282:ARG:HB3	2.45	0.46
3:D:1393:GLN:HB2	3:D:1398:TRP:HZ2	1.80	0.46
3:D:1400:VAL:HG11	9:D:2388:HOH:O	2.14	0.46
3:D:18:ILE:HG21	3:D:516:ALA:O	2.16	0.46
3:D:441:ARG:HB3	3:D:443:VAL:HG23	1.98	0.46
3:D:396:VAL:CG2	3:D:447:VAL:HB	2.42	0.46
3:D:702:LEU:HB3	3:D:745:MET:HE3	1.96	0.46
3:D:810:GLU:HA	3:D:813:LEU:HD23	1.98	0.46
3:D:829:VAL:HG11	9:D:9902:HOH:O	2.16	0.46
1:B:150:TYR:HD2	3:D:857:ILE:HG13	1.80	0.46
3:D:972:LEU:HD23	3:D:973:GLN:N	2.31	0.46
5:F:282:LEU:HD12	5:F:284:ARG:O	2.16	0.46
5:F:361:LEU:CD2	5:F:362:SER:H	2.21	0.46
1:L:117:VAL:HA	9:L:3956:HOH:O	2.16	0.46
1:L:197:LEU:HD11	1:L:199:ILE:HD11	1.97	0.46
1:L:45:LEU:HB2	9:L:3651:HOH:O	2.14	0.46
2:M:1040:LEU:HG	2:M:1045:ALA:HB3	1.97	0.46
2:M:139:GLN:HB3	2:M:334:ARG:HB2	1.98	0.46
2:M:139:GLN:NE2	2:M:334:ARG:HH11	2.10	0.46
2:M:352:ALA:HA	2:M:355:VAL:CG1	2.46	0.46
2:M:134:ARG:NH2	2:M:393:GLN:HA	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:496:ILE:HD12	2:M:496:ILE:H	1.80	0.46
2:M:535:SER:O	2:M:538:GLN:HG2	2.15	0.46
2:M:537:LYS:HE3	2:M:905:ILE:HD11	1.97	0.46
2:M:78:PHE:HB2	2:M:88:LEU:HD21	1.97	0.46
2:M:912:PRO:HB2	9:M:2025:HOH:O	2.14	0.46
3:N:1111:ASP:HB2	3:N:1203:LYS:HG3	1.98	0.46
3:N:136:ASP:HB3	3:N:137:PRO:CD	2.35	0.46
3:N:459:GLU:HG3	3:N:460:ALA:N	2.30	0.46
3:N:953:ASP:O	3:N:955:VAL:HG23	2.15	0.46
1:A:189:ARG:HD2	9:A:9741:HOH:O	2.15	0.46
1:A:48:ILE:HG22	1:A:173:PRO:CD	2.45	0.46
1:B:185:ARG:HG2	9:B:9526:HOH:O	2.16	0.46
2:C:1049:LEU:HG	2:C:1053:LEU:HD11	1.97	0.46
2:C:129:ILE:HG12	2:C:386:PHE:O	2.15	0.46
2:C:503:LEU:HD13	2:C:507:ARG:O	2.15	0.46
2:C:645:VAL:HA	9:C:9913:HOH:O	2.16	0.46
2:C:565:GLN:OE1	2:C:842:ARG:HG2	2.16	0.46
3:D:38:LYS:HE3	9:D:9903:HOH:O	2.16	0.46
3:D:656:PHE:HB3	3:D:694:VAL:CG1	2.44	0.46
3:D:736:PHE:O	3:D:738:ALA:N	2.48	0.46
3:D:781:PRO:HB3	3:D:785:ILE:HB	1.97	0.46
3:D:850:LEU:HD22	3:D:884:ARG:NH2	2.29	0.46
5:F:278:LEU:HB2	5:F:286:PRO:HG2	1.98	0.46
2:C:1021:LEU:HD13	5:F:332:PHE:HA	1.98	0.46
1:L:146:ARG:HB3	9:L:4052:HOH:O	2.14	0.46
1:L:24:VAL:HG22	1:L:196:THR:HB	1.98	0.46
2:M:260:LEU:HA	2:M:291:ALA:CB	2.46	0.46
2:M:595:LEU:HG	9:M:2074:HOH:O	2.14	0.46
2:M:869:VAL:HB	9:M:2014:HOH:O	2.15	0.46
3:N:1383:ASP:HB3	3:N:1416:ALA:H	1.79	0.46
3:N:175:VAL:HG11	3:N:218:LYS:H	1.80	0.46
3:N:702:LEU:HD23	3:N:716:PHE:CD1	2.51	0.46
3:N:789:LEU:O	3:N:792:ILE:HG23	2.16	0.46
3:N:950:GLY:O	3:N:953:ASP:N	2.35	0.46
4:O:50:THR:HB	9:O:4388:HOH:O	2.16	0.46
4:O:51:LEU:HA	9:O:6073:HOH:O	2.15	0.46
1:A:220:GLU:HG2	9:A:9635:HOH:O	2.14	0.46
1:B:152:PRO:HB2	9:B:9614:HOH:O	2.15	0.46
2:C:113:VAL:HG11	2:C:373:VAL:CB	2.44	0.46
2:C:191:PHE:HE2	2:C:196:LEU:HD21	1.80	0.46
2:C:170:PRO:HG2	2:C:258:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:GLY:HA2	2:C:341:THR:OG1	2.16	0.46
2:C:473:ARG:HA	2:C:531:PHE:CD1	2.50	0.46
2:C:571:LEU:HD21	2:C:669:GLY:H	1.80	0.46
2:C:943:VAL:HG11	2:C:973:VAL:CG2	2.46	0.46
3:D:119:SER:HB2	3:D:123:LEU:CB	2.37	0.46
3:D:1213:ARG:HE	3:D:1213:ARG:N	2.06	0.46
3:D:1393:GLN:CB	3:D:1398:TRP:HE1	2.29	0.46
3:D:19:ARG:HD2	9:D:9854:HOH:O	2.15	0.46
3:D:56:TYR:O	3:D:80:VAL:HG21	2.15	0.46
3:D:723:GLY:HA3	9:D:9564:HOH:O	2.15	0.46
5:F:256:ARG:CD	5:F:260:ILE:HD12	2.46	0.46
1:K:101:LEU:HD23	1:K:113:ASP:O	2.15	0.46
1:K:49:PRO:HB3	1:K:148:VAL:HG22	1.97	0.46
1:K:45:LEU:HD23	9:K:3684:HOH:O	2.15	0.46
1:L:100:LEU:O	1:L:115:LEU:HG	2.16	0.46
1:L:128:HIS:CE1	1:L:131:THR:HG23	2.50	0.46
1:L:58:ILE:HD13	1:L:140:MET:HB2	1.97	0.46
2:M:1091:GLU:HA	3:N:520:LEU:HD13	1.97	0.46
2:M:333:ILE:HD13	2:M:467:ILE:HD11	1.98	0.46
2:M:966:LEU:HD21	2:M:986:PRO:HG3	1.97	0.46
3:N:1112:CYS:HB2	3:N:1195:GLN:CD	2.36	0.46
3:N:1115:THR:HG22	3:N:1117:TYR:CD2	2.51	0.46
3:N:1153:VAL:HG21	9:N:9815:HOH:O	2.15	0.46
9:N:2022:HOH:O	5:P:94:LEU:HD22	2.15	0.46
1:A:117:VAL:HG12	9:A:9578:HOH:O	2.16	0.46
1:A:54:THR:CG2	1:A:158:ILE:HG13	2.42	0.46
2:C:1056:LYS:HD3	3:D:623:VAL:HG13	1.98	0.46
2:C:285:LEU:HD23	2:C:285:LEU:O	2.16	0.46
2:C:29:ALA:HB1	2:C:340:MET:CE	2.46	0.46
2:C:42:VAL:HG12	2:C:43:GLY:N	2.27	0.46
2:C:328:LEU:HD22	2:C:433:THR:O	2.15	0.46
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.50	0.46
2:C:843:HIS:CD2	2:C:884:GLN:HA	2.51	0.46
3:D:1348:LEU:HD13	3:D:1348:LEU:HA	1.81	0.46
3:D:1486:VAL:HG11	4:E:26:ARG:HD3	1.98	0.46
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.97	0.46
5:F:253:ASP:HA	5:F:259:ARG:NH1	2.30	0.46
5:F:335:ASP:CG	5:F:338:LEU:HD12	2.36	0.46
1:K:211:LEU:O	1:K:215:VAL:HG13	2.15	0.46
1:K:217:ILE:HA	1:K:220:GLU:CD	2.36	0.46
1:L:123:MET:O	1:L:125:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:143:ARG:NH1	1:L:158:ILE:HG23	2.30	0.46
2:M:157:ARG:HB3	9:M:2062:HOH:O	2.14	0.46
2:M:289:THR:HG22	2:M:290:LEU:H	1.80	0.46
2:M:503:LEU:HD13	2:M:507:ARG:O	2.16	0.46
3:N:10:ILE:HG13	3:N:1434:TRP:CZ2	2.51	0.46
3:N:9:ARG:HG3	3:N:1455:LYS:C	2.36	0.46
3:N:168:THR:CB	3:N:393:ILE:HD12	2.46	0.46
3:N:8:VAL:HG21	9:N:2132:HOH:O	2.15	0.46
3:N:890:VAL:HG13	3:N:926:LYS:HG2	1.98	0.46
4:O:48:MET:HB3	4:O:54:LEU:HB2	1.98	0.46
5:P:223:ALA:HB2	5:P:242:TRP:HB2	1.97	0.46
1:B:19:GLU:O	1:B:200:TRP:HA	2.16	0.46
2:C:110:GLU:H	2:C:368:THR:CG2	2.27	0.46
2:C:218:VAL:HG22	2:C:221:LEU:HD23	1.98	0.46
2:C:340:MET:HB2	9:C:9586:HOH:O	2.16	0.46
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.97	0.46
2:C:747:ALA:O	2:C:799:ILE:HA	2.16	0.46
3:D:1243:THR:HG22	3:D:1244:GLY:H	1.81	0.46
3:D:1290:LEU:CD2	3:D:1291:SER:H	2.28	0.46
3:D:175:VAL:HG12	3:D:176:ASP:OD1	2.15	0.46
3:D:460:ALA:O	3:D:464:LEU:HG	2.15	0.46
3:D:823:LEU:HG	9:D:9797:HOH:O	2.15	0.46
3:D:770:LEU:HG	3:D:919:PHE:CD1	2.51	0.46
4:E:86:GLN:HB2	9:E:9579:HOH:O	2.16	0.46
1:L:133:GLU:HG3	1:L:134:GLU:HG2	1.98	0.46
1:L:218:LEU:O	1:L:222:LEU:HG	2.16	0.46
1:L:65:PHE:CD1	3:N:813:LEU:HD13	2.50	0.46
2:M:355:VAL:HB	9:M:9797:HOH:O	2.14	0.46
2:M:798:GLY:HA2	9:M:9603:HOH:O	2.16	0.46
2:M:876:VAL:O	2:M:879:ARG:O	2.34	0.46
3:N:1278:ASP:HA	3:N:1319:VAL:O	2.16	0.46
3:N:1278:ASP:HB2	3:N:1318:TYR:OH	2.16	0.46
3:N:1297:GLU:HG3	9:N:2208:HOH:O	2.15	0.46
3:N:861:GLN:N	3:N:861:GLN:CD	2.68	0.46
3:N:9:ARG:HG3	3:N:1455:LYS:O	2.16	0.46
5:P:217:ASN:O	5:P:221:ILE:HG13	2.16	0.46
5:P:252:ALA:HA	9:P:3803:HOH:O	2.16	0.46
5:P:396:ARG:HH11	5:P:399:GLN:HE22	1.62	0.46
1:A:176:ARG:HD3	1:A:200:TRP:CE3	2.50	0.46
1:B:228:PRO:O	1:B:229:GLN:HG3	2.16	0.46
1:A:42:ARG:NH2	1:B:34:VAL:HB	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1101:THR:C	2:C:1102:LEU:HD12	2.36	0.46
2:C:547:ILE:HB	2:C:550:LEU:HD13	1.98	0.46
2:C:630:ARG:NH2	2:C:706:GLU:C	2.69	0.46
2:C:710:ILE:HD12	2:C:790:LEU:HD13	1.98	0.46
2:C:716:LYS:HA	9:C:2391:HOH:O	2.16	0.46
2:C:79:PRO:O	2:C:83:CYS:SG	2.72	0.46
3:D:103:TRP:HA	9:D:9830:HOH:O	2.16	0.46
3:D:1150:ALA:HA	9:D:2165:HOH:O	2.14	0.46
3:D:213:VAL:HG22	3:D:214:GLU:H	1.80	0.46
3:D:813:LEU:O	3:D:839:LEU:HD11	2.15	0.46
5:F:162:LYS:HA	9:F:9569:HOH:O	2.15	0.46
1:K:227:ASN:ND2	1:K:227:ASN:H	2.13	0.46
2:M:84:ARG:NH2	2:M:128:ILE:HD11	2.31	0.46
2:M:224:GLU:HB3	2:M:227:PHE:CD1	2.51	0.46
3:N:1078:ARG:NH1	3:N:1078:ARG:HG3	2.30	0.46
3:N:1212:ALA:HA	9:N:2149:HOH:O	2.16	0.46
3:N:1301:LYS:HE3	3:N:1301:LYS:HA	1.97	0.46
3:N:131:LYS:CG	3:N:568:ARG:HG2	2.46	0.46
3:N:99:ALA:HA	3:N:575:GLN:NE2	2.31	0.46
3:N:653:PHE:CD1	3:N:653:PHE:N	2.85	0.46
3:N:417:PRO:HA	5:P:168:LYS:NZ	2.30	0.46
5:P:323:ASP:CB	5:P:325:LYS:HE2	2.45	0.46
5:P:419:ARG:O	5:P:421:PHE:N	2.48	0.46
1:A:40:LEU:O	1:A:44:LEU:HD12	2.16	0.45
1:B:75:VAL:O	1:B:79:ILE:HG23	2.15	0.45
2:C:172:ILE:N	2:C:172:ILE:HD12	2.29	0.45
2:C:437:ARG:HG2	2:C:467:ILE:O	2.16	0.45
2:C:441:VAL:HG12	2:C:559:LEU:HA	1.96	0.45
2:C:626:ARG:H	2:C:639:GLN:HE21	1.62	0.45
3:D:1012:GLU:HG3	9:D:2626:HOH:O	2.14	0.45
3:D:1153:VAL:HG12	3:D:1155:VAL:CG2	2.44	0.45
3:D:1318:TYR:HD1	3:D:1319:VAL:N	2.14	0.45
3:D:1320:GLU:HG2	3:D:1339:LYS:NZ	2.31	0.45
3:D:1330:ILE:HB	3:D:1347:TYR:CE1	2.51	0.45
3:D:369:ALA:HB2	9:D:9672:HOH:O	2.16	0.45
3:D:566:ILE:CG1	5:F:192:LEU:HD11	2.46	0.45
5:F:105:LYS:NZ	5:F:179:GLU:HB3	2.31	0.45
1:K:2:LEU:HD13	9:K:6158:HOH:O	2.15	0.45
1:K:50:GLY:O	1:K:146:ARG:HA	2.15	0.45
2:M:131:GLY:HA2	9:M:9630:HOH:O	2.16	0.45
2:M:162:ILE:HD12	2:M:172:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:24:GLU:HB2	9:M:2039:HOH:O	2.16	0.45
2:M:881:ASN:H	2:M:881:ASN:HD22	1.64	0.45
2:M:914:ILE:HD11	2:M:918:LEU:HD13	1.98	0.45
3:N:119:SER:HB2	3:N:123:LEU:CB	2.37	0.45
3:N:1312:LEU:N	9:N:2252:HOH:O	2.48	0.45
3:N:434:ARG:HB2	3:N:447:VAL:CG2	2.46	0.45
3:N:787:LEU:HD21	3:N:947:ILE:HD11	1.98	0.45
5:P:181:GLU:O	5:P:184:ARG:HB3	2.16	0.45
5:P:306:GLU:O	5:P:310:ILE:HG13	2.16	0.45
1:A:189:ARG:HB3	9:A:9569:HOH:O	2.16	0.45
1:A:24:VAL:HG22	1:A:196:THR:CG2	2.45	0.45
1:B:49:PRO:HB3	1:B:148:VAL:HG13	1.97	0.45
2:C:195:LEU:HG	2:C:238:LEU:HD12	1.98	0.45
2:C:512:ARG:HB2	9:C:9776:HOH:O	2.16	0.45
2:C:721:ARG:HG2	2:C:820:ARG:HH12	1.81	0.45
2:C:958:THR:HG23	2:C:961:GLU:CG	2.46	0.45
2:C:862:PRO:HA	2:C:975:TYR:CE1	2.51	0.45
3:D:1293:PHE:CD2	3:D:1302:GLU:HA	2.51	0.45
3:D:1371:VAL:HG12	3:D:1375:MET:CE	2.46	0.45
3:D:28:LYS:CB	3:D:41:ARG:HD2	2.41	0.45
3:D:653:PHE:CD1	3:D:653:PHE:N	2.84	0.45
3:D:899:LEU:HB3	3:D:917:GLN:HG2	1.99	0.45
1:K:101:LEU:HD22	1:K:102:LYS:H	1.79	0.45
2:M:189:ARG:HG3	2:M:190:LYS:N	2.31	0.45
2:M:278:GLU:HG3	2:M:283:ILE:HA	1.97	0.45
2:M:287:GLY:HA3	9:M:2054:HOH:O	2.16	0.45
2:M:260:LEU:HA	2:M:291:ALA:HB2	1.98	0.45
2:M:419:THR:HG22	9:M:9836:HOH:O	2.16	0.45
2:M:510:ALA:HB3	2:M:513:VAL:CG2	2.46	0.45
2:M:610:ARG:HH11	2:M:612:VAL:HG23	1.80	0.45
2:M:853:LEU:HB2	2:M:858:MET:HE3	1.98	0.45
3:N:1003:VAL:O	3:N:1007:VAL:HG13	2.16	0.45
3:N:1272:ALA:CA	3:N:1326:THR:HB	2.44	0.45
3:N:134:VAL:O	3:N:134:VAL:HG23	2.17	0.45
3:N:141:ILE:HD13	3:N:450:TYR:CB	2.43	0.45
3:N:1103:HIS:HD2	3:N:1462:LEU:N	2.14	0.45
3:N:1498:ALA:HA	3:N:1501:GLU:OE2	2.16	0.45
3:N:486:ARG:HA	3:N:489:ARG:HG2	1.97	0.45
3:N:486:ARG:NH2	9:N:2166:HOH:O	2.48	0.45
3:N:658:LEU:HD22	3:N:670:VAL:HG13	1.98	0.45
2:M:1083:GLU:OE2	3:N:87:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:197:SER:O	5:P:200:LYS:HB3	2.16	0.45
5:P:210:LEU:HA	5:P:213:ILE:HD12	1.98	0.45
5:P:410:TYR:HB3	9:P:4652:HOH:O	2.16	0.45
1:A:161:ARG:HB2	1:A:161:ARG:CZ	2.46	0.45
1:B:101:LEU:HD12	1:B:114:PHE:CE1	2.51	0.45
2:C:1060:ILE:CG2	2:C:1061:GLU:N	2.79	0.45
2:C:229:MET:HE3	9:C:2102:HOH:O	2.15	0.45
2:C:430:VAL:HG13	3:D:1075:HIS:HA	1.98	0.45
2:C:48:PHE:HB3	9:C:2027:HOH:O	2.16	0.45
2:C:603:VAL:H	2:C:647:GLN:H	1.64	0.45
2:C:636:ALA:C	2:C:637:LEU:HD23	2.37	0.45
3:D:1037:GLN:OE1	3:D:1042:ARG:HB3	2.15	0.45
3:D:183:GLU:HA	3:D:186:VAL:CG1	2.46	0.45
3:D:572:ARG:NH2	5:F:83:GLN:HG3	2.31	0.45
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.36	0.45
3:D:631:ILE:HG21	3:D:745:MET:SD	2.56	0.45
4:E:33:HIS:HB2	4:E:37:ASN:HD21	1.82	0.45
4:E:86:GLN:O	4:E:90:GLU:HG3	2.16	0.45
5:F:140:ARG:HA	9:F:9735:HOH:O	2.15	0.45
5:F:287:THR:O	5:F:289:GLU:N	2.49	0.45
5:F:332:PHE:HB2	9:F:9704:HOH:O	2.14	0.45
1:L:50:GLY:O	1:L:146:ARG:HA	2.16	0.45
1:L:209:GLU:HB3	9:L:4456:HOH:O	2.16	0.45
2:M:139:GLN:HG3	2:M:140:ILE:N	2.27	0.45
2:M:422:ARG:NH1	9:M:9984:HOH:O	2.49	0.45
2:M:437:ARG:NH1	2:M:488:ALA:HA	2.31	0.45
2:M:460:ARG:HD2	2:M:485:TYR:CD2	2.51	0.45
2:M:571:LEU:HA	2:M:701:THR:O	2.16	0.45
2:M:8:ARG:HG3	2:M:10:ARG:HH21	1.81	0.45
2:M:921:ALA:HB2	9:M:9641:HOH:O	2.16	0.45
2:M:979:THR:HG23	2:M:981:GLU:HB2	1.97	0.45
3:N:1109:GLU:HG2	3:N:1201:CYS:CA	2.47	0.45
3:N:1124:GLN:HE21	3:N:1133:ARG:CD	2.24	0.45
3:N:1471:LEU:HD12	3:N:1472:ILE:H	1.80	0.45
3:N:1498:ALA:HB3	9:N:2275:HOH:O	2.17	0.45
3:N:116:LEU:CD2	3:N:468:LEU:HD11	2.47	0.45
3:N:573:MET:SD	5:P:210:LEU:HD22	2.56	0.45
3:N:76:CYS:HB2	9:N:9715:HOH:O	2.16	0.45
3:N:799:LYS:N	3:N:826:PRO:HG2	2.30	0.45
3:N:990:ASP:HB2	9:N:9775:HOH:O	2.15	0.45
5:P:214:GLN:O	5:P:217:ASN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:OE1	2:C:605:LYS:HB2	2.16	0.45
1:B:101:LEU:HG	1:B:114:PHE:CA	2.45	0.45
2:C:14:PRO:HB3	2:C:586:ARG:HH21	1.80	0.45
3:D:1242:HIS:HE1	3:D:1266:ARG:HB3	1.81	0.45
3:D:1372:VAL:O	3:D:1375:MET:HB2	2.16	0.45
3:D:1412:LYS:HE2	3:D:1414:PRO:HG3	1.97	0.45
3:D:1431:THR:OG1	3:D:1432:LYS:N	2.49	0.45
3:D:178:LEU:HG	3:D:200:ASP:H	1.80	0.45
3:D:553:ARG:CZ	9:F:9685:HOH:O	2.64	0.45
3:D:722:GLU:HB3	9:D:9664:HOH:O	2.14	0.45
5:F:353:GLU:OE2	5:F:356:LYS:HD2	2.15	0.45
1:K:61:VAL:HG13	1:K:66:SER:OG	2.16	0.45
1:K:97:VAL:HG12	1:K:99:LEU:HD12	1.98	0.45
2:M:148:PHE:CZ	2:M:281:LEU:HD13	2.52	0.45
2:M:770:GLU:HB3	9:M:2326:HOH:O	2.16	0.45
2:M:897:LEU:HD13	9:M:9641:HOH:O	2.17	0.45
3:N:1339:LYS:O	3:N:1339:LYS:HG3	2.16	0.45
3:N:1418:LYS:HB2	9:N:2727:HOH:O	2.15	0.45
3:N:598:ARG:HH11	3:N:598:ARG:HG2	1.82	0.45
3:N:950:GLY:C	3:N:952:ASP:N	2.65	0.45
5:P:408:LEU:O	5:P:412:GLU:HG2	2.16	0.45
1:A:106:PRO:HG3	1:A:133:GLU:O	2.17	0.45
1:B:89:PHE:CD1	1:B:120:VAL:HG13	2.51	0.45
1:B:92:PRO:HA	1:B:146:ARG:CZ	2.46	0.45
1:B:50:GLY:O	1:B:146:ARG:HA	2.15	0.45
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.99	0.45
2:C:163:ILE:HG13	2:C:171:TRP:CH2	2.50	0.45
2:C:137:VAL:O	2:C:391:LEU:HD11	2.16	0.45
2:C:901:TYR:N	2:C:901:TYR:CD1	2.83	0.45
2:C:911:GLU:O	2:C:915:LYS:HG2	2.16	0.45
2:C:971:LYS:HD2	2:C:986:PRO:HB2	1.98	0.45
3:D:1155:VAL:CG1	3:D:1177:ALA:HB1	2.47	0.45
3:D:1382:THR:HA	9:D:2920:HOH:O	2.15	0.45
3:D:1393:GLN:N	9:D:9959:HOH:O	2.49	0.45
3:D:1501:GLU:HB2	9:D:2754:HOH:O	2.16	0.45
3:D:28:LYS:O	3:D:43:GLY:HA2	2.16	0.45
3:D:465:LEU:HD21	3:D:509:PRO:HB2	1.99	0.45
3:D:563:PRO:CG	3:D:566:ILE:HD12	2.46	0.45
3:D:860:LEU:HA	3:D:877:PRO:HB2	1.98	0.45
3:D:95:LEU:HA	3:D:551:ASN:OD1	2.16	0.45
3:D:974:ILE:HG22	9:D:9882:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:88:ILE:CD1	5:F:193:ARG:HB2	2.37	0.45
5:F:231:ARG:HB3	5:F:233:PHE:CZ	2.52	0.45
5:F:396:ARG:HA	9:F:9581:HOH:O	2.16	0.45
1:K:107:LYS:HB2	9:K:4981:HOH:O	2.17	0.45
1:K:127:LEU:HD12	1:K:127:LEU:C	2.37	0.45
1:K:19:GLU:O	1:K:200:TRP:HA	2.16	0.45
1:K:43:ILE:HD11	1:L:35:THR:HG21	1.99	0.45
2:M:273:GLY:HA2	2:M:276:LYS:HD3	1.98	0.45
2:M:39:ARG:HE	2:M:39:ARG:HA	1.82	0.45
2:M:400:PRO:HG3	9:M:9799:HOH:O	2.15	0.45
2:M:68:PHE:CZ	2:M:71:TYR:HB3	2.52	0.45
2:M:905:ILE:HG22	2:M:906:PHE:HD1	1.81	0.45
3:N:1258:ARG:HH21	3:N:1351:GLU:CG	2.29	0.45
3:N:1314:LYS:HZ3	3:N:1317:ASP:H	1.63	0.45
3:N:186:VAL:HG11	3:N:213:VAL:HB	1.99	0.45
3:N:23:TYR:O	3:N:49:ILE:HG23	2.16	0.45
3:N:27:GLU:N	9:N:9589:HOH:O	2.47	0.45
3:N:364:GLY:N	9:N:2883:HOH:O	2.49	0.45
3:N:487:ALA:N	9:N:2856:HOH:O	2.49	0.45
4:O:45:ARG:HD2	4:O:47:LYS:HE3	1.99	0.45
4:O:83:ASP:HB3	9:O:4879:HOH:O	2.17	0.45
5:P:332:PHE:N	5:P:332:PHE:HD1	2.15	0.45
5:P:366:ALA:HB3	5:P:367:MET:CE	2.46	0.45
1:A:195:LEU:HD11	1:A:197:LEU:HD22	1.97	0.45
1:A:85:LEU:HD12	1:A:86:VAL:N	2.32	0.45
1:B:125:PRO:HB3	9:B:9731:HOH:O	2.17	0.45
1:B:65:PHE:HD1	3:D:813:LEU:HD22	1.82	0.45
2:C:127:PHE:O	2:C:133:ASP:HA	2.17	0.45
2:C:601:GLY:HA3	2:C:615:TYR:HA	1.97	0.45
2:C:732:ALA:HA	2:C:735:ARG:NH2	2.31	0.45
2:C:773:LEU:HG	2:C:777:ILE:HD11	1.98	0.45
3:D:1332:PRO:HB3	3:D:1348:LEU:HD21	1.99	0.45
3:D:66:GLN:HB3	9:D:9848:HOH:O	2.16	0.45
5:F:243:ILE:HB	9:F:9669:HOH:O	2.16	0.45
5:F:278:LEU:CB	5:F:286:PRO:HG2	2.46	0.45
5:F:412:GLU:OE1	5:F:418:LEU:HD13	2.17	0.45
1:L:11:PHE:HD1	1:L:25:LEU:HD13	1.81	0.45
1:L:9:PRO:HB3	1:L:25:LEU:HG	1.97	0.45
2:M:51:THR:CB	2:M:348:LEU:HD23	2.47	0.45
2:M:64:LEU:HB2	2:M:359:MET:SD	2.56	0.45
2:M:462:ASP:OD1	2:M:466:PHE:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:52:PHE:O	2:M:54:ILE:N	2.50	0.45
2:M:52:PHE:HB3	2:M:53:PRO:HD3	1.98	0.45
2:M:575:GLN:OE1	2:M:670:GLN:HB3	2.17	0.45
2:M:805:ARG:HB3	9:M:2157:HOH:O	2.16	0.45
3:N:111:LYS:HD3	3:N:1452:ILE:HD13	1.97	0.45
3:N:1156:LEU:CD1	3:N:1176:LYS:HD2	2.46	0.45
3:N:1162:GLU:HG2	3:N:1163:GLY:N	2.31	0.45
3:N:1280:VAL:HG12	3:N:1316:GLY:O	2.16	0.45
3:N:567:ILE:C	3:N:571:LYS:HZ2	2.20	0.45
3:N:129:PHE:CZ	3:N:587:ARG:HD3	2.51	0.45
3:N:633:VAL:HG22	3:N:635:PRO:CD	2.46	0.45
3:N:701:LEU:O	3:N:747:VAL:HA	2.16	0.45
3:N:764:LEU:HD23	3:N:767:HIS:NE2	2.32	0.45
3:N:971:LEU:HD11	3:N:992:ILE:HG23	1.98	0.45
5:P:413:SER:HA	5:P:416:ARG:HD3	1.97	0.45
1:A:112:ARG:HB2	9:A:9722:HOH:O	2.17	0.45
1:A:18:ARG:NH1	9:A:9718:HOH:O	2.49	0.45
1:B:71:VAL:HG22	1:B:132:LEU:HD12	1.98	0.45
2:C:203:ASP:OD1	2:C:205:GLU:HG3	2.16	0.45
2:C:281:LEU:HB2	2:C:309:TYR:CD1	2.52	0.45
2:C:367:LEU:O	2:C:371:LYS:HB3	2.17	0.45
2:C:410:ILE:HD12	2:C:410:ILE:N	2.31	0.45
2:C:580:MET:HB3	2:C:584:GLU:OE1	2.16	0.45
2:C:640:ARG:HB3	9:C:9670:HOH:O	2.16	0.45
2:C:3:ILE:HD13	2:C:900:ARG:O	2.16	0.45
3:D:1043:GLY:O	3:D:1056:PRO:HB3	2.15	0.45
3:D:1462:LEU:HD13	3:D:1472:ILE:CG2	2.46	0.45
3:D:209:ARG:HG3	9:D:2664:HOH:O	2.16	0.45
3:D:190:GLU:HG3	3:D:210:ARG:CD	2.46	0.45
3:D:57:GLU:HG3	3:D:64:LYS:HE3	1.97	0.45
1:L:149:GLY:O	1:L:171:PHE:HB2	2.15	0.45
1:L:219:ARG:O	1:L:223:THR:HG23	2.16	0.45
1:L:95:GLN:H	1:L:95:GLN:NE2	2.13	0.45
2:M:146:VAL:HG13	2:M:161:SER:O	2.16	0.45
2:M:287:GLY:HA2	9:M:9726:HOH:O	2.17	0.45
2:M:368:THR:HB	2:M:369:PRO:HD3	1.99	0.45
3:N:1176:LYS:HD3	3:N:1176:LYS:O	2.17	0.45
3:N:118:LEU:O	3:N:120:ALA:N	2.49	0.45
3:N:1468:LEU:HG	9:N:2132:HOH:O	2.17	0.45
3:N:1481:VAL:HG11	4:O:18:ARG:CA	2.40	0.45
3:N:810:GLU:HA	3:N:813:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:350:LEU:HG	5:P:354:LEU:HD11	1.98	0.45
2:C:1091:GLU:O	2:C:1094:ALA:HB3	2.16	0.45
2:C:214:TYR:HB3	9:C:2050:HOH:O	2.17	0.45
2:C:374:ASN:ND2	2:C:377:PRO:HD3	2.32	0.45
2:C:640:ARG:HG3	9:C:2078:HOH:O	2.17	0.45
2:C:695:LEU:HG	9:C:9871:HOH:O	2.15	0.45
2:C:983:ILE:HG22	2:C:983:ILE:O	2.16	0.45
3:D:1101:VAL:HG22	3:D:1428:ALA:HB2	1.97	0.45
3:D:118:LEU:O	3:D:120:ALA:N	2.50	0.45
3:D:180:LYS:HG3	9:D:9629:HOH:O	2.15	0.45
3:D:517:VAL:HG11	3:D:581:LEU:HD21	1.99	0.45
3:D:605:ASP:HB3	9:D:9653:HOH:O	2.16	0.45
3:D:880:ILE:O	3:D:883:ALA:HB3	2.17	0.45
4:E:9:LEU:HD22	4:E:19:LEU:HD11	1.98	0.45
4:E:26:ARG:HD2	4:E:29:GLN:CD	2.37	0.45
5:F:361:LEU:CD1	5:F:408:LEU:HD21	2.47	0.45
1:L:145:ASP:O	1:L:171:PHE:HE1	2.00	0.45
2:M:1040:LEU:HG	2:M:1045:ALA:CB	2.46	0.45
2:M:321:GLU:HB3	9:M:9616:HOH:O	2.16	0.45
2:M:890:LEU:HA	2:M:914:ILE:CD1	2.45	0.45
2:M:966:LEU:HD21	2:M:986:PRO:CG	2.47	0.45
3:N:1465:ASN:HD22	3:N:1465:ASN:HA	1.54	0.45
3:N:170:PRO:HA	9:N:2270:HOH:O	2.16	0.45
3:N:56:TYR:N	9:N:9683:HOH:O	2.50	0.45
3:N:844:ALA:HB1	3:N:867:ARG:NH1	2.32	0.45
3:N:970:LYS:HB2	3:N:970:LYS:NZ	2.32	0.45
5:P:215:GLU:HA	5:P:215:GLU:OE1	2.17	0.45
5:P:409:LYS:HE3	5:P:410:TYR:CE1	2.52	0.45
1:A:161:ARG:HB2	1:A:161:ARG:HH11	1.81	0.45
1:A:30:ARG:HD3	1:A:191:ASP:OD2	2.17	0.45
1:A:48:ILE:HD11	1:A:210:ALA:O	2.17	0.45
1:A:88:ARG:HG2	1:A:88:ARG:O	2.16	0.45
1:B:94:LEU:HD11	1:B:119:ASP:CB	2.46	0.45
2:C:1008:ARG:HH12	2:C:1011:GLY:CA	2.30	0.45
2:C:158:TYR:HD1	9:C:9658:HOH:O	2.00	0.45
2:C:352:ALA:C	2:C:355:VAL:HG12	2.38	0.45
2:C:480:THR:HG22	2:C:481:ASP:N	2.32	0.45
2:C:577:PRO:HG3	2:C:993:PHE:CE2	2.51	0.45
2:C:605:LYS:HG3	2:C:612:VAL:HB	1.98	0.45
3:D:1057:VAL:HG21	9:D:9822:HOH:O	2.16	0.45
3:D:1161:GLU:HG2	3:D:1161:GLU:H	1.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:574:LEU:O	3:D:577:ALA:HB3	2.17	0.45
3:D:581:LEU:CD1	3:D:603:LEU:HD12	2.47	0.45
3:D:724:GLN:HB2	3:D:724:GLN:HE21	1.59	0.45
3:D:863:VAL:HA	9:D:9665:HOH:O	2.17	0.45
3:D:420:VAL:HG13	5:F:164:LYS:HZ3	1.81	0.45
1:L:165:ILE:HG13	1:L:165:ILE:O	2.17	0.45
2:M:310:LEU:HD21	9:M:9821:HOH:O	2.16	0.45
2:M:59:LYS:HB3	9:M:9796:HOH:O	2.16	0.45
2:M:625:LEU:HD22	2:M:639:GLN:CB	2.47	0.45
2:M:793:PRO:HB3	9:M:2101:HOH:O	2.16	0.45
2:M:831:ARG:HH11	2:M:831:ARG:HG2	1.81	0.45
3:N:18:ILE:HG21	3:N:516:ALA:HB1	1.99	0.45
3:N:477:LEU:O	3:N:481:MET:HB2	2.15	0.45
3:N:520:LEU:CD1	3:N:521:PRO:HD2	2.36	0.45
2:M:1008:ARG:HD2	3:N:624:ASP:O	2.17	0.45
3:N:628:ARG:O	3:N:628:ARG:HD2	2.17	0.45
3:N:690:ALA:O	3:N:694:VAL:HG23	2.16	0.45
3:N:710:ARG:HD2	3:N:772:PRO:HG2	1.99	0.45
3:N:792:ILE:O	3:N:878:GLY:HA3	2.17	0.45
3:N:831:GLY:HA3	9:N:9579:HOH:O	2.16	0.45
5:P:113:ILE:HG23	5:P:127:ILE:HG22	1.97	0.45
5:P:336:GLU:HA	9:P:5536:HOH:O	2.17	0.45
1:A:176:ARG:O	1:A:200:TRP:HE3	2.00	0.45
1:A:192:LEU:HA	9:A:9561:HOH:O	2.17	0.45
1:A:77:GLU:O	1:A:80:LEU:HB3	2.17	0.45
1:A:92:PRO:HD3	9:A:9646:HOH:O	2.16	0.45
1:B:103:ALA:HB1	1:B:107:LYS:HD2	1.99	0.45
2:C:313:LEU:HD13	2:C:321:GLU:O	2.16	0.45
2:C:359:MET:HB2	9:C:9719:HOH:O	2.16	0.45
2:C:952:LEU:HB3	2:C:966:LEU:CD1	2.47	0.45
3:D:783:ARG:NH2	3:D:1029:ARG:CZ	2.80	0.45
2:C:516:ARG:NE	3:D:1068:LEU:HD13	2.32	0.45
3:D:1145:TYR:HD2	3:D:1168:MET:SD	2.40	0.45
3:D:1352:ILE:HG22	3:D:1368:ILE:HD13	1.98	0.45
3:D:1402:ALA:HB2	3:D:1415:VAL:HG23	1.98	0.45
3:D:1441:GLN:HB2	9:D:2106:HOH:O	2.16	0.45
3:D:154:THR:HG23	3:D:157:GLU:H	1.81	0.45
3:D:827:ILE:H	3:D:828:LYS:HZ1	1.65	0.45
1:K:72:LYS:HB3	1:K:73:GLU:OE2	2.16	0.45
1:L:111:ALA:HB3	1:L:124:ASN:O	2.18	0.45
1:L:71:VAL:HG22	1:L:132:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1038:TRP:HD1	2:M:1041:GLU:OE1	2.00	0.45
2:M:207:LEU:HD23	2:M:211:LEU:HD23	1.98	0.45
2:M:267:TYR:H	2:M:267:TYR:HD2	1.65	0.45
2:M:365:ASP:O	2:M:367:LEU:HD12	2.17	0.45
2:M:747:ALA:O	2:M:799:ILE:HA	2.17	0.45
3:N:1045:MET:HE3	9:N:9946:HOH:O	2.17	0.45
3:N:191:LEU:HA	3:N:191:LEU:HD23	1.82	0.45
3:N:397:LYS:HZ1	3:N:399:ARG:HH21	1.65	0.45
3:N:659:LYS:O	3:N:663:GLU:HG3	2.17	0.45
5:P:142:ARG:HB2	9:P:3557:HOH:O	2.17	0.45
5:P:154:LYS:HD3	9:P:3717:HOH:O	2.16	0.45
5:P:184:ARG:O	5:P:188:ILE:HG13	2.16	0.45
5:P:287:THR:O	5:P:289:GLU:N	2.49	0.45
2:C:1033:GLY:O	2:C:1037:VAL:HG23	2.17	0.44
2:C:114:PHE:HD1	2:C:114:PHE:N	2.13	0.44
2:C:479:VAL:HG23	2:C:506:ASN:O	2.17	0.44
2:C:876:VAL:HG21	3:D:949:ILE:HG13	1.98	0.44
3:D:1023:MET:O	3:D:1028:ALA:HB3	2.17	0.44
3:D:1066:THR:OG1	3:D:1067:VAL:N	2.50	0.44
3:D:1109:GLU:HG2	3:D:1202:GLN:H	1.81	0.44
3:D:1280:VAL:O	3:D:1294:VAL:HA	2.17	0.44
3:D:33:ASN:HD21	3:D:35:ARG:NE	2.15	0.44
3:D:396:VAL:HG13	3:D:446:VAL:O	2.17	0.44
3:D:828:LYS:HD3	3:D:828:LYS:N	2.32	0.44
5:F:300:ASP:HA	9:F:9583:HOH:O	2.17	0.44
2:M:167:LYS:HD3	2:M:168:ARG:N	2.32	0.44
2:M:458:TYR:CD2	2:M:470:PRO:HG3	2.52	0.44
2:M:52:PHE:HB3	9:M:2228:HOH:O	2.16	0.44
2:M:704:HIS:HB2	2:M:831:ARG:NE	2.24	0.44
3:N:1500:LYS:HB3	9:N:9903:HOH:O	2.16	0.44
5:P:308:LEU:O	5:P:312:GLN:HG3	2.17	0.44
5:P:393:THR:O	5:P:397:ILE:HG13	2.17	0.44
1:A:115:LEU:O	1:A:115:LEU:HD12	2.16	0.44
1:A:31:GLY:HA2	2:C:938:LYS:HE2	1.99	0.44
1:A:46:SER:HB3	2:C:856:GLU:CG	2.48	0.44
1:A:97:VAL:HG12	1:A:99:LEU:HD12	1.99	0.44
2:C:1051:GLU:HG3	2:C:1055:LEU:HD12	2.00	0.44
2:C:1103:ASP:N	2:C:1107:ASN:O	2.50	0.44
2:C:181:VAL:HG12	2:C:182:VAL:N	2.32	0.44
2:C:216:GLU:HA	9:C:2087:HOH:O	2.16	0.44
2:C:288:ARG:HD2	2:C:288:ARG:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:110:GLU:N	2:C:368:THR:HG21	2.27	0.44
2:C:462:ASP:CG	2:C:468:ARG:HD2	2.37	0.44
2:C:810:ASP:HA	2:C:811:PRO:HD3	1.79	0.44
2:C:707:ARG:HG3	2:C:826:TYR:CE1	2.52	0.44
3:D:220:ARG:HA	9:D:2217:HOH:O	2.16	0.44
3:D:611:GLN:HB2	9:D:2875:HOH:O	2.16	0.44
3:D:965:GLU:O	3:D:968:ASP:HB2	2.17	0.44
4:E:55:PHE:N	9:E:9537:HOH:O	2.50	0.44
5:F:323:ASP:C	5:F:325:LYS:H	2.21	0.44
5:F:361:LEU:HD22	5:F:366:ALA:HB2	1.99	0.44
1:K:59:GLU:HG3	1:K:139:ASN:O	2.16	0.44
1:K:161:ARG:HH11	1:K:161:ARG:HB2	1.79	0.44
1:K:34:VAL:HG23	9:K:4850:HOH:O	2.18	0.44
2:M:167:LYS:HA	9:M:2164:HOH:O	2.15	0.44
2:M:257:VAL:HG13	9:M:9979:HOH:O	2.17	0.44
2:M:309:TYR:O	2:M:313:LEU:HB3	2.17	0.44
2:M:338:GLU:O	2:M:341:THR:HG22	2.17	0.44
2:M:438:ILE:HG22	2:M:439:CYS:O	2.17	0.44
2:M:515:ALA:O	2:M:516:ARG:HD3	2.18	0.44
2:M:607:ASP:HB3	2:M:609:ASN:H	1.81	0.44
2:M:72:ARG:HG3	9:M:2023:HOH:O	2.16	0.44
3:N:1124:GLN:HA	3:N:1125:PRO:HD3	1.73	0.44
3:N:1242:HIS:HE1	3:N:1266:ARG:CZ	2.30	0.44
3:N:1263:PHE:CE2	3:N:1371:VAL:HG11	2.52	0.44
3:N:1310:ARG:HB2	9:N:2073:HOH:O	2.17	0.44
3:N:196:VAL:HG13	3:N:202:VAL:HG11	1.99	0.44
3:N:112:ILE:HG22	3:N:512:MET:SD	2.57	0.44
1:A:153:ALA:HA	1:A:156:HIS:NE2	2.32	0.44
2:C:274:ARG:HB2	2:C:285:LEU:CD1	2.48	0.44
3:D:1284:GLU:HG3	3:D:1293:PHE:HE1	1.82	0.44
3:D:187:LYS:HA	3:D:187:LYS:HD3	1.76	0.44
3:D:85:VAL:HG12	3:D:89:ARG:NE	2.32	0.44
5:F:416:ARG:NH1	5:F:419:ARG:HB2	2.32	0.44
1:K:221:HIS:HA	1:K:224:TYR:CD2	2.52	0.44
1:L:104:GLU:HB3	9:L:3981:HOH:O	2.17	0.44
1:L:112:ARG:HH12	1:L:125:PRO:HB2	1.82	0.44
1:L:13:VAL:HG13	1:L:23:PHE:CD1	2.53	0.44
2:M:148:PHE:HB2	2:M:313:LEU:HD13	1.98	0.44
2:M:411:SER:HA	2:M:452:ILE:HA	1.98	0.44
2:M:554:ASP:OD2	2:M:556:ASN:HB3	2.17	0.44
2:M:586:ARG:CZ	2:M:590:ASP:OD2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1031:ASN:OD1	3:N:1033:GLN:N	2.49	0.44
3:N:891:GLU:OE1	3:N:891:GLU:HA	2.17	0.44
3:N:1495:ILE:HG21	4:O:80:VAL:HG13	1.98	0.44
4:O:96:GLU:HG3	9:O:4005:HOH:O	2.17	0.44
9:M:9721:HOH:O	5:P:374:GLY:HA2	2.17	0.44
1:B:20:TYR:HB3	9:B:9575:HOH:O	2.18	0.44
2:C:1067:TYR:CB	5:F:341:PRO:HB3	2.47	0.44
2:C:1100:GLN:HB3	9:C:9972:HOH:O	2.17	0.44
2:C:137:VAL:HG22	2:C:391:LEU:O	2.17	0.44
2:C:254:VAL:HG22	9:C:9577:HOH:O	2.16	0.44
2:C:366:SER:HA	9:C:9836:HOH:O	2.18	0.44
2:C:437:ARG:HB3	2:C:467:ILE:HB	1.98	0.44
2:C:780:GLU:O	2:C:782:ALA:N	2.50	0.44
2:C:795:GLY:HA3	2:C:1004:LYS:HD2	2.00	0.44
3:D:1106:VAL:CG2	3:D:1474:ALA:HB2	2.47	0.44
3:D:1425:THR:CG2	3:D:1426:LYS:N	2.81	0.44
3:D:23:TYR:HB2	3:D:49:ILE:O	2.17	0.44
3:D:932:ASP:HA	3:D:935:LYS:HE2	2.00	0.44
4:E:44:GLU:C	4:E:45:ARG:HG3	2.36	0.44
3:D:1491:THR:HG21	4:E:89:MET:SD	2.58	0.44
2:C:773:LEU:HD13	5:F:373:LYS:HG3	1.99	0.44
1:K:63:HIS:CD2	1:K:65:PHE:H	2.36	0.44
1:K:79:ILE:HD11	9:M:2040:HOH:O	2.16	0.44
2:M:1034:GLU:HA	2:M:1037:VAL:CG2	2.46	0.44
2:M:1102:LEU:HB2	3:N:7:LYS:HB2	1.99	0.44
2:M:110:GLU:HG2	2:M:369:PRO:HG3	1.98	0.44
2:M:140:ILE:HD12	2:M:140:ILE:H	1.82	0.44
2:M:177:GLU:HB2	9:M:2552:HOH:O	2.17	0.44
2:M:290:LEU:HD22	2:M:302:VAL:HG11	2.00	0.44
2:M:139:GLN:OE1	2:M:415:PRO:HD2	2.18	0.44
2:M:63:GLY:O	2:M:103:LYS:HE2	2.16	0.44
2:M:722:ILE:HD11	2:M:756:VAL:HG11	1.99	0.44
3:N:101:HIS:CD2	3:N:582:LEU:HD13	2.53	0.44
3:N:1148:VAL:HG13	3:N:1163:GLY:O	2.17	0.44
2:M:1091:GLU:OE1	3:N:613:ARG:HG2	2.17	0.44
3:N:607:LEU:HD22	3:N:614:PHE:CE2	2.51	0.44
3:N:67:ARG:HD2	3:N:67:ARG:HA	1.75	0.44
2:M:1090:LYS:HZ2	3:N:90:MET:HG3	1.80	0.44
5:P:142:ARG:HH11	5:P:142:ARG:CB	2.26	0.44
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.50	0.44
2:C:1003:ASP:O	2:C:1005:MET:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1052:MET:SD	2:C:1056:LYS:HD3	2.56	0.44
2:C:1060:ILE:CG2	2:C:1061:GLU:H	2.30	0.44
2:C:395:LYS:NZ	2:C:407:LYS:HZ2	2.16	0.44
2:C:444:PRO:CD	2:C:452:ILE:HG13	2.48	0.44
2:C:48:PHE:HA	2:C:348:LEU:CD2	2.47	0.44
2:C:751:PRO:HA	2:C:792:VAL:HB	2.00	0.44
2:C:952:LEU:HB3	2:C:966:LEU:HD11	1.99	0.44
3:D:1073:SER:HB2	9:D:9940:HOH:O	2.18	0.44
3:D:432:TYR:HA	3:D:448:GLU:O	2.18	0.44
3:D:696:HIS:HD2	4:E:59:ASN:HB2	1.83	0.44
3:D:860:LEU:HD23	3:D:877:PRO:HB2	2.00	0.44
5:F:363:GLU:HG2	9:F:9732:HOH:O	2.17	0.44
5:F:365:GLU:OE1	5:F:400:ILE:HD12	2.17	0.44
5:F:395:GLU:OE1	5:F:395:GLU:HA	2.16	0.44
1:K:176:ARG:HG3	1:K:200:TRP:CE3	2.52	0.44
1:K:9:PRO:HB3	1:K:25:LEU:HG	1.99	0.44
2:M:1088:LEU:HD13	9:N:2483:HOH:O	2.18	0.44
2:M:230:ARG:HG3	9:M:9597:HOH:O	2.17	0.44
2:M:342:ASP:O	2:M:345:ARG:HG2	2.17	0.44
2:M:420:ARG:HG2	2:M:422:ARG:HG2	1.99	0.44
2:M:564:MET:SD	2:M:846:LYS:HG3	2.58	0.44
2:M:726:ILE:O	2:M:726:ILE:HG22	2.18	0.44
3:N:1394:VAL:HB	3:N:1397:LYS:CD	2.47	0.44
3:N:573:MET:HG2	9:N:9585:HOH:O	2.18	0.44
2:M:1005:MET:CE	3:N:648:MET:HB2	2.48	0.44
3:N:702:LEU:N	3:N:702:LEU:HD22	2.33	0.44
3:N:87:ARG:HB3	3:N:523:ASP:CB	2.48	0.44
3:N:693:GLU:HG3	4:O:48:MET:SD	2.57	0.44
1:A:128:HIS:HE1	9:A:9698:HOH:O	2.01	0.44
1:A:23:PHE:CE1	1:A:211:LEU:HD23	2.53	0.44
1:B:163:ASN:HA	9:B:9544:HOH:O	2.17	0.44
2:C:352:ALA:CA	2:C:355:VAL:HG12	2.46	0.44
2:C:54:ILE:CD1	2:C:356:ARG:HG2	2.46	0.44
2:C:369:PRO:CG	2:C:370:ALA:H	2.30	0.44
2:C:435:TYR:C	2:C:437:ARG:H	2.21	0.44
2:C:582:GLY:N	2:C:584:GLU:OE2	2.45	0.44
2:C:879:ARG:HB3	9:C:9575:HOH:O	2.17	0.44
3:D:1090:ASP:C	3:D:1092:GLY:N	2.69	0.44
3:D:1326:THR:HA	9:D:9899:HOH:O	2.17	0.44
1:L:62:LEU:H	1:L:62:LEU:HD12	1.82	0.44
2:M:309:TYR:HA	9:M:9614:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:679:PHE:HD2	2:M:682:TYR:HD2	1.65	0.44
2:M:754:ILE:HD12	9:M:2146:HOH:O	2.18	0.44
3:N:1128:VAL:O	3:N:1129:THR:C	2.55	0.44
3:N:135:LEU:HD11	3:N:139:GLY:HA3	1.99	0.44
3:N:1462:LEU:CD2	3:N:1473:PRO:HD2	2.48	0.44
3:N:488:ARG:CZ	3:N:488:ARG:HB3	2.47	0.44
3:N:18:ILE:HD12	3:N:518:PRO:HD3	1.99	0.44
3:N:631:ILE:O	3:N:632:VAL:HG23	2.18	0.44
3:N:754:PHE:CE2	3:N:1476:THR:HG21	2.52	0.44
3:N:863:VAL:HG12	9:N:9691:HOH:O	2.18	0.44
3:N:960:LYS:HG2	3:N:964:LEU:HD12	2.00	0.44
4:O:62:THR:HA	4:O:65:MET:CE	2.46	0.44
5:P:301:ALA:N	9:P:3676:HOH:O	2.51	0.44
1:A:69:PRO:O	1:A:71:VAL:HG23	2.18	0.44
2:C:198:ARG:NH2	9:C:2102:HOH:O	2.50	0.44
2:C:707:ARG:NH2	2:C:824:ARG:HH11	2.15	0.44
3:D:1164:ARG:HG3	3:D:1164:ARG:NH1	2.32	0.44
3:D:1145:TYR:HE2	3:D:1168:MET:HB2	1.82	0.44
3:D:1209:LEU:HD21	4:E:16:LYS:HZ3	1.81	0.44
3:D:1321:ALA:O	3:D:1339:LYS:HD3	2.18	0.44
3:D:135:LEU:HD11	3:D:139:GLY:HA3	2.00	0.44
3:D:140:ALA:HB2	9:D:2414:HOH:O	2.17	0.44
3:D:505:SER:HB3	9:D:2397:HOH:O	2.17	0.44
3:D:539:ASP:HB3	9:D:9656:HOH:O	2.17	0.44
2:C:1039:ALA:HB2	3:D:707:THR:HG21	1.99	0.44
3:D:74:GLU:HG3	9:D:2222:HOH:O	2.18	0.44
1:K:48:ILE:HD12	1:K:174:VAL:HG21	1.99	0.44
1:L:110:LYS:NZ	1:L:110:LYS:HB2	2.33	0.44
1:K:9:PRO:CB	1:L:224:TYR:HB3	2.43	0.44
2:M:1063:ARG:O	2:M:1066:ALA:HB3	2.17	0.44
2:M:310:LEU:O	2:M:313:LEU:HD23	2.17	0.44
2:M:401:LEU:HD12	2:M:587:VAL:HG11	2.00	0.44
2:M:465:GLY:N	9:M:9933:HOH:O	2.51	0.44
2:M:575:GLN:HA	2:M:662:GLU:CD	2.38	0.44
2:M:611:ILE:N	2:M:611:ILE:HD12	2.33	0.44
2:M:640:ARG:HG2	2:M:640:ARG:NH1	2.32	0.44
3:N:1025:GLN:HB3	9:N:9833:HOH:O	2.16	0.44
3:N:1435:LEU:HD23	3:N:1464:GLU:HB2	2.00	0.44
3:N:421:LEU:HD11	3:N:437:VAL:CG2	2.48	0.44
3:N:777:PRO:HD2	3:N:912:LYS:HG2	2.00	0.44
3:N:864:VAL:HG12	3:N:865:THR:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1090:LYS:NZ	3:N:90:MET:CG	2.80	0.44
1:A:66:SER:O	1:A:75:VAL:HG23	2.18	0.44
1:B:45:LEU:HD23	1:B:174:VAL:HG12	2.00	0.44
2:C:1026:GLN:HA	9:C:9758:HOH:O	2.18	0.44
2:C:127:PHE:CE1	2:C:386:PHE:HE2	2.36	0.44
2:C:197:LEU:HD12	2:C:207:LEU:HD11	1.99	0.44
2:C:488:ALA:O	2:C:491:GLU:HG2	2.16	0.44
2:C:693:GLU:HA	2:C:696:LYS:CG	2.48	0.44
2:C:722:ILE:HG21	2:C:821:GLU:OE2	2.18	0.44
2:C:726:ILE:HG23	2:C:787:ASP:OD2	2.18	0.44
2:C:94:LEU:HD12	2:C:95:TYR:N	2.32	0.44
3:D:126:VAL:HG22	9:D:9864:HOH:O	2.17	0.44
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	2.00	0.44
3:D:1496:GLU:HG2	9:D:2624:HOH:O	2.17	0.44
3:D:651:GLU:HA	3:D:651:GLU:OE1	2.18	0.44
3:D:659:LYS:C	3:D:659:LYS:HD3	2.38	0.44
3:D:710:ARG:NH2	9:D:2362:HOH:O	2.51	0.44
3:D:868:TYR:CG	3:D:869:MET:N	2.85	0.44
1:K:175:ARG:NE	1:K:202:ASP:HA	2.32	0.44
1:L:112:ARG:HB2	9:L:5043:HOH:O	2.17	0.44
1:L:20:TYR:OH	1:L:198:ARG:HD2	2.17	0.44
1:L:7:LYS:HZ2	1:L:186:LEU:HD21	1.83	0.44
2:M:129:ILE:HG22	2:M:130:ASN:N	2.31	0.44
2:M:207:LEU:HD22	2:M:221:LEU:CD2	2.47	0.44
2:M:338:GLU:HA	2:M:341:THR:HG22	1.99	0.44
2:M:881:ASN:ND2	2:M:881:ASN:H	2.15	0.44
2:M:972:VAL:HG23	2:M:974:LEU:CD1	2.48	0.44
3:N:957:PRO:CG	3:N:1007:VAL:HA	2.48	0.44
3:N:1149:LEU:CD2	3:N:1166:LEU:HD22	2.48	0.44
3:N:1292:VAL:O	3:N:1303:TYR:HB2	2.18	0.44
3:N:1283:ILE:HD12	3:N:1315:ASP:CG	2.38	0.44
3:N:1345:GLU:H	3:N:1345:GLU:HG2	1.70	0.44
3:N:1364:HIS:CE1	3:N:1366:LYS:H	2.35	0.44
3:N:1432:LYS:HB2	9:N:9954:HOH:O	2.18	0.44
3:N:598:ARG:HG2	3:N:598:ARG:NH1	2.33	0.44
9:M:9863:HOH:O	3:N:89:ARG:HG3	2.16	0.44
4:O:16:LYS:HD3	4:O:17:TYR:HE2	1.83	0.44
4:O:76:GLY:N	4:O:79:LEU:HD22	2.33	0.44
5:P:287:THR:HG23	5:P:289:GLU:HB2	2.00	0.44
1:A:95:GLN:HB3	9:A:9650:HOH:O	2.18	0.44
1:B:176:ARG:HG3	1:B:200:TRP:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1109:VAL:HG22	3:D:3:LYS:CG	2.47	0.44
2:C:157:ARG:HD3	2:C:158:TYR:N	2.33	0.44
2:C:279:GLU:HG3	2:C:280:LYS:N	2.32	0.44
2:C:302:VAL:O	2:C:306:THR:HG23	2.18	0.44
2:C:572:ILE:HG13	2:C:573:ARG:N	2.33	0.44
3:D:1132:LEU:HA	3:D:1132:LEU:HD12	1.86	0.44
3:D:1242:HIS:CE1	3:D:1266:ARG:HB3	2.53	0.44
3:D:1310:ARG:NH1	3:D:1327:ARG:HD3	2.33	0.44
3:D:1394:VAL:HB	3:D:1397:LYS:CD	2.46	0.44
3:D:569:ASN:HD21	5:F:210:LEU:HD22	1.83	0.44
3:D:983:LEU:HD13	3:D:991:GLN:OE1	2.18	0.44
5:F:127:ILE:HD11	9:F:9677:HOH:O	2.17	0.44
5:F:196:VAL:HG13	5:F:213:ILE:CD1	2.48	0.44
1:K:173:PRO:HA	1:K:202:ASP:OD1	2.17	0.44
1:K:32:PHE:N	9:K:4770:HOH:O	2.49	0.44
1:L:208:LEU:HG	9:L:6488:HOH:O	2.17	0.44
2:M:475:VAL:HB	9:M:9558:HOH:O	2.17	0.44
2:M:644:VAL:HG22	9:M:9667:HOH:O	2.18	0.44
2:M:688:ILE:CD1	2:M:847:GLY:HA3	2.47	0.44
2:M:814:GLU:HA	9:M:2144:HOH:O	2.18	0.44
2:M:814:GLU:HG3	2:M:814:GLU:O	2.18	0.44
2:M:821:GLU:HG2	2:M:822:VAL:N	2.33	0.44
3:N:1014:ASN:HB3	9:N:9933:HOH:O	2.18	0.44
3:N:1231:GLU:HB3	3:N:1232:PRO:HD3	2.00	0.44
3:N:1280:VAL:O	3:N:1294:VAL:HA	2.17	0.44
3:N:1282:ARG:HD3	3:N:1295:GLU:OE1	2.18	0.44
3:N:1489:GLN:O	3:N:1493:LYS:HG2	2.18	0.44
3:N:760:ARG:HH21	4:O:3:GLU:CD	2.22	0.44
4:O:42:PRO:HG2	9:O:4104:HOH:O	2.17	0.44
4:O:59:ASN:HD22	4:O:59:ASN:HA	1.61	0.44
5:P:113:ILE:HB	9:P:4593:HOH:O	2.17	0.44
5:P:208:SER:HB2	5:P:211:ASP:CG	2.38	0.44
1:B:149:GLY:O	1:B:171:PHE:HB2	2.18	0.43
2:C:1005:MET:HB2	9:C:9600:HOH:O	2.18	0.43
2:C:289:THR:O	2:C:291:ALA:N	2.51	0.43
2:C:342:ASP:HA	2:C:345:ARG:HG2	2.00	0.43
2:C:64:LEU:HD13	2:C:359:MET:HG3	2.00	0.43
2:C:437:ARG:HE	2:C:469:THR:H	1.66	0.43
2:C:528:GLU:O	2:C:530:GLU:HG3	2.18	0.43
2:C:690:ILE:CG2	2:C:852:ILE:HG23	2.47	0.43
3:D:115:LEU:HD22	3:D:502:PHE:HE1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:141:ILE:HD13	3:D:449:SER:HA	2.00	0.43
3:D:754:PHE:HE2	3:D:1476:THR:HG21	1.83	0.43
3:D:472:ALA:HB1	9:D:2893:HOH:O	2.18	0.43
3:D:875:THR:HG22	3:D:879:ARG:HB2	1.99	0.43
2:C:886:LEU:CD2	3:D:951:ILE:HG13	2.48	0.43
3:D:983:LEU:HB2	9:D:9941:HOH:O	2.18	0.43
4:E:51:LEU:HB3	9:E:9581:HOH:O	2.18	0.43
4:E:70:THR:HG22	4:E:71:GLY:N	2.33	0.43
5:F:198:ILE:HD11	9:F:9857:HOH:O	2.17	0.43
5:F:256:ARG:HA	9:F:9900:HOH:O	2.17	0.43
1:K:162:ILE:HG13	1:K:163:ASN:N	2.33	0.43
2:M:137:VAL:HG23	2:M:391:LEU:CD1	2.47	0.43
2:M:480:THR:HG22	2:M:481:ASP:N	2.33	0.43
2:M:854:PRO:C	2:M:856:GLU:N	2.70	0.43
2:M:861:LEU:HD23	2:M:862:PRO:CD	2.46	0.43
3:N:1365:ASP:O	3:N:1369:GLU:HG3	2.18	0.43
3:N:1459:LEU:HD22	3:N:1465:ASN:HA	1.99	0.43
3:N:179:VAL:O	3:N:183:GLU:HB2	2.18	0.43
3:N:464:LEU:HD11	9:N:9914:HOH:O	2.18	0.43
3:N:598:ARG:NH2	5:P:319:THR:HA	2.33	0.43
3:N:78:VAL:HG12	3:N:78:VAL:O	2.17	0.43
4:O:20:THR:N	9:O:3658:HOH:O	2.50	0.43
4:O:29:GLN:HB2	4:O:33:HIS:NE2	2.33	0.43
5:P:150:THR:HG23	9:P:3557:HOH:O	2.18	0.43
1:A:95:GLN:HG2	1:A:146:ARG:HH12	1.83	0.43
1:B:156:HIS:CE1	1:B:158:ILE:H	2.36	0.43
1:B:67:THR:HB	1:B:74:ASP:OD1	2.18	0.43
2:C:1057:SER:HB2	3:D:622:ARG:O	2.18	0.43
2:C:326:ASP:HA	9:C:9742:HOH:O	2.18	0.43
2:C:502:PRO:HB2	2:C:509:ALA:HB3	2.00	0.43
2:C:51:THR:O	2:C:51:THR:HG22	2.19	0.43
2:C:536:PRO:HB2	2:C:905:ILE:HD13	2.00	0.43
2:C:683:ASN:N	2:C:683:ASN:OD1	2.50	0.43
3:D:1120:VAL:HA	3:D:1121:PRO:HD3	1.76	0.43
3:D:1147:ARG:HH12	3:D:1190:SER:HB2	1.83	0.43
3:D:1164:ARG:HG3	3:D:1164:ARG:HH11	1.82	0.43
3:D:13:ALA:O	3:D:511:TRP:HB3	2.18	0.43
3:D:493:ARG:HA	9:D:2197:HOH:O	2.19	0.43
3:D:527:MET:CE	5:F:258:ILE:HD11	2.48	0.43
3:D:984:THR:CG2	3:D:987:GLU:H	2.30	0.43
5:F:163:LEU:HB3	5:F:174:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:2010:HOH:O	5:F:326:ASP:HA	2.18	0.43
1:K:43:ILE:HD13	9:L:5637:HOH:O	2.18	0.43
2:M:19:THR:HG21	2:M:125:GLY:HA3	2.00	0.43
2:M:243:ARG:HB3	9:M:2252:HOH:O	2.18	0.43
2:M:260:LEU:HD23	2:M:293:PHE:HB3	2.01	0.43
2:M:369:PRO:HD2	9:M:9605:HOH:O	2.17	0.43
2:M:721:ARG:HG3	9:M:9649:HOH:O	2.18	0.43
2:M:810:ASP:HA	2:M:811:PRO:HD3	1.90	0.43
3:N:1293:PHE:C	9:N:9607:HOH:O	2.56	0.43
3:N:133:ILE:HG12	3:N:133:ILE:H	1.47	0.43
3:N:138:LYS:HB2	3:N:138:LYS:NZ	2.33	0.43
3:N:1438:ALA:N	3:N:1446:VAL:HG11	2.33	0.43
3:N:1468:LEU:HD23	3:N:1468:LEU:O	2.17	0.43
3:N:465:LEU:HD13	3:N:509:PRO:O	2.18	0.43
2:M:1005:MET:HE2	3:N:648:MET:CE	2.47	0.43
3:N:799:LYS:O	3:N:799:LYS:HD3	2.18	0.43
4:O:5:GLY:HA3	4:O:8:LYS:HD2	2.00	0.43
5:P:203:THR:HG22	5:P:204:GLY:N	2.34	0.43
3:N:388:HIS:H	5:P:97:GLU:HG3	1.83	0.43
1:B:101:LEU:HG	1:B:113:ASP:C	2.38	0.43
1:B:122:ILE:HD11	9:B:9749:HOH:O	2.18	0.43
2:C:104:ASP:HA	9:C:9858:HOH:O	2.18	0.43
2:C:101:ILE:HD12	2:C:107:LEU:HD22	2.00	0.43
2:C:196:LEU:O	2:C:199:VAL:HB	2.19	0.43
2:C:236:ILE:O	2:C:239:PHE:HB2	2.19	0.43
2:C:257:VAL:HG22	9:C:2287:HOH:O	2.18	0.43
2:C:264:PRO:HB3	2:C:289:THR:CG2	2.46	0.43
2:C:260:LEU:HA	2:C:291:ALA:CB	2.47	0.43
2:C:389:SER:C	2:C:391:LEU:H	2.20	0.43
2:C:413:LEU:HD12	2:C:413:LEU:N	2.33	0.43
2:C:50:GLU:HB2	9:C:9766:HOH:O	2.17	0.43
2:C:516:ARG:NH2	3:D:1068:LEU:HB3	2.33	0.43
2:C:54:ILE:CG2	2:C:66:LEU:HB3	2.48	0.43
2:C:801:VAL:HG12	9:C:9826:HOH:O	2.19	0.43
2:C:839:LEU:HD21	2:C:849:VAL:CG2	2.48	0.43
2:C:979:THR:HG23	2:C:981:GLU:HB2	1.99	0.43
3:D:175:VAL:HG11	3:D:218:LYS:H	1.84	0.43
3:D:400:VAL:HA	3:D:442:ASN:O	2.19	0.43
3:D:525:ARG:HB2	3:D:541:ASN:ND2	2.32	0.43
3:D:829:VAL:H	3:D:835:SER:HB2	1.83	0.43
3:D:867:ARG:CG	3:D:867:ARG:HH11	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:891:GLU:HG3	9:D:2312:HOH:O	2.18	0.43
3:D:899:LEU:CB	3:D:917:GLN:HG2	2.47	0.43
3:D:924:MET:HB3	4:E:7:ASP:OD1	2.18	0.43
5:F:114:LYS:O	5:F:118:GLU:HG3	2.18	0.43
5:F:205:ARG:CD	5:F:251:ILE:HG21	2.47	0.43
1:K:133:GLU:HG3	9:M:2288:HOH:O	2.17	0.43
1:K:44:LEU:HD21	1:K:199:ILE:HD13	2.00	0.43
1:L:7:LYS:NZ	1:L:186:LEU:HD21	2.33	0.43
1:L:95:GLN:HG2	9:L:6455:HOH:O	2.18	0.43
2:M:1015:LEU:HB3	2:M:1016:ILE:HD13	2.00	0.43
2:M:226:VAL:HG21	9:M:9691:HOH:O	2.18	0.43
2:M:189:ARG:HH22	2:M:243:ARG:HG2	1.83	0.43
2:M:411:SER:OG	2:M:452:ILE:HG23	2.19	0.43
2:M:464:LEU:HA	2:M:464:LEU:HD12	1.81	0.43
2:M:602:GLU:HG2	2:M:603:VAL:N	2.33	0.43
2:M:603:VAL:H	2:M:647:GLN:H	1.66	0.43
2:M:654:LEU:HD13	2:M:664:GLY:N	2.33	0.43
2:M:695:LEU:HD22	2:M:832:LYS:HG2	2.00	0.43
1:L:30:ARG:CZ	2:M:854:PRO:HG3	2.48	0.43
1:K:46:SER:HB3	2:M:856:GLU:HG2	1.99	0.43
2:M:82:GLU:OE2	2:M:86:LYS:HD3	2.19	0.43
2:M:877:PRO:HG3	3:N:1023:MET:CE	2.48	0.43
3:N:1026:SER:C	3:N:1028:ALA:H	2.21	0.43
3:N:12:LEU:HD23	3:N:13:ALA:N	2.28	0.43
3:N:1441:GLN:HE21	3:N:1441:GLN:HB3	1.69	0.43
2:M:1085:PHE:CE2	3:N:1468:LEU:HA	2.52	0.43
3:N:171:LEU:HD21	9:N:2196:HOH:O	2.17	0.43
3:N:27:GLU:C	3:N:28:LYS:HD2	2.38	0.43
3:N:567:ILE:HG22	3:N:571:LYS:CE	2.49	0.43
3:N:683:ILE:HD12	3:N:683:ILE:N	2.33	0.43
3:N:988:ARG:HH11	3:N:992:ILE:HD11	1.83	0.43
4:O:8:LYS:HD2	4:O:69:LEU:HD11	2.01	0.43
5:P:226:LYS:HB2	5:P:238:TYR:OH	2.18	0.43
5:P:321:ILE:O	5:P:327:SER:HB3	2.17	0.43
5:P:80:PRO:HA	5:P:83:GLN:HB2	2.00	0.43
2:C:332:ARG:HE	2:C:464:LEU:CD1	2.29	0.43
2:C:115:LEU:HA	2:C:375:SER:CB	2.48	0.43
2:C:52:PHE:HB3	2:C:53:PRO:HD3	1.99	0.43
2:C:717:LEU:HB3	9:C:9827:HOH:O	2.18	0.43
2:C:726:ILE:HG22	2:C:726:ILE:O	2.18	0.43
2:C:876:VAL:HA	9:C:9650:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:877:PRO:HG3	3:D:1020:LEU:HD12	2.00	0.43
2:C:949:LYS:HE2	3:D:828:LYS:HE3	2.01	0.43
3:D:1038:LEU:O	3:D:1060:SER:HB2	2.18	0.43
3:D:1157:GLY:HA3	9:D:9683:HOH:O	2.16	0.43
3:D:1213:ARG:HB2	3:D:1214:PRO:HD3	1.99	0.43
3:D:1232:PRO:HB3	3:D:1361:VAL:CG2	2.48	0.43
3:D:1478:SER:OG	3:D:1481:VAL:HG23	2.18	0.43
3:D:42:ASP:HA	3:D:46:ASP:OD1	2.18	0.43
3:D:524:LEU:C	3:D:526:PRO:HD3	2.39	0.43
3:D:633:VAL:O	3:D:633:VAL:HG13	2.18	0.43
5:F:212:LEU:HD23	5:F:247:ILE:HG23	2.00	0.43
5:F:295:MET:HB3	5:F:299:TRP:CD1	2.54	0.43
5:F:321:ILE:O	5:F:327:SER:HB3	2.18	0.43
5:F:406:ARG:HA	5:F:409:LYS:HG2	1.99	0.43
1:K:110:LYS:HB3	1:K:112:ARG:HD3	2.00	0.43
1:K:188:GLN:HB2	9:K:6263:HOH:O	2.18	0.43
2:M:1118:LYS:HG2	9:M:2038:HOH:O	2.18	0.43
2:M:333:ILE:HG22	2:M:465:GLY:HA3	2.00	0.43
2:M:396:ASP:CA	2:M:633:GLN:HE22	2.28	0.43
2:M:63:GLY:HA3	2:M:103:LYS:CG	2.48	0.43
2:M:773:LEU:HG	2:M:777:ILE:HD11	2.00	0.43
3:N:1000:THR:HG23	3:N:1001:GLU:N	2.33	0.43
3:N:1147:ARG:HB3	3:N:1188:VAL:CG1	2.49	0.43
3:N:1219:GLU:HA	4:O:17:TYR:CE1	2.54	0.43
3:N:1263:PHE:HA	3:N:1375:MET:CE	2.48	0.43
3:N:153:LEU:HD11	3:N:158:TYR:CA	2.48	0.43
3:N:444:VAL:HG22	3:N:444:VAL:O	2.18	0.43
3:N:488:ARG:H	3:N:488:ARG:HG2	1.49	0.43
3:N:95:LEU:CD2	3:N:574:LEU:HD11	2.47	0.43
3:N:806:PHE:CG	3:N:806:PHE:O	2.71	0.43
3:N:80:VAL:HG12	3:N:81:THR:H	1.83	0.43
3:N:895:VAL:HG11	3:N:922:LEU:HD21	1.99	0.43
4:O:81:PRO:HB3	9:O:3911:HOH:O	2.18	0.43
5:P:218:GLN:HG3	9:P:3800:HOH:O	2.18	0.43
5:P:370:LYS:C	5:P:370:LYS:HD2	2.38	0.43
5:P:392:VAL:HG12	5:P:396:ARG:HB2	1.98	0.43
1:A:157:GLY:HA3	9:A:9582:HOH:O	2.19	0.43
1:A:53:VAL:HG12	1:A:167:VAL:HG21	1.99	0.43
1:B:56:VAL:HG13	1:B:142:VAL:HG12	2.01	0.43
2:C:1076:VAL:CG2	3:D:752:SER:HA	2.48	0.43
2:C:1094:ALA:HB1	3:D:603:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1117:SER:HB3	9:C:2289:HOH:O	2.18	0.43
2:C:428:ARG:HD3	2:C:449:ILE:HG23	2.00	0.43
2:C:612:VAL:HG22	2:C:622:GLU:HB2	2.00	0.43
2:C:631:SER:HB3	2:C:637:LEU:HD21	2.01	0.43
2:C:700:TYR:HA	9:C:9842:HOH:O	2.19	0.43
2:C:73:LEU:N	2:C:73:LEU:HD23	2.33	0.43
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.99	0.43
3:D:1191:PRO:HB3	3:D:1370:ILE:HD13	1.99	0.43
3:D:212:ARG:HD2	9:D:9717:HOH:O	2.18	0.43
3:D:3:LYS:H	3:D:3:LYS:CD	2.31	0.43
4:E:63:TRP:O	4:E:67:GLU:HG3	2.19	0.43
1:L:88:ARG:NH1	1:L:88:ARG:HG2	2.32	0.43
2:M:1089:VAL:O	2:M:1093:GLN:HG3	2.19	0.43
2:M:42:VAL:HG12	2:M:43:GLY:H	1.83	0.43
2:M:56:GLU:HA	2:M:56:GLU:OE1	2.18	0.43
3:N:1012:GLU:HA	9:N:9575:HOH:O	2.17	0.43
3:N:119:SER:H	3:N:123:LEU:CD1	2.29	0.43
3:N:1423:GLY:HA3	9:N:9705:HOH:O	2.19	0.43
3:N:152:LEU:CD2	3:N:152:LEU:H	2.24	0.43
3:N:207:PHE:CB	3:N:208:PRO:HD2	2.37	0.43
3:N:209:ARG:NH2	9:N:9622:HOH:O	2.50	0.43
3:N:400:VAL:HA	3:N:442:ASN:O	2.18	0.43
3:N:455:ARG:NH1	3:N:455:ARG:HG2	2.33	0.43
3:N:571:LYS:HZ2	3:N:571:LYS:HB2	1.83	0.43
3:N:666:ILE:HG23	9:N:2719:HOH:O	2.18	0.43
3:N:770:LEU:HD21	3:N:919:PHE:CG	2.54	0.43
3:N:777:PRO:HA	9:N:9909:HOH:O	2.18	0.43
1:A:205:VAL:HG23	1:A:206:THR:H	1.82	0.43
1:B:151:VAL:HB	1:B:169:ALA:HB3	1.99	0.43
2:C:102:HIS:HD2	9:C:2260:HOH:O	2.00	0.43
2:C:115:LEU:HD12	2:C:378:LEU:HD22	1.98	0.43
2:C:7:GLY:HA3	2:C:907:ASP:CG	2.39	0.43
3:D:1026:SER:C	3:D:1028:ALA:H	2.20	0.43
3:D:1280:VAL:HG12	3:D:1316:GLY:O	2.18	0.43
2:C:1109:VAL:HG13	3:D:3:LYS:HG2	2.01	0.43
3:D:141:ILE:CD1	3:D:449:SER:HA	2.49	0.43
3:D:478:LEU:HD21	3:D:500:ARG:HH21	1.80	0.43
3:D:525:ARG:HB2	3:D:541:ASN:HD21	1.82	0.43
3:D:531:ASP:C	3:D:533:GLY:N	2.67	0.43
3:D:806:PHE:O	3:D:807:ALA:C	2.57	0.43
3:D:799:LYS:N	3:D:826:PRO:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:193:ARG:NH2	9:F:9899:HOH:O	2.51	0.43
1:K:216:GLU:O	1:K:220:GLU:HG3	2.19	0.43
1:K:66:SER:O	1:K:75:VAL:HG23	2.18	0.43
2:M:172:ILE:N	2:M:172:ILE:HD12	2.33	0.43
2:M:26:TYR:CE1	2:M:30:LEU:HD11	2.53	0.43
2:M:383:ARG:HD3	9:M:2458:HOH:O	2.19	0.43
2:M:414:GLY:O	2:M:416:GLY:N	2.51	0.43
2:M:503:LEU:HD12	2:M:505:GLY:O	2.19	0.43
1:K:67:THR:N	2:M:627:ARG:HH21	2.14	0.43
2:M:687:ALA:C	2:M:688:ILE:HD12	2.38	0.43
2:M:879:ARG:CZ	9:M:9982:HOH:O	2.66	0.43
2:M:881:ASN:N	2:M:881:ASN:ND2	2.66	0.43
2:M:958:THR:HG22	9:M:9918:HOH:O	2.18	0.43
3:N:108:VAL:HG23	3:N:109:PRO:HD3	2.00	0.43
3:N:1108:ARG:HG3	3:N:1108:ARG:O	2.19	0.43
3:N:1394:VAL:HG21	3:N:1397:LYS:HE3	1.99	0.43
3:N:36:THR:O	3:N:38:LYS:N	2.49	0.43
3:N:169:TYR:HA	3:N:392:SER:HA	2.01	0.43
3:N:422:ALA:O	3:N:427:VAL:HG21	2.18	0.43
3:N:396:VAL:CG2	3:N:447:VAL:HB	2.44	0.43
3:N:470:LEU:HG	3:N:470:LEU:H	1.60	0.43
3:N:130:SER:O	3:N:568:ARG:NH2	2.51	0.43
3:N:636:GLN:HB3	9:N:9859:HOH:O	2.19	0.43
3:N:629:SER:HG	3:N:726:ILE:HG13	1.83	0.43
9:L:4624:HOH:O	3:N:821:VAL:HG22	2.18	0.43
5:P:155:THR:O	5:P:159:ILE:HG13	2.18	0.43
5:P:408:LEU:HA	5:P:411:HIS:CE1	2.54	0.43
1:A:213:GLN:O	1:A:217:ILE:HG13	2.18	0.43
1:B:83:LYS:HE3	1:B:167:VAL:HG12	2.00	0.43
2:C:64:LEU:CD2	2:C:359:MET:HG3	2.36	0.43
2:C:427:VAL:HG21	9:C:9712:HOH:O	2.17	0.43
2:C:577:PRO:HG3	2:C:993:PHE:CD2	2.54	0.43
2:C:693:GLU:OE1	2:C:696:LYS:HG3	2.19	0.43
2:C:97:ARG:HG3	9:C:2099:HOH:O	2.17	0.43
3:D:797:LYS:NZ	3:D:1016:PRO:HB3	2.34	0.43
3:D:1045:MET:O	3:D:1053:PHE:HD1	2.01	0.43
3:D:1072:ILE:HG22	9:D:9822:HOH:O	2.18	0.43
3:D:1129:THR:HA	9:D:9689:HOH:O	2.18	0.43
3:D:1164:ARG:HH21	3:D:1170:ASP:CG	2.22	0.43
3:D:1197:ARG:CG	3:D:1198:TYR:H	2.32	0.43
3:D:1396:GLU:O	3:D:1400:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:191:LEU:HB2	3:D:211:VAL:CG2	2.49	0.43
3:D:519:VAL:HG13	3:D:544:TYR:CZ	2.54	0.43
3:D:785:ILE:HG22	3:D:789:LEU:HD12	2.01	0.43
3:D:789:LEU:O	3:D:792:ILE:HG23	2.19	0.43
3:D:827:ILE:H	3:D:828:LYS:NZ	2.16	0.43
5:F:74:LYS:HA	9:F:9750:HOH:O	2.18	0.43
1:K:128:HIS:CE1	1:K:131:THR:HG23	2.54	0.43
1:K:1:MET:N	1:K:1:MET:SD	2.91	0.43
9:K:4324:HOH:O	1:L:11:PHE:HB2	2.18	0.43
1:L:23:PHE:CE1	1:L:208:LEU:HD13	2.54	0.43
2:M:1000:MET:HB3	2:M:1002:GLU:CG	2.49	0.43
2:M:191:PHE:HD2	2:M:195:LEU:HD23	1.82	0.43
2:M:262:ALA:HB3	9:M:9979:HOH:O	2.18	0.43
2:M:252:LYS:HZ2	2:M:296:GLY:HA3	1.83	0.43
2:M:282:GLY:HA2	2:M:308:ARG:HH21	1.82	0.43
2:M:136:ILE:HG21	2:M:336:VAL:HG13	2.00	0.43
2:M:498:GLN:O	2:M:532:MET:SD	2.76	0.43
2:M:636:ALA:HB2	2:M:703:ILE:CG2	2.47	0.43
2:M:717:LEU:HB3	9:M:9709:HOH:O	2.17	0.43
3:N:1267:ARG:HH11	3:N:1267:ARG:CB	2.31	0.43
3:N:1285:GLU:HG2	3:N:1286:THR:N	2.33	0.43
3:N:1403:LEU:O	3:N:1407:LEU:HB2	2.19	0.43
3:N:475:LYS:HA	3:N:478:LEU:HD12	2.01	0.43
3:N:493:ARG:HG3	3:N:494:LYS:N	2.33	0.43
3:N:546:ARG:HA	9:N:9938:HOH:O	2.19	0.43
3:N:60:CYS:HA	9:N:9716:HOH:O	2.18	0.43
3:N:87:ARG:HG3	3:N:88:TYR:CD2	2.53	0.43
5:P:361:LEU:HD13	5:P:366:ALA:CB	2.49	0.43
5:P:398:ARG:NH1	9:P:5295:HOH:O	2.52	0.43
1:A:49:PRO:O	1:A:173:PRO:HG3	2.18	0.43
2:C:474:VAL:HG13	2:C:530:GLU:O	2.19	0.43
2:C:585:GLU:HB2	9:C:9822:HOH:O	2.19	0.43
3:D:1098:LEU:N	3:D:1098:LEU:HD12	2.33	0.43
3:D:1087:ARG:CG	3:D:1234:THR:HA	2.47	0.43
3:D:119:SER:CB	3:D:123:LEU:H	2.27	0.43
3:D:1366:LYS:O	3:D:1369:GLU:HB2	2.18	0.43
3:D:1468:LEU:HD22	3:D:1470:ARG:CB	2.43	0.43
3:D:178:LEU:CD1	3:D:200:ASP:H	2.32	0.43
3:D:498:VAL:HG12	9:D:2771:HOH:O	2.19	0.43
3:D:501:ALA:HA	3:D:504:ASP:HB2	2.00	0.43
2:C:1033:GLY:HA2	3:D:619:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:805:GLU:O	3:D:805:GLU:OE1	2.37	0.43
3:D:838:ARG:HD3	3:D:874:GLU:HB3	1.99	0.43
3:D:925:GLU:HA	9:D:9640:HOH:O	2.18	0.43
3:D:984:THR:HG22	3:D:987:GLU:CD	2.39	0.43
4:E:58:PRO:HB2	9:E:9513:HOH:O	2.19	0.43
5:F:243:ILE:O	5:F:247:ILE:HG13	2.19	0.43
5:F:366:ALA:HB3	5:F:367:MET:CE	2.48	0.43
5:F:400:ILE:HG23	9:F:9566:HOH:O	2.19	0.43
1:K:32:PHE:HZ	1:L:47:SER:HG	1.65	0.43
2:M:1007:ALA:HB2	3:N:648:MET:HE2	2.00	0.43
2:M:232:GLU:O	2:M:235:LEU:HB2	2.18	0.43
2:M:289:THR:O	2:M:291:ALA:N	2.52	0.43
2:M:110:GLU:CG	2:M:369:PRO:HG3	2.49	0.43
2:M:413:LEU:N	2:M:413:LEU:HD12	2.33	0.43
2:M:139:GLN:CG	2:M:418:LEU:HD22	2.48	0.43
2:M:431:HIS:CD2	2:M:433:THR:H	2.36	0.43
2:M:933:GLY:HA2	9:M:9651:HOH:O	2.17	0.43
3:N:216:VAL:O	3:N:217:LYS:O	2.36	0.43
3:N:440:VAL:HG12	3:N:441:ARG:N	2.34	0.43
3:N:519:VAL:HG13	3:N:544:TYR:CE1	2.53	0.43
3:N:637:LEU:HD12	3:N:641:GLN:OE1	2.18	0.43
3:N:907:GLU:OE1	3:N:909:ASN:HB2	2.18	0.43
3:N:911:LEU:O	3:N:915:VAL:HG23	2.18	0.43
5:P:163:LEU:HB3	5:P:174:LEU:HD11	2.00	0.43
5:P:214:GLN:HA	5:P:214:GLN:OE1	2.19	0.43
5:P:324:GLU:HB3	9:P:6625:HOH:O	2.19	0.43
1:A:93:SER:HB2	9:A:9647:HOH:O	2.19	0.43
1:B:102:LYS:HZ1	1:B:137:ARG:NH2	2.17	0.43
1:B:111:ALA:HB3	1:B:124:ASN:O	2.19	0.43
2:C:121:MET:HA	2:C:127:PHE:CD2	2.54	0.43
2:C:193:LEU:HD11	9:C:9698:HOH:O	2.18	0.43
2:C:199:VAL:HG13	2:C:235:LEU:HD21	1.99	0.43
2:C:22:GLN:NE2	2:C:336:VAL:HG21	2.34	0.43
2:C:139:GLN:HA	2:C:411:SER:O	2.18	0.43
2:C:52:PHE:O	2:C:54:ILE:N	2.52	0.43
2:C:546:LEU:HD21	2:C:587:VAL:CG2	2.46	0.43
2:C:549:PHE:HB3	2:C:552:HIS:CD2	2.54	0.43
3:D:1209:LEU:HD22	3:D:1211:MET:CG	2.47	0.43
3:D:1472:ILE:HG22	3:D:1474:ALA:O	2.18	0.43
3:D:441:ARG:O	3:D:443:VAL:HG23	2.19	0.43
3:D:473:LEU:HD21	3:D:495:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:58:CYS:SG	3:D:60:CYS:N	2.92	0.43
3:D:420:VAL:HA	5:F:164:LYS:HZ1	1.83	0.43
5:F:358:LEU:HD23	9:F:9758:HOH:O	2.19	0.43
2:M:242:LEU:HB3	9:M:2128:HOH:O	2.18	0.43
2:M:29:ALA:HB3	2:M:30:LEU:HD12	2.00	0.43
2:M:309:TYR:HD2	9:M:9616:HOH:O	2.02	0.43
2:M:640:ARG:HG2	2:M:640:ARG:HH11	1.84	0.43
2:M:778:PHE:HE1	9:P:3891:HOH:O	2.02	0.43
2:M:877:PRO:HB3	3:N:1020:LEU:CD1	2.49	0.43
3:N:1293:PHE:CE2	3:N:1302:GLU:HB2	2.54	0.43
3:N:1336:LEU:CD1	3:N:1341:PRO:HG3	2.48	0.43
3:N:1397:LYS:O	3:N:1400:VAL:HB	2.18	0.43
3:N:1412:LYS:C	3:N:1414:PRO:HD3	2.38	0.43
2:M:1118:LYS:HB3	3:N:23:TYR:CE1	2.54	0.43
3:N:552:ASN:HA	3:N:555:LYS:HE3	2.01	0.43
2:M:1007:ALA:HB1	3:N:652:LEU:HD13	2.01	0.43
3:N:682:ASP:HB2	9:N:9692:HOH:O	2.18	0.43
3:N:699:VAL:HG12	3:N:717:GLN:CA	2.46	0.43
3:N:699:VAL:H	3:N:756:GLN:HE21	1.62	0.43
3:N:822:ALA:HB2	9:N:2411:HOH:O	2.18	0.43
3:N:827:ILE:HG23	3:N:837:GLY:HA2	2.01	0.43
3:N:950:GLY:O	3:N:951:ILE:C	2.56	0.43
4:O:72:ARG:HA	9:O:5993:HOH:O	2.18	0.43
5:P:126:LEU:O	5:P:130:VAL:HG23	2.19	0.43
5:P:350:LEU:HA	5:P:422:LEU:CD1	2.49	0.43
1:B:117:VAL:HG13	9:B:9600:HOH:O	2.18	0.43
2:C:102:HIS:HB2	2:C:106:GLY:O	2.19	0.43
2:C:94:LEU:HB3	2:C:118:ILE:HD11	2.01	0.43
2:C:474:VAL:O	2:C:474:VAL:HG22	2.19	0.43
2:C:724:ARG:CG	2:C:740:GLU:HA	2.49	0.43
3:D:1462:LEU:CD2	3:D:1473:PRO:HD2	2.45	0.43
1:K:26:GLU:HG3	1:K:184:THR:HG21	2.01	0.43
1:K:44:LEU:O	1:K:174:VAL:HG21	2.18	0.43
1:L:169:ALA:HB1	1:L:171:PHE:CD2	2.53	0.43
2:M:1092:LEU:HD22	2:M:1099:VAL:CG2	2.49	0.43
2:M:139:GLN:HE21	2:M:334:ARG:NH1	2.11	0.43
2:M:211:LEU:CD1	2:M:308:ARG:HG3	2.49	0.43
2:M:310:LEU:O	2:M:314:THR:HG23	2.19	0.43
2:M:704:HIS:C	2:M:705:ILE:HG13	2.38	0.43
2:M:807:ARG:HH11	2:M:807:ARG:HB2	1.83	0.43
2:M:549:PHE:CZ	2:M:886:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:948:GLU:HG2	2:M:953:VAL:CG2	2.47	0.43
3:N:1120:VAL:HA	3:N:1121:PRO:HD3	1.82	0.43
3:N:1136:LYS:HE3	3:N:1139:ASP:OD2	2.19	0.43
3:N:1274:ILE:HG12	3:N:1334:GLN:CD	2.38	0.43
3:N:1353:GLN:HG2	3:N:1368:ILE:HD12	2.00	0.43
3:N:1390:LEU:HD11	9:N:9817:HOH:O	2.18	0.43
3:N:450:TYR:HB3	9:N:2011:HOH:O	2.19	0.43
3:N:575:GLN:O	3:N:576:GLU:C	2.57	0.43
3:N:630:VAL:HG12	3:N:631:ILE:N	2.33	0.43
3:N:703:ASN:HD22	3:N:713:ILE:HG13	1.84	0.43
3:N:833:GLU:HB2	9:N:2032:HOH:O	2.19	0.43
3:N:863:VAL:HG21	9:N:2211:HOH:O	2.18	0.43
5:P:134:LYS:HD3	5:P:134:LYS:HA	1.87	0.43
5:P:337:HIS:H	5:P:337:HIS:HD2	1.66	0.43
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.40	0.42
2:C:333:ILE:N	2:C:333:ILE:HD12	2.34	0.42
2:C:461:VAL:HB	9:C:9892:HOH:O	2.18	0.42
2:C:501:THR:HG22	2:C:513:VAL:HG22	2.01	0.42
2:C:897:LEU:CD1	2:C:921:ALA:HA	2.48	0.42
2:C:927:GLY:HA2	2:C:930:LYS:HE3	1.99	0.42
3:D:107:ASP:O	3:D:108:VAL:C	2.56	0.42
3:D:1123:PHE:HB2	9:D:2629:HOH:O	2.18	0.42
3:D:1152:GLU:HG3	3:D:1159:ARG:HH12	1.84	0.42
3:D:1281:VAL:HG21	3:D:1313:VAL:CG2	2.49	0.42
3:D:1406:ARG:HG3	3:D:1412:LYS:HG3	2.01	0.42
3:D:1429:LEU:HG	3:D:1441:GLN:OE1	2.18	0.42
3:D:1431:THR:HG21	9:D:9674:HOH:O	2.18	0.42
3:D:170:PRO:HA	9:D:2060:HOH:O	2.19	0.42
3:D:62:LYS:HE2	3:D:75:ARG:HH12	1.84	0.42
3:D:770:LEU:HD23	3:D:777:PRO:HA	2.00	0.42
3:D:916:TYR:CE2	3:D:920:LEU:HD13	2.52	0.42
5:F:204:GLY:HA2	9:F:9554:HOH:O	2.19	0.42
3:D:675:ARG:HH22	5:F:420:ASP:HA	1.84	0.42
1:L:41:ARG:HE	1:L:45:LEU:HD11	1.84	0.42
2:M:1005:MET:HE2	3:N:648:MET:HB2	2.01	0.42
2:M:164:PRO:HD2	2:M:170:PRO:O	2.19	0.42
2:M:253:ALA:O	2:M:256:TYR:HB2	2.19	0.42
2:M:486:MET:CE	2:M:491:GLU:HA	2.49	0.42
2:M:624:PRO:HB3	9:M:9892:HOH:O	2.19	0.42
2:M:557:ARG:HH12	2:M:879:ARG:NH1	2.17	0.42
2:M:95:TYR:N	2:M:95:TYR:CD1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:565:GLN:HG2	2:M:995:MET:CE	2.49	0.42
3:N:100:ALA:HB2	9:N:9680:HOH:O	2.19	0.42
3:N:1482:ARG:HB2	3:N:1483:PHE:CE1	2.53	0.42
3:N:172:PRO:HA	3:N:173:PRO:HD3	1.63	0.42
3:N:749:VAL:HA	3:N:750:PRO:HD3	1.87	0.42
5:P:292:ALA:HB2	9:P:3676:HOH:O	2.18	0.42
1:B:165:ILE:O	1:B:165:ILE:HG13	2.19	0.42
1:B:79:ILE:HG13	1:B:80:LEU:N	2.33	0.42
2:C:1085:PHE:CE1	2:C:1111:ILE:HG21	2.54	0.42
2:C:48:PHE:HA	2:C:348:LEU:HD22	2.01	0.42
2:C:395:LYS:H	2:C:632:ASN:ND2	2.17	0.42
2:C:674:VAL:HB	2:C:869:VAL:CG1	2.49	0.42
2:C:689:VAL:O	2:C:869:VAL:HG23	2.19	0.42
2:C:813:VAL:HG13	9:C:9710:HOH:O	2.19	0.42
2:C:876:VAL:HB	3:D:949:ILE:HG13	2.01	0.42
2:C:890:LEU:HD21	2:C:901:TYR:CD1	2.53	0.42
2:C:89:THR:O	2:C:89:THR:HG23	2.19	0.42
2:C:95:TYR:CD1	2:C:95:TYR:N	2.87	0.42
3:D:1378:TYR:CD1	3:D:1378:TYR:N	2.87	0.42
3:D:1381:VAL:HG11	9:D:2302:HOH:O	2.19	0.42
3:D:173:PRO:HB3	9:D:2093:HOH:O	2.19	0.42
3:D:704:ARG:HH11	3:D:738:ALA:HB2	1.83	0.42
2:C:1045:ALA:HB2	3:D:763:MET:SD	2.59	0.42
3:D:953:ASP:O	3:D:955:VAL:HG23	2.18	0.42
1:K:115:LEU:HB3	9:K:4284:HOH:O	2.19	0.42
1:L:44:LEU:O	1:L:174:VAL:HG21	2.19	0.42
1:L:23:PHE:O	1:L:196:THR:HA	2.19	0.42
2:M:165:LEU:HA	2:M:166:PRO:O	2.20	0.42
2:M:165:LEU:HD12	2:M:165:LEU:HA	1.89	0.42
3:N:1047:LYS:HB3	3:N:1048:PRO:HD2	1.99	0.42
3:N:1133:ARG:HB2	9:N:2201:HOH:O	2.19	0.42
3:N:176:ASP:HB3	9:N:9934:HOH:O	2.18	0.42
3:N:191:LEU:HB2	3:N:211:VAL:CG2	2.49	0.42
3:N:46:ASP:HB3	3:N:49:ILE:HD12	2.01	0.42
3:N:474:GLU:HG3	3:N:496:LEU:HD11	2.00	0.42
2:M:1009:SER:OG	3:N:655:PRO:HD3	2.19	0.42
2:M:1043:TYR:CE2	3:N:763:MET:HA	2.54	0.42
5:P:191:ASN:HA	9:P:3565:HOH:O	2.18	0.42
5:P:267:THR:O	5:P:271:LEU:HD12	2.19	0.42
5:P:278:LEU:CB	5:P:286:PRO:HG2	2.48	0.42
5:P:402:ASN:O	5:P:406:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD13	9:A:9621:HOH:O	2.18	0.42
1:A:83:LYS:HE2	1:A:167:VAL:HG12	2.00	0.42
2:C:1060:ILE:HG23	2:C:1061:GLU:HG3	2.01	0.42
2:C:1092:LEU:HD22	2:C:1099:VAL:CG2	2.50	0.42
2:C:196:LEU:HB2	9:C:2392:HOH:O	2.19	0.42
2:C:322:VAL:HG13	9:C:2040:HOH:O	2.20	0.42
2:C:334:ARG:O	2:C:339:LEU:HD11	2.19	0.42
2:C:340:MET:HE3	2:C:341:THR:N	2.34	0.42
2:C:405:ARG:HA	2:C:408:ARG:CG	2.49	0.42
2:C:41:ASN:HA	2:C:45:GLN:OE1	2.19	0.42
2:C:51:THR:HB	2:C:348:LEU:HD23	2.01	0.42
2:C:571:LEU:HD22	2:C:571:LEU:H	1.84	0.42
3:D:1008:PHE:HB3	9:D:9863:HOH:O	2.20	0.42
3:D:1243:THR:HB	3:D:1253:THR:HG22	2.00	0.42
3:D:174:GLY:HA3	9:D:9618:HOH:O	2.19	0.42
3:D:452:ILE:CG2	9:D:9938:HOH:O	2.66	0.42
3:D:555:LYS:HD3	9:D:2656:HOH:O	2.19	0.42
3:D:574:LEU:O	3:D:578:VAL:HG23	2.18	0.42
4:E:37:ASN:HD22	4:E:89:MET:HE3	1.84	0.42
5:F:139:ALA:HB1	5:F:152:ASP:HB3	2.02	0.42
3:D:553:ARG:HH22	5:F:211:ASP:CG	2.23	0.42
2:M:101:ILE:HG22	2:M:102:HIS:H	1.84	0.42
2:M:154:ARG:HE	2:M:154:ARG:HB3	1.58	0.42
2:M:191:PHE:CD2	2:M:195:LEU:HD23	2.54	0.42
2:M:142:ARG:HH12	2:M:325:ILE:HG12	1.83	0.42
2:M:439:CYS:HB2	2:M:541:SER:HB2	2.00	0.42
2:M:508:ILE:HG22	9:M:9646:HOH:O	2.18	0.42
2:M:724:ARG:HB2	9:M:9783:HOH:O	2.20	0.42
2:M:816:LYS:HB2	2:M:819:VAL:CG2	2.48	0.42
3:N:1018:ASN:HB3	3:N:1021:TYR:CB	2.48	0.42
3:N:1020:LEU:HA	3:N:1023:MET:HE2	2.02	0.42
3:N:1033:GLN:NE2	3:N:1036:ARG:HD3	2.32	0.42
3:N:1390:LEU:HD11	9:N:2607:HOH:O	2.19	0.42
3:N:1399:ASP:O	3:N:1403:LEU:HD12	2.20	0.42
3:N:1491:THR:HG23	9:O:3910:HOH:O	2.19	0.42
3:N:417:PRO:O	5:P:168:LYS:HE3	2.20	0.42
3:N:567:ILE:HG13	3:N:567:ILE:H	1.58	0.42
2:M:1044:GLY:N	3:N:762:GLN:OE1	2.52	0.42
3:N:824:ASN:HA	3:N:824:ASN:HD22	1.59	0.42
3:N:90:MET:HE3	3:N:518:PRO:HB3	2.01	0.42
1:A:143:ARG:HG2	9:A:9755:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LYS:HE3	9:B:9561:HOH:O	2.18	0.42
2:C:1038:TRP:HB3	3:D:1223:ILE:HG21	2.02	0.42
2:C:226:VAL:HG12	9:C:9620:HOH:O	2.19	0.42
2:C:367:LEU:HB3	2:C:371:LYS:HG2	2.01	0.42
2:C:626:ARG:CB	2:C:639:GLN:HE21	2.32	0.42
2:C:578:VAL:HG13	2:C:671:ASN:OD1	2.20	0.42
2:C:836:GLY:HA2	3:D:725:SER:OG	2.19	0.42
3:D:1109:GLU:CG	3:D:1202:GLN:H	2.33	0.42
3:D:455:ARG:HG3	9:D:9918:HOH:O	2.18	0.42
3:D:566:ILE:HD13	5:F:217:ASN:HB3	2.02	0.42
3:D:576:GLU:HA	3:D:579:ASP:OD2	2.20	0.42
3:D:864:VAL:HA	9:D:9946:HOH:O	2.19	0.42
2:C:1083:GLU:CD	3:D:88:TYR:HH	2.23	0.42
9:D:9642:HOH:O	4:E:48:MET:HE2	2.18	0.42
4:E:54:LEU:HB3	9:E:9537:HOH:O	2.19	0.42
5:F:128:ARG:HA	9:F:9837:HOH:O	2.19	0.42
5:F:421:PHE:C	5:F:423:ASP:N	2.71	0.42
1:K:209:GLU:O	1:K:213:GLN:HG3	2.20	0.42
1:L:112:ARG:HH11	1:L:112:ARG:HB3	1.85	0.42
2:M:1000:MET:SD	2:M:1001:VAL:N	2.87	0.42
2:M:1008:ARG:HH21	2:M:1028:GLY:HA2	1.83	0.42
2:M:274:ARG:HB2	2:M:285:LEU:CD1	2.49	0.42
2:M:330:ASN:O	2:M:331:ARG:C	2.57	0.42
2:M:350:ARG:HB3	9:M:9765:HOH:O	2.19	0.42
2:M:958:THR:HG23	2:M:961:GLU:CG	2.49	0.42
3:N:1409:ALA:HB1	9:N:2070:HOH:O	2.19	0.42
3:N:416:ALA:HA	3:N:442:ASN:HD22	1.83	0.42
3:N:18:ILE:HD12	3:N:518:PRO:CG	2.49	0.42
3:N:660:LYS:HA	3:N:663:GLU:OE2	2.19	0.42
3:N:789:LEU:HD13	9:N:9875:HOH:O	2.19	0.42
3:N:794:GLN:HB3	3:N:794:GLN:HE21	1.66	0.42
3:N:80:VAL:HG13	9:N:9871:HOH:O	2.19	0.42
2:C:165:LEU:HA	2:C:166:PRO:O	2.20	0.42
2:C:313:LEU:HD13	2:C:321:GLU:HB2	2.00	0.42
2:C:925:TYR:C	2:C:925:TYR:CD1	2.93	0.42
1:A:30:ARG:HD2	2:C:938:LYS:NZ	2.34	0.42
3:D:1123:PHE:HD1	3:D:1133:ARG:O	2.02	0.42
3:D:1432:LYS:HD2	3:D:1433:SER:N	2.34	0.42
3:D:10:ILE:CD1	3:D:1434:TRP:NE1	2.83	0.42
3:D:674:ARG:HG2	3:D:674:ARG:HH11	1.85	0.42
3:D:796:ARG:O	3:D:828:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:827:ILE:HG23	3:D:837:GLY:HA2	2.02	0.42
3:D:853:VAL:HA	3:D:858:VAL:O	2.20	0.42
3:D:844:ALA:HA	3:D:867:ARG:NH1	2.35	0.42
5:F:202:TYR:OH	5:F:244:ARG:HD2	2.19	0.42
5:F:319:THR:HG23	9:F:9846:HOH:O	2.19	0.42
1:K:143:ARG:HG3	1:K:144:VAL:N	2.34	0.42
1:L:12:THR:OG1	1:L:24:VAL:HB	2.19	0.42
1:L:143:ARG:HG3	9:L:4737:HOH:O	2.19	0.42
2:M:1012:PRO:HD2	2:M:1021:LEU:O	2.18	0.42
2:M:1068:GLU:OE1	5:P:345:ALA:HA	2.19	0.42
2:M:409:ARG:HA	2:M:454:SER:CA	2.35	0.42
2:M:405:ARG:HD3	2:M:543:ASN:CG	2.39	0.42
2:M:589:ARG:HD2	9:M:9978:HOH:O	2.19	0.42
2:M:4:LYS:HE3	2:M:6:PHE:HE2	1.84	0.42
2:M:821:GLU:HG3	9:M:2312:HOH:O	2.20	0.42
2:M:756:VAL:HG21	2:M:823:VAL:CG1	2.49	0.42
2:M:969:GLN:HB3	2:M:969:GLN:HE21	1.66	0.42
3:N:1123:PHE:HA	3:N:1135:ARG:N	2.35	0.42
3:N:171:LEU:HB2	3:N:390:PRO:CA	2.49	0.42
3:N:432:TYR:HA	3:N:448:GLU:O	2.18	0.42
3:N:591:VAL:HG12	3:N:592:THR:O	2.19	0.42
5:P:277:GLN:O	5:P:280:GLN:HB3	2.18	0.42
9:M:9906:HOH:O	5:P:354:LEU:HD13	2.20	0.42
5:P:93:LEU:HB2	9:P:4152:HOH:O	2.18	0.42
2:C:390:GLN:O	7:C:8001:RBT:H142	2.20	0.42
2:C:397:GLU:HB3	2:C:631:SER:HB2	2.02	0.42
2:C:519:GLY:O	3:D:1053:PHE:HE2	2.02	0.42
2:C:575:GLN:C	2:C:667:ALA:HB1	2.39	0.42
2:C:721:ARG:HH11	2:C:721:ARG:HG3	1.85	0.42
2:C:831:ARG:HG2	2:C:831:ARG:NH1	2.32	0.42
2:C:565:GLN:HG2	2:C:995:MET:CE	2.50	0.42
3:D:1197:ARG:HG3	3:D:1198:TYR:H	1.84	0.42
3:D:1286:THR:HB	9:D:2814:HOH:O	2.19	0.42
3:D:1434:TRP:CZ3	3:D:1455:LYS:HB3	2.54	0.42
3:D:154:THR:HG22	3:D:157:GLU:OE2	2.20	0.42
3:D:528:VAL:HG13	9:D:2844:HOH:O	2.18	0.42
3:D:894:LYS:HD2	9:D:2034:HOH:O	2.20	0.42
4:E:49:GLN:HA	4:E:51:LEU:O	2.20	0.42
4:E:93:TYR:HA	4:E:94:PRO:HD3	1.78	0.42
5:F:328:PHE:HD2	5:F:328:PHE:HA	1.72	0.42
2:M:139:GLN:CG	2:M:140:ILE:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:195:LEU:HD12	9:M:2147:HOH:O	2.18	0.42
2:M:19:THR:HG22	2:M:19:THR:O	2.19	0.42
2:M:325:ILE:HG22	2:M:331:ARG:HG3	2.02	0.42
2:M:432:ARG:CD	2:M:519:GLY:HA3	2.47	0.42
2:M:722:ILE:HD11	2:M:756:VAL:CG1	2.50	0.42
3:N:1209:LEU:HG	3:N:1219:GLU:OE2	2.19	0.42
3:N:1435:LEU:HB2	3:N:1457:ASP:OD2	2.19	0.42
3:N:404:GLU:HB3	3:N:414:ARG:CD	2.49	0.42
3:N:412:GLY:O	3:N:421:LEU:HB3	2.19	0.42
3:N:421:LEU:O	3:N:421:LEU:HD23	2.20	0.42
3:N:543:LEU:HD21	3:N:600:LEU:HD13	2.01	0.42
3:N:639:LEU:N	3:N:729:HIS:CD2	2.87	0.42
2:M:1083:GLU:OE2	3:N:87:ARG:NH1	2.52	0.42
1:B:25:LEU:HD23	1:B:28:LEU:HD21	2.01	0.42
1:B:61:VAL:HG11	1:B:75:VAL:HG21	2.01	0.42
1:B:83:LYS:HE3	1:B:167:VAL:CG1	2.50	0.42
2:C:129:ILE:HB	2:C:134:ARG:HG3	2.02	0.42
2:C:162:ILE:HB	2:C:172:ILE:HD13	2.01	0.42
2:C:313:LEU:CB	2:C:321:GLU:HG3	2.50	0.42
2:C:328:LEU:HB2	2:C:488:ALA:CB	2.46	0.42
2:C:328:LEU:HB2	2:C:433:THR:HG21	2.02	0.42
2:C:61:LYS:HD3	9:C:2241:HOH:O	2.19	0.42
2:C:704:HIS:CD2	2:C:705:ILE:H	2.36	0.42
2:C:724:ARG:HG3	2:C:740:GLU:HA	2.00	0.42
2:C:876:VAL:O	2:C:879:ARG:O	2.38	0.42
2:C:554:ASP:HB2	2:C:880:MET:O	2.20	0.42
2:C:881:ASN:HD22	2:C:881:ASN:N	2.12	0.42
3:D:1057:VAL:HA	3:D:1069:GLU:HG2	2.02	0.42
3:D:16:GLU:HA	9:D:9854:HOH:O	2.18	0.42
3:D:435:VAL:HG22	3:D:446:VAL:HG13	2.01	0.42
3:D:724:GLN:HG3	3:D:725:SER:N	2.35	0.42
4:E:29:GLN:HB2	4:E:33:HIS:CD2	2.55	0.42
5:F:153:PRO:CG	5:F:154:LYS:H	2.33	0.42
2:M:318:PRO:HB3	9:M:2297:HOH:O	2.19	0.42
2:M:331:ARG:HD2	9:M:2020:HOH:O	2.19	0.42
2:M:362:GLY:HA3	2:M:367:LEU:CD2	2.44	0.42
2:M:100:LEU:CD2	2:M:368:THR:HA	2.46	0.42
2:M:380:ALA:CA	2:M:383:ARG:HG2	2.50	0.42
2:M:414:GLY:C	2:M:416:GLY:H	2.23	0.42
2:M:772:ARG:NH1	2:M:772:ARG:HB2	2.34	0.42
3:N:1262:LEU:HD11	3:N:1351:GLU:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:152:LEU:N	3:N:152:LEU:CD2	2.82	0.42
3:N:507:ASN:HA	9:N:9633:HOH:O	2.19	0.42
3:N:93:ILE:CD1	3:N:548:ILE:HD11	2.49	0.42
3:N:574:LEU:O	3:N:577:ALA:HB3	2.19	0.42
3:N:625:TYR:N	3:N:625:TYR:CD1	2.87	0.42
3:N:633:VAL:C	3:N:635:PRO:HD3	2.40	0.42
4:O:18:ARG:O	4:O:22:VAL:HG23	2.19	0.42
5:P:132:ARG:HD3	5:P:181:GLU:OE1	2.20	0.42
3:N:573:MET:CE	5:P:210:LEU:HD22	2.50	0.42
5:P:77:THR:O	5:P:81:VAL:HG23	2.19	0.42
1:B:205:VAL:HG12	9:B:9565:HOH:O	2.19	0.42
2:C:176:VAL:O	2:C:178:PRO:HD3	2.19	0.42
2:C:188:LYS:HG3	9:C:2493:HOH:O	2.19	0.42
2:C:25:SER:OG	2:C:337:GLY:N	2.52	0.42
2:C:265:ARG:HB2	9:C:9833:HOH:O	2.20	0.42
2:C:48:PHE:O	2:C:52:PHE:HB2	2.20	0.42
2:C:674:VAL:O	2:C:989:VAL:HA	2.20	0.42
2:C:686:ASP:OD2	2:C:879:ARG:NH2	2.53	0.42
2:C:713:ARG:HG3	2:C:713:ARG:NH1	2.35	0.42
2:C:78:PHE:CB	2:C:88:LEU:HD21	2.49	0.42
3:D:953:ASP:OD1	3:D:1019:PRO:HG2	2.20	0.42
3:D:124:GLU:HG2	3:D:128:TYR:CE1	2.55	0.42
3:D:1290:LEU:HD22	3:D:1291:SER:H	1.83	0.42
3:D:1382:THR:CG2	3:D:1418:LYS:HE3	2.49	0.42
3:D:159:ARG:HB2	3:D:159:ARG:NH1	2.35	0.42
3:D:412:GLY:O	3:D:421:LEU:HB3	2.20	0.42
3:D:444:VAL:HG22	3:D:444:VAL:O	2.19	0.42
3:D:448:GLU:HG3	9:D:9766:HOH:O	2.19	0.42
3:D:23:TYR:O	3:D:49:ILE:HG23	2.20	0.42
1:K:9:PRO:HB3	1:K:25:LEU:CG	2.49	0.42
1:L:101:LEU:HD12	1:L:114:PHE:CE1	2.55	0.42
1:L:165:ILE:HA	1:L:166:PRO:HD3	1.94	0.42
2:M:1091:GLU:O	2:M:1094:ALA:HB3	2.19	0.42
2:M:172:ILE:HA	2:M:185:LYS:O	2.19	0.42
2:M:222:MET:H	2:M:222:MET:HG2	1.64	0.42
2:M:27:ARG:HG3	2:M:27:ARG:HH11	1.85	0.42
2:M:321:GLU:CB	9:M:9616:HOH:O	2.68	0.42
2:M:136:ILE:HB	2:M:336:VAL:HG13	2.01	0.42
2:M:433:THR:CG2	2:M:488:ALA:HB1	2.49	0.42
2:M:582:GLY:N	9:M:2487:HOH:O	2.53	0.42
2:M:605:LYS:HD3	2:M:610:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:64:LEU:HD12	9:M:9772:HOH:O	2.19	0.42
2:M:578:VAL:HG13	2:M:671:ASN:OD1	2.20	0.42
2:M:73:LEU:HD22	2:M:118:ILE:HD11	2.01	0.42
2:M:794:PRO:HB2	2:M:1027:PHE:CE2	2.54	0.42
3:N:1378:TYR:CE2	3:N:1394:VAL:HG22	2.54	0.42
3:N:42:ASP:O	3:N:46:ASP:HB2	2.20	0.42
3:N:893:GLU:O	3:N:896:ALA:HB3	2.19	0.42
3:N:948:THR:O	3:N:1019:PRO:HG2	2.19	0.42
5:P:262:VAL:O	5:P:265:VAL:HB	2.20	0.42
5:P:358:LEU:HD11	5:P:370:LYS:CD	2.50	0.42
1:A:98:THR:HG22	1:A:100:LEU:CD1	2.50	0.42
1:B:2:LEU:HA	1:B:6:LEU:HD22	2.01	0.42
2:C:1019:GLN:HB3	2:C:1019:GLN:HE21	1.63	0.42
2:C:1054:THR:HG23	2:C:1059:ASP:HB2	2.00	0.42
2:C:138:SER:HB2	2:C:410:ILE:HG13	2.02	0.42
2:C:274:ARG:HB2	2:C:285:LEU:HD12	2.01	0.42
2:C:29:ALA:HB2	2:C:337:GLY:HA2	2.00	0.42
2:C:390:GLN:NE2	7:C:8001:RBT:H131	2.35	0.42
2:C:584:GLU:H	2:C:584:GLU:CD	2.23	0.42
1:A:72:LYS:O	2:C:608:GLY:CA	2.68	0.42
2:C:707:ARG:NH2	2:C:824:ARG:NH1	2.68	0.42
2:C:760:SER:O	2:C:785:VAL:HG22	2.18	0.42
2:C:924:VAL:HG21	9:C:9996:HOH:O	2.19	0.42
3:D:1211:MET:HE1	3:D:1216:SER:OG	2.20	0.42
3:D:210:ARG:NH1	9:D:9792:HOH:O	2.52	0.42
3:D:214:GLU:OE2	3:D:390:PRO:HB2	2.20	0.42
3:D:646:LYS:HE2	3:D:722:GLU:OE2	2.19	0.42
3:D:795:VAL:HG12	3:D:796:ARG:N	2.34	0.42
3:D:866:VAL:HG12	3:D:867:ARG:N	2.34	0.42
3:D:9:ARG:HG2	3:D:9:ARG:O	2.20	0.42
5:F:163:LEU:HD13	5:F:174:LEU:HD21	2.02	0.42
5:F:282:LEU:HB2	5:F:284:ARG:H	1.85	0.42
5:F:302:LYS:HE3	9:F:9749:HOH:O	2.20	0.42
5:F:366:ALA:HB1	9:F:9610:HOH:O	2.19	0.42
5:F:408:LEU:HD22	9:F:9858:HOH:O	2.19	0.42
1:K:219:ARG:HB2	1:K:219:ARG:HH11	1.84	0.42
1:K:2:LEU:O	1:K:6:LEU:HB3	2.20	0.42
2:M:1115:LEU:HD12	2:M:1115:LEU:H	1.80	0.42
2:M:167:LYS:HD3	2:M:167:LYS:C	2.40	0.42
2:M:174:LEU:HD22	2:M:193:LEU:HG	2.01	0.42
2:M:191:PHE:CE2	2:M:238:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:219:GLN:HB3	9:M:2554:HOH:O	2.19	0.42
2:M:479:VAL:HG22	2:M:508:ILE:CD1	2.49	0.42
2:M:699:PHE:HD1	9:M:2289:HOH:O	2.02	0.42
2:M:783:ARG:HG2	2:M:785:VAL:HG12	2.02	0.42
2:M:835:VAL:HA	2:M:849:VAL:HG12	2.02	0.42
3:N:1074:SER:O	3:N:1077:ALA:HB3	2.19	0.42
3:N:1083:ASP:O	3:N:1087:ARG:HD3	2.20	0.42
3:N:23:TYR:HB2	3:N:49:ILE:O	2.19	0.42
3:N:426:LYS:HD2	3:N:428:LYS:HZ1	1.84	0.42
3:N:591:VAL:CG1	3:N:597:ASP:HA	2.50	0.42
3:N:826:PRO:HD2	3:N:829:VAL:HG22	2.01	0.42
3:N:826:PRO:HD3	9:N:2300:HOH:O	2.20	0.42
1:A:195:LEU:HD12	1:A:196:THR:N	2.35	0.42
1:A:70:GLY:O	1:A:132:LEU:HA	2.19	0.42
1:B:103:ALA:HB2	9:B:9543:HOH:O	2.20	0.42
1:B:23:PHE:CE1	1:B:208:LEU:HD22	2.55	0.42
2:C:243:ARG:HD2	9:C:2185:HOH:O	2.19	0.42
2:C:282:GLY:HA2	2:C:308:ARG:NH2	2.35	0.42
2:C:525:SER:OG	2:C:528:GLU:HG3	2.20	0.42
2:C:854:PRO:C	2:C:856:GLU:N	2.72	0.42
2:C:861:LEU:HD23	2:C:862:PRO:N	2.35	0.42
3:D:1063:GLU:HB3	9:D:9565:HOH:O	2.19	0.42
3:D:112:ILE:HB	9:D:2195:HOH:O	2.20	0.42
3:D:1264:GLU:CD	3:D:1425:THR:HG22	2.40	0.42
3:D:208:PRO:HB2	3:D:395:VAL:HG13	2.01	0.42
3:D:455:ARG:HG2	3:D:455:ARG:NH1	2.35	0.42
3:D:517:VAL:HG21	3:D:547:LEU:HD21	2.01	0.42
3:D:519:VAL:HA	3:D:544:TYR:CZ	2.54	0.42
3:D:528:VAL:HG23	3:D:536:ALA:O	2.20	0.42
3:D:679:ARG:HD2	9:D:9589:HOH:O	2.20	0.42
3:D:52:PRO:HG3	3:D:78:VAL:HG13	2.01	0.42
3:D:806:PHE:O	3:D:806:PHE:CD1	2.73	0.42
3:D:817:GLU:HG2	3:D:840:LYS:HZ1	1.85	0.42
3:D:898:GLU:HA	9:D:2157:HOH:O	2.19	0.42
3:D:770:LEU:HG	3:D:919:PHE:CE1	2.55	0.42
4:E:33:HIS:ND1	4:E:33:HIS:N	2.68	0.42
3:D:760:ARG:NH1	4:E:59:ASN:HD21	2.18	0.42
3:D:32:ILE:O	5:F:258:ILE:HD12	2.20	0.42
5:F:287:THR:HG23	5:F:289:GLU:H	1.84	0.42
1:K:128:HIS:HE1	1:K:131:THR:HG23	1.84	0.42
1:L:140:MET:HG2	1:L:142:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:143:ARG:HD3	9:L:6404:HOH:O	2.19	0.42
2:M:274:ARG:HB2	2:M:285:LEU:HD13	2.02	0.42
2:M:290:LEU:HB3	2:M:302:VAL:HG12	2.00	0.42
2:M:304:LEU:HG	2:M:305:PRO:N	2.35	0.42
2:M:352:ALA:C	2:M:355:VAL:HG12	2.40	0.42
2:M:435:TYR:N	9:M:9588:HOH:O	2.53	0.42
2:M:617:ASP:OD1	2:M:619:ARG:HB2	2.20	0.42
2:M:783:ARG:C	2:M:785:VAL:H	2.23	0.42
2:M:841:ASN:ND2	2:M:841:ASN:C	2.73	0.42
2:M:688:ILE:HD11	2:M:847:GLY:HA3	2.02	0.42
2:M:916:GLU:O	2:M:919:ALA:HB3	2.20	0.42
3:N:1005:GLN:HG2	9:N:9941:HOH:O	2.20	0.42
3:N:161:LEU:HD13	3:N:452:ILE:HD13	2.02	0.42
3:N:473:LEU:HD23	3:N:499:VAL:HG21	2.01	0.42
3:N:50:PHE:CB	3:N:522:PRO:HG2	2.50	0.42
3:N:719:VAL:HG22	9:N:9830:HOH:O	2.19	0.42
3:N:785:ILE:HG23	3:N:938:GLY:HA3	2.01	0.42
3:N:985:ASP:HB2	9:N:9696:HOH:O	2.20	0.42
1:A:79:ILE:HG13	1:A:80:LEU:N	2.34	0.41
1:B:14:ARG:NH2	1:B:24:VAL:HG21	2.35	0.41
2:C:108:ILE:HD13	2:C:365:ASP:O	2.19	0.41
2:C:260:LEU:HA	2:C:291:ALA:HB2	2.01	0.41
2:C:267:TYR:N	2:C:267:TYR:CD2	2.88	0.41
2:C:310:LEU:HD12	2:C:310:LEU:HA	1.86	0.41
2:C:366:SER:O	2:C:367:LEU:HD23	2.20	0.41
2:C:459:ALA:HB1	2:C:467:ILE:CG2	2.50	0.41
2:C:735:ARG:NH1	2:C:735:ARG:HG2	2.35	0.41
2:C:773:LEU:HD11	9:F:9748:HOH:O	2.19	0.41
2:C:979:THR:HG23	2:C:981:GLU:N	2.17	0.41
3:D:1283:ILE:HB	3:D:1315:ASP:OD2	2.20	0.41
3:D:131:LYS:HE2	3:D:568:ARG:HB2	2.01	0.41
3:D:1303:TYR:HD1	3:D:1325:LEU:HD23	1.85	0.41
3:D:897:TRP:CZ2	3:D:902:LEU:HD21	2.55	0.41
4:E:91:ARG:NE	9:E:9529:HOH:O	2.53	0.41
5:F:292:ALA:HB1	5:F:299:TRP:O	2.20	0.41
5:F:348:SER:OG	5:F:349:LEU:N	2.53	0.41
5:F:416:ARG:HD2	5:F:419:ARG:HB3	2.02	0.41
1:L:128:HIS:HB3	9:L:6378:HOH:O	2.20	0.41
1:L:30:ARG:NH1	1:L:30:ARG:HG2	2.34	0.41
2:M:191:PHE:CD2	2:M:195:LEU:HB3	2.55	0.41
2:M:194:VAL:HG21	2:M:221:LEU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:244:PRO:HD2	2:M:245:GLY:N	2.29	0.41
2:M:285:LEU:O	2:M:285:LEU:HD23	2.20	0.41
2:M:264:PRO:HB3	2:M:289:THR:CB	2.50	0.41
2:M:575:GLN:C	2:M:667:ALA:HB1	2.40	0.41
2:M:724:ARG:O	2:M:734:LEU:HD21	2.20	0.41
2:M:826:TYR:N	2:M:826:TYR:CD1	2.88	0.41
2:M:939:ARG:HB3	2:M:982:PRO:HG3	2.02	0.41
3:N:1008:PHE:O	3:N:1012:GLU:HB2	2.20	0.41
3:N:1185:GLU:HB2	9:N:9824:HOH:O	2.20	0.41
3:N:1478:SER:HG	3:N:1480:PHE:HB3	1.84	0.41
3:N:782:SER:O	3:N:786:ILE:HG13	2.20	0.41
3:N:894:LYS:O	3:N:898:GLU:HG3	2.20	0.41
5:P:194:LEU:O	5:P:198:ILE:HG13	2.20	0.41
1:A:221:HIS:HE1	9:B:9596:HOH:O	2.03	0.41
2:C:196:LEU:HD22	2:C:303:PHE:CZ	2.56	0.41
2:C:22:GLN:HE21	2:C:22:GLN:HB3	1.62	0.41
2:C:415:PRO:C	2:C:417:GLY:H	2.24	0.41
2:C:598:GLU:HB2	2:C:615:TYR:OH	2.20	0.41
2:C:668:LEU:HD12	2:C:668:LEU:H	1.85	0.41
2:C:684:PHE:HD2	3:D:740:PHE:HE1	1.67	0.41
2:C:707:ARG:N	9:C:2428:HOH:O	2.53	0.41
1:A:46:SER:HB3	2:C:856:GLU:HG2	2.00	0.41
2:C:8:ARG:NE	2:C:8:ARG:HA	2.34	0.41
3:D:1089:ALA:HA	9:D:2262:HOH:O	2.20	0.41
3:D:1168:MET:O	3:D:1168:MET:HE3	2.20	0.41
3:D:1462:LEU:HD13	3:D:1472:ILE:HG21	2.01	0.41
3:D:172:PRO:HB3	3:D:178:LEU:HB3	2.02	0.41
3:D:186:VAL:HG13	3:D:187:LYS:N	2.34	0.41
3:D:584:ASN:HA	9:D:2212:HOH:O	2.19	0.41
3:D:814:ALA:HB1	3:D:818:ARG:NH2	2.34	0.41
3:D:916:TYR:C	3:D:916:TYR:CD2	2.94	0.41
2:C:988:VAL:HG13	3:D:948:THR:OG1	2.21	0.41
5:F:110:MET:HB2	9:F:9606:HOH:O	2.20	0.41
1:K:20:TYR:HE2	1:K:198:ARG:HB3	1.85	0.41
1:K:89:PHE:HB2	1:K:94:LEU:HD13	2.01	0.41
2:M:103:LYS:HB2	9:M:9621:HOH:O	2.20	0.41
2:M:1059:ASP:OD2	2:M:1062:GLY:HA3	2.20	0.41
2:M:520:GLU:HA	2:M:521:PRO:HD3	1.91	0.41
2:M:15:LEU:CD2	2:M:583:LEU:HD21	2.50	0.41
3:N:1032:PRO:HD3	9:N:9814:HOH:O	2.20	0.41
3:N:133:ILE:HD13	3:N:456:MET:SD	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1488:ASP:OD1	3:N:1488:ASP:N	2.52	0.41
3:N:123:LEU:HG	3:N:152:LEU:CD1	2.50	0.41
3:N:208:PRO:CB	3:N:395:VAL:HG13	2.47	0.41
3:N:30:GLU:HB3	3:N:40:GLU:CG	2.50	0.41
3:N:135:LEU:HA	3:N:453:ASP:O	2.20	0.41
3:N:461:ILE:HD13	3:N:461:ILE:N	2.34	0.41
3:N:581:LEU:HG	3:N:582:LEU:N	2.34	0.41
3:N:63:TYR:HB3	3:N:68:PHE:CE1	2.55	0.41
3:N:785:ILE:HD12	3:N:785:ILE:N	2.35	0.41
3:N:806:PHE:O	3:N:807:ALA:C	2.58	0.41
3:N:880:ILE:O	3:N:883:ALA:HB3	2.20	0.41
4:O:16:LYS:HA	9:O:3678:HOH:O	2.20	0.41
1:B:102:LYS:HE3	1:B:139:ASN:HB2	2.01	0.41
2:C:1072:LYS:HB3	9:C:9787:HOH:O	2.20	0.41
2:C:334:ARG:HA	2:C:338:GLU:OE2	2.20	0.41
2:C:395:LYS:H	2:C:632:ASN:HD22	1.69	0.41
2:C:436:GLY:O	2:C:459:ALA:HB2	2.21	0.41
3:D:1048:PRO:HD2	9:D:2426:HOH:O	2.19	0.41
3:D:1167:SER:O	3:D:1171:VAL:HG23	2.19	0.41
3:D:1243:THR:CB	3:D:1253:THR:HB	2.50	0.41
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	2.20	0.41
3:D:134:VAL:O	3:D:134:VAL:HG23	2.20	0.41
3:D:1351:GLU:HA	3:D:1354:LYS:HG2	2.02	0.41
3:D:1468:LEU:HB3	3:D:1470:ARG:HB2	2.02	0.41
3:D:214:GLU:CD	3:D:390:PRO:HB2	2.40	0.41
3:D:179:VAL:HG22	3:D:389:GLU:CD	2.41	0.41
3:D:41:ARG:CD	3:D:42:ASP:H	2.26	0.41
3:D:458:ALA:HB1	9:D:2526:HOH:O	2.20	0.41
3:D:572:ARG:NH1	5:F:80:PRO:HD3	2.35	0.41
2:C:1087:VAL:HG11	3:D:613:ARG:HH21	1.84	0.41
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.45	0.41
3:D:789:LEU:HD22	3:D:882:PHE:CE1	2.56	0.41
5:F:113:ILE:HG12	9:F:9837:HOH:O	2.20	0.41
5:F:91:VAL:HG12	9:F:9932:HOH:O	2.19	0.41
1:K:100:LEU:CD2	1:K:141:GLU:HG2	2.50	0.41
1:K:154:GLU:H	1:K:154:GLU:CD	2.24	0.41
1:K:178:ALA:HB3	1:K:198:ARG:HD3	2.03	0.41
1:L:95:GLN:N	1:L:95:GLN:HE21	2.14	0.41
2:M:1090:LYS:HG2	2:M:1112:PHE:HZ	1.83	0.41
2:M:233:GLU:HB2	9:M:2176:HOH:O	2.20	0.41
2:M:459:ALA:HB1	2:M:467:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:524:VAL:HG22	2:M:528:GLU:HB2	2.03	0.41
2:M:405:ARG:HD3	2:M:543:ASN:CB	2.50	0.41
2:M:73:LEU:O	2:M:73:LEU:HD12	2.20	0.41
2:M:816:LYS:O	2:M:819:VAL:HB	2.20	0.41
3:N:1031:ASN:HA	9:N:9814:HOH:O	2.20	0.41
3:N:1031:ASN:HB3	3:N:1034:GLN:HB2	2.00	0.41
3:N:1122:LEU:O	3:N:1135:ARG:N	2.49	0.41
3:N:1399:ASP:O	3:N:1403:LEU:HB2	2.21	0.41
3:N:998:GLU:O	3:N:1002:LYS:HG3	2.19	0.41
1:A:47:SER:HG	1:B:32:PHE:HZ	1.66	0.41
1:B:178:ALA:C	1:B:197:LEU:HD12	2.40	0.41
2:C:172:ILE:HA	2:C:185:LYS:O	2.19	0.41
2:C:18:LEU:HD21	2:C:542:VAL:HG11	2.02	0.41
2:C:571:LEU:N	2:C:571:LEU:HD22	2.35	0.41
2:C:623:TYR:N	9:C:9615:HOH:O	2.53	0.41
2:C:780:GLU:HG3	2:C:781:LYS:H	1.85	0.41
2:C:97:ARG:HB3	9:C:9753:HOH:O	2.21	0.41
3:D:1014:ASN:O	3:D:1016:PRO:HD3	2.19	0.41
3:D:1089:ALA:HB2	9:D:9966:HOH:O	2.19	0.41
3:D:1253:THR:HG23	9:D:9622:HOH:O	2.18	0.41
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.86	0.41
3:D:36:THR:HB	3:D:38:LYS:CD	2.51	0.41
3:D:209:ARG:HB2	3:D:395:VAL:O	2.20	0.41
3:D:400:VAL:HG23	9:D:9594:HOH:O	2.21	0.41
3:D:553:ARG:NE	9:F:9685:HOH:O	2.53	0.41
3:D:661:MET:CE	3:D:677:LEU:HD11	2.51	0.41
3:D:815:ALA:HA	9:D:2515:HOH:O	2.20	0.41
1:K:181:VAL:HG12	2:M:938:LYS:NZ	2.35	0.41
1:K:71:VAL:HG21	1:K:138:LEU:HD23	2.02	0.41
1:L:151:VAL:HB	1:L:169:ALA:HB3	2.01	0.41
2:M:1002:GLU:HG3	2:M:1002:GLU:H	1.43	0.41
2:M:66:LEU:CD1	2:M:100:LEU:HB3	2.51	0.41
2:M:288:ARG:HB2	9:M:9837:HOH:O	2.20	0.41
2:M:460:ARG:HB3	2:M:460:ARG:HH11	1.85	0.41
2:M:577:PRO:HD2	2:M:580:MET:HG2	2.02	0.41
2:M:68:PHE:HB3	9:M:2228:HOH:O	2.19	0.41
2:M:862:PRO:HG3	2:M:975:TYR:HE1	1.85	0.41
3:N:1312:LEU:HB3	9:N:2390:HOH:O	2.20	0.41
3:N:1466:VAL:HG23	3:N:1472:ILE:CD1	2.49	0.41
3:N:1106:VAL:CG2	3:N:1474:ALA:HB2	2.49	0.41
3:N:560:GLN:O	5:P:184:ARG:NH2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:629:SER:C	3:N:744:GLN:HG2	2.40	0.41
4:O:45:ARG:H	4:O:47:LYS:NZ	2.18	0.41
1:A:170:VAL:HG11	9:C:9860:HOH:O	2.21	0.41
1:A:79:ILE:HD11	9:A:9704:HOH:O	2.21	0.41
1:B:27:PRO:C	1:B:28:LEU:HD23	2.40	0.41
1:B:51:THR:HA	1:B:145:ASP:O	2.21	0.41
2:C:1029:GLY:O	3:D:622:ARG:NH1	2.54	0.41
2:C:191:PHE:CE2	2:C:196:LEU:HD11	2.55	0.41
2:C:117:HIS:HB2	2:C:379:GLU:OE2	2.20	0.41
2:C:380:ALA:O	2:C:384:GLU:HB2	2.21	0.41
2:C:504:GLU:CD	2:C:509:ALA:HB2	2.41	0.41
2:C:791:ARG:O	2:C:793:PRO:HD3	2.20	0.41
2:C:815:LEU:HD21	2:C:820:ARG:O	2.21	0.41
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.61	0.41
2:C:890:LEU:HD23	2:C:890:LEU:C	2.40	0.41
2:C:900:ARG:NH1	9:C:2088:HOH:O	2.52	0.41
3:D:100:ALA:H	3:D:575:GLN:HE22	1.69	0.41
3:D:1031:ASN:HB3	3:D:1034:GLN:CD	2.41	0.41
3:D:1090:ASP:O	3:D:1093:TYR:HB3	2.20	0.41
3:D:1135:ARG:HB3	3:D:1140:ILE:HG13	2.03	0.41
3:D:1389:LEU:CG	3:D:1390:LEU:N	2.83	0.41
3:D:432:TYR:HE2	9:D:9631:HOH:O	2.03	0.41
3:D:543:LEU:CD2	3:D:600:LEU:HD12	2.51	0.41
3:D:565:ILE:HB	5:F:84:TYR:HD2	1.85	0.41
3:D:690:ALA:O	3:D:693:GLU:HB3	2.20	0.41
3:D:848:GLU:HA	3:D:851:LEU:CD1	2.50	0.41
3:D:89:ARG:O	3:D:521:PRO:HG3	2.20	0.41
5:F:302:LYS:HG3	5:F:303:ARG:N	2.35	0.41
1:K:11:PHE:CD1	1:L:225:PHE:HA	2.55	0.41
1:L:88:ARG:HB3	1:L:121:GLU:OE1	2.20	0.41
1:L:137:ARG:HH11	1:L:137:ARG:HB3	1.81	0.41
1:L:86:VAL:HG12	1:L:124:ASN:CG	2.40	0.41
2:M:63:GLY:HA3	2:M:103:LYS:HD2	2.02	0.41
2:M:1050:GLN:HA	2:M:1053:LEU:HD12	2.03	0.41
2:M:1095:LEU:O	2:M:1096:ALA:C	2.58	0.41
2:M:157:ARG:HA	2:M:157:ARG:NE	2.36	0.41
2:M:165:LEU:HB2	9:M:9613:HOH:O	2.20	0.41
2:M:231:PRO:HG3	9:M:2224:HOH:O	2.19	0.41
2:M:138:SER:OG	2:M:335:THR:HA	2.19	0.41
2:M:339:LEU:HD13	2:M:391:LEU:HD21	2.03	0.41
2:M:620:LEU:N	2:M:620:LEU:HD13	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:721:ARG:O	2:M:758:ARG:HA	2.21	0.41
2:M:890:LEU:HD21	2:M:901:TYR:HD1	1.85	0.41
3:N:1123:PHE:HA	3:N:1134:LEU:HA	2.03	0.41
3:N:1290:LEU:HA	9:N:2475:HOH:O	2.20	0.41
3:N:129:PHE:O	3:N:572:ARG:HG2	2.21	0.41
3:N:199:LEU:N	9:N:9629:HOH:O	2.53	0.41
3:N:416:ALA:H	3:N:417:PRO:CD	2.33	0.41
3:N:793:THR:O	3:N:879:ARG:NH1	2.50	0.41
5:P:421:PHE:C	5:P:423:ASP:H	2.22	0.41
1:A:211:LEU:O	1:A:214:ALA:HB3	2.21	0.41
1:B:71:VAL:HG22	1:B:132:LEU:CD1	2.51	0.41
2:C:1008:ARG:HB2	2:C:1027:PHE:HB2	2.03	0.41
2:C:1083:GLU:O	2:C:1087:VAL:HB	2.20	0.41
2:C:95:TYR:CD2	2:C:114:PHE:HB3	2.55	0.41
2:C:14:PRO:HB3	2:C:586:ARG:NH2	2.34	0.41
2:C:525:SER:O	2:C:529:VAL:HG23	2.19	0.41
2:C:569:VAL:HG11	2:C:996:LYS:HE2	2.03	0.41
2:C:630:ARG:HH12	2:C:707:ARG:HB2	1.85	0.41
2:C:597:ALA:CB	2:C:655:LEU:HD21	2.48	0.41
2:C:705:ILE:HG23	2:C:827:VAL:O	2.21	0.41
2:C:710:ILE:HD11	2:C:758:ARG:HE	1.85	0.41
2:C:713:ARG:HH11	2:C:713:ARG:HG3	1.85	0.41
2:C:723:THR:HB	9:C:2334:HOH:O	2.20	0.41
2:C:929:ARG:HH11	2:C:929:ARG:HG3	1.86	0.41
3:D:1299:PHE:N	3:D:1299:PHE:CD2	2.88	0.41
3:D:1389:LEU:HD13	9:D:2920:HOH:O	2.20	0.41
3:D:169:TYR:HA	3:D:392:SER:HA	2.03	0.41
3:D:493:ARG:HH12	3:D:1390:LEU:CB	2.32	0.41
3:D:54:LYS:HD3	3:D:57:GLU:OE2	2.21	0.41
3:D:699:VAL:HA	3:D:718:PRO:HD3	2.02	0.41
3:D:783:ARG:HH21	3:D:1029:ARG:NH1	2.18	0.41
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.56	0.41
4:E:68:LEU:HA	4:E:73:LEU:HD13	2.03	0.41
5:F:401:GLU:HA	9:F:9597:HOH:O	2.20	0.41
5:F:421:PHE:C	5:F:423:ASP:H	2.24	0.41
1:L:206:THR:HG22	1:L:209:GLU:CG	2.50	0.41
1:L:86:VAL:O	1:L:86:VAL:HG13	2.21	0.41
2:M:1018:GLN:HB3	2:M:1060:ILE:HD11	2.03	0.41
2:M:63:GLY:HA3	2:M:103:LYS:CD	2.50	0.41
2:M:139:GLN:CD	2:M:418:LEU:HD22	2.41	0.41
2:M:14:PRO:HA	9:M:2059:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:342:ASP:HA	2:M:345:ARG:HG2	2.03	0.41
2:M:674:VAL:O	2:M:989:VAL:HA	2.20	0.41
3:N:1136:LYS:O	3:N:1139:ASP:HB2	2.20	0.41
3:N:1305:LEU:HD21	3:N:1326:THR:OG1	2.20	0.41
3:N:528:VAL:HG12	3:N:529:GLN:N	2.35	0.41
3:N:704:ARG:CG	3:N:736:PHE:HB3	2.44	0.41
3:N:897:TRP:CH2	3:N:902:LEU:HD21	2.56	0.41
3:N:1481:VAL:HG11	4:O:18:ARG:CB	2.51	0.41
5:P:358:LEU:CD2	5:P:370:LYS:HG3	2.51	0.41
2:C:175:GLU:HB3	2:C:183:SER:HG	1.86	0.41
2:C:232:GLU:O	2:C:235:LEU:HB2	2.20	0.41
2:C:338:GLU:O	2:C:341:THR:HG22	2.21	0.41
2:C:34:VAL:HG22	9:C:2353:HOH:O	2.19	0.41
2:C:536:PRO:O	2:C:539:VAL:HG23	2.20	0.41
2:C:597:ALA:HB2	2:C:655:LEU:CD2	2.47	0.41
2:C:668:LEU:O	2:C:993:PHE:CZ	2.74	0.41
2:C:670:GLN:HE22	2:C:699:PHE:C	2.24	0.41
2:C:816:LYS:O	2:C:819:VAL:HB	2.21	0.41
2:C:76:PRO:HB3	2:C:90:TYR:HE1	1.86	0.41
2:C:916:GLU:O	2:C:919:ALA:HB3	2.21	0.41
2:C:932:GLU:CB	9:C:2388:HOH:O	2.68	0.41
2:C:973:VAL:HG13	9:C:9633:HOH:O	2.21	0.41
3:D:127:LEU:HD21	3:D:461:ILE:CD1	2.50	0.41
3:D:389:GLU:HG2	9:D:9755:HOH:O	2.20	0.41
3:D:420:VAL:HA	5:F:164:LYS:HE3	2.01	0.41
3:D:776:GLU:HB2	9:D:2369:HOH:O	2.20	0.41
3:D:882:PHE:HA	3:D:885:ILE:HD12	2.02	0.41
2:C:1075:ASP:HB3	4:E:32:ARG:CZ	2.51	0.41
5:F:74:LYS:HD3	5:F:74:LYS:HA	1.92	0.41
1:L:27:PRO:HG2	1:L:186:LEU:HD13	2.01	0.41
1:L:46:SER:HB2	9:L:3651:HOH:O	2.19	0.41
2:M:100:LEU:HD11	2:M:368:THR:OG1	2.21	0.41
2:M:1013:TYR:CZ	2:M:1063:ARG:HD2	2.56	0.41
2:M:1102:LEU:HA	2:M:1107:ASN:O	2.21	0.41
2:M:1115:LEU:N	2:M:1115:LEU:CD1	2.83	0.41
2:M:203:ASP:OD1	2:M:206:THR:HG22	2.20	0.41
2:M:239:PHE:HZ	9:M:9883:HOH:O	2.04	0.41
2:M:253:ALA:HB3	9:M:9883:HOH:O	2.20	0.41
2:M:261:ILE:HG22	2:M:262:ALA:N	2.36	0.41
2:M:311:PHE:HB3	9:M:9648:HOH:O	2.21	0.41
2:M:543:ASN:O	2:M:546:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:54:ILE:HG22	2:M:66:LEU:HB3	2.02	0.41
2:M:950:LEU:HB3	2:M:952:LEU:HD23	2.03	0.41
3:N:1123:PHE:CA	3:N:1133:ARG:O	2.69	0.41
3:N:1482:ARG:HB2	3:N:1483:PHE:CD1	2.56	0.41
3:N:1492:LEU:HD12	9:N:9749:HOH:O	2.20	0.41
3:N:165:LYS:NZ	3:N:166:GLN:HE22	2.19	0.41
3:N:456:MET:C	9:N:9968:HOH:O	2.59	0.41
3:N:586:ARG:HG2	9:N:2177:HOH:O	2.21	0.41
3:N:62:LYS:HE2	3:N:75:ARG:HH11	1.86	0.41
3:N:82:LYS:HG2	5:P:337:HIS:HB3	2.02	0.41
2:M:1090:LYS:NZ	3:N:90:MET:HG3	2.36	0.41
3:N:933:ALA:O	3:N:937:TYR:HD1	2.04	0.41
3:N:971:LEU:HD13	3:N:995:LEU:HD23	2.01	0.41
4:O:25:LYS:HE3	9:O:6116:HOH:O	2.20	0.41
4:O:49:GLN:HA	4:O:51:LEU:O	2.20	0.41
5:P:93:LEU:HD22	5:P:102:LEU:HD11	2.02	0.41
1:A:44:LEU:HD23	1:A:174:VAL:HG21	2.02	0.41
1:A:18:ARG:NH1	1:A:88:ARG:NE	2.69	0.41
1:B:19:GLU:HG3	1:B:201:THR:O	2.20	0.41
2:C:1015:LEU:HD12	9:C:9582:HOH:O	2.21	0.41
2:C:8:ARG:NE	2:C:10:ARG:HH21	2.19	0.41
2:C:233:GLU:HB2	9:C:9837:HOH:O	2.20	0.41
2:C:272:ALA:HB1	9:C:2186:HOH:O	2.21	0.41
2:C:349:ALA:O	2:C:353:ARG:HB2	2.21	0.41
3:D:1133:ARG:HG2	3:D:1134:LEU:N	2.35	0.41
3:D:1205:TYR:HE1	3:D:1221:VAL:CG1	2.33	0.41
3:D:1258:ARG:HH21	3:D:1351:GLU:CG	2.34	0.41
3:D:1326:THR:CA	9:D:9899:HOH:O	2.69	0.41
3:D:639:LEU:CD1	3:D:639:LEU:N	2.76	0.41
3:D:675:ARG:NH2	5:F:420:ASP:HA	2.36	0.41
3:D:688:TRP:HA	3:D:688:TRP:CE3	2.56	0.41
3:D:786:ILE:H	3:D:786:ILE:HG13	1.63	0.41
3:D:818:ARG:HD2	9:D:2824:HOH:O	2.20	0.41
3:D:847:ASP:HA	3:D:850:LEU:CD1	2.51	0.41
3:D:847:ASP:O	3:D:851:LEU:HG	2.21	0.41
4:E:87:LYS:NZ	4:E:91:ARG:HH21	2.19	0.41
5:F:265:VAL:HG11	9:F:9667:HOH:O	2.20	0.41
1:L:19:GLU:O	1:L:200:TRP:HA	2.21	0.41
2:M:1050:GLN:CG	2:M:1079:PRO:HG2	2.47	0.41
2:M:157:ARG:HD3	2:M:314:THR:HG22	2.02	0.41
2:M:165:LEU:HD12	2:M:166:PRO:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:218:VAL:HG22	2:M:221:LEU:HD21	2.03	0.41
2:M:191:PHE:CD2	2:M:238:LEU:HD21	2.55	0.41
2:M:285:LEU:HD22	9:M:9952:HOH:O	2.20	0.41
2:M:252:LYS:HZ3	2:M:296:GLY:HA3	1.86	0.41
2:M:473:ARG:HG2	2:M:473:ARG:NH1	2.36	0.41
2:M:802:ARG:NH2	9:M:2540:HOH:O	2.54	0.41
2:M:824:ARG:HE	2:M:824:ARG:HB2	1.73	0.41
3:N:1007:VAL:O	3:N:1010:ASN:HB3	2.20	0.41
3:N:1036:ARG:HH21	3:N:1043:GLY:N	2.18	0.41
2:M:882:LEU:HD21	3:N:1038:LEU:HD23	2.02	0.41
3:N:1171:VAL:HG12	3:N:1171:VAL:O	2.21	0.41
3:N:128:TYR:HB3	3:N:129:PHE:CD1	2.56	0.41
3:N:1275:SER:HB3	3:N:1325:LEU:CD1	2.50	0.41
3:N:1401:GLU:OE1	3:N:1415:VAL:HG11	2.21	0.41
3:N:396:VAL:HG13	3:N:447:VAL:HA	2.02	0.41
2:M:1101:THR:HB	3:N:5:VAL:HG13	2.03	0.41
3:N:830:ALA:HA	9:N:9989:HOH:O	2.20	0.41
5:P:169:GLU:H	5:P:169:GLU:CD	2.24	0.41
2:M:1015:LEU:HD12	5:P:334:PRO:O	2.19	0.41
1:A:109:VAL:O	1:A:129:ILE:HB	2.20	0.41
1:A:29:GLU:HB3	1:A:30:ARG:H	1.72	0.41
1:A:64:GLU:O	1:A:64:GLU:HG2	2.19	0.41
1:B:124:ASN:OD1	1:B:127:LEU:HD22	2.21	0.41
1:B:23:PHE:HE1	1:B:208:LEU:HD22	1.86	0.41
2:C:1069:ALA:O	2:C:1074:GLU:HB3	2.21	0.41
2:C:304:LEU:HD21	9:C:9585:HOH:O	2.20	0.41
2:C:304:LEU:HD23	2:C:305:PRO:HD3	2.03	0.41
2:C:44:ILE:HD11	2:C:340:MET:SD	2.61	0.41
2:C:358:ARG:HH12	2:C:374:ASN:HB3	1.85	0.41
2:C:520:GLU:HA	2:C:521:PRO:HD3	1.93	0.41
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.55	0.41
2:C:710:ILE:CD1	2:C:758:ARG:HE	2.34	0.41
2:C:799:ILE:N	2:C:799:ILE:HD13	2.35	0.41
3:D:1093:TYR:HE1	3:D:1097:LYS:HZ3	1.68	0.41
3:D:112:ILE:O	3:D:116:LEU:HB2	2.21	0.41
3:D:1169:ASP:HA	9:D:2794:HOH:O	2.21	0.41
3:D:1331:ASP:OD1	3:D:1333:HIS:HB2	2.20	0.41
3:D:459:GLU:HB2	9:D:9714:HOH:O	2.20	0.41
3:D:757:ALA:CB	4:E:24:ALA:HB2	2.51	0.41
5:F:149:GLU:HB2	9:F:9715:HOH:O	2.21	0.41
1:K:224:TYR:HB3	1:L:9:PRO:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:249:LYS:HG2	2:M:249:LYS:H	1.74	0.41
2:M:211:LEU:CD1	2:M:308:ARG:HA	2.51	0.41
2:M:19:THR:HG23	2:M:407:LYS:HE2	2.03	0.41
2:M:557:ARG:NH1	2:M:879:ARG:HH11	2.18	0.41
3:N:1033:GLN:HE21	3:N:1036:ARG:NH1	1.94	0.41
3:N:1042:ARG:HB2	9:N:2155:HOH:O	2.20	0.41
3:N:1071:PHE:O	3:N:1071:PHE:HD1	2.04	0.41
3:N:1225:ALA:HA	3:N:1367:HIS:ND1	2.36	0.41
3:N:1243:THR:CB	3:N:1253:THR:HB	2.50	0.41
3:N:1440:PHE:HB3	9:N:9766:HOH:O	2.19	0.41
3:N:139:GLY:N	3:N:147:VAL:HG21	2.36	0.41
3:N:1485:GLN:HG2	3:N:1485:GLN:H	1.69	0.41
3:N:601:ARG:NH2	3:N:612:GLY:HA2	2.35	0.41
3:N:658:LEU:O	3:N:661:MET:HB2	2.20	0.41
3:N:675:ARG:O	3:N:678:GLU:HG2	2.20	0.41
3:N:649:ALA:CB	3:N:720:LEU:HD21	2.51	0.41
3:N:729:HIS:ND1	3:N:730:PRO:HD2	2.36	0.41
3:N:853:VAL:HA	3:N:858:VAL:O	2.20	0.41
4:O:93:TYR:HA	4:O:94:PRO:HD3	1.81	0.41
5:P:195:VAL:HG21	5:P:217:ASN:HA	2.03	0.41
5:P:247:ILE:O	5:P:251:ILE:HG13	2.21	0.41
5:P:372:ARG:HD3	9:P:4888:HOH:O	2.21	0.41
1:B:101:LEU:HD12	1:B:114:PHE:CD1	2.56	0.41
1:A:32:PHE:CZ	1:B:43:ILE:HD12	2.56	0.41
1:B:95:GLN:HB2	1:B:95:GLN:HE21	1.65	0.41
2:C:254:VAL:O	2:C:257:VAL:HG23	2.20	0.41
2:C:252:LYS:HB3	2:C:298:PHE:HZ	1.84	0.41
2:C:413:LEU:H	2:C:413:LEU:CD1	2.32	0.41
2:C:437:ARG:HA	2:C:467:ILE:CG2	2.47	0.41
2:C:455:LEU:H	2:C:455:LEU:CD2	2.34	0.41
2:C:589:ARG:HB3	9:C:9581:HOH:O	2.21	0.41
2:C:899:GLN:HG3	2:C:901:TYR:CZ	2.56	0.41
2:C:521:PRO:CB	3:D:1055:VAL:HB	2.48	0.41
3:D:1152:GLU:CG	3:D:1159:ARG:HH12	2.33	0.41
3:D:177:ALA:HB1	3:D:199:LEU:HB3	2.03	0.41
3:D:421:LEU:HD23	3:D:421:LEU:O	2.20	0.41
3:D:480:GLU:OE1	3:D:484:PRO:HG2	2.21	0.41
3:D:604:THR:C	3:D:606:ILE:N	2.74	0.41
3:D:61:GLY:O	3:D:64:LYS:HD2	2.21	0.41
3:D:916:TYR:C	3:D:916:TYR:HD2	2.24	0.41
3:D:779:ALA:HB1	3:D:931:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:10:PHE:CE2	4:E:16:LYS:HG3	2.55	0.41
3:D:696:HIS:HB2	4:E:48:MET:HE1	2.03	0.41
9:D:9710:HOH:O	5:F:164:LYS:HG2	2.21	0.41
1:K:108:GLU:OE1	1:K:110:LYS:HE3	2.21	0.41
1:K:58:ILE:HD13	1:K:140:MET:HB2	2.02	0.41
1:K:179:PHE:CD2	1:K:179:PHE:N	2.89	0.41
1:K:192:LEU:HD21	9:K:6176:HOH:O	2.20	0.41
1:L:72:LYS:HE3	1:L:72:LYS:HB2	1.94	0.41
2:M:118:ILE:HA	2:M:119:PRO:HD3	1.99	0.41
2:M:216:GLU:HB2	9:M:9791:HOH:O	2.19	0.41
2:M:242:LEU:HD21	9:M:2213:HOH:O	2.20	0.41
2:M:157:ARG:HD3	2:M:314:THR:CG2	2.50	0.41
3:N:1117:TYR:N	3:N:1117:TYR:CD2	2.88	0.41
3:N:1406:ARG:HG2	3:N:1406:ARG:NH1	2.36	0.41
3:N:587:ARG:NH1	3:N:587:ARG:HB3	2.35	0.41
2:M:1030:GLN:HB2	3:N:626:SER:HB2	2.03	0.41
3:N:683:ILE:HG23	3:N:687:VAL:CG2	2.51	0.41
3:N:708:LEU:HD23	3:N:708:LEU:HA	1.84	0.41
2:M:1115:LEU:HD23	3:N:85:VAL:CA	2.51	0.41
3:N:884:ARG:HD3	3:N:888:GLU:CD	2.41	0.41
3:N:907:GLU:HG2	3:N:908:LYS:H	1.82	0.41
4:O:3:GLU:HA	9:O:4620:HOH:O	2.21	0.41
4:O:54:LEU:HG	9:O:3710:HOH:O	2.19	0.41
4:O:82:GLU:HG3	9:O:3831:HOH:O	2.20	0.41
5:P:135:ILE:O	5:P:135:ILE:HD13	2.20	0.41
5:P:201:LYS:HG2	9:P:4854:HOH:O	2.20	0.41
5:P:317:LEU:HD21	5:P:333:ILE:HD12	2.02	0.41
1:A:161:ARG:HG2	9:A:9594:HOH:O	2.21	0.41
2:C:108:ILE:H	2:C:108:ILE:HD12	1.85	0.41
2:C:585:GLU:HB2	9:C:9765:HOH:O	2.21	0.41
2:C:612:VAL:HG22	2:C:622:GLU:CA	2.46	0.41
2:C:699:PHE:N	9:C:9889:HOH:O	2.54	0.41
2:C:720:GLU:HG2	2:C:760:SER:HB3	2.03	0.41
2:C:897:LEU:HB3	2:C:899:GLN:HG2	2.03	0.41
2:C:926:PHE:HA	2:C:929:ARG:HB2	2.02	0.41
3:D:1103:HIS:CG	3:D:1104:GLU:N	2.89	0.41
3:D:115:LEU:HD22	3:D:502:PHE:CE1	2.56	0.41
3:D:1319:VAL:HG23	3:D:1319:VAL:O	2.21	0.41
3:D:1346:ARG:HG2	3:D:1346:ARG:HH11	1.86	0.41
3:D:1458:GLU:OE2	3:D:1458:GLU:HA	2.21	0.41
3:D:483:HIS:HB2	9:D:2535:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:561:GLY:HA3	5:F:184:ARG:NH1	2.35	0.41
3:D:653:PHE:HD1	3:D:653:PHE:N	2.18	0.41
3:D:867:ARG:CB	3:D:867:ARG:HH11	2.33	0.41
5:F:123:ASP:N	5:F:126:LEU:HD22	2.36	0.41
5:F:373:LYS:HD3	5:F:378:GLY:C	2.41	0.41
1:K:127:LEU:HD12	1:K:128:HIS:N	2.37	0.41
1:K:150:TYR:CD1	2:M:696:LYS:HG2	2.56	0.41
1:K:74:ASP:OD1	1:K:77:GLU:N	2.52	0.41
1:L:29:GLU:HB3	1:L:30:ARG:H	1.61	0.41
2:M:12:VAL:HG22	2:M:13:ILE:HG23	2.02	0.41
2:M:168:ARG:HD2	2:M:168:ARG:H	1.85	0.41
2:M:202:TYR:HE2	2:M:304:LEU:HB3	1.86	0.41
2:M:395:LYS:HG2	2:M:397:GLU:HG2	2.03	0.41
2:M:401:LEU:HD13	2:M:666:LEU:HD22	2.02	0.41
2:M:520:GLU:O	2:M:522:VAL:HG23	2.21	0.41
2:M:669:GLY:C	2:M:670:GLN:HG2	2.41	0.41
2:M:815:LEU:HD21	2:M:820:ARG:O	2.21	0.41
2:M:86:LYS:CG	2:M:813:VAL:HG12	2.51	0.41
3:N:1042:ARG:O	3:N:1057:VAL:HB	2.21	0.41
3:N:416:ALA:HB3	3:N:417:PRO:HD3	2.02	0.41
3:N:506:GLY:HA3	9:N:9591:HOH:O	2.21	0.41
3:N:65:ARG:HH11	3:N:65:ARG:HG2	1.86	0.41
3:N:882:PHE:CE1	3:N:906:GLN:HG3	2.56	0.41
4:O:35:PHE:HZ	4:O:60:ALA:HA	1.86	0.41
5:P:353:GLU:OE2	5:P:356:LYS:HE2	2.21	0.41
1:B:32:PHE:O	1:B:36:LEU:HD12	2.21	0.40
1:B:86:VAL:HG13	1:B:86:VAL:O	2.20	0.40
2:C:1034:GLU:CA	2:C:1037:VAL:HG23	2.50	0.40
2:C:170:PRO:HG2	2:C:258:TYR:CD2	2.56	0.40
2:C:524:VAL:HG22	2:C:528:GLU:CD	2.41	0.40
2:C:534:VAL:N	2:C:538:GLN:NE2	2.69	0.40
2:C:569:VAL:HA	2:C:570:PRO:HD3	1.97	0.40
2:C:681:GLY:C	3:D:635:PRO:CG	2.89	0.40
2:C:858:MET:SD	2:C:867:VAL:O	2.79	0.40
2:C:837:ASP:HA	2:C:999:HIS:CE1	2.56	0.40
3:D:1109:GLU:HG2	3:D:1201:CYS:CA	2.47	0.40
3:D:1160:LEU:HD11	3:D:1174:LEU:CD2	2.37	0.40
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.57	0.40
3:D:187:LYS:NZ	3:D:213:VAL:HG12	2.36	0.40
3:D:135:LEU:HA	3:D:453:ASP:O	2.21	0.40
3:D:543:LEU:HA	3:D:546:ARG:CG	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:719:VAL:O	3:D:719:VAL:HG23	2.20	0.40
5:F:172:ARG:O	5:F:176:ILE:HD13	2.20	0.40
5:F:295:MET:HB3	5:F:299:TRP:CG	2.56	0.40
5:F:298:GLY:N	9:F:9729:HOH:O	2.54	0.40
1:K:1:MET:O	1:K:6:LEU:HB2	2.22	0.40
1:K:37:GLY:HA3	1:K:179:PHE:CD1	2.56	0.40
2:M:292:ARG:CB	2:M:299:LYS:HE2	2.50	0.40
2:M:304:LEU:O	2:M:308:ARG:HB2	2.20	0.40
2:M:539:VAL:HB	2:M:540:PHE:CD1	2.56	0.40
3:N:1044:LEU:HA	9:N:9900:HOH:O	2.21	0.40
3:N:1156:LEU:HG	3:N:1177:ALA:HB2	2.02	0.40
3:N:1182:GLU:HG2	9:N:9782:HOH:O	2.21	0.40
3:N:1197:ARG:HD2	3:N:1198:TYR:HE1	1.86	0.40
3:N:1238:MET:HG2	3:N:1256:LEU:HD23	2.02	0.40
3:N:1273:VAL:O	3:N:1273:VAL:HG23	2.21	0.40
3:N:1346:ARG:HA	3:N:1346:ARG:NE	2.36	0.40
3:N:639:LEU:HD12	3:N:640:HIS:H	1.86	0.40
3:N:666:ILE:N	3:N:666:ILE:HD12	2.27	0.40
3:N:728:LEU:HD12	3:N:729:HIS:H	1.85	0.40
2:C:1100:GLN:HG3	2:C:1101:THR:O	2.22	0.40
2:C:218:VAL:HG22	2:C:221:LEU:CD2	2.51	0.40
2:C:305:PRO:HA	2:C:308:ARG:NE	2.36	0.40
2:C:841:ASN:HD21	2:C:845:ASN:H	1.69	0.40
1:A:178:ALA:HB1	2:C:864:GLY:H	1.85	0.40
2:C:83:CYS:CA	2:C:88:LEU:HB3	2.47	0.40
2:C:839:LEU:HD12	2:C:994:ILE:HG21	2.03	0.40
3:D:1103:HIS:C	9:D:9709:HOH:O	2.59	0.40
3:D:455:ARG:HG2	3:D:455:ARG:HH11	1.85	0.40
3:D:57:GLU:HG2	3:D:58:CYS:O	2.22	0.40
3:D:644:LEU:HD23	3:D:718:PRO:HB3	2.03	0.40
3:D:647:ARG:HD3	3:D:647:ARG:O	2.22	0.40
3:D:62:LYS:HE2	3:D:75:ARG:HH22	1.85	0.40
3:D:420:VAL:HG13	5:F:164:LYS:NZ	2.36	0.40
5:F:181:GLU:O	5:F:184:ARG:HB3	2.21	0.40
3:D:561:GLY:CA	5:F:184:ARG:HH12	2.34	0.40
5:F:309:LYS:NZ	9:F:9939:HOH:O	2.54	0.40
5:F:316:SER:C	5:F:318:GLU:N	2.75	0.40
2:C:1021:LEU:CD1	5:F:332:PHE:HA	2.51	0.40
5:F:82:ARG:HG2	5:F:86:HIS:CD2	2.56	0.40
1:K:111:ALA:HB3	1:K:124:ASN:O	2.22	0.40
1:K:9:PRO:HD2	1:L:224:TYR:CE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:146:VAL:HG11	2:M:306:THR:HG22	2.02	0.40
2:M:343:GLN:NE2	2:M:343:GLN:HA	2.36	0.40
2:M:360:LEU:HD12	9:M:9853:HOH:O	2.21	0.40
2:M:393:GLN:OE1	2:M:406:HIS:NE2	2.52	0.40
2:M:460:ARG:HD2	2:M:485:TYR:CE2	2.57	0.40
2:M:542:VAL:HG13	2:M:583:LEU:HD23	2.03	0.40
2:M:929:ARG:HH11	2:M:929:ARG:HG3	1.86	0.40
2:M:961:GLU:OE2	2:M:961:GLU:HA	2.20	0.40
3:N:1087:ARG:CG	3:N:1238:MET:HB2	2.51	0.40
3:N:1296:SER:HA	9:N:9818:HOH:O	2.21	0.40
1:L:152:PRO:HG2	3:N:857:ILE:HD12	2.02	0.40
3:N:866:VAL:HG12	3:N:867:ARG:N	2.36	0.40
5:P:137:GLY:HA3	9:P:3900:HOH:O	2.21	0.40
5:P:304:VAL:HG22	9:P:4835:HOH:O	2.21	0.40
3:N:34:TYR:CD1	5:P:310:ILE:HD13	2.55	0.40
1:A:102:LYS:HG3	1:A:139:ASN:HB2	2.03	0.40
1:A:76:VAL:HB	9:A:9703:HOH:O	2.20	0.40
1:A:9:PRO:HG2	1:B:224:TYR:CD2	2.56	0.40
2:C:1005:MET:HB3	3:D:629:SER:CB	2.51	0.40
2:C:147:TYR:HE2	2:C:280:LYS:NZ	2.18	0.40
2:C:224:GLU:HB3	2:C:227:PHE:CD1	2.56	0.40
2:C:264:PRO:HA	9:C:9831:HOH:O	2.21	0.40
2:C:256:TYR:CE1	2:C:293:PHE:HB2	2.57	0.40
2:C:124:ASP:HB2	2:C:407:LYS:HZ3	1.87	0.40
2:C:598:GLU:HB2	2:C:615:TYR:CZ	2.56	0.40
9:A:9703:HOH:O	2:C:628:PHE:HZ	2.05	0.40
2:C:395:LYS:N	2:C:632:ASN:HD22	2.19	0.40
2:C:578:VAL:N	2:C:671:ASN:OD1	2.54	0.40
2:C:717:LEU:N	2:C:717:LEU:HD23	2.36	0.40
3:D:1010:ASN:HA	9:D:9981:HOH:O	2.21	0.40
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.36	0.40
3:D:1295:GLU:HB3	3:D:1300:SER:CB	2.52	0.40
3:D:135:LEU:HD21	3:D:138:LYS:C	2.41	0.40
3:D:206:ARG:O	3:D:206:ARG:HD3	2.22	0.40
3:D:445:ARG:HH11	3:D:445:ARG:CB	2.31	0.40
3:D:951:ILE:HD13	3:D:951:ILE:O	2.21	0.40
5:F:84:TYR:CD2	5:F:192:LEU:HD13	2.56	0.40
5:F:235:PHE:CA	9:F:9866:HOH:O	2.66	0.40
5:F:363:GLU:CA	5:F:367:MET:HG2	2.51	0.40
1:K:83:LYS:HE2	1:K:168:ASP:HB2	2.03	0.40
1:K:219:ARG:HG3	9:K:6366:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:ARG:HG3	9:L:3590:HOH:O	2.20	0.40
1:L:97:VAL:HG22	9:L:5813:HOH:O	2.22	0.40
2:M:27:ARG:HG3	9:M:2339:HOH:O	2.21	0.40
2:M:142:ARG:HH11	2:M:325:ILE:HG23	1.86	0.40
2:M:490:GLU:HG2	2:M:494:TYR:CE1	2.56	0.40
2:M:713:ARG:O	2:M:720:GLU:HG3	2.22	0.40
2:M:762:LYS:HD3	2:M:771:GLU:OE2	2.20	0.40
2:M:884:GLN:HG2	2:M:885:ILE:N	2.37	0.40
2:M:987:ILE:HG12	3:N:948:THR:CG2	2.47	0.40
2:M:671:ASN:HD22	2:M:993:PHE:HA	1.87	0.40
3:N:1109:GLU:HG2	3:N:1202:GLN:N	2.36	0.40
3:N:1398:TRP:HH2	9:N:9689:HOH:O	2.02	0.40
3:N:1478:SER:C	3:N:1480:PHE:N	2.74	0.40
4:O:45:ARG:HG2	4:O:45:ARG:NH1	2.36	0.40
5:P:244:ARG:O	5:P:248:ASN:ND2	2.55	0.40
9:N:9917:HOH:O	5:P:325:LYS:HG3	2.21	0.40
5:P:85:LEU:HD13	5:P:193:ARG:NH1	2.29	0.40
1:A:216:GLU:O	1:A:220:GLU:HG3	2.21	0.40
1:A:30:ARG:HD3	1:A:191:ASP:OD1	2.22	0.40
1:A:58:ILE:HG21	1:A:68:ILE:CD1	2.51	0.40
1:A:89:PHE:HB3	1:A:120:VAL:HG23	2.04	0.40
2:C:139:GLN:HE22	2:C:415:PRO:CD	2.34	0.40
2:C:238:LEU:HD23	2:C:238:LEU:O	2.22	0.40
2:C:26:TYR:CE2	2:C:30:LEU:HD21	2.57	0.40
2:C:479:VAL:HG22	2:C:508:ILE:CD1	2.51	0.40
2:C:695:LEU:N	9:C:9871:HOH:O	2.54	0.40
2:C:958:THR:HG23	2:C:961:GLU:HG3	2.03	0.40
3:D:1166:LEU:CD1	3:D:1171:VAL:HG22	2.43	0.40
3:D:1155:VAL:CG1	3:D:1183:ILE:HD11	2.52	0.40
3:D:786:ILE:HD13	3:D:908:LYS:HB3	2.03	0.40
5:F:147:LEU:HD23	9:F:9589:HOH:O	2.21	0.40
5:F:171:LYS:HE3	5:F:175:HIS:NE2	2.36	0.40
5:F:279:GLN:HB2	9:F:9736:HOH:O	2.22	0.40
1:K:101:LEU:HD11	1:K:109:VAL:CG1	2.51	0.40
1:K:106:PRO:HD3	9:K:5912:HOH:O	2.21	0.40
1:K:68:ILE:HD13	1:K:138:LEU:CD2	2.52	0.40
2:M:1097:LEU:HD22	2:M:1097:LEU:N	2.36	0.40
2:M:154:ARG:HB3	9:M:9876:HOH:O	2.21	0.40
2:M:21:ILE:HD12	2:M:21:ILE:N	2.37	0.40
2:M:230:ARG:HB2	9:M:2176:HOH:O	2.22	0.40
2:M:19:THR:O	2:M:23:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:486:MET:HG2	9:M:9856:HOH:O	2.21	0.40
2:M:535:SER:H	2:M:538:GLN:HE21	1.68	0.40
2:M:728:HIS:O	2:M:729:LEU:HD12	2.21	0.40
2:M:777:ILE:HG22	9:P:3891:HOH:O	2.22	0.40
2:M:876:VAL:HG22	2:M:884:GLN:NE2	2.37	0.40
3:N:12:LEU:HD22	3:N:511:TRP:HB2	2.02	0.40
3:N:1459:LEU:HD22	3:N:1465:ASN:ND2	2.37	0.40
3:N:668:PRO:HD2	3:N:672:ALA:CB	2.52	0.40
4:O:78:ASN:HB3	9:O:3963:HOH:O	2.22	0.40
5:P:228:GLU:HG2	9:P:5612:HOH:O	2.21	0.40
5:P:363:GLU:CA	5:P:367:MET:HG2	2.49	0.40
5:P:399:GLN:HE21	5:P:399:GLN:HB3	1.65	0.40
1:A:111:ALA:HB3	1:A:124:ASN:O	2.21	0.40
1:A:222:LEU:HD12	1:B:215:VAL:CB	2.46	0.40
1:B:89:PHE:HD1	1:B:120:VAL:HG13	1.85	0.40
1:B:84:GLU:HG3	1:B:127:LEU:HD21	2.04	0.40
1:B:142:VAL:HG23	1:B:142:VAL:O	2.21	0.40
2:C:1083:GLU:OE1	2:C:1083:GLU:HA	2.21	0.40
2:C:1095:LEU:O	2:C:1096:ALA:C	2.59	0.40
2:C:116:GLY:HA3	2:C:378:LEU:HD23	2.02	0.40
2:C:195:LEU:CD1	2:C:234:ALA:HB1	2.51	0.40
2:C:139:GLN:NE2	2:C:415:PRO:HD3	2.36	0.40
2:C:420:ARG:HG2	2:C:422:ARG:HG2	2.03	0.40
2:C:588:VAL:HG23	2:C:589:ARG:N	2.36	0.40
2:C:597:ALA:HB1	9:C:9597:HOH:O	2.21	0.40
2:C:77:PRO:HD2	2:C:91:GLN:O	2.21	0.40
2:C:811:PRO:HD3	9:C:2160:HOH:O	2.21	0.40
2:C:839:LEU:HB2	2:C:994:ILE:CG2	2.52	0.40
1:A:46:SER:HB3	2:C:856:GLU:CD	2.42	0.40
3:D:1047:LYS:HA	3:D:1053:PHE:CZ	2.57	0.40
3:D:1045:MET:CG	3:D:1073:SER:HA	2.29	0.40
3:D:50:PHE:HB3	3:D:522:PRO:HG2	2.03	0.40
5:F:161:GLN:NE2	9:F:9682:HOH:O	2.51	0.40
1:K:159:LYS:HD3	9:K:5879:HOH:O	2.21	0.40
1:L:176:ARG:HH22	3:N:884:ARG:HH21	1.68	0.40
2:M:114:PHE:HB2	9:M:9731:HOH:O	2.21	0.40
2:M:157:ARG:HD3	9:M:2062:HOH:O	2.22	0.40
2:M:690:ILE:CG2	2:M:852:ILE:HG13	2.51	0.40
3:N:147:VAL:HG13	9:N:9901:HOH:O	2.21	0.40
3:N:77:GLY:O	3:N:78:VAL:HG23	2.22	0.40
4:O:16:LYS:HG2	4:O:17:TYR:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:151:LEU:HB3	5:P:155:THR:H	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	8	14
1	B	227/315 (72%)	201 (88%)	21 (9%)	5 (2%)	6	10
1	K	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	8	14
1	L	227/315 (72%)	205 (90%)	18 (8%)	4 (2%)	8	14
2	C	1117/1119 (100%)	911 (82%)	153 (14%)	53 (5%)	2	2
2	M	1117/1119 (100%)	904 (81%)	168 (15%)	45 (4%)	3	3
3	D	1388/1524 (91%)	1112 (80%)	202 (15%)	74 (5%)	2	2
3	N	1388/1524 (91%)	1118 (80%)	195 (14%)	75 (5%)	2	2
4	E	93/99 (94%)	74 (80%)	15 (16%)	4 (4%)	2	3
4	O	93/99 (94%)	76 (82%)	13 (14%)	4 (4%)	2	3
5	F	341/423 (81%)	286 (84%)	40 (12%)	15 (4%)	2	3
5	P	341/423 (81%)	290 (85%)	37 (11%)	14 (4%)	3	3
All	All	6786/7590 (89%)	5585 (82%)	900 (13%)	301 (4%)	2	3

All (301) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE

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Mol	Chain	Res	Type
2	C	152	PRO
2	C	156	GLY
2	C	178	PRO
2	C	231	PRO
2	C	244	PRO
2	C	261	ILE
2	C	262	ALA
2	C	369	PRO
2	C	444	PRO
2	C	462	ASP
2	C	465	GLY
2	C	548	PRO
2	C	864	GLY
2	C	908	GLY
3	D	40	GLU
3	D	43	GLY
3	D	55	ASP
3	D	82	LYS
3	D	137	PRO
3	D	208	PRO
3	D	209	ARG
3	D	238	PRO
3	D	246	PRO
3	D	370	ALA
3	D	373	PRO
3	D	381	ALA
3	D	385	VAL
3	D	440	VAL
3	D	451	ASP
3	D	705	ALA
3	D	832	ARG
3	D	844	ALA
3	D	1028	ALA
3	D	1129	THR
3	D	1208	ASP
3	D	1243	THR
4	E	42	PRO
4	E	58	PRO
5	F	147	LEU
5	F	153	PRO
5	F	341	PRO
5	F	390	PHE

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Mol	Chain	Res	Type
1	K	29	GLU
1	L	29	GLU
2	M	152	PRO
2	M	178	PRO
2	M	231	PRO
2	M	244	PRO
2	M	261	ILE
2	M	262	ALA
2	M	290	LEU
2	M	369	PRO
2	M	444	PRO
2	M	462	ASP
2	M	465	GLY
2	M	548	PRO
2	M	864	GLY
2	M	908	GLY
3	N	40	GLU
3	N	43	GLY
3	N	55	ASP
3	N	137	PRO
3	N	208	PRO
3	N	209	ARG
3	N	217	LYS
3	N	238	PRO
3	N	246	PRO
3	N	370	ALA
3	N	373	PRO
3	N	385	VAL
3	N	440	VAL
3	N	451	ASP
3	N	705	ALA
3	N	832	ARG
3	N	844	ALA
3	N	1028	ALA
3	N	1125	PRO
3	N	1129	THR
3	N	1208	ASP
3	N	1243	THR
4	O	42	PRO
4	O	58	PRO
5	P	147	LEU
5	P	153	PRO

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Mol	Chain	Res	Type
5	P	390	PHE
1	B	187	GLY
2	C	59	LYS
2	C	170	PRO
2	C	268	ASP
2	C	288	ARG
2	C	290	LEU
2	C	363	SER
2	C	626	ARG
2	C	680	ASP
2	C	781	LYS
2	C	1004	LYS
2	C	1097	LEU
3	D	31	THR
3	D	98	PRO
3	D	120	ALA
3	D	165	LYS
3	D	231	VAL
3	D	415	VAL
3	D	417	PRO
3	D	504	ASP
3	D	594	PRO
3	D	609	GLY
3	D	803	GLY
3	D	822	ALA
3	D	1389	LEU
3	D	1441	GLN
4	E	53	GLY
5	F	324	GLU
5	F	326	ASP
5	F	420	ASP
1	K	187	GLY
1	L	187	GLY
2	M	59	LYS
2	M	156	GLY
2	M	164	PRO
2	M	170	PRO
2	M	268	ASP
2	M	288	ARG
2	M	363	SER
2	M	626	ARG
2	M	680	ASP

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Mol	Chain	Res	Type
2	M	705	ILE
2	M	727	PRO
2	M	781	LYS
3	N	31	THR
3	N	96	ALA
3	N	98	PRO
3	N	165	LYS
3	N	231	VAL
3	N	381	ALA
3	N	417	PRO
3	N	504	ASP
3	N	594	PRO
3	N	609	GLY
3	N	803	GLY
3	N	822	ALA
3	N	1342	GLU
3	N	1389	LEU
3	N	1441	GLN
3	N	1446	VAL
4	O	53	GLY
5	P	288	TYR
5	P	324	GLU
5	P	326	ASP
5	P	341	PRO
1	A	187	GLY
2	C	18	LEU
2	C	164	PRO
2	C	422	ARG
2	C	424	GLY
2	C	517	ARG
2	C	627	ARG
2	C	727	PRO
2	C	1106	ASP
3	D	37	LEU
3	D	96	ALA
3	D	162	ARG
3	D	170	PRO
3	D	217	LYS
3	D	387	LEU
3	D	424	GLY
3	D	522	PRO
3	D	539	ASP

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Mol	Chain	Res	Type
3	D	766	ALA
3	D	1020	LEU
3	D	1213	ARG
3	D	1446	VAL
5	F	232	ARG
5	F	259	ARG
5	F	288	TYR
2	M	422	ARG
2	M	517	ARG
2	M	1097	LEU
2	M	1106	ASP
3	N	37	LEU
3	N	83	SER
3	N	120	ALA
3	N	170	PRO
3	N	415	VAL
3	N	424	GLY
3	N	539	ASP
3	N	1019	PRO
3	N	1213	ARG
5	P	232	ARG
5	P	420	ASP
1	A	106	PRO
1	A	188	GLN
1	B	106	PRO
2	C	180	GLY
2	C	272	ALA
2	C	425	PHE
2	C	705	ILE
2	C	835	VAL
3	D	219	GLU
3	D	416	ALA
3	D	526	PRO
3	D	924	MET
3	D	1019	PRO
3	D	1248	GLY
3	D	1287	GLU
3	D	1288	GLU
3	D	1385	GLY
5	F	286	PRO
1	K	106	PRO
1	K	188	GLN

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Mol	Chain	Res	Type
2	M	74	GLY
2	M	180	GLY
2	M	272	ALA
2	M	425	PHE
3	N	82	LYS
3	N	219	GLU
3	N	387	LEU
3	N	416	ALA
3	N	522	PRO
3	N	696	HIS
3	N	833	GLU
3	N	1248	GLY
3	N	1268	PRO
3	N	1287	GLU
3	N	1385	GLY
5	P	97	GLU
5	P	286	PRO
2	C	40	GLU
2	C	74	GLY
2	C	144	PRO
2	C	400	PRO
3	D	696	HIS
3	D	808	THR
3	D	833	GLU
3	D	1197	ARG
3	D	1241	PHE
5	F	97	GLU
5	F	297	PRO
5	F	393	THR
1	L	106	PRO
2	M	40	GLU
2	M	223	ASP
2	M	415	PRO
2	M	443	THR
2	M	529	VAL
2	M	627	ARG
3	N	509	PRO
3	N	526	PRO
3	N	808	THR
3	N	924	MET
3	N	1064	GLY
5	P	297	PRO

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Mol	Chain	Res	Type
5	P	393	THR
1	B	188	GLN
2	C	80	GLN
2	C	443	THR
2	C	529	VAL
3	D	136	ASP
3	D	173	PRO
3	D	509	PRO
3	D	1064	GLY
3	D	1432	LYS
1	L	188	GLN
2	M	779	GLY
2	M	1079	PRO
3	N	173	PRO
3	N	533	GLY
3	N	766	ALA
3	N	1241	PHE
2	C	336	VAL
2	C	779	GLY
3	D	1349	VAL
3	N	1341	PRO
2	C	415	PRO
2	C	669	GLY
3	D	368	VAL
2	M	835	VAL
3	N	530	VAL
3	N	1050	GLY
3	N	1349	VAL
5	P	167	PRO
2	C	79	PRO
2	C	377	PRO
2	C	1079	PRO
3	D	407	VAL
3	D	530	VAL
3	D	670	VAL
3	D	1050	GLY
2	M	377	PRO
3	N	169	TYR
3	N	368	VAL
3	N	670	VAL
4	O	5	GLY
2	C	905	ILE

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Mol	Chain	Res	Type
4	E	5	GLY
5	F	167	PRO
2	M	79	PRO
3	N	136	ASP

### 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	202/273 (74%)	148 (73%)	54 (27%)	0	0
1	B	202/273 (74%)	164 (81%)	38 (19%)	1	2
1	K	202/273 (74%)	144 (71%)	58 (29%)	0	0
1	L	202/273 (74%)	159 (79%)	43 (21%)	1	2
2	C	941/941 (100%)	738 (78%)	203 (22%)	1	1
2	M	941/941 (100%)	737 (78%)	204 (22%)	1	1
3	D	1123/1279 (88%)	841 (75%)	282 (25%)	0	1
3	N	1123/1279 (88%)	865 (77%)	258 (23%)	1	1
4	E	83/87 (95%)	67 (81%)	16 (19%)	1	2
4	O	83/87 (95%)	61 (74%)	22 (26%)	0	0
5	F	295/370 (80%)	235 (80%)	60 (20%)	1	2
5	P	295/370 (80%)	247 (84%)	48 (16%)	2	4
All	All	5692/6446 (88%)	4406 (77%)	1286 (23%)	1	1

All (1286) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LYS
1	A	9	PRO
1	A	12	THR
1	A	15	THR
1	A	19	GLU

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Mol	Chain	Res	Type
1	A	20	TYR
1	A	26	GLU
1	A	32	PHE
1	A	34	VAL
1	A	40	LEU
1	A	44	LEU
1	A	47	SER
1	A	73	GLU
1	A	74	ASP
1	A	77	GLU
1	A	86	VAL
1	A	89	PHE
1	A	92	PRO
1	A	96	THR
1	A	101	LEU
1	A	104	GLU
1	A	112	ARG
1	A	113	ASP
1	A	119	ASP
1	A	120	VAL
1	A	121	GLU
1	A	126	ASP
1	A	127	LEU
1	A	137	ARG
1	A	139	ASN
1	A	142	VAL
1	A	145	ASP
1	A	156	HIS
1	A	161	ARG
1	A	163	ASN
1	A	167	VAL
1	A	168	ASP
1	A	170	VAL
1	A	176	ARG
1	A	180	GLN
1	A	183	ASP
1	A	186	LEU
1	A	188	GLN
1	A	191	ASP
1	A	193	ASP
1	A	197	LEU
1	A	206	THR

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Mol	Chain	Res	Type
1	A	211	LEU
1	A	216	GLU
1	A	222	LEU
1	A	223	THR
1	A	227	ASN
1	A	229	GLN
1	B	1	MET
1	B	5	LYS
1	B	7	LYS
1	B	25	LEU
1	B	26	GLU
1	B	29	GLU
1	B	65	PHE
1	B	68	ILE
1	B	73	GLU
1	B	77	GLU
1	B	80	LEU
1	B	81	ASN
1	B	87	VAL
1	B	88	ARG
1	B	89	PHE
1	B	92	PRO
1	B	94	LEU
1	B	95	GLN
1	B	96	THR
1	B	101	LEU
1	B	112	ARG
1	B	119	ASP
1	B	124	ASN
1	B	138	LEU
1	B	140	MET
1	B	141	GLU
1	B	148	VAL
1	B	159	LYS
1	B	176	ARG
1	B	180	GLN
1	B	196	THR
1	B	200	TRP
1	B	208	LEU
1	B	209	GLU
1	B	220	GLU
1	B	222	LEU

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Mol	Chain	Res	Type
1	B	224	TYR
1	B	227	ASN
2	C	1	MET
2	C	5	ARG
2	C	9	ILE
2	C	10	ARG
2	C	20	GLU
2	C	22	GLN
2	C	26	TYR
2	C	30	LEU
2	C	31	GLN
2	C	34	VAL
2	C	39	ARG
2	C	41	ASN
2	C	48	PHE
2	C	49	ARG
2	C	71	TYR
2	C	73	LEU
2	C	75	GLU
2	C	87	ASP
2	C	95	TYR
2	C	98	LEU
2	C	99	GLN
2	C	100	LEU
2	C	104	ASP
2	C	108	ILE
2	C	110	GLU
2	C	114	PHE
2	C	115	LEU
2	C	118	ILE
2	C	133	ASP
2	C	140	ILE
2	C	141	HIS
2	C	149	THR
2	C	152	PRO
2	C	157	ARG
2	C	158	TYR
2	C	163	ILE
2	C	168	ARG
2	C	170	PRO
2	C	178	PRO
2	C	184	MET

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Mol	Chain	Res	Type
2	C	193	LEU
2	C	198	ARG
2	C	205	GLU
2	C	209	ARG
2	C	211	LEU
2	C	216	GLU
2	C	221	LEU
2	C	223	ASP
2	C	229	MET
2	C	237	ARG
2	C	243	ARG
2	C	250	ARG
2	C	252	LYS
2	C	257	VAL
2	C	260	LEU
2	C	267	TYR
2	C	271	GLU
2	C	275	TYR
2	C	279	GLU
2	C	281	LEU
2	C	285	LEU
2	C	290	LEU
2	C	293	PHE
2	C	297	GLU
2	C	303	PHE
2	C	304	LEU
2	C	321	GLU
2	C	323	ASP
2	C	342	ASP
2	C	343	GLN
2	C	345	ARG
2	C	357	GLU
2	C	359	MET
2	C	360	LEU
2	C	365	ASP
2	C	371	LYS
2	C	384	GLU
2	C	388	ARG
2	C	392	SER
2	C	394	PHE
2	C	399	ASN
2	C	408	ARG

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Mol	Chain	Res	Type
2	C	413	LEU
2	C	419	THR
2	C	420	ARG
2	C	421	GLU
2	C	425	PHE
2	C	432	ARG
2	C	443	THR
2	C	448	ASN
2	C	451	LEU
2	C	452	ILE
2	C	460	ARG
2	C	474	VAL
2	C	479	VAL
2	C	482	GLU
2	C	486	MET
2	C	491	GLU
2	C	492	ASP
2	C	496	ILE
2	C	503	LEU
2	C	504	GLU
2	C	508	ILE
2	C	524	VAL
2	C	527	GLU
2	C	533	ASP
2	C	539	VAL
2	C	543	ASN
2	C	549	PHE
2	C	557	ARG
2	C	559	LEU
2	C	564	MET
2	C	565	GLN
2	C	571	LEU
2	C	620	LEU
2	C	622	GLU
2	C	633	GLN
2	C	640	ARG
2	C	645	VAL
2	C	650	ARG
2	C	654	LEU
2	C	655	LEU
2	C	657	ASP
2	C	668	LEU

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Mol	Chain	Res	Type
2	C	671	ASN
2	C	672	VAL
2	C	679	PHE
2	C	684	PHE
2	C	690	ILE
2	C	693	GLU
2	C	697	ARG
2	C	698	ASP
2	C	699	PHE
2	C	707	ARG
2	C	717	LEU
2	C	724	ARG
2	C	725	ASP
2	C	727	PRO
2	C	729	LEU
2	C	730	SER
2	C	737	LEU
2	C	740	GLU
2	C	744	ARG
2	C	750	LYS
2	C	775	ARG
2	C	780	GLU
2	C	785	VAL
2	C	791	ARG
2	C	794	PRO
2	C	799	ILE
2	C	802	ARG
2	C	804	VAL
2	C	808	ARG
2	C	814	GLU
2	C	821	GLU
2	C	829	GLN
2	C	834	GLN
2	C	837	ASP
2	C	839	LEU
2	C	841	ASN
2	C	857	ASP
2	C	858	MET
2	C	862	PRO
2	C	863	ASP
2	C	870	ILE
2	C	881	ASN

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Mol	Chain	Res	Type
2	C	882	LEU
2	C	900	ARG
2	C	901	TYR
2	C	904	PRO
2	C	905	ILE
2	C	907	ASP
2	C	923	GLU
2	C	925	TYR
2	C	929	ARG
2	C	932	GLU
2	C	934	PHE
2	C	937	ASP
2	C	950	LEU
2	C	952	LEU
2	C	953	VAL
2	C	958	THR
2	C	959	PRO
2	C	971	LYS
2	C	975	TYR
2	C	984	GLU
2	C	993	PHE
2	C	995	MET
2	C	1002	GLU
2	C	1008	ARG
2	C	1016	ILE
2	C	1017	THR
2	C	1019	GLN
2	C	1021	LEU
2	C	1035	MET
2	C	1036	GLU
2	C	1052	MET
2	C	1076	VAL
2	C	1079	PRO
2	C	1084	SER
2	C	1087	VAL
2	C	1092	LEU
2	C	1098	ASP
3	D	3	LYS
3	D	4	GLU
3	D	6	ARG
3	D	9	ARG
3	D	14	SER

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Mol	Chain	Res	Type
3	D	16	GLU
3	D	17	LYS
3	D	25	GLU
3	D	27	GLU
3	D	29	PRO
3	D	32	ILE
3	D	38	LYS
3	D	41	ARG
3	D	47	GLU
3	D	48	ARG
3	D	53	ILE
3	D	55	ASP
3	D	56	TYR
3	D	58	CYS
3	D	62	LYS
3	D	71	LYS
3	D	76	CYS
3	D	80	VAL
3	D	82	LYS
3	D	85	VAL
3	D	86	ARG
3	D	87	ARG
3	D	89	ARG
3	D	98	PRO
3	D	101	HIS
3	D	102	ILE
3	D	103	TRP
3	D	107	ASP
3	D	112	ILE
3	D	115	LEU
3	D	118	LEU
3	D	122	GLU
3	D	123	LEU
3	D	130	SER
3	D	133	ILE
3	D	145	VAL
3	D	153	LEU
3	D	155	ASP
3	D	156	GLU
3	D	162	ARG
3	D	166	GLN
3	D	170	PRO

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Mol	Chain	Res	Type
3	D	171	LEU
3	D	183	GLU
3	D	185	VAL
3	D	199	LEU
3	D	200	ASP
3	D	205	TYR
3	D	206	ARG
3	D	208	PRO
3	D	209	ARG
3	D	210	ARG
3	D	389	GLU
3	D	394	LEU
3	D	395	VAL
3	D	405	ASP
3	D	411	THR
3	D	413	ASP
3	D	421	LEU
3	D	432	TYR
3	D	444	VAL
3	D	445	ARG
3	D	455	ARG
3	D	456	MET
3	D	465	LEU
3	D	475	LYS
3	D	481	MET
3	D	482	LYS
3	D	483	HIS
3	D	493	ARG
3	D	494	LYS
3	D	502	PHE
3	D	504	ASP
3	D	513	ILE
3	D	521	PRO
3	D	525	ARG
3	D	529	GLN
3	D	531	ASP
3	D	535	PHE
3	D	537	THR
3	D	540	LEU
3	D	546	ARG
3	D	549	ASN
3	D	565	ILE

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Mol	Chain	Res	Type
3	D	571	LYS
3	D	573	MET
3	D	590	PRO
3	D	594	PRO
3	D	597	ASP
3	D	598	ARG
3	D	605	ASP
3	D	613	ARG
3	D	614	PHE
3	D	615	ARG
3	D	617	ASN
3	D	624	ASP
3	D	636	GLN
3	D	638	LYS
3	D	639	LEU
3	D	641	GLN
3	D	651	GLU
3	D	661	MET
3	D	666	ILE
3	D	668	PRO
3	D	675	ARG
3	D	676	MET
3	D	681	ARG
3	D	682	ASP
3	D	685	ASP
3	D	688	TRP
3	D	692	GLU
3	D	701	LEU
3	D	702	LEU
3	D	704	ARG
3	D	709	HIS
3	D	713	ILE
3	D	721	VAL
3	D	724	GLN
3	D	732	VAL
3	D	734	GLU
3	D	739	ASP
3	D	749	VAL
3	D	754	PHE
3	D	767	HIS
3	D	784	ASP
3	D	792	ILE

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Mol	Chain	Res	Type
3	D	793	THR
3	D	794	GLN
3	D	796	ARG
3	D	797	LYS
3	D	800	LYS
3	D	805	GLU
3	D	808	THR
3	D	828	LYS
3	D	829	VAL
3	D	832	ARG
3	D	833	GLU
3	D	838	ARG
3	D	847	ASP
3	D	848	GLU
3	D	851	LEU
3	D	858	VAL
3	D	863	VAL
3	D	864	VAL
3	D	865	THR
3	D	867	ARG
3	D	879	ARG
3	D	880	ILE
3	D	888	GLU
3	D	893	GLU
3	D	897	TRP
3	D	901	GLN
3	D	902	LEU
3	D	904	VAL
3	D	910	SER
3	D	914	LEU
3	D	916	TYR
3	D	920	LEU
3	D	922	LEU
3	D	927	THR
3	D	944	THR
3	D	951	ILE
3	D	957	PRO
3	D	959	GLU
3	D	972	LEU
3	D	983	LEU
3	D	984	THR
3	D	985	ASP

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Mol	Chain	Res	Type
3	D	987	GLU
3	D	988	ARG
3	D	1001	GLU
3	D	1020	LEU
3	D	1029	ARG
3	D	1038	LEU
3	D	1042	ARG
3	D	1045	MET
3	D	1049	SER
3	D	1051	GLU
3	D	1052	THR
3	D	1058	ARG
3	D	1060	SER
3	D	1062	ARG
3	D	1065	LEU
3	D	1068	LEU
3	D	1079	LYS
3	D	1084	THR
3	D	1087	ARG
3	D	1093	TYR
3	D	1095	THR
3	D	1096	ARG
3	D	1109	GLU
3	D	1112	CYS
3	D	1114	THR
3	D	1127	GLU
3	D	1129	THR
3	D	1130	ARG
3	D	1135	ARG
3	D	1152	GLU
3	D	1159	ARG
3	D	1160	LEU
3	D	1161	GLU
3	D	1164	ARG
3	D	1174	LEU
3	D	1176	LYS
3	D	1182	GLU
3	D	1183	ILE
3	D	1188	VAL
3	D	1191	PRO
3	D	1195	GLN
3	D	1197	ARG

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Mol	Chain	Res	Type
3	D	1207	TYR
3	D	1208	ASP
3	D	1210	SER
3	D	1213	ARG
3	D	1236	LEU
3	D	1238	MET
3	D	1242	HIS
3	D	1243	THR
3	D	1251	ASP
3	D	1252	ILE
3	D	1258	ARG
3	D	1260	ILE
3	D	1264	GLU
3	D	1267	ARG
3	D	1269	LYS
3	D	1274	ILE
3	D	1280	VAL
3	D	1285	GLU
3	D	1287	GLU
3	D	1288	GLU
3	D	1290	LEU
3	D	1295	GLU
3	D	1299	PHE
3	D	1302	GLU
3	D	1307	LYS
3	D	1310	ARG
3	D	1314	LYS
3	D	1318	TYR
3	D	1331	ASP
3	D	1336	LEU
3	D	1337	GLU
3	D	1344	VAL
3	D	1345	GLU
3	D	1346	ARG
3	D	1348	LEU
3	D	1350	GLU
3	D	1359	GLN
3	D	1363	LEU
3	D	1378	TYR
3	D	1382	THR
3	D	1389	LEU
3	D	1403	LEU

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Mol	Chain	Res	Type
3	D	1406	ARG
3	D	1415	VAL
3	D	1419	PRO
3	D	1420	LEU
3	D	1424	VAL
3	D	1431	THR
3	D	1432	LYS
3	D	1435	LEU
3	D	1439	SER
3	D	1440	PHE
3	D	1444	THR
3	D	1455	LYS
3	D	1460	ILE
3	D	1463	LYS
3	D	1464	GLU
3	D	1465	ASN
3	D	1466	VAL
3	D	1470	ARG
3	D	1479	ASP
3	D	1483	PHE
3	D	1485	GLN
3	D	1488	ASP
3	D	1491	THR
3	D	1492	LEU
3	D	1496	GLU
4	E	12	MET
4	E	14	ASP
4	E	28	GLN
4	E	31	LEU
4	E	33	HIS
4	E	40	LEU
4	E	42	PRO
4	E	43	GLU
4	E	45	ARG
4	E	52	GLU
4	E	56	ASP
4	E	57	ASP
4	E	61	GLU
4	E	67	GLU
4	E	75	PHE
4	E	81	PRO
5	F	75	ILE

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Mol	Chain	Res	Type
5	F	78	SER
5	F	80	PRO
5	F	83	GLN
5	F	84	TYR
5	F	87	GLU
5	F	91	VAL
5	F	101	GLU
5	F	120	THR
5	F	125	ASP
5	F	126	LEU
5	F	135	ILE
5	F	136	LEU
5	F	142	ARG
5	F	149	GLU
5	F	150	THR
5	F	154	LYS
5	F	161	GLN
5	F	174	LEU
5	F	181	GLU
5	F	187	LEU
5	F	192	LEU
5	F	209	PHE
5	F	212	LEU
5	F	220	LEU
5	F	225	GLU
5	F	228	GLU
5	F	233	PHE
5	F	240	THR
5	F	249	ARG
5	F	280	GLN
5	F	282	LEU
5	F	295	MET
5	F	297	PRO
5	F	302	LYS
5	F	306	GLU
5	F	313	GLU
5	F	316	SER
5	F	328	PHE
5	F	329	TYR
5	F	331	ASP
5	F	340	SER
5	F	341	PRO

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Mol	Chain	Res	Type
5	F	342	VAL
5	F	343	ASP
5	F	347	GLN
5	F	349	LEU
5	F	355	GLU
5	F	360	LYS
5	F	362	SER
5	F	365	GLU
5	F	370	LYS
5	F	393	THR
5	F	395	GLU
5	F	398	ARG
5	F	399	GLN
5	F	403	LYS
5	F	405	LEU
5	F	410	TYR
5	F	420	ASP
1	K	2	LEU
1	K	5	LYS
1	K	9	PRO
1	K	14	ARG
1	K	15	THR
1	K	16	GLN
1	K	18	ARG
1	K	26	GLU
1	K	30	ARG
1	K	44	LEU
1	K	45	LEU
1	K	54	THR
1	K	60	ASP
1	K	62	LEU
1	K	66	SER
1	K	73	GLU
1	K	76	VAL
1	K	80	LEU
1	K	88	ARG
1	K	89	PHE
1	K	90	LEU
1	K	92	PRO
1	K	94	LEU
1	K	101	LEU
1	K	108	GLU

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Mol	Chain	Res	Type
1	K	112	ARG
1	K	113	ASP
1	K	115	LEU
1	K	119	ASP
1	K	121	GLU
1	K	127	LEU
1	K	133	GLU
1	K	138	LEU
1	K	140	MET
1	K	142	VAL
1	K	143	ARG
1	K	146	ARG
1	K	156	HIS
1	K	160	ASP
1	K	161	ARG
1	K	165	ILE
1	K	167	VAL
1	K	176	ARG
1	K	179	PHE
1	K	180	GLN
1	K	184	THR
1	K	186	LEU
1	K	189	ARG
1	K	190	THR
1	K	196	THR
1	K	198	ARG
1	K	201	THR
1	K	211	LEU
1	K	216	GLU
1	K	219	ARG
1	K	223	THR
1	K	227	ASN
1	K	229	GLN
1	L	1	MET
1	L	2	LEU
1	L	3	ASP
1	L	5	LYS
1	L	7	LYS
1	L	9	PRO
1	L	19	GLU
1	L	25	LEU
1	L	29	GLU

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Mol	Chain	Res	Type
1	L	36	LEU
1	L	38	ASN
1	L	41	ARG
1	L	47	SER
1	L	55	SER
1	L	62	LEU
1	L	65	PHE
1	L	73	GLU
1	L	81	ASN
1	L	84	GLU
1	L	88	ARG
1	L	89	PHE
1	L	95	GLN
1	L	101	LEU
1	L	110	LYS
1	L	112	ARG
1	L	113	ASP
1	L	121	GLU
1	L	124	ASN
1	L	134	GLU
1	L	137	ARG
1	L	140	MET
1	L	145	ASP
1	L	146	ARG
1	L	159	LYS
1	L	160	ASP
1	L	162	ILE
1	L	182	GLU
1	L	191	ASP
1	L	197	LEU
1	L	204	SER
1	L	206	THR
1	L	213	GLN
1	L	227	ASN
2	M	5	ARG
2	M	9	ILE
2	M	22	GLN
2	M	27	ARG
2	M	30	LEU
2	M	31	GLN
2	M	39	ARG
2	M	42	VAL

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Mol	Chain	Res	Type
2	M	48	PHE
2	M	49	ARG
2	M	51	THR
2	M	71	TYR
2	M	82	GLU
2	M	91	GLN
2	M	95	TYR
2	M	98	LEU
2	M	102	HIS
2	M	103	LYS
2	M	104	ASP
2	M	107	LEU
2	M	111	ASP
2	M	114	PHE
2	M	115	LEU
2	M	117	HIS
2	M	123	GLU
2	M	133	ASP
2	M	140	ILE
2	M	141	HIS
2	M	143	SER
2	M	147	TYR
2	M	152	PRO
2	M	157	ARG
2	M	158	TYR
2	M	163	ILE
2	M	168	ARG
2	M	175	GLU
2	M	178	PRO
2	M	182	VAL
2	M	193	LEU
2	M	198	ARG
2	M	205	GLU
2	M	209	ARG
2	M	221	LEU
2	M	222	MET
2	M	229	MET
2	M	235	LEU
2	M	237	ARG
2	M	238	LEU
2	M	239	PHE
2	M	241	LEU

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Mol	Chain	Res	Type
2	M	243	ARG
2	M	251	ASP
2	M	252	LYS
2	M	254	VAL
2	M	257	VAL
2	M	260	LEU
2	M	267	TYR
2	M	269	LEU
2	M	279	GLU
2	M	290	LEU
2	M	293	PHE
2	M	294	GLU
2	M	297	GLU
2	M	303	PHE
2	M	304	LEU
2	M	309	TYR
2	M	313	LEU
2	M	321	GLU
2	M	322	VAL
2	M	327	HIS
2	M	333	ILE
2	M	335	THR
2	M	348	LEU
2	M	358	ARG
2	M	359	MET
2	M	360	LEU
2	M	365	ASP
2	M	367	LEU
2	M	371	LYS
2	M	388	ARG
2	M	393	GLN
2	M	397	GLU
2	M	399	ASN
2	M	400	PRO
2	M	413	LEU
2	M	420	ARG
2	M	422	ARG
2	M	425	PHE
2	M	426	ASP
2	M	429	ASP
2	M	443	THR
2	M	451	LEU

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Mol	Chain	Res	Type
2	M	452	ILE
2	M	455	LEU
2	M	460	ARG
2	M	469	THR
2	M	479	VAL
2	M	496	ILE
2	M	503	LEU
2	M	507	ARG
2	M	508	ILE
2	M	524	VAL
2	M	530	GLU
2	M	540	PHE
2	M	563	ASN
2	M	564	MET
2	M	579	VAL
2	M	584	GLU
2	M	586	ARG
2	M	588	VAL
2	M	606	VAL
2	M	607	ASP
2	M	620	LEU
2	M	626	ARG
2	M	630	ARG
2	M	633	GLN
2	M	635	THR
2	M	637	LEU
2	M	639	GLN
2	M	640	ARG
2	M	644	VAL
2	M	645	VAL
2	M	648	ARG
2	M	650	ARG
2	M	654	LEU
2	M	663	ASN
2	M	668	LEU
2	M	672	VAL
2	M	680	ASP
2	M	685	GLU
2	M	689	VAL
2	M	699	PHE
2	M	705	ILE
2	M	713	ARG

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Mol	Chain	Res	Type
2	M	714	ASP
2	M	716	LYS
2	M	717	LEU
2	M	727	PRO
2	M	729	LEU
2	M	737	LEU
2	M	748	GLU
2	M	753	ASP
2	M	765	SER
2	M	772	ARG
2	M	775	ARG
2	M	780	GLU
2	M	785	VAL
2	M	790	LEU
2	M	791	ARG
2	M	799	ILE
2	M	802	ARG
2	M	807	ARG
2	M	821	GLU
2	M	822	VAL
2	M	824	ARG
2	M	834	GLN
2	M	835	VAL
2	M	837	ASP
2	M	839	LEU
2	M	841	ASN
2	M	853	LEU
2	M	860	HIS
2	M	862	PRO
2	M	870	ILE
2	M	881	ASN
2	M	884	GLN
2	M	886	LEU
2	M	900	ARG
2	M	907	ASP
2	M	910	LYS
2	M	911	GLU
2	M	925	TYR
2	M	934	PHE
2	M	937	ASP
2	M	950	LEU
2	M	953	VAL

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Mol	Chain	Res	Type
2	M	958	THR
2	M	960	GLU
2	M	963	LEU
2	M	968	LEU
2	M	975	TYR
2	M	981	GLU
2	M	988	VAL
2	M	998	TYR
2	M	1000	MET
2	M	1002	GLU
2	M	1008	ARG
2	M	1016	ILE
2	M	1019	GLN
2	M	1035	MET
2	M	1051	GLU
2	M	1054	THR
2	M	1058	ASP
2	M	1067	TYR
2	M	1074	GLU
2	M	1079	PRO
2	M	1092	LEU
2	M	1098	ASP
2	M	1099	VAL
2	M	1100	GLN
2	M	1103	ASP
2	M	1109	VAL
2	M	1111	ILE
2	M	1118	LYS
3	N	3	LYS
3	N	4	GLU
3	N	6	ARG
3	N	12	LEU
3	N	15	PRO
3	N	22	SER
3	N	31	THR
3	N	32	ILE
3	N	34	TYR
3	N	36	THR
3	N	55	ASP
3	N	56	TYR
3	N	66	GLN
3	N	68	PHE

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Mol	Chain	Res	Type
3	N	71	LYS
3	N	76	CYS
3	N	80	VAL
3	N	82	LYS
3	N	86	ARG
3	N	87	ARG
3	N	95	LEU
3	N	101	HIS
3	N	102	ILE
3	N	103	TRP
3	N	107	ASP
3	N	108	VAL
3	N	112	ILE
3	N	123	LEU
3	N	127	LEU
3	N	128	TYR
3	N	133	ILE
3	N	142	LEU
3	N	145	VAL
3	N	152	LEU
3	N	153	LEU
3	N	159	ARG
3	N	160	GLU
3	N	162	ARG
3	N	166	GLN
3	N	168	THR
3	N	170	PRO
3	N	171	LEU
3	N	185	VAL
3	N	199	LEU
3	N	200	ASP
3	N	206	ARG
3	N	208	PRO
3	N	210	ARG
3	N	389	GLU
3	N	393	ILE
3	N	395	VAL
3	N	408	GLU
3	N	413	ASP
3	N	419	ASP
3	N	421	LEU
3	N	427	VAL

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Mol	Chain	Res	Type
3	N	429	SER
3	N	430	ASP
3	N	432	TYR
3	N	441	ARG
3	N	442	ASN
3	N	444	VAL
3	N	449	SER
3	N	450	TYR
3	N	453	ASP
3	N	455	ARG
3	N	456	MET
3	N	459	GLU
3	N	481	MET
3	N	486	ARG
3	N	488	ARG
3	N	493	ARG
3	N	494	LYS
3	N	502	PHE
3	N	518	PRO
3	N	530	VAL
3	N	535	PHE
3	N	551	ASN
3	N	554	LEU
3	N	571	LYS
3	N	581	LEU
3	N	584	ASN
3	N	594	PRO
3	N	597	ASP
3	N	598	ARG
3	N	602	SER
3	N	605	ASP
3	N	613	ARG
3	N	624	ASP
3	N	625	TYR
3	N	626	SER
3	N	639	LEU
3	N	641	GLN
3	N	651	GLU
3	N	669	ASN
3	N	676	MET
3	N	688	TRP
3	N	695	ILE

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Mol	Chain	Res	Type
3	N	701	LEU
3	N	702	LEU
3	N	704	ARG
3	N	710	ARG
3	N	713	ILE
3	N	717	GLN
3	N	734	GLU
3	N	739	ASP
3	N	741	ASP
3	N	749	VAL
3	N	754	PHE
3	N	758	GLU
3	N	770	LEU
3	N	778	LEU
3	N	780	LYS
3	N	781	PRO
3	N	783	ARG
3	N	786	ILE
3	N	787	LEU
3	N	792	ILE
3	N	794	GLN
3	N	796	ARG
3	N	797	LYS
3	N	799	LYS
3	N	800	LYS
3	N	804	LEU
3	N	805	GLU
3	N	824	ASN
3	N	828	LYS
3	N	829	VAL
3	N	833	GLU
3	N	841	TYR
3	N	846	PRO
3	N	851	LEU
3	N	863	VAL
3	N	865	THR
3	N	874	GLU
3	N	876	SER
3	N	879	ARG
3	N	880	ILE
3	N	886	VAL
3	N	888	GLU

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Mol	Chain	Res	Type
3	N	892	ASP
3	N	897	TRP
3	N	939	PHE
3	N	951	ILE
3	N	952	ASP
3	N	959	GLU
3	N	964	LEU
3	N	965	GLU
3	N	972	LEU
3	N	984	THR
3	N	988	ARG
3	N	990	ASP
3	N	994	GLN
3	N	1005	GLN
3	N	1029	ARG
3	N	1032	PRO
3	N	1042	ARG
3	N	1052	THR
3	N	1058	ARG
3	N	1060	SER
3	N	1062	ARG
3	N	1065	LEU
3	N	1068	LEU
3	N	1071	PHE
3	N	1084	THR
3	N	1087	ARG
3	N	1093	TYR
3	N	1095	THR
3	N	1096	ARG
3	N	1109	GLU
3	N	1112	CYS
3	N	1116	ASN
3	N	1119	SER
3	N	1120	VAL
3	N	1127	GLU
3	N	1129	THR
3	N	1130	ARG
3	N	1131	SER
3	N	1133	ARG
3	N	1134	LEU
3	N	1144	LEU
3	N	1151	ARG

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Mol	Chain	Res	Type
3	N	1161	GLU
3	N	1166	LEU
3	N	1169	ASP
3	N	1182	GLU
3	N	1183	ILE
3	N	1195	GLN
3	N	1202	GLN
3	N	1207	TYR
3	N	1210	SER
3	N	1219	GLU
3	N	1231	GLU
3	N	1238	MET
3	N	1239	ARG
3	N	1243	THR
3	N	1252	ILE
3	N	1254	GLN
3	N	1262	LEU
3	N	1264	GLU
3	N	1267	ARG
3	N	1278	ASP
3	N	1280	VAL
3	N	1284	GLU
3	N	1285	GLU
3	N	1287	GLU
3	N	1299	PHE
3	N	1301	LYS
3	N	1305	LEU
3	N	1306	PRO
3	N	1307	LYS
3	N	1314	LYS
3	N	1331	ASP
3	N	1332	PRO
3	N	1337	GLU
3	N	1344	VAL
3	N	1345	GLU
3	N	1346	ARG
3	N	1348	LEU
3	N	1350	GLU
3	N	1353	GLN
3	N	1355	VAL
3	N	1359	GLN
3	N	1362	LYS

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Mol	Chain	Res	Type
3	N	1365	ASP
3	N	1372	VAL
3	N	1373	ARG
3	N	1376	MET
3	N	1382	THR
3	N	1388	ARG
3	N	1396	GLU
3	N	1401	GLU
3	N	1415	VAL
3	N	1418	LYS
3	N	1419	PRO
3	N	1420	LEU
3	N	1424	VAL
3	N	1432	LYS
3	N	1433	SER
3	N	1435	LEU
3	N	1439	SER
3	N	1440	PHE
3	N	1441	GLN
3	N	1442	ASN
3	N	1447	LEU
3	N	1452	ILE
3	N	1460	ILE
3	N	1463	LYS
3	N	1465	ASN
3	N	1466	VAL
3	N	1467	ILE
3	N	1478	SER
3	N	1481	VAL
3	N	1483	PHE
3	N	1485	GLN
3	N	1488	ASP
3	N	1492	LEU
3	N	1501	GLU
4	O	6	ILE
4	O	10	PHE
4	O	12	MET
4	O	14	ASP
4	O	15	SER
4	O	28	GLN
4	O	32	ARG
4	O	42	PRO

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Mol	Chain	Res	Type
4	O	43	GLU
4	O	45	ARG
4	O	47	LYS
4	O	51	LEU
4	O	54	LEU
4	O	57	ASP
4	O	59	ASN
4	O	61	GLU
4	O	66	LYS
4	O	69	LEU
4	O	84	ARG
4	O	85	LEU
4	O	86	GLN
4	O	89	MET
5	P	83	GLN
5	P	84	TYR
5	P	85	LEU
5	P	86	HIS
5	P	87	GLU
5	P	90	GLN
5	P	91	VAL
5	P	96	LEU
5	P	108	GLU
5	P	125	ASP
5	P	126	LEU
5	P	135	ILE
5	P	142	ARG
5	P	150	THR
5	P	151	LEU
5	P	161	GLN
5	P	174	LEU
5	P	176	ILE
5	P	185	GLN
5	P	187	LEU
5	P	207	LEU
5	P	214	GLN
5	P	271	LEU
5	P	277	GLN
5	P	280	GLN
5	P	295	MET
5	P	300	ASP
5	P	307	THR

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Mol	Chain	Res	Type
5	P	317	LEU
5	P	318	GLU
5	P	325	LYS
5	P	328	PHE
5	P	336	GLU
5	P	337	HIS
5	P	341	PRO
5	P	347	GLN
5	P	349	LEU
5	P	350	LEU
5	P	353	GLU
5	P	358	LEU
5	P	365	GLU
5	P	370	LYS
5	P	393	THR
5	P	396	ARG
5	P	399	GLN
5	P	403	LYS
5	P	419	ARG
5	P	420	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (174) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	81	ASN
1	A	124	ASN
1	A	139	ASN
1	A	156	HIS
1	A	163	ASN
1	A	180	GLN
1	A	227	ASN
1	B	81	ASN
1	B	95	GLN
1	B	139	ASN
1	B	163	ASN
1	B	212	ASN
1	B	213	GLN
1	B	227	ASN
2	C	22	GLN
2	C	31	GLN
2	C	41	ASN

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Mol	Chain	Res	Type
2	C	117	HIS
2	C	130	ASN
2	C	204	GLN
2	C	343	GLN
2	C	374	ASN
2	C	399	ASN
2	C	431	HIS
2	C	538	GLN
2	C	545	ASN
2	C	563	ASN
2	C	632	ASN
2	C	639	GLN
2	C	663	ASN
2	C	670	GLN
2	C	671	ASN
2	C	728	HIS
2	C	834	GLN
2	C	841	ASN
2	C	881	ASN
2	C	889	HIS
2	C	899	GLN
2	C	920	GLN
2	C	969	GLN
2	C	1019	GLN
2	C	1047	HIS
2	C	1107	ASN
3	D	33	ASN
3	D	66	GLN
3	D	151	GLN
3	D	166	GLN
3	D	189	GLN
3	D	462	GLN
3	D	507	ASN
3	D	529	GLN
3	D	549	ASN
3	D	727	GLN
3	D	756	GLN
3	D	768	ASN
3	D	994	GLN
3	D	1010	ASN
3	D	1014	ASN
3	D	1033	GLN

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Mol	Chain	Res	Type
3	D	1103	HIS
3	D	1116	ASN
3	D	1124	GLN
3	D	1184	GLN
3	D	1323	GLN
3	D	1353	GLN
3	D	1359	GLN
3	D	1374	GLN
3	D	1404	ASN
3	D	1465	ASN
4	E	28	GLN
4	E	37	ASN
5	F	83	GLN
5	F	90	GLN
5	F	161	GLN
5	F	217	ASN
5	F	218	GLN
5	F	269	ASN
5	F	277	GLN
5	F	312	GLN
5	F	337	HIS
1	K	63	HIS
1	K	81	ASN
1	K	128	HIS
1	K	156	HIS
1	K	163	ASN
1	K	212	ASN
1	K	213	GLN
1	K	227	ASN
1	L	16	GLN
1	L	38	ASN
1	L	95	GLN
1	L	124	ASN
1	L	128	HIS
1	L	139	ASN
1	L	163	ASN
1	L	188	GLN
1	L	212	ASN
2	M	22	GLN
2	M	91	GLN
2	M	99	GLN
2	M	102	HIS

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Mol	Chain	Res	Type
2	M	117	HIS
2	M	139	GLN
2	M	204	GLN
2	M	327	HIS
2	M	330	ASN
2	M	431	HIS
2	M	434	HIS
2	M	448	ASN
2	M	506	ASN
2	M	552	HIS
2	M	563	ASN
2	M	609	ASN
2	M	633	GLN
2	M	663	ASN
2	M	671	ASN
2	M	834	GLN
2	M	841	ASN
2	M	843	HIS
2	M	881	ASN
2	M	920	GLN
2	M	969	GLN
2	M	1018	GLN
2	M	1019	GLN
2	M	1050	GLN
2	M	1100	GLN
2	M	1107	ASN
3	N	151	GLN
3	N	166	GLN
3	N	549	ASN
3	N	551	ASN
3	N	560	GLN
3	N	569	ASN
3	N	616	GLN
3	N	636	GLN
3	N	669	ASN
3	N	703	ASN
3	N	717	GLN
3	N	727	GLN
3	N	748	HIS
3	N	756	GLN
3	N	768	ASN
3	N	824	ASN

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Mol	Chain	Res	Type
3	N	845	ASN
3	N	855	HIS
3	N	909	ASN
3	N	917	GLN
3	N	976	GLN
3	N	994	GLN
3	N	1033	GLN
3	N	1103	HIS
3	N	1116	ASN
3	N	1124	GLN
3	N	1202	GLN
3	N	1323	GLN
3	N	1333	HIS
3	N	1334	GLN
3	N	1353	GLN
3	N	1359	GLN
3	N	1374	GLN
3	N	1404	ASN
3	N	1441	GLN
3	N	1465	ASN
3	N	1485	GLN
4	O	29	GLN
4	O	59	ASN
4	O	86	GLN
5	P	83	GLN
5	P	90	GLN
5	P	186	HIS
5	P	269	ASN
5	P	337	HIS
5	P	399	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 568 ligands modelled in this entry, 566 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
7	RBT	C	8001	6	61,66,66	2.90	22 (36%)	86,101,101	1.87	19 (22%)
7	RBT	M	8002	-	61,66,66	2.86	24 (39%)	86,101,101	1.95	18 (20%)

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
7	RBT	C	8001	6	-	18/59/116/116	0/5/6/6
7	RBT	M	8002	-	-	16/59/116/116	0/5/6/6

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	8001	RBT	C9-C8	8.84	1.58	1.41
7	M	8002	RBT	C9-C8	8.54	1.57	1.41
7	M	8002	RBT	C8-C7	7.03	1.54	1.40
7	C	8001	RBT	C8-C7	6.71	1.54	1.40
7	C	8001	RBT	C5-C6	6.59	1.48	1.39
7	C	8001	RBT	C10-C9	6.51	1.56	1.41
7	M	8002	RBT	C10-C9	6.22	1.55	1.41
7	M	8002	RBT	C5-C6	6.22	1.48	1.39
7	C	8001	RBT	O6-C27	5.87	1.58	1.43
7	M	8002	RBT	O6-C27	5.83	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	8002	RBT	O5-C29	5.38	1.53	1.39
7	C	8001	RBT	O5-C29	5.24	1.53	1.39
7	C	8001	RBT	C43-N4	5.17	1.56	1.47
7	C	8001	RBT	C10-C5	5.06	1.52	1.41
7	M	8002	RBT	O1-C1	4.98	1.33	1.23
7	C	8001	RBT	O1-C1	4.88	1.33	1.23
7	M	8002	RBT	C10-C5	4.68	1.52	1.41
7	C	8001	RBT	C42-N4	3.96	1.57	1.46
7	M	8002	RBT	C43-N4	3.91	1.54	1.47
7	M	8002	RBT	C42-N4	3.86	1.57	1.46
7	M	8002	RBT	C41-N4	3.78	1.57	1.46
7	C	8001	RBT	C41-N4	3.74	1.57	1.46
7	M	8002	RBT	C24-C25	3.72	1.63	1.54
7	C	8001	RBT	C24-C25	3.64	1.63	1.54
7	C	8001	RBT	O4-C11	3.63	1.27	1.21
7	M	8002	RBT	O5-C12	3.58	1.58	1.42
7	M	8002	RBT	O2-C8	-3.53	1.28	1.37
7	C	8001	RBT	O5-C12	3.17	1.56	1.42
7	M	8002	RBT	O4-C11	2.87	1.26	1.21
7	C	8001	RBT	O7-C25	2.86	1.49	1.44
7	C	8001	RBT	O2-C8	-2.69	1.30	1.37
7	C	8001	RBT	C27-C28	2.65	1.59	1.50
7	M	8002	RBT	C32-C22	2.60	1.58	1.53
7	M	8002	RBT	C27-C28	2.58	1.59	1.50
7	M	8002	RBT	C2-N1	2.54	1.46	1.41
7	C	8001	RBT	C9-C1	2.50	1.52	1.46
7	C	8001	RBT	O7-C35	2.49	1.40	1.35
7	M	8002	RBT	C18-C17	2.41	1.50	1.43
7	C	8001	RBT	O6-C37	2.29	1.50	1.42
7	C	8001	RBT	C32-C22	2.24	1.58	1.53
7	M	8002	RBT	O7-C25	2.24	1.48	1.44
7	M	8002	RBT	C9-C1	2.20	1.52	1.46
7	M	8002	RBT	C17-C16	2.18	1.40	1.34
7	M	8002	RBT	C5-C11	-2.06	1.40	1.46
7	M	8002	RBT	O7-C35	2.04	1.39	1.35
7	C	8001	RBT	C17-C16	2.02	1.40	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	8002	RBT	C42-C40-C38	7.37	122.58	112.64
7	C	8001	RBT	C42-C40-C38	7.35	122.55	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	8002	RBT	C41-C39-C38	7.18	122.32	112.64
7	C	8001	RBT	C41-C39-C38	7.09	122.20	112.64
7	M	8002	RBT	C39-C38-N3	-5.00	106.87	111.42
7	C	8001	RBT	O3-C6-C5	-4.81	111.08	114.36
7	M	8002	RBT	O3-C6-C5	-4.73	111.13	114.36
7	C	8001	RBT	C1-C2-N1	4.01	124.66	115.28
7	M	8002	RBT	C40-C38-N3	-3.91	107.86	111.42
7	M	8002	RBT	C1-C2-N1	3.84	124.27	115.28
7	C	8001	RBT	C24-C23-C22	3.50	121.28	115.43
7	M	8002	RBT	C20-C21-C22	3.25	121.59	114.96
7	C	8001	RBT	C39-C38-N3	-3.10	108.61	111.42
7	M	8002	RBT	C24-C23-C22	3.07	120.58	115.43
7	M	8002	RBT	C2-C3-N2	3.02	133.58	127.95
7	C	8001	RBT	C20-C21-C22	2.92	120.92	114.96
7	M	8002	RBT	C31-C20-C19	-2.91	102.95	109.99
7	C	8001	RBT	C9-C10-C5	-2.85	116.06	119.90
7	C	8001	RBT	O11-C15-N1	2.77	127.68	122.86
7	M	8002	RBT	C34-C26-C25	-2.76	106.45	111.40
7	M	8002	RBT	C9-C10-C5	-2.74	116.21	119.90
7	M	8002	RBT	C25-O7-C35	2.67	121.84	117.72
7	C	8001	RBT	C31-C20-C19	-2.59	103.72	109.99
7	M	8002	RBT	C5-C6-C7	2.56	127.34	125.33
7	C	8001	RBT	C5-C6-C7	2.55	127.33	125.33
7	C	8001	RBT	C25-O7-C35	2.52	121.62	117.72
7	C	8001	RBT	C40-C38-N3	-2.46	109.18	111.42
7	C	8001	RBT	C34-C26-C25	-2.36	107.17	111.40
7	C	8001	RBT	C2-C3-N2	2.24	132.13	127.95
7	M	8002	RBT	O11-C15-N1	2.23	126.74	122.86
7	C	8001	RBT	C37-O6-C27	2.19	118.27	113.01
7	C	8001	RBT	C32-C22-C23	-2.18	106.98	111.39
7	C	8001	RBT	C12-O5-C29	2.13	123.12	117.84
7	M	8002	RBT	C9-C8-C7	-2.05	118.96	122.33
7	M	8002	RBT	C18-C17-C16	2.04	132.59	126.61
7	C	8001	RBT	C26-C27-C28	2.03	116.56	112.13
7	M	8002	RBT	C31-C20-C21	2.02	115.53	111.31

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	8001	RBT	C1-C2-N1-C15
7	C	8001	RBT	C3-C2-N1-C15

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Mol	Chain	Res	Type	Atoms
7	C	8001	RBT	C16-C17-C18-C19
7	C	8001	RBT	C26-C27-C28-C29
7	C	8001	RBT	C26-C27-O6-C37
7	M	8002	RBT	C1-C2-N1-C15
7	M	8002	RBT	C26-C27-O6-C37
7	M	8002	RBT	N4-C43-C44-C46
7	C	8001	RBT	N4-C43-C44-C45
7	M	8002	RBT	N4-C43-C44-C45
7	C	8001	RBT	N4-C43-C44-C46
7	M	8002	RBT	C16-C17-C18-C19
7	C	8001	RBT	C19-C20-C21-C22
7	M	8002	RBT	C19-C20-C21-C22
7	M	8002	RBT	C31-C20-C21-C22
7	C	8001	RBT	C28-C27-O6-C37
7	M	8002	RBT	C28-C27-O6-C37
7	C	8001	RBT	C18-C19-C20-C31
7	C	8001	RBT	O6-C27-C28-C29
7	M	8002	RBT	O6-C27-C28-C29
7	C	8001	RBT	C23-C24-C25-C26
7	M	8002	RBT	C31-C20-C21-O10
7	C	8001	RBT	C33-C24-C25-C26
7	M	8002	RBT	C3-C2-N1-C15
7	C	8001	RBT	C44-C43-N4-C41
7	M	8002	RBT	C26-C27-C28-C29
7	M	8002	RBT	C44-C43-N4-C41
7	C	8001	RBT	C44-C43-N4-C42
7	M	8002	RBT	C44-C43-N4-C42
7	C	8001	RBT	C31-C20-C21-C22
7	C	8001	RBT	C18-C19-C20-C21
7	M	8002	RBT	C19-C20-C21-O10
7	C	8001	RBT	C28-C29-O5-C12
7	M	8002	RBT	C18-C19-C20-C31

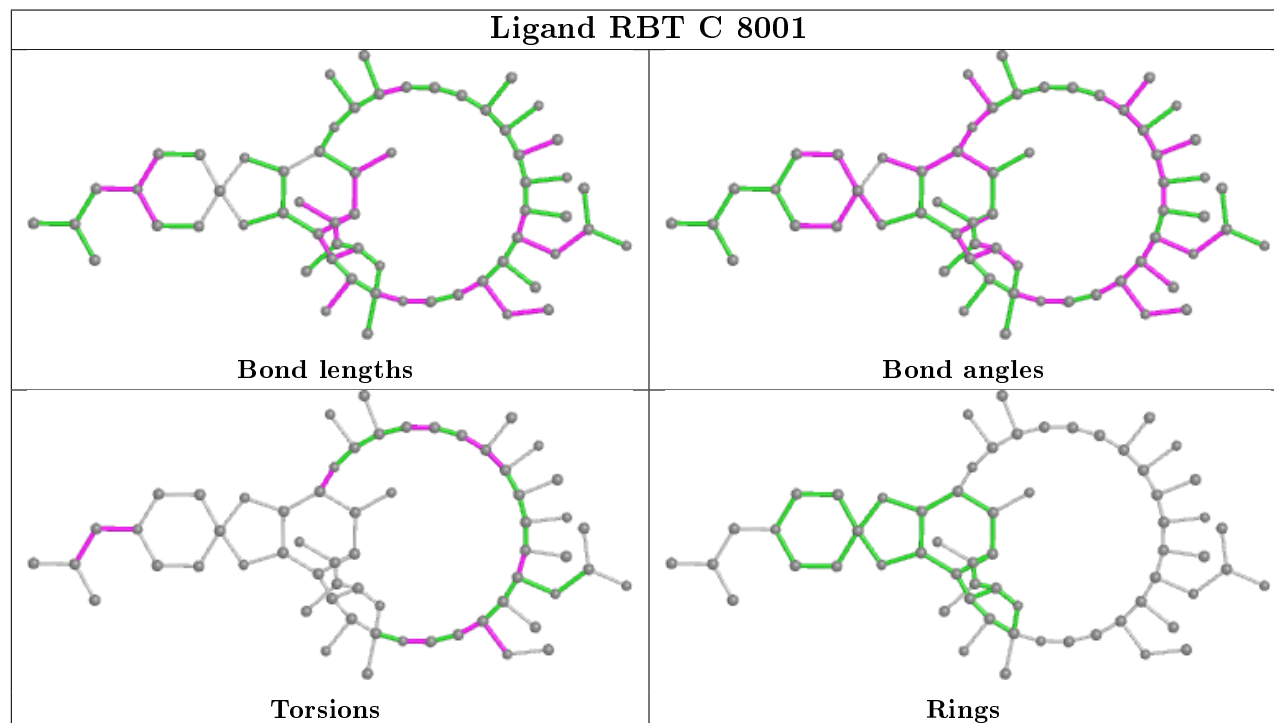
There are no ring outliers.

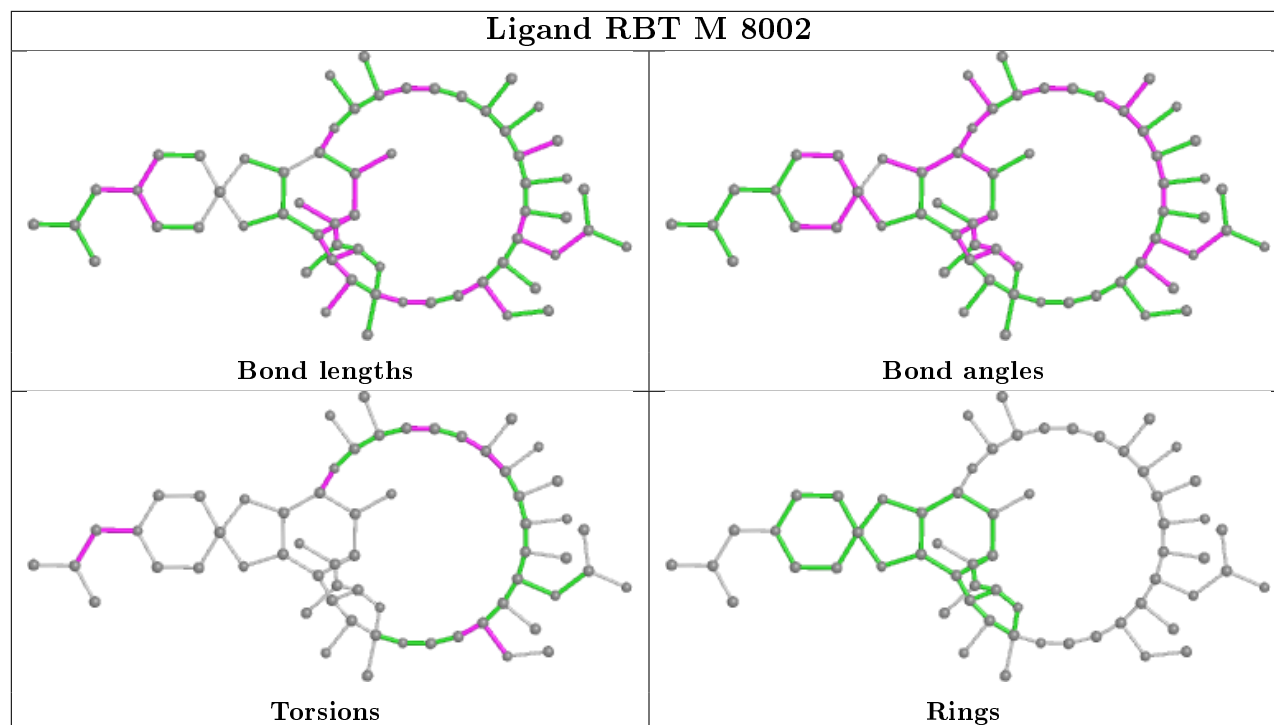
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	8001	RBT	3	0
7	M	8002	RBT	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	229/315 (72%)	-0.40	1 (0%) 92 93	29, 60, 84, 110	0
1	B	229/315 (72%)	-0.13	13 (5%) 23 25	44, 89, 114, 118	0
1	K	229/315 (72%)	-0.40	2 (0%) 84 86	33, 58, 89, 120	0
1	L	229/315 (72%)	-0.25	8 (3%) 44 47	49, 89, 109, 119	0
2	C	1119/1119 (100%)	-0.39	10 (0%) 84 86	14, 74, 102, 117	0
2	M	1119/1119 (100%)	-0.39	12 (1%) 80 82	19, 71, 103, 119	0
3	D	1392/1524 (91%)	-0.36	17 (1%) 79 80	19, 62, 107, 125	0
3	N	1392/1524 (91%)	-0.36	24 (1%) 70 72	23, 65, 107, 131	0
4	E	95/99 (95%)	-0.40	2 (2%) 63 66	41, 77, 107, 120	0
4	O	95/99 (95%)	-0.44	1 (1%) 80 82	33, 72, 94, 103	0
5	F	345/423 (81%)	-0.39	7 (2%) 65 68	46, 81, 104, 118	0
5	P	345/423 (81%)	-0.30	8 (2%) 60 63	53, 81, 108, 123	0
All	All	6818/7590 (89%)	-0.36	105 (1%) 73 75	14, 70, 105, 131	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	P	145	PRO	5.8
3	N	1243	THR	5.8
2	M	269	LEU	5.2
3	D	1244	GLY	4.8
3	D	1240	THR	4.8
1	B	130	ALA	4.7
1	L	6	LEU	4.5
3	N	802	ALA	4.5
1	L	135	GLY	4.4
3	N	1248	GLY	4.4
1	L	130	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
2	C	813	VAL	4.1
3	D	1238	MET	4.0
3	N	1241	PHE	4.0
3	N	1249	ALA	4.0
3	N	1398	TRP	3.9
3	D	177	ALA	3.8
3	D	1245	GLY	3.7
5	P	357	ALA	3.7
2	C	351	LEU	3.7
1	B	62	LEU	3.6
1	L	109	VAL	3.5
5	P	163	LEU	3.5
3	D	247	GLU	3.4
5	F	144	ILE	3.4
3	D	803	GLY	3.4
1	B	92	PRO	3.3
2	M	101	ILE	3.3
3	D	1241	PHE	3.3
3	N	242	LEU	3.3
3	N	369	ALA	3.2
3	N	1244	GLY	3.2
2	M	211	LEU	3.2
5	P	147	LEU	3.2
1	B	129	ILE	3.2
1	B	82	LEU	3.1
1	B	118	ALA	3.1
1	A	1	MET	3.1
3	N	205	TYR	3.1
3	D	802	ALA	3.0
3	N	178	LEU	3.0
3	N	1240	THR	3.0
2	C	311	PHE	2.9
3	D	244	GLU	2.9
1	L	1	MET	2.9
1	B	58	ILE	2.9
2	M	207	LEU	2.9
3	N	1242	HIS	2.9
2	C	819	VAL	2.8
1	B	93	SER	2.8
2	M	100	LEU	2.8
3	N	186	VAL	2.8
5	F	386	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	281	LEU	2.7
1	B	6	LEU	2.7
3	D	228	ALA	2.6
3	N	169	TYR	2.6
3	D	592	THR	2.6
1	L	82	LEU	2.6
2	C	38	LYS	2.6
2	C	153	ALA	2.5
2	C	180	GLY	2.5
3	N	381	ALA	2.5
3	N	379	ALA	2.5
2	M	186	VAL	2.5
2	C	333	ILE	2.5
3	D	1409	ALA	2.4
1	B	2	LEU	2.4
5	F	145	PRO	2.4
3	N	184	GLU	2.4
1	B	70	GLY	2.3
3	N	177	ALA	2.3
2	M	372	LEU	2.3
3	D	1243	THR	2.3
3	N	1246	VAL	2.3
3	N	1407	LEU	2.2
3	N	401	TYR	2.2
5	P	153	PRO	2.2
2	M	226	VAL	2.2
3	D	407	VAL	2.2
3	N	836	VAL	2.2
1	L	71	VAL	2.2
2	M	65	VAL	2.2
3	D	444	VAL	2.2
2	M	270	GLY	2.2
4	E	85	LEU	2.2
4	O	85	LEU	2.2
5	P	278	LEU	2.2
3	D	439	LEU	2.1
3	N	371	ILE	2.1
4	E	93	TYR	2.1
5	P	378	GLY	2.1
2	C	307	LEU	2.1
1	K	6	LEU	2.1
1	B	61	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	4	SER	2.0
5	F	147	LEU	2.0
5	F	139	ALA	2.0
5	P	90	GLN	2.0
2	M	217	LEU	2.0
1	L	11	PHE	2.0
5	F	388	ALA	2.0
5	F	130	VAL	2.0
1	B	78	ILE	2.0
2	M	152	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	B	9163	1/1	0.92	0.06	44,44,44,44	0
6	MG	N	9538	1/1	0.92	0.10	42,42,42,42	0
6	MG	L	9258	1/1	0.94	0.10	47,47,47,47	0
6	MG	M	9364	1/1	0.94	0.08	37,37,37,37	0
6	MG	F	9410	1/1	0.94	0.12	47,47,47,47	0
6	MG	N	9354	1/1	0.95	0.07	42,42,42,42	0
6	MG	N	9235	1/1	0.95	0.12	63,63,63,63	0
6	MG	C	9068	1/1	0.95	0.12	37,37,37,37	0
8	ZN	D	7058	1/1	0.95	0.07	100,100,100,100	0
6	MG	B	9199	1/1	0.95	0.10	52,52,52,52	0
6	MG	C	9398	1/1	0.95	0.10	44,44,44,44	0
6	MG	N	9250	1/1	0.95	0.16	61,61,61,61	0
6	MG	N	9503	1/1	0.96	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9349	1/1	0.96	0.06	37,37,37,37	0
6	MG	M	9261	1/1	0.96	0.10	45,45,45,45	0
6	MG	O	9359	1/1	0.96	0.08	57,57,57,57	0
6	MG	P	9322	1/1	0.96	0.12	43,43,43,43	0
6	MG	A	9062	1/1	0.96	0.11	45,45,45,45	0
6	MG	D	9084	1/1	0.96	0.10	47,47,47,47	0
6	MG	M	9383	1/1	0.96	0.09	46,46,46,46	0
6	MG	K	9257	1/1	0.96	0.12	57,57,57,57	0
6	MG	D	9147	1/1	0.96	0.09	40,40,40,40	0
6	MG	D	9520	1/1	0.96	0.14	46,46,46,46	0
6	MG	D	9155	1/1	0.96	0.12	56,56,56,56	0
6	MG	C	9190	1/1	0.96	0.07	40,40,40,40	0
6	MG	A	9514	1/1	0.96	0.12	42,42,42,42	0
7	RBT	M	8002	61/61	0.96	0.18	28,39,48,54	0
6	MG	F	9048	1/1	0.96	0.16	50,50,50,50	0
6	MG	D	9111	1/1	0.96	0.09	43,43,43,43	0
6	MG	N	9474	1/1	0.96	0.13	56,56,56,56	0
6	MG	M	9255	1/1	0.96	0.13	58,58,58,58	0
6	MG	C	9177	1/1	0.96	0.09	40,40,40,40	0
6	MG	N	9253	1/1	0.96	0.08	39,39,39,39	0
6	MG	A	9413	1/1	0.96	0.10	46,46,46,46	0
6	MG	M	9267	1/1	0.96	0.12	41,41,41,41	0
6	MG	M	9220	1/1	0.96	0.13	45,45,45,45	0
6	MG	C	9399	1/1	0.96	0.10	43,43,43,43	0
6	MG	K	9351	1/1	0.97	0.09	37,37,37,37	0
6	MG	M	9334	1/1	0.97	0.09	44,44,44,44	0
6	MG	N	9358	1/1	0.97	0.12	48,48,48,48	0
6	MG	N	9230	1/1	0.97	0.09	40,40,40,40	0
6	MG	E	9467	1/1	0.97	0.12	52,52,52,52	0
6	MG	M	9325	1/1	0.97	0.10	44,44,44,44	0
6	MG	A	9430	1/1	0.97	0.11	35,35,35,35	0
6	MG	N	9539	1/1	0.97	0.10	57,57,57,57	0
6	MG	D	9095	1/1	0.97	0.06	40,40,40,40	0
6	MG	D	9548	1/1	0.97	0.12	51,51,51,51	0
6	MG	D	9543	1/1	0.97	0.12	46,46,46,46	0
6	MG	D	9423	1/1	0.97	0.09	44,44,44,44	0
6	MG	D	9042	1/1	0.97	0.12	47,47,47,47	0
6	MG	P	9304	1/1	0.97	0.10	57,57,57,57	0
6	MG	M	9259	1/1	0.97	0.17	57,57,57,57	0
6	MG	C	9414	1/1	0.97	0.07	41,41,41,41	0
6	MG	N	9486	1/1	0.97	0.09	44,44,44,44	0
6	MG	D	9523	1/1	0.97	0.11	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9208	1/1	0.97	0.12	35,35,35,35	0
6	MG	C	9455	1/1	0.97	0.12	61,61,61,61	0
6	MG	N	9244	1/1	0.97	0.08	37,37,37,37	0
6	MG	A	9107	1/1	0.97	0.07	40,40,40,40	0
6	MG	A	9145	1/1	0.97	0.11	45,45,45,45	0
6	MG	D	9518	1/1	0.97	0.11	55,55,55,55	0
6	MG	M	9312	1/1	0.97	0.10	37,37,37,37	0
6	MG	K	9363	1/1	0.97	0.09	47,47,47,47	0
6	MG	C	9081	1/1	0.97	0.13	52,52,52,52	0
6	MG	N	9327	1/1	0.97	0.11	54,54,54,54	0
6	MG	L	9249	1/1	0.97	0.07	51,51,51,51	0
7	RBT	C	8001	61/61	0.97	0.19	25,37,42,48	0
6	MG	D	9096	1/1	0.97	0.14	43,43,43,43	0
6	MG	A	9559	1/1	0.97	0.12	45,45,45,45	0
6	MG	O	9209	1/1	0.97	0.11	37,37,37,37	0
6	MG	N	9246	1/1	0.97	0.13	49,49,49,49	0
6	MG	N	9555	1/1	0.97	0.11	56,56,56,56	0
6	MG	N	9247	1/1	0.97	0.08	29,29,29,29	0
6	MG	C	9023	1/1	0.97	0.09	44,44,44,44	0
6	MG	A	9050	1/1	0.97	0.10	41,41,41,41	0
6	MG	D	9066	1/1	0.97	0.11	49,49,49,49	0
6	MG	N	9508	1/1	0.97	0.11	41,41,41,41	0
6	MG	L	9346	1/1	0.97	0.14	52,52,52,52	0
6	MG	C	9047	1/1	0.97	0.06	47,47,47,47	0
6	MG	L	9483	1/1	0.97	0.15	44,44,44,44	0
6	MG	P	9284	1/1	0.97	0.10	51,51,51,51	0
6	MG	F	9010	1/1	0.97	0.17	57,57,57,57	0
6	MG	C	9156	1/1	0.97	0.12	43,43,43,43	0
6	MG	D	9152	1/1	0.97	0.11	32,32,32,32	0
6	MG	M	9348	1/1	0.97	0.11	63,63,63,63	0
6	MG	M	9473	1/1	0.97	0.11	42,42,42,42	0
6	MG	D	9026	1/1	0.97	0.12	37,37,37,37	0
6	MG	N	9551	1/1	0.97	0.08	40,40,40,40	0
6	MG	E	9184	1/1	0.97	0.16	48,48,48,48	0
6	MG	M	9332	1/1	0.97	0.13	54,54,54,54	0
6	MG	N	9554	1/1	0.97	0.11	45,45,45,45	0
6	MG	C	9192	1/1	0.97	0.10	55,55,55,55	0
6	MG	D	9067	1/1	0.97	0.12	49,49,49,49	0
6	MG	N	9381	1/1	0.97	0.07	35,35,35,35	0
6	MG	F	9461	1/1	0.97	0.12	52,52,52,52	0
6	MG	C	9549	1/1	0.98	0.11	48,48,48,48	0
6	MG	N	9490	1/1	0.98	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9498	1/1	0.98	0.09	45,45,45,45	0
6	MG	N	9207	1/1	0.98	0.10	30,30,30,30	0
6	MG	C	9007	1/1	0.98	0.11	34,34,34,34	0
6	MG	D	9172	1/1	0.98	0.10	35,35,35,35	0
6	MG	D	9401	1/1	0.98	0.12	40,40,40,40	0
6	MG	M	9283	1/1	0.98	0.14	35,35,35,35	0
6	MG	D	9202	1/1	0.98	0.18	61,61,61,61	0
6	MG	N	9342	1/1	0.98	0.07	48,48,48,48	0
6	MG	D	9445	1/1	0.98	0.13	48,48,48,48	0
6	MG	P	9558	1/1	0.98	0.09	44,44,44,44	0
6	MG	A	9097	1/1	0.98	0.09	41,41,41,41	0
6	MG	D	9123	1/1	0.98	0.14	37,37,37,37	0
6	MG	M	9347	1/1	0.98	0.11	37,37,37,37	0
6	MG	P	9541	1/1	0.98	0.10	44,44,44,44	0
6	MG	N	9365	1/1	0.98	0.12	43,43,43,43	0
6	MG	D	9466	1/1	0.98	0.10	57,57,57,57	0
6	MG	D	9168	1/1	0.98	0.06	38,38,38,38	0
6	MG	C	9546	1/1	0.98	0.06	49,49,49,49	0
6	MG	N	9314	1/1	0.98	0.11	38,38,38,38	0
6	MG	C	9124	1/1	0.98	0.08	33,33,33,33	0
6	MG	N	9301	1/1	0.98	0.08	50,50,50,50	0
6	MG	D	9003	1/1	0.98	0.06	43,43,43,43	0
6	MG	M	9377	1/1	0.98	0.12	39,39,39,39	0
6	MG	A	9001	1/1	0.98	0.18	26,26,26,26	0
6	MG	N	9295	1/1	0.98	0.05	48,48,48,48	0
6	MG	N	9504	1/1	0.98	0.10	32,32,32,32	0
6	MG	D	9002	1/1	0.98	0.16	29,29,29,29	0
6	MG	E	9131	1/1	0.98	0.08	47,47,47,47	0
6	MG	N	9297	1/1	0.98	0.13	48,48,48,48	0
6	MG	B	9092	1/1	0.98	0.11	50,50,50,50	0
6	MG	L	9505	1/1	0.98	0.10	58,58,58,58	0
6	MG	A	9078	1/1	0.98	0.13	34,34,34,34	0
6	MG	D	9424	1/1	0.98	0.14	50,50,50,50	0
6	MG	N	9313	1/1	0.98	0.09	39,39,39,39	0
6	MG	M	9478	1/1	0.98	0.06	35,35,35,35	0
6	MG	D	9449	1/1	0.98	0.07	29,29,29,29	0
6	MG	M	9219	1/1	0.98	0.10	39,39,39,39	0
6	MG	B	9101	1/1	0.98	0.08	40,40,40,40	0
6	MG	N	9242	1/1	0.98	0.12	36,36,36,36	0
6	MG	C	9515	1/1	0.98	0.08	41,41,41,41	0
6	MG	D	9397	1/1	0.98	0.12	31,31,31,31	0
6	MG	N	9319	1/1	0.98	0.11	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	9457	1/1	0.98	0.10	40,40,40,40	0
6	MG	M	9233	1/1	0.98	0.15	38,38,38,38	0
6	MG	C	9157	1/1	0.98	0.16	44,44,44,44	0
6	MG	B	9395	1/1	0.98	0.11	56,56,56,56	0
6	MG	C	9063	1/1	0.98	0.10	32,32,32,32	0
6	MG	P	9317	1/1	0.98	0.18	53,53,53,53	0
6	MG	D	9012	1/1	0.98	0.06	39,39,39,39	0
6	MG	B	9389	1/1	0.98	0.10	37,37,37,37	0
6	MG	N	9310	1/1	0.98	0.08	36,36,36,36	0
6	MG	D	9015	1/1	0.98	0.12	37,37,37,37	0
6	MG	K	9553	1/1	0.98	0.09	50,50,50,50	0
6	MG	D	9039	1/1	0.98	0.11	40,40,40,40	0
6	MG	E	9151	1/1	0.98	0.05	48,48,48,48	0
6	MG	C	9396	1/1	0.98	0.14	57,57,57,57	0
6	MG	K	9214	1/1	0.98	0.20	31,31,31,31	0
6	MG	N	9228	1/1	0.98	0.08	49,49,49,49	0
6	MG	D	9447	1/1	0.98	0.10	50,50,50,50	0
6	MG	M	9293	1/1	0.98	0.11	43,43,43,43	0
6	MG	N	9526	1/1	0.98	0.10	30,30,30,30	0
6	MG	D	9112	1/1	0.98	0.13	39,39,39,39	0
6	MG	F	9153	1/1	0.98	0.07	39,39,39,39	0
6	MG	F	9429	1/1	0.98	0.12	57,57,57,57	0
6	MG	D	9059	1/1	0.98	0.10	40,40,40,40	0
6	MG	D	9099	1/1	0.98	0.07	38,38,38,38	0
6	MG	D	9516	1/1	0.98	0.05	51,51,51,51	0
6	MG	D	9140	1/1	0.98	0.13	43,43,43,43	0
6	MG	C	9014	1/1	0.98	0.14	45,45,45,45	0
6	MG	N	9281	1/1	0.98	0.09	50,50,50,50	0
6	MG	C	9458	1/1	0.98	0.09	38,38,38,38	0
6	MG	A	9102	1/1	0.98	0.09	38,38,38,38	0
6	MG	K	9344	1/1	0.98	0.12	55,55,55,55	0
6	MG	C	9191	1/1	0.98	0.13	44,44,44,44	0
6	MG	N	9534	1/1	0.98	0.09	54,54,54,54	0
6	MG	L	9213	1/1	0.98	0.23	49,49,49,49	0
6	MG	C	9141	1/1	0.98	0.12	45,45,45,45	0
6	MG	N	9499	1/1	0.98	0.08	38,38,38,38	0
6	MG	M	9290	1/1	0.98	0.12	48,48,48,48	0
6	MG	M	9285	1/1	0.98	0.13	43,43,43,43	0
6	MG	N	9262	1/1	0.98	0.14	49,49,49,49	0
6	MG	D	9432	1/1	0.98	0.10	47,47,47,47	0
6	MG	M	9211	1/1	0.98	0.10	28,28,28,28	0
6	MG	D	9019	1/1	0.98	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	M	9540	1/1	0.98	0.16	63,63,63,63	0
6	MG	D	9110	1/1	0.98	0.13	38,38,38,38	0
6	MG	N	9315	1/1	0.98	0.11	41,41,41,41	0
6	MG	N	9245	1/1	0.98	0.12	28,28,28,28	0
6	MG	M	9276	1/1	0.98	0.14	54,54,54,54	0
6	MG	L	9311	1/1	0.98	0.07	33,33,33,33	0
6	MG	B	9419	1/1	0.98	0.11	46,46,46,46	0
6	MG	B	9079	1/1	0.98	0.11	28,28,28,28	0
6	MG	M	9485	1/1	0.98	0.06	42,42,42,42	0
6	MG	D	9041	1/1	0.98	0.10	32,32,32,32	0
6	MG	C	9083	1/1	0.98	0.11	48,48,48,48	0
6	MG	L	9378	1/1	0.98	0.14	47,47,47,47	0
6	MG	A	9522	1/1	0.98	0.11	57,57,57,57	0
6	MG	D	9009	1/1	0.98	0.12	53,53,53,53	0
6	MG	D	9057	1/1	0.98	0.11	33,33,33,33	0
6	MG	B	9427	1/1	0.98	0.11	42,42,42,42	0
6	MG	M	9557	1/1	0.98	0.09	54,54,54,54	0
6	MG	D	9036	1/1	0.98	0.13	41,41,41,41	0
6	MG	C	9076	1/1	0.98	0.11	37,37,37,37	0
6	MG	N	9266	1/1	0.98	0.08	36,36,36,36	0
6	MG	D	9104	1/1	0.98	0.09	35,35,35,35	0
6	MG	L	9532	1/1	0.98	0.08	51,51,51,51	0
6	MG	D	9451	1/1	0.98	0.09	37,37,37,37	0
6	MG	N	9341	1/1	0.98	0.13	38,38,38,38	0
6	MG	N	9506	1/1	0.98	0.10	56,56,56,56	0
6	MG	D	9034	1/1	0.98	0.16	37,37,37,37	0
6	MG	O	9362	1/1	0.98	0.04	49,49,49,49	0
6	MG	F	9206	1/1	0.98	0.12	33,33,33,33	0
6	MG	B	9148	1/1	0.98	0.15	54,54,54,54	0
6	MG	K	9217	1/1	0.98	0.06	36,36,36,36	0
6	MG	M	9229	1/1	0.98	0.09	35,35,35,35	0
6	MG	N	9338	1/1	0.98	0.12	42,42,42,42	0
6	MG	D	9055	1/1	0.98	0.09	51,51,51,51	0
6	MG	K	9484	1/1	0.98	0.11	30,30,30,30	0
6	MG	C	9183	1/1	0.98	0.16	44,44,44,44	0
6	MG	N	9529	1/1	0.98	0.08	55,55,55,55	0
6	MG	D	9108	1/1	0.98	0.11	51,51,51,51	0
6	MG	F	9167	1/1	0.98	0.12	59,59,59,59	0
6	MG	M	9488	1/1	0.98	0.12	42,42,42,42	0
6	MG	A	9109	1/1	0.98	0.09	33,33,33,33	0
6	MG	M	9350	1/1	0.98	0.09	37,37,37,37	0
6	MG	F	9448	1/1	0.98	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9292	1/1	0.98	0.16	52,52,52,52	0
6	MG	F	9437	1/1	0.98	0.09	47,47,47,47	0
6	MG	M	9309	1/1	0.98	0.15	35,35,35,35	0
6	MG	C	9406	1/1	0.98	0.10	47,47,47,47	0
6	MG	M	9227	1/1	0.98	0.10	44,44,44,44	0
6	MG	L	9556	1/1	0.98	0.09	58,58,58,58	0
6	MG	K	9367	1/1	0.98	0.09	38,38,38,38	0
6	MG	D	9441	1/1	0.98	0.10	46,46,46,46	0
6	MG	B	9150	1/1	0.98	0.10	43,43,43,43	0
6	MG	M	9243	1/1	0.98	0.11	45,45,45,45	0
6	MG	M	9298	1/1	0.98	0.12	43,43,43,43	0
6	MG	N	9232	1/1	0.98	0.10	33,33,33,33	0
6	MG	A	9165	1/1	0.98	0.11	65,65,65,65	0
6	MG	N	9288	1/1	0.98	0.10	33,33,33,33	0
6	MG	D	9517	1/1	0.99	0.09	45,45,45,45	0
6	MG	C	9521	1/1	0.99	0.12	45,45,45,45	0
6	MG	F	9072	1/1	0.99	0.07	40,40,40,40	0
6	MG	D	9446	1/1	0.99	0.10	36,36,36,36	0
6	MG	N	9256	1/1	0.99	0.09	41,41,41,41	0
6	MG	O	9355	1/1	0.99	0.14	36,36,36,36	0
6	MG	B	9137	1/1	0.99	0.09	35,35,35,35	0
6	MG	F	9135	1/1	0.99	0.14	42,42,42,42	0
6	MG	N	9379	1/1	0.99	0.06	56,56,56,56	0
6	MG	N	9475	1/1	0.99	0.07	43,43,43,43	0
6	MG	C	9088	1/1	0.99	0.12	36,36,36,36	0
6	MG	M	9340	1/1	0.99	0.10	43,43,43,43	0
6	MG	N	9280	1/1	0.99	0.09	34,34,34,34	0
6	MG	N	9218	1/1	0.99	0.12	32,32,32,32	0
6	MG	C	9462	1/1	0.99	0.12	50,50,50,50	0
6	MG	D	9454	1/1	0.99	0.08	42,42,42,42	0
6	MG	E	9438	1/1	0.99	0.10	38,38,38,38	0
6	MG	K	9265	1/1	0.99	0.13	37,37,37,37	0
6	MG	F	9054	1/1	0.99	0.07	37,37,37,37	0
6	MG	F	9197	1/1	0.99	0.10	39,39,39,39	0
6	MG	C	9422	1/1	0.99	0.13	41,41,41,41	0
6	MG	B	9180	1/1	0.99	0.09	36,36,36,36	0
6	MG	C	9029	1/1	0.99	0.12	36,36,36,36	0
6	MG	N	9273	1/1	0.99	0.17	30,30,30,30	0
6	MG	P	9274	1/1	0.99	0.11	45,45,45,45	0
6	MG	F	9435	1/1	0.99	0.08	40,40,40,40	0
6	MG	N	9376	1/1	0.99	0.13	31,31,31,31	0
6	MG	N	9226	1/1	0.99	0.07	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	9011	1/1	0.99	0.10	39,39,39,39	0
6	MG	N	9320	1/1	0.99	0.11	41,41,41,41	0
6	MG	N	9248	1/1	0.99	0.06	47,47,47,47	0
6	MG	E	9186	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9154	1/1	0.99	0.12	31,31,31,31	0
6	MG	C	9545	1/1	0.99	0.10	45,45,45,45	0
6	MG	D	9169	1/1	0.99	0.12	45,45,45,45	0
6	MG	L	9471	1/1	0.99	0.10	33,33,33,33	0
6	MG	M	9384	1/1	0.99	0.10	35,35,35,35	0
6	MG	P	9333	1/1	0.99	0.07	28,28,28,28	0
6	MG	D	9189	1/1	0.99	0.10	34,34,34,34	0
6	MG	M	9336	1/1	0.99	0.10	31,31,31,31	0
6	MG	M	9287	1/1	0.99	0.08	36,36,36,36	0
6	MG	D	9463	1/1	0.99	0.11	32,32,32,32	0
6	MG	F	9407	1/1	0.99	0.07	32,32,32,32	0
6	MG	D	9122	1/1	0.99	0.10	31,31,31,31	0
6	MG	D	9119	1/1	0.99	0.09	44,44,44,44	0
6	MG	B	9103	1/1	0.99	0.09	37,37,37,37	0
6	MG	D	9077	1/1	0.99	0.10	32,32,32,32	0
6	MG	C	9439	1/1	0.99	0.10	35,35,35,35	0
6	MG	N	9356	1/1	0.99	0.14	29,29,29,29	0
6	MG	P	9326	1/1	0.99	0.08	39,39,39,39	0
6	MG	M	9321	1/1	0.99	0.13	40,40,40,40	0
6	MG	P	9502	1/1	0.99	0.07	43,43,43,43	0
6	MG	D	9519	1/1	0.99	0.12	55,55,55,55	0
6	MG	A	9560	1/1	0.99	0.13	49,49,49,49	0
6	MG	C	9044	1/1	0.99	0.08	37,37,37,37	0
6	MG	L	9300	1/1	0.99	0.07	58,58,58,58	0
6	MG	D	9038	1/1	0.99	0.11	35,35,35,35	0
6	MG	C	9196	1/1	0.99	0.13	30,30,30,30	0
6	MG	C	9205	1/1	0.99	0.12	53,53,53,53	0
6	MG	C	9025	1/1	0.99	0.10	39,39,39,39	0
6	MG	D	9393	1/1	0.99	0.13	35,35,35,35	0
6	MG	F	9164	1/1	0.99	0.11	29,29,29,29	0
6	MG	B	9146	1/1	0.99	0.09	44,44,44,44	0
6	MG	N	9335	1/1	0.99	0.10	33,33,33,33	0
6	MG	B	9512	1/1	0.99	0.20	53,53,53,53	0
6	MG	E	9115	1/1	0.99	0.08	39,39,39,39	0
6	MG	C	9121	1/1	0.99	0.15	43,43,43,43	0
6	MG	D	9175	1/1	0.99	0.09	40,40,40,40	0
6	MG	F	9053	1/1	0.99	0.10	34,34,34,34	0
6	MG	D	9159	1/1	0.99	0.11	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	P	9329	1/1	0.99	0.07	46,46,46,46	0
6	MG	B	9391	1/1	0.99	0.12	27,27,27,27	0
6	MG	D	9100	1/1	0.99	0.07	31,31,31,31	0
6	MG	C	9415	1/1	0.99	0.11	38,38,38,38	0
6	MG	M	9251	1/1	0.99	0.13	33,33,33,33	0
6	MG	D	9021	1/1	0.99	0.12	34,34,34,34	0
6	MG	N	9375	1/1	0.99	0.10	43,43,43,43	0
6	MG	A	9178	1/1	0.99	0.09	28,28,28,28	0
6	MG	N	9307	1/1	0.99	0.09	38,38,38,38	0
6	MG	A	9411	1/1	0.99	0.10	31,31,31,31	0
6	MG	M	9481	1/1	0.99	0.09	37,37,37,37	0
6	MG	D	9561	1/1	0.99	0.06	38,38,38,38	0
8	ZN	N	7113	1/1	0.99	0.11	79,79,79,79	0
6	MG	D	9416	1/1	0.99	0.09	48,48,48,48	0
6	MG	D	9136	1/1	0.99	0.10	41,41,41,41	0
6	MG	D	9073	1/1	0.99	0.15	38,38,38,38	0
6	MG	N	9289	1/1	0.99	0.09	35,35,35,35	0
6	MG	C	9144	1/1	0.99	0.09	39,39,39,39	0
6	MG	D	9166	1/1	0.99	0.08	49,49,49,49	0
6	MG	D	9049	1/1	0.99	0.14	31,31,31,31	0
6	MG	D	9203	1/1	0.99	0.09	46,46,46,46	0
6	MG	N	9368	1/1	0.99	0.09	41,41,41,41	0
6	MG	A	9139	1/1	0.99	0.10	35,35,35,35	0
6	MG	C	9074	1/1	0.99	0.13	30,30,30,30	0
6	MG	N	9509	1/1	0.99	0.11	31,31,31,31	0
6	MG	D	9443	1/1	0.99	0.07	47,47,47,47	0
6	MG	C	9071	1/1	0.99	0.13	39,39,39,39	0
6	MG	C	9456	1/1	0.99	0.07	37,37,37,37	0
6	MG	C	9420	1/1	0.99	0.07	37,37,37,37	0
6	MG	M	9366	1/1	0.99	0.10	41,41,41,41	0
6	MG	C	9020	1/1	0.99	0.14	28,28,28,28	0
6	MG	E	9187	1/1	0.99	0.12	39,39,39,39	0
6	MG	A	9018	1/1	0.99	0.14	31,31,31,31	0
6	MG	D	9065	1/1	0.99	0.14	44,44,44,44	0
6	MG	L	9272	1/1	0.99	0.10	29,29,29,29	0
6	MG	D	9562	1/1	0.99	0.17	49,49,49,49	0
6	MG	M	9252	1/1	0.99	0.12	37,37,37,37	0
6	MG	M	9472	1/1	0.99	0.06	51,51,51,51	0
6	MG	D	9417	1/1	0.99	0.11	35,35,35,35	0
6	MG	P	9296	1/1	0.99	0.07	42,42,42,42	0
6	MG	D	9129	1/1	0.99	0.09	38,38,38,38	0
6	MG	F	9032	1/1	0.99	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	9428	1/1	0.99	0.12	42,42,42,42	0
6	MG	D	9094	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9090	1/1	0.99	0.11	48,48,48,48	0
6	MG	F	9035	1/1	0.99	0.10	40,40,40,40	0
6	MG	A	9394	1/1	0.99	0.10	46,46,46,46	0
6	MG	D	9544	1/1	0.99	0.11	49,49,49,49	0
6	MG	L	9271	1/1	0.99	0.09	39,39,39,39	0
6	MG	B	9033	1/1	0.99	0.10	44,44,44,44	0
6	MG	K	9496	1/1	0.99	0.09	42,42,42,42	0
6	MG	N	9316	1/1	0.99	0.09	32,32,32,32	0
6	MG	C	9028	1/1	0.99	0.07	41,41,41,41	0
6	MG	N	9476	1/1	0.99	0.06	44,44,44,44	0
6	MG	M	9222	1/1	0.99	0.09	33,33,33,33	0
6	MG	M	9323	1/1	0.99	0.10	37,37,37,37	0
6	MG	L	9236	1/1	0.99	0.08	41,41,41,41	0
6	MG	F	9045	1/1	0.99	0.10	40,40,40,40	0
6	MG	D	9016	1/1	0.99	0.07	38,38,38,38	0
6	MG	P	9536	1/1	0.99	0.07	41,41,41,41	0
6	MG	M	9361	1/1	0.99	0.10	51,51,51,51	0
6	MG	N	9282	1/1	0.99	0.06	38,38,38,38	0
6	MG	M	9500	1/1	0.99	0.09	46,46,46,46	0
6	MG	M	9268	1/1	0.99	0.11	37,37,37,37	0
6	MG	M	9385	1/1	0.99	0.10	29,29,29,29	0
6	MG	C	9130	1/1	0.99	0.14	42,42,42,42	0
6	MG	L	9345	1/1	0.99	0.12	42,42,42,42	0
6	MG	D	9460	1/1	0.99	0.14	38,38,38,38	0
6	MG	C	9198	1/1	0.99	0.11	36,36,36,36	0
6	MG	F	9513	1/1	0.99	0.14	43,43,43,43	0
6	MG	A	9194	1/1	0.99	0.09	40,40,40,40	0
6	MG	F	9465	1/1	0.99	0.06	36,36,36,36	0
6	MG	N	9291	1/1	0.99	0.15	55,55,55,55	0
6	MG	D	9093	1/1	0.99	0.11	34,34,34,34	0
6	MG	D	9060	1/1	0.99	0.11	35,35,35,35	0
6	MG	P	9353	1/1	0.99	0.11	44,44,44,44	0
6	MG	D	9091	1/1	0.99	0.14	47,47,47,47	0
6	MG	F	9525	1/1	0.99	0.08	54,54,54,54	0
6	MG	N	9277	1/1	0.99	0.09	37,37,37,37	0
6	MG	D	9425	1/1	0.99	0.09	44,44,44,44	0
6	MG	N	9215	1/1	0.99	0.10	40,40,40,40	0
6	MG	M	9216	1/1	0.99	0.12	44,44,44,44	0
6	MG	C	9431	1/1	0.99	0.06	42,42,42,42	0
6	MG	N	9270	1/1	0.99	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	M	9489	1/1	0.99	0.09	43,43,43,43	0
6	MG	P	9275	1/1	0.99	0.09	32,32,32,32	0
6	MG	A	9126	1/1	0.99	0.10	39,39,39,39	0
6	MG	N	9324	1/1	0.99	0.08	39,39,39,39	0
6	MG	C	9524	1/1	0.99	0.08	45,45,45,45	0
6	MG	D	9125	1/1	0.99	0.10	35,35,35,35	0
6	MG	A	9200	1/1	0.99	0.10	49,49,49,49	0
6	MG	C	9056	1/1	0.99	0.06	34,34,34,34	0
6	MG	D	9405	1/1	0.99	0.10	38,38,38,38	0
6	MG	C	9193	1/1	0.99	0.09	37,37,37,37	0
6	MG	M	9373	1/1	0.99	0.12	38,38,38,38	0
6	MG	L	9479	1/1	0.99	0.10	48,48,48,48	0
6	MG	E	9402	1/1	0.99	0.12	39,39,39,39	0
6	MG	M	9497	1/1	0.99	0.12	43,43,43,43	0
6	MG	N	9221	1/1	0.99	0.10	30,30,30,30	0
6	MG	A	9024	1/1	0.99	0.10	29,29,29,29	0
6	MG	C	9098	1/1	0.99	0.09	52,52,52,52	0
6	MG	L	9530	1/1	0.99	0.10	58,58,58,58	0
6	MG	F	9133	1/1	0.99	0.10	42,42,42,42	0
6	MG	D	9403	1/1	0.99	0.16	30,30,30,30	0
6	MG	K	9493	1/1	0.99	0.09	38,38,38,38	0
6	MG	P	9240	1/1	0.99	0.11	38,38,38,38	0
6	MG	A	9440	1/1	0.99	0.10	53,53,53,53	0
6	MG	D	9418	1/1	0.99	0.08	47,47,47,47	0
6	MG	M	9224	1/1	0.99	0.06	38,38,38,38	0
6	MG	C	9170	1/1	0.99	0.10	36,36,36,36	0
6	MG	C	9185	1/1	0.99	0.18	60,60,60,60	0
6	MG	D	9452	1/1	0.99	0.10	32,32,32,32	0
6	MG	D	9128	1/1	0.99	0.11	35,35,35,35	0
6	MG	D	9070	1/1	0.99	0.10	46,46,46,46	0
6	MG	D	9052	1/1	0.99	0.09	36,36,36,36	0
6	MG	C	9408	1/1	0.99	0.12	38,38,38,38	0
6	MG	K	9492	1/1	0.99	0.10	40,40,40,40	0
6	MG	A	9173	1/1	0.99	0.10	41,41,41,41	0
6	MG	N	9343	1/1	0.99	0.09	45,45,45,45	0
6	MG	N	9237	1/1	0.99	0.14	40,40,40,40	0
6	MG	N	9305	1/1	0.99	0.09	42,42,42,42	0
6	MG	B	9442	1/1	0.99	0.12	47,47,47,47	0
6	MG	C	9161	1/1	0.99	0.07	40,40,40,40	0
6	MG	N	9386	1/1	0.99	0.08	46,46,46,46	0
6	MG	C	9171	1/1	0.99	0.09	33,33,33,33	0
6	MG	L	9374	1/1	0.99	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9459	1/1	0.99	0.10	33,33,33,33	0
6	MG	L	9234	1/1	0.99	0.07	41,41,41,41	0
6	MG	D	9082	1/1	0.99	0.11	30,30,30,30	0
6	MG	N	9550	1/1	0.99	0.09	34,34,34,34	0
6	MG	D	9436	1/1	0.99	0.09	46,46,46,46	0
6	MG	N	9501	1/1	0.99	0.08	47,47,47,47	0
6	MG	D	9120	1/1	0.99	0.07	34,34,34,34	0
6	MG	M	9382	1/1	0.99	0.09	33,33,33,33	0
6	MG	N	9357	1/1	0.99	0.09	41,41,41,41	0
6	MG	D	9158	1/1	0.99	0.08	31,31,31,31	0
6	MG	N	9286	1/1	0.99	0.12	46,46,46,46	0
6	MG	D	9142	1/1	0.99	0.11	40,40,40,40	0
8	ZN	D	7112	1/1	0.99	0.13	72,72,72,72	0
6	MG	D	9174	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9433	1/1	0.99	0.12	46,46,46,46	0
6	MG	D	9051	1/1	0.99	0.07	36,36,36,36	0
6	MG	D	9181	1/1	0.99	0.06	36,36,36,36	0
6	MG	C	9113	1/1	0.99	0.16	47,47,47,47	0
6	MG	A	9116	1/1	0.99	0.12	47,47,47,47	0
6	MG	D	9132	1/1	0.99	0.10	33,33,33,33	0
6	MG	K	9507	1/1	0.99	0.14	45,45,45,45	0
6	MG	C	9031	1/1	0.99	0.12	43,43,43,43	0
6	MG	N	9263	1/1	0.99	0.08	37,37,37,37	0
6	MG	N	9371	1/1	0.99	0.10	30,30,30,30	0
6	MG	M	9318	1/1	0.99	0.14	51,51,51,51	0
6	MG	M	9328	1/1	0.99	0.09	48,48,48,48	0
6	MG	N	9294	1/1	0.99	0.07	49,49,49,49	0
6	MG	M	9210	1/1	0.99	0.13	35,35,35,35	0
6	MG	M	9369	1/1	0.99	0.09	35,35,35,35	0
6	MG	F	9542	1/1	0.99	0.19	50,50,50,50	0
6	MG	C	9005	1/1	0.99	0.08	31,31,31,31	0
6	MG	C	9204	1/1	0.99	0.12	41,41,41,41	0
6	MG	L	9480	1/1	0.99	0.13	36,36,36,36	0
6	MG	D	9138	1/1	0.99	0.12	38,38,38,38	0
6	MG	B	9434	1/1	0.99	0.11	35,35,35,35	0
6	MG	K	9279	1/1	0.99	0.11	36,36,36,36	0
6	MG	P	9388	1/1	0.99	0.08	45,45,45,45	0
6	MG	M	9223	1/1	0.99	0.10	48,48,48,48	0
6	MG	D	9134	1/1	0.99	0.10	40,40,40,40	0
6	MG	N	9238	1/1	0.99	0.16	29,29,29,29	0
6	MG	L	9260	1/1	0.99	0.09	41,41,41,41	0
6	MG	M	9535	1/1	0.99	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	A	9117	1/1	0.99	0.07	32,32,32,32	0
6	MG	M	9537	1/1	0.99	0.13	38,38,38,38	0
6	MG	K	9370	1/1	0.99	0.06	46,46,46,46	0
6	MG	D	9118	1/1	0.99	0.12	34,34,34,34	0
6	MG	D	9085	1/1	0.99	0.10	32,32,32,32	0
6	MG	N	9533	1/1	0.99	0.12	33,33,33,33	0
6	MG	F	9089	1/1	0.99	0.10	48,48,48,48	0
6	MG	C	9004	1/1	0.99	0.09	30,30,30,30	0
6	MG	D	9061	1/1	0.99	0.11	35,35,35,35	0
6	MG	M	9372	1/1	0.99	0.09	47,47,47,47	0
6	MG	D	9017	1/1	0.99	0.07	37,37,37,37	0
6	MG	P	9269	1/1	0.99	0.09	41,41,41,41	0
6	MG	D	9008	1/1	0.99	0.13	37,37,37,37	0
6	MG	D	9058	1/1	0.99	0.11	41,41,41,41	0
6	MG	N	9482	1/1	0.99	0.14	52,52,52,52	0
6	MG	D	9464	1/1	0.99	0.12	38,38,38,38	0
6	MG	C	9426	1/1	0.99	0.06	47,47,47,47	0
6	MG	K	9487	1/1	0.99	0.12	36,36,36,36	0
6	MG	P	9494	1/1	0.99	0.10	50,50,50,50	0
6	MG	N	9552	1/1	0.99	0.11	46,46,46,46	0
6	MG	N	9303	1/1	0.99	0.12	35,35,35,35	0
6	MG	D	9114	1/1	0.99	0.10	32,32,32,32	0
6	MG	D	9162	1/1	0.99	0.11	44,44,44,44	0
6	MG	L	9330	1/1	0.99	0.09	41,41,41,41	0
6	MG	N	9387	1/1	0.99	0.07	28,28,28,28	0
6	MG	D	9105	1/1	0.99	0.07	48,48,48,48	0
6	MG	M	9254	1/1	0.99	0.08	34,34,34,34	0
6	MG	C	9046	1/1	0.99	0.09	31,31,31,31	0
6	MG	D	9392	1/1	0.99	0.09	46,46,46,46	0
6	MG	C	9444	1/1	0.99	0.09	40,40,40,40	0
6	MG	A	9412	1/1	0.99	0.12	33,33,33,33	0
6	MG	B	9040	1/1	0.99	0.16	29,29,29,29	0
6	MG	B	9450	1/1	0.99	0.08	46,46,46,46	0
6	MG	N	9225	1/1	0.99	0.08	40,40,40,40	0
6	MG	N	9306	1/1	0.99	0.13	30,30,30,30	0
6	MG	N	9339	1/1	0.99	0.11	34,34,34,34	0
6	MG	C	9400	1/1	0.99	0.12	49,49,49,49	0
6	MG	D	9064	1/1	0.99	0.11	41,41,41,41	0
6	MG	D	9188	1/1	0.99	0.09	37,37,37,37	0
6	MG	K	9495	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9075	1/1	0.99	0.11	39,39,39,39	0
6	MG	N	9352	1/1	0.99	0.05	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	F	9080	1/1	0.99	0.12	30,30,30,30	0
6	MG	C	9086	1/1	0.99	0.10	34,34,34,34	0
6	MG	C	9022	1/1	0.99	0.12	28,28,28,28	0
6	MG	N	9528	1/1	0.99	0.10	40,40,40,40	0
6	MG	C	9409	1/1	0.99	0.12	49,49,49,49	0
6	MG	C	9201	1/1	0.99	0.08	45,45,45,45	0
6	MG	D	9037	1/1	1.00	0.08	31,31,31,31	0
6	MG	C	9390	1/1	1.00	0.12	30,30,30,30	0
6	MG	B	9176	1/1	1.00	0.09	41,41,41,41	0
8	ZN	N	7059	1/1	1.00	0.12	83,83,83,83	0
6	MG	D	9195	1/1	1.00	0.08	32,32,32,32	0
6	MG	E	9511	1/1	1.00	0.12	42,42,42,42	0
6	MG	L	9299	1/1	1.00	0.07	36,36,36,36	0
6	MG	D	9510	1/1	1.00	0.12	51,51,51,51	0
6	MG	D	9043	1/1	1.00	0.11	28,28,28,28	0
6	MG	F	9547	1/1	1.00	0.09	52,52,52,52	0
6	MG	N	9527	1/1	1.00	0.14	42,42,42,42	0
6	MG	N	9531	1/1	1.00	0.10	38,38,38,38	0
6	MG	F	9030	1/1	1.00	0.11	36,36,36,36	0
6	MG	D	9006	1/1	1.00	0.14	30,30,30,30	0
6	MG	P	9239	1/1	1.00	0.11	33,33,33,33	0
6	MG	K	9264	1/1	1.00	0.09	36,36,36,36	0
6	MG	N	9308	1/1	1.00	0.12	31,31,31,31	0
6	MG	D	9453	1/1	1.00	0.12	31,31,31,31	0
6	MG	O	9337	1/1	1.00	0.08	34,34,34,34	0
6	MG	D	9182	1/1	1.00	0.07	46,46,46,46	0
6	MG	D	9087	1/1	1.00	0.09	27,27,27,27	0
6	MG	N	9302	1/1	1.00	0.14	48,48,48,48	0
6	MG	N	9468	1/1	1.00	0.11	35,35,35,35	0
6	MG	N	9470	1/1	1.00	0.15	27,27,27,27	0
6	MG	N	9360	1/1	1.00	0.05	39,39,39,39	0
6	MG	C	9160	1/1	1.00	0.12	46,46,46,46	0
6	MG	N	9491	1/1	1.00	0.11	43,43,43,43	0
6	MG	M	9380	1/1	1.00	0.08	32,32,32,32	0
6	MG	M	9241	1/1	1.00	0.09	35,35,35,35	0
6	MG	K	9212	1/1	1.00	0.08	33,33,33,33	0
6	MG	F	9421	1/1	1.00	0.13	30,30,30,30	0
6	MG	L	9278	1/1	1.00	0.08	46,46,46,46	0
6	MG	A	9404	1/1	1.00	0.16	55,55,55,55	0
6	MG	D	9149	1/1	1.00	0.13	42,42,42,42	0
6	MG	C	9027	1/1	1.00	0.12	28,28,28,28	0
6	MG	C	9106	1/1	1.00	0.09	37,37,37,37	0

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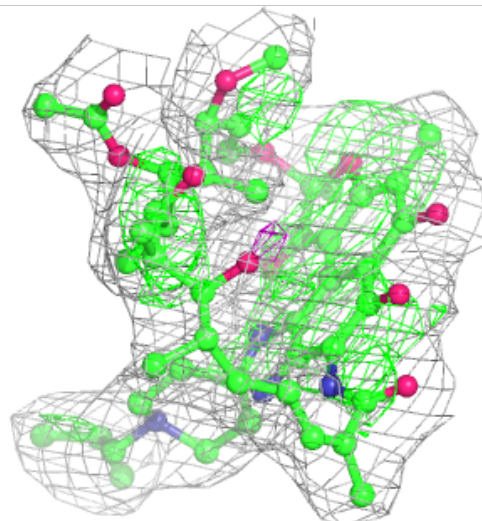
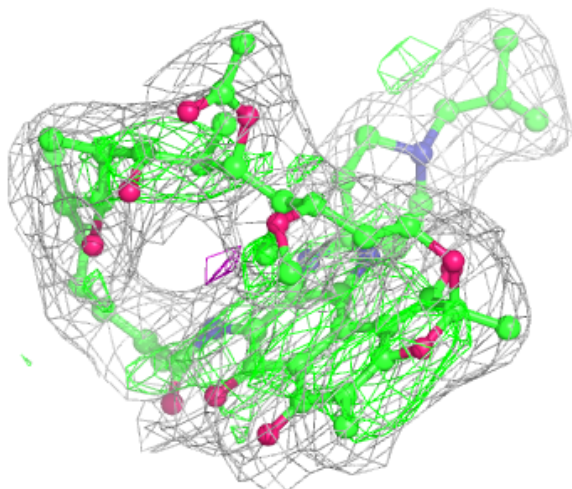
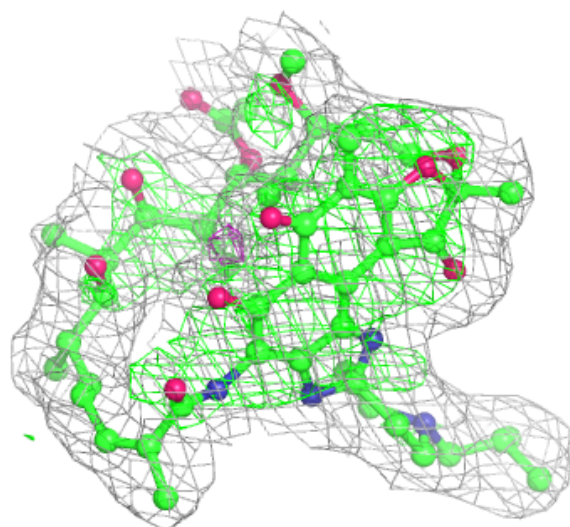
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	O	9231	1/1	1.00	0.15	41,41,41,41	0
6	MG	D	9179	1/1	1.00	0.09	30,30,30,30	0
6	MG	M	9469	1/1	1.00	0.14	39,39,39,39	0
6	MG	D	9069	1/1	1.00	0.12	32,32,32,32	0
6	MG	K	9477	1/1	1.00	0.11	38,38,38,38	0
6	MG	M	9331	1/1	1.00	0.08	49,49,49,49	0
6	MG	C	9127	1/1	1.00	0.10	41,41,41,41	0
6	MG	D	9143	1/1	1.00	0.14	35,35,35,35	0
6	MG	D	9013	1/1	1.00	0.09	34,34,34,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

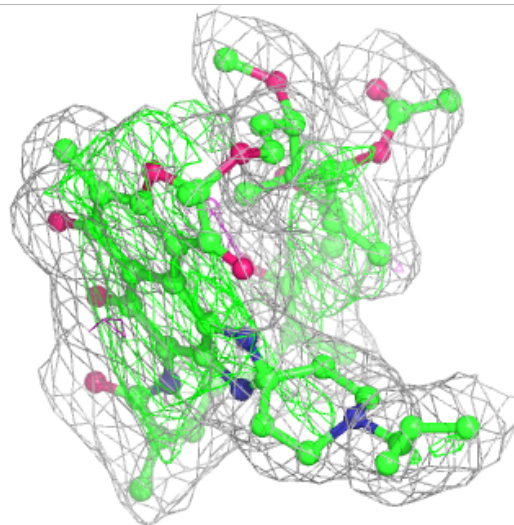
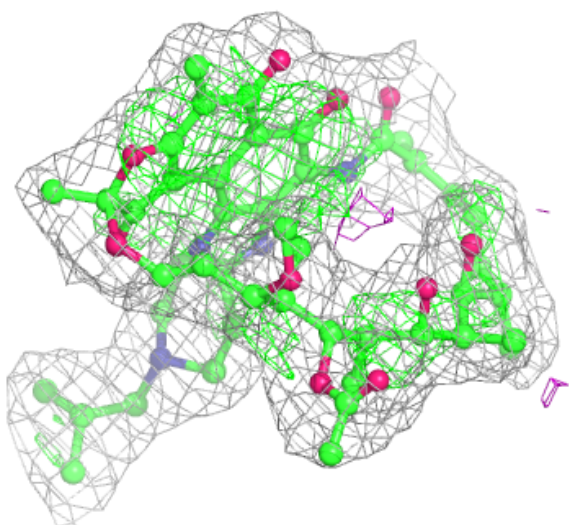
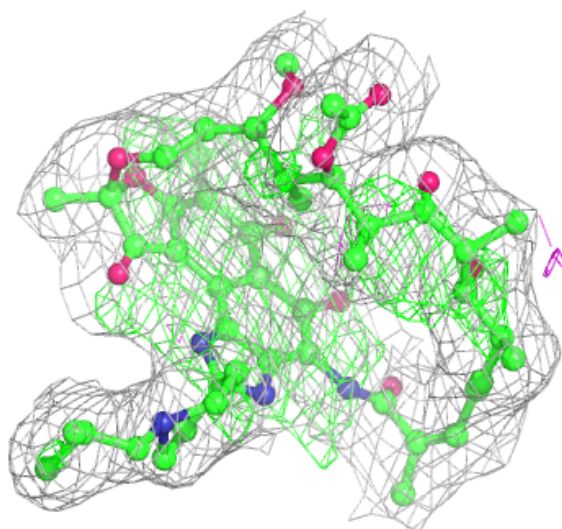
**Electron density around RBT M 8002:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around RBT C 8001:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.