



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 09:43 AM EDT

PDB ID : 1SMY  
Title : Structural basis for transcription regulation by alarmone ppGpp  
Authors : Artsimovitch, I.; Patlan, V.; Sekine, S.; Vassylyeva, M.N.; Hosaka, T.; Ochi, K.; Yokoyama, S.; Vassylyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2004-03-10  
Resolution : 2.70 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.

The types of validation reports are described at

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

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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 : 2.36  
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) : 2.36

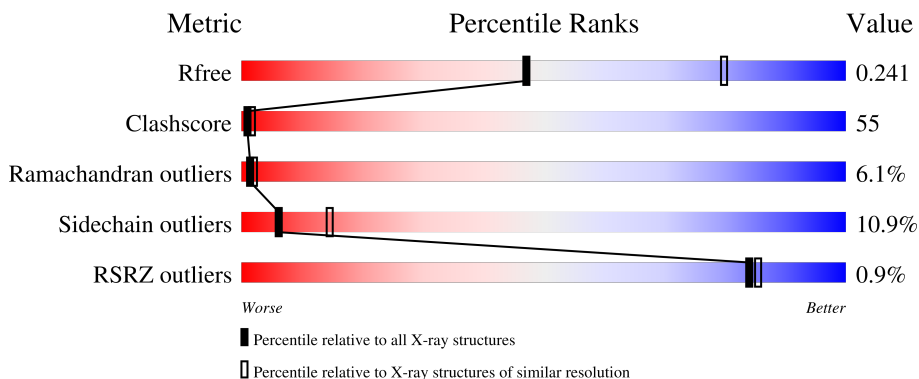
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.




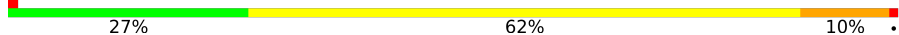

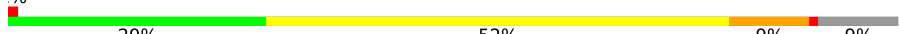
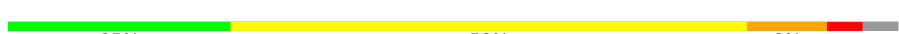

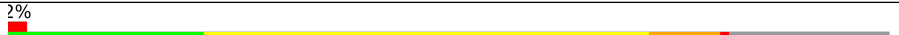
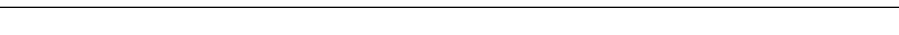
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 21% 44% 8% 27%
1	B	315	 21% 46% 5% 27%
1	K	315	 21% 46% 5% 27%
1	L	315	 23% 46% 5% 27%

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Mol	Chain	Length	Quality of chain
2	C	1119	 28% 59% 12% .
2	M	1119	 % 27% 62% 10% .
3	D	1524	 % 27% 53% 10% . 9%
3	N	1524	 % 29% 52% 9% . 9%
4	E	99	 25% 58% 9% . .
4	O	99	 33% 51% 8% . .
5	F	423	 2% 22% 50% 8% . 18%
5	P	423	 21% 52% 7% 18%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 63021 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
			Total	C	N	O	S			
1	A	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	B	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	K	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	L	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1119	Total 8828	C 5581	N 1577	O 1646	S 24	0	0	0
2	M	1119	Total 8828	C 5581	N 1577	O 1646	S 24	0	0	0

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

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

- Molecule 4 is a protein called RNA POLYMERASE OMEGA SUBUNIT.

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

- Molecule 5 is a protein called principal sigma factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	345	Total 2770	C 1744	N 504	O 518	S 4	0	0	0
5	P	345	Total 2770	C 1744	N 504	O 518	S 4	0	0	0

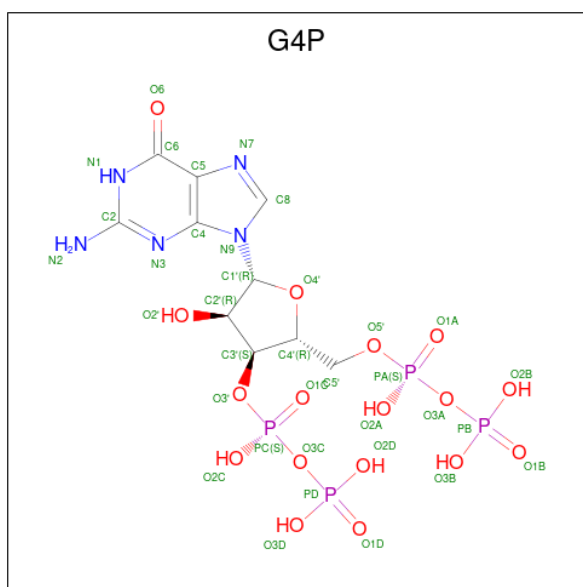
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total 29	Mg 29	0	0
6	B	22	Total 22	Mg 22	0	0
6	C	92	Total 92	Mg 92	0	0
6	D	150	Total 150	Mg 150	0	0
6	E	17	Total 17	Mg 17	0	0
6	F	49	Total 49	Mg 49	0	0
6	M	1	Total 1	Mg 1	0	0
6	N	2	Total 2	Mg 2	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>5</sub>O<sub>17</sub>P<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	N	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
8	N	1	Total	C	N	O	P	0	0
			36	10	5	17	4		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	296	Total	O	0	0
			296	296		
9	B	307	Total	O	0	0
			307	307		
9	C	1308	Total	O	0	0
			1308	1308		
9	D	1745	Total	O	0	0
			1745	1745		
9	E	160	Total	O	0	0
			160	160		
9	F	619	Total	O	0	0
			619	619		
9	K	316	Total	O	0	0
			316	316		
9	L	341	Total	O	0	0
			341	341		
9	M	1401	Total	O	0	0
			1401	1401		
9	N	1794	Total	O	0	0
			1794	1794		

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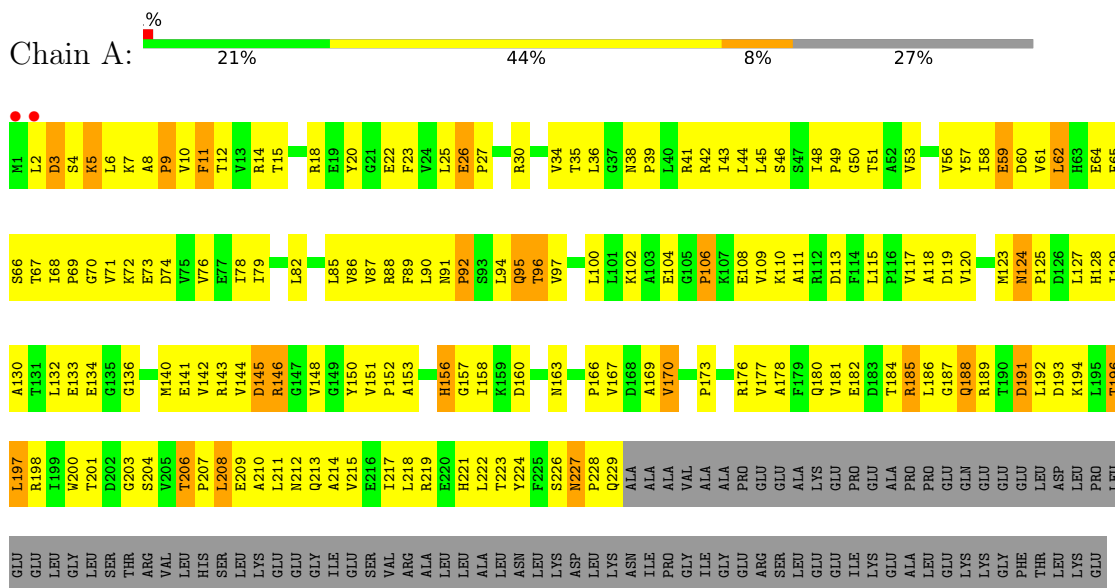
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
9	O	203	Total 203	O 203	0	0
9	P	541	Total 541	O 541	0	0

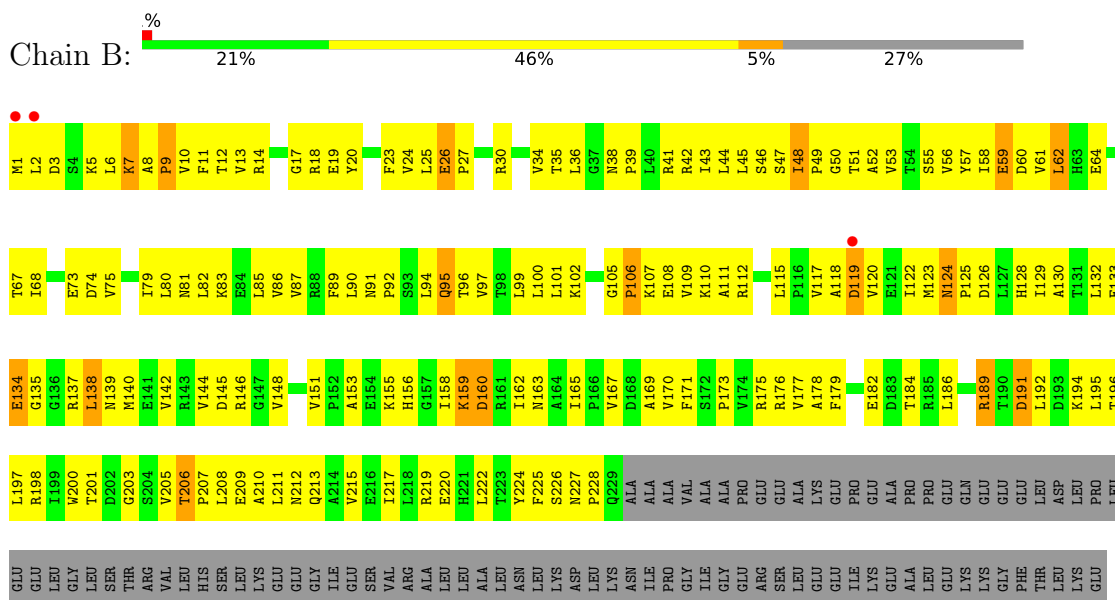
### 3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase alpha chain

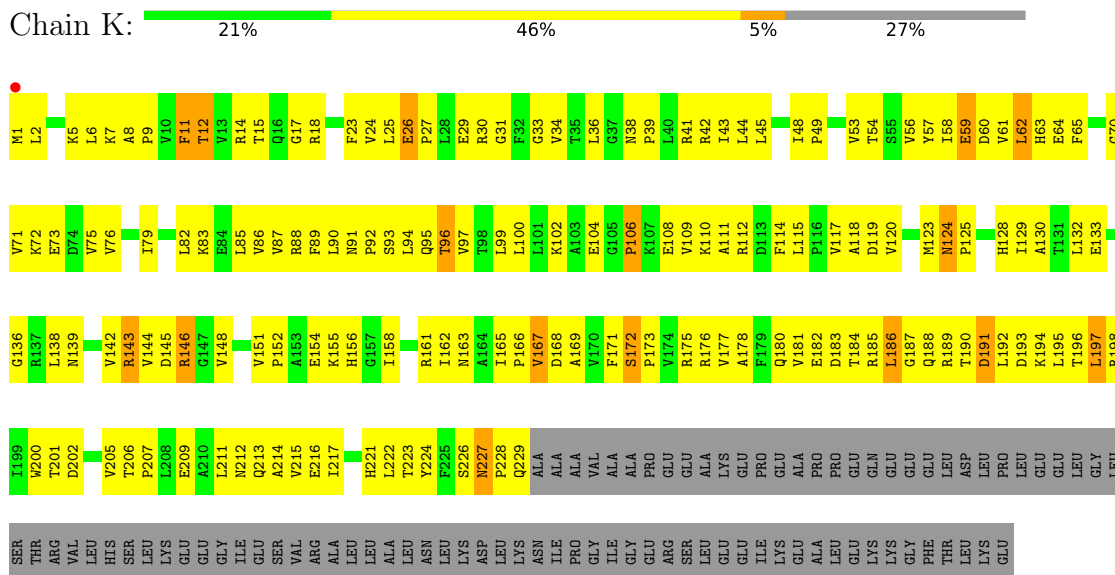


- Molecule 1: DNA-directed RNA polymerase alpha chain





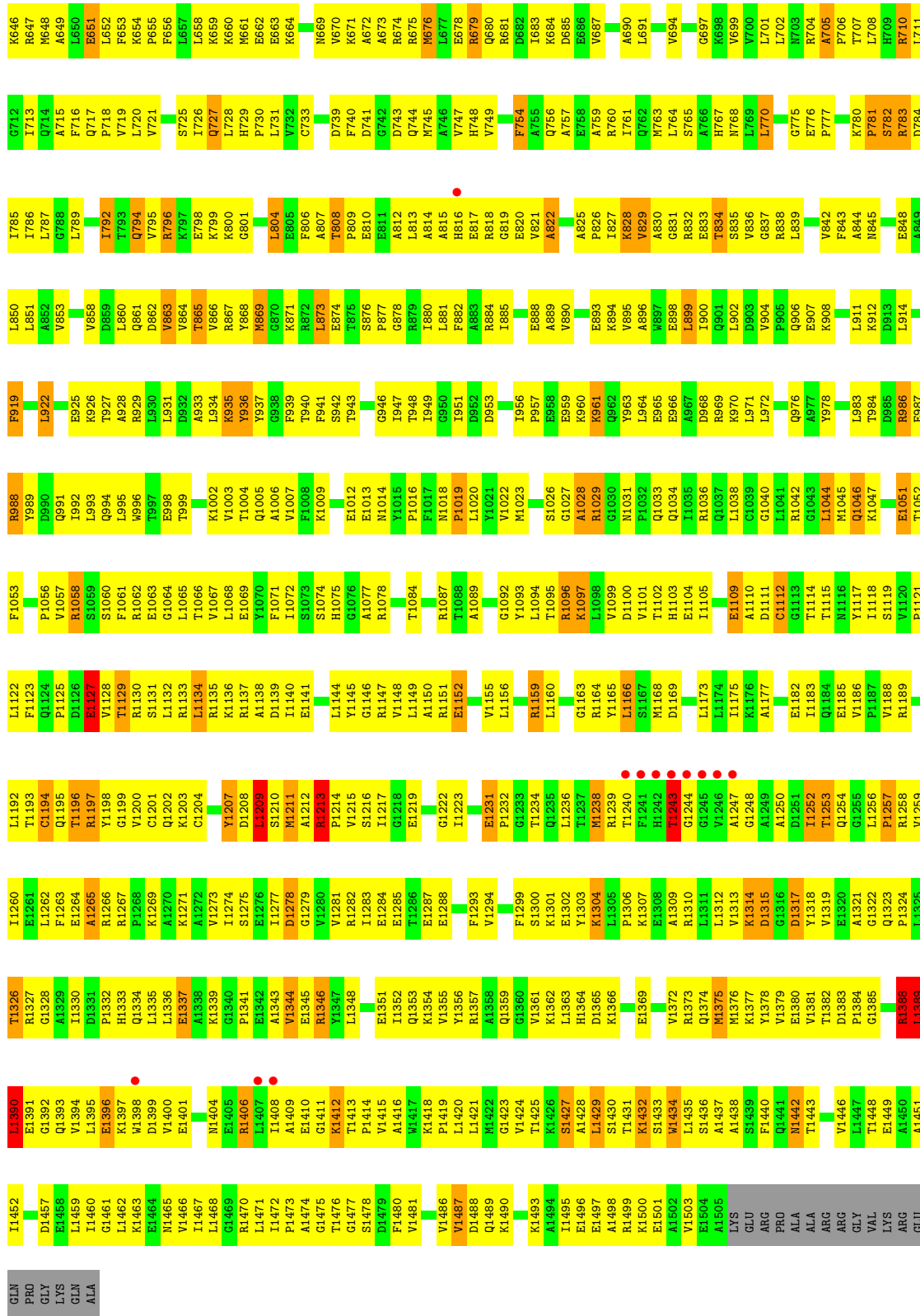
- Molecule 1: DNA-directed RNA polymerase alpha chain







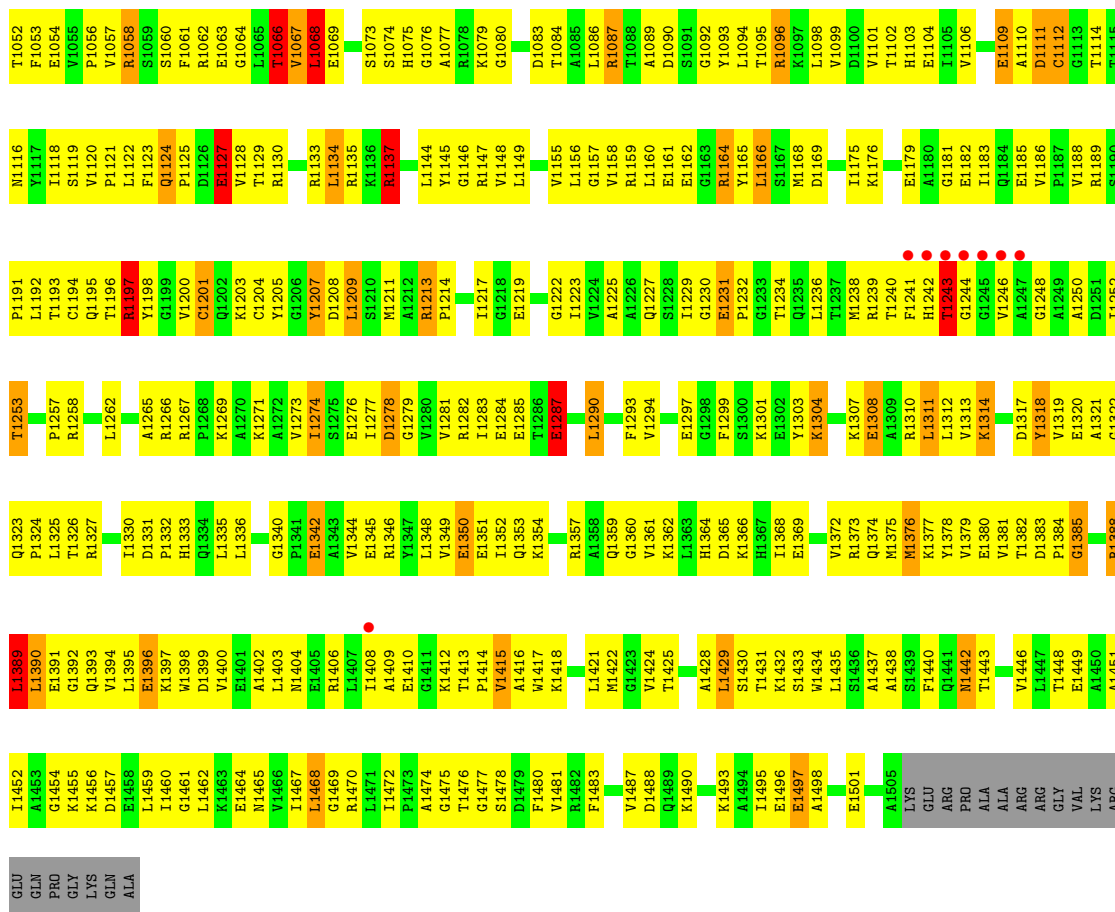




• Molecule 3: DNA-directed RNA polymerase beta' chain



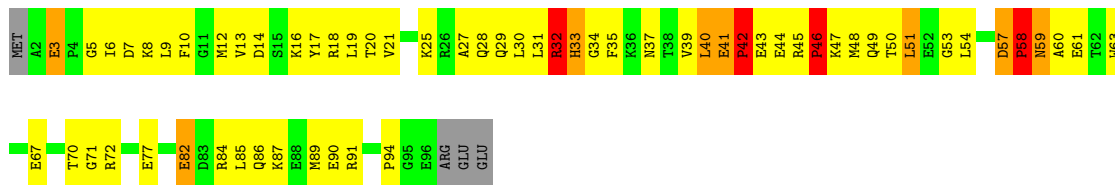
I992	A918	L850	G788	V719	L652	G585	A516	D453	I393	ALA	LEU	G188	Q125	K64	MET	
L993	F919	L851	L789	L720	F653	R586	F517	A454	L394	GLU	GLU	Q189	V126	K65	K2	
A994	A920	A852	I792	V721	K654	R587	P518	R455	V395	GLU	GLU	E190	L127	K66	K3	
L995	R921	V853	I793	E722	P655	G588	F519	R456	V396	GLU	GLU	L191	Y128	K67	E4	
A996	L922	A854	T793	G723	F656	A589	L520	C457	K397	GLY	ALA	A192	F129	V5	V5	
E998	E925	V858	Q794	Q724	L657	P590	F921	A458	A398	GLU	PHE	P193	S130	R6	R6	
T999	K926	D859	V795	Q725	L658	G591	P522	E459	R399	THR	LEU	G194	K131	K7	K7	
T1000	R927	D860	R796	L728	K659	P594	D523	A460	V400	VAL	VAL	Y132	K131	V8	V8	
E1001	R928	Q861	G797	H729	G660	G595	L524	I461	Y401	TYR	LEU	Y196	I133	R9	R9	
K1002	A928	D862	F798	G732	M661	S596	R525	Q462	P402	THR	ARG	S197	V134	I10	I10	
T1003	R930	K800	K799	V732	E662	D597	F526	Q463	F403	THR	ARG	R198	L135	A11	A11	
V1004	L931	V863	G800	G733	E663	R598	M527	L464	E494	LEU	GLU	L199	D136	L12	L12	
Q1005	L931	T865	G801	E734	K664	P599	V528	L465	D495	PHE	ASP	D200	P137	A13	A13	
A1006	K935	V866	L804	A735	N669	L600	F535	K466	D496	LEU	GLU	G201	K138	S14	S14	
V1007	R936	F736	E805	F736	V670	R601	A536	E467	Y497	GLU	PRO	V202	G139	P15	P15	
F1008	F807	A738	F807	M737	V671	S602	A536	L468	E408	TRP	VAL	A203	G139	E16	E16	
F939	M869	A738	A807	A738	K671	L603	T537	D469	V409	THR	ALA	L204	L141	K17	K17	
N1010	G870	T808	T808	D739	A672	T604	S538	L470	S410	GLU	THR	Y205	L142	I18	I18	
F1011	G871	T809	T809	D743	A673	D605	D539	E471	T411	PRO	TYR	R206	N143	R19	R19	
T943	K871	R871	E810	D743	R674	I606	L543	A472	G412	LYS	PHE	F207	G144	S20	S20	
T944	L873	R872	E811	Q744	R675	S608	L544	L473	D413	ASP	THR	F208	V145	W21	W21	
N1013	L873	R873	E812	M745	M676	G609	R544	E474	R414	TYR	PRO	R209	P146	R84	R84	
N1014	E845	R874	A812	A746	G609	G609	R545	R475	V415	ARG	VAL	R210	V147	R85	R85	
Y1015	G946	T875	L813	A747	R679	G610	R546	E476	A416	VAL	GLY	V211	V147	R86	R86	
I947	A814	S876	G814	H748	Q680	O611	L547	L477	P417	GLN	MET	R212	E148	R87	R87	
T948	A815	R877	A815	V749	R681	G612	L548	L478	G416	PRO	THR	V213	K149	E25	E25	
N1018	H816	G878	H816	F750	D682	R622	M549	E479	D419	HIS	PRO	E214	R156	V26	V26	
I951	E817	R879	L751	L751	I683	F614	R550	E480	V420	MET	LEU	Y215	Q151	R90	R90	
D952	R818	I880	R818	S752	K684	R622	M551	M481	L421	ASN	VAL	L152	L152	E91	E91	
N953	G819	S753	S753	S753	D685	L619	N552	A422	A422	VAL	VAL	K217	T154	H92	H92	
A954	E820	F754	E686	F754	E686	G620	R553	D423	D423	VAL	HIS	D421	D155	I32	I32	
I955	V821	A755	V687	A755	V687	K620	L554	S485	G424	VAL	GLY	A221	E156	L95	L95	
N956	A822	Q756	G688	Q756	G688	R622	K555	R486	G425	PRO	GLY	P226	E157	A96	A96	
P957	L823	A757	D689	A757	D689	G623	K556	A487	V427	GLU	ILE	L227	R162	P98	P98	
E958	N824	E758	A690	E758	A690	D624	L557	R488	R428	ALA	GLU	P238	R161	A99	A99	
E959	A825	A759	L691	A759	L691	Y625	L558	R489	S429	ALA	ARG	V231	R162	A100	A100	
P826	P826	R692	E692	R692	E692	G625	A559	A490	D430	VAL	GLY	E232	K165	H101	H101	
D922	I827	D922	E693	R628	E693	R628	Q560	A490	D430	VAL	GLY	E232	K166	E40	E40	
E893	K828	K894	G629	S629	K394	V630	R493	R493	V432	ALA	PRO	E234	Q166	R41	R41	
K894	V829	R894	V630	V630	K394	V630	R495	R495	G433	G364	LEU	E234	T168	D42	D42	
V895	A830	V895	L631	L631	K698	V632	L496	L496	R434	I367	ALA	P238	Y169	F104	F104	
A896	G831	A896	V632	V632	V699	V632	L496	L496	R434	I367	ALA	P238	Y169	V105	V105	
V897	R832	R832	V633	V633	V700	V633	L567	E497	V435	ALA	GLY	G239	P170	L44	L44	
E898	E833	E833	G634	G634	L701	G634	R568	V498	E436	ALA	GLY	L171	L171	F45	F45	
L899	T834	T834	P635	P635	L702	P635	R569	V499	V437	LYS	LYS	L245	P172	D46	D46	
I900	N703	N703	Q636	Q636	N703	Q636	E570	R500	D438	GLY	GLY	P246	P173	E47	E47	
Q901	R704	R704	L637	L637	R704	L637	K571	A501	V440	LEU	LEU	G174	G174	S10	S10	
D903	A705	A705	K638	K638	P706	K638	F502	L503	R441	ARG	ARG	D176	D176	I49	I49	
V904	T707	T707	O641	O641	T707	O641	L574	D504	M442	MET	MET	A177	A177	G51	G51	
Q905	L708	L708	G642	G642	L708	G642	Q575	D504	M442	PRO	PRO	ALA	L176	P52	P52	
Q906	H709	H709	G643	G643	H709	G643	M507	R507	V444	ARG	ARG	ALA	L176	D55	D55	
E907	R710	R710	L644	L644	R710	L644	R508	R445	V444	ARG	GLU	GLU	L116	D55	D55	
K908	L711	L711	P645	P645	L711	P645	R508	R445	V444	ARG	GLU	GLU	L116	D17	D17	
N909	G712	G712	R646	R646	G712	R646	E510	P509	V446	VAL	VAL	GLY	D181	L18	L18	
N845	L713	L713	R647	R647	L713	R647	E511	D510	V447	ARG	ARG	VAL	G182	S119	S119	
N846	Q714	Q714	M648	M648	L713	R647	E511	D510	V447	ARG	ARG	VAL	G182	S119	S119	
F846	L911	L911	M648	M648	Q714	M648	E511	D510	V447	ARG	ARG	VAL	G182	S119	S119	
D847	R912	R912	A649	A649	L911	M648	E511	D510	V447	ARG	ARG	VAL	G182	S119	S119	
E848	F716	F716	L650	L650	L912	M649	E512	L513	A391	ALA	ALA	GLU	E184	G60	G60	
A849	L787	L787	E651	E651	L912	M649	E512	L513	A391	ALA	ALA	GLU	E184	G61	G61	
															K62	K62
															L123	L123
															E124	E124



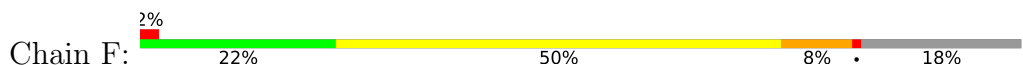
• Molecule 4: RNA POLYMERASE OMEGA SUBUNIT



• Molecule 4: RNA POLYMERASE OMEGA SUBUNIT



• Molecule 5: principal sigma factor







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	236.35Å 236.35Å 249.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 50.12 – 2.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.70) 97.1 (50.12-2.71)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.73Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.186 , 0.266 0.186 , 0.241	Depositor DCC
$R_{free}$ test set	14873 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 59.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.086 for h,-h-k,-l 0.086 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	63021	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, G4P, 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	0.68	0/1838	0.70	0/2498
1	B	0.68	0/1838	0.68	0/2498
1	K	0.68	0/1838	0.72	1/2498 (0.0%)
1	L	0.68	0/1838	0.67	1/2498 (0.0%)
2	C	0.75	0/8996	0.79	4/12164 (0.0%)
2	M	0.74	0/8996	0.78	4/12164 (0.0%)
3	D	0.74	0/10975	0.81	10/14836 (0.1%)
3	N	0.73	0/10975	0.81	14/14836 (0.1%)
4	E	0.74	0/783	0.81	0/1054
4	O	0.75	0/783	0.81	0/1054
5	F	0.65	0/2811	0.75	1/3781 (0.0%)
5	P	0.64	0/2811	0.74	1/3781 (0.0%)
All	All	0.72	0/54482	0.78	36/73662 (0.0%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	243	ARG	C-N-CD	-9.21	100.34	120.60
3	D	199	LEU	CA-CB-CG	-8.95	94.72	115.30
3	N	199	LEU	CA-CB-CG	-8.85	94.94	115.30
1	K	197	LEU	CA-CB-CG	8.22	134.21	115.30
2	C	243	ARG	C-N-CD	-7.23	104.69	120.60
3	D	804	LEU	CA-CB-CG	6.65	130.59	115.30
5	P	136	LEU	CA-CB-CG	6.29	129.78	115.30
2	M	950	LEU	CA-CB-CG	6.07	129.27	115.30
5	F	84	TYR	CA-CB-CG	6.06	124.92	113.40
3	N	783	ARG	NE-CZ-NH2	6.00	123.30	120.30
3	D	783	ARG	NE-CZ-NH1	5.99	123.29	120.30
3	N	813	LEU	CA-CB-CG	5.64	128.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	197	LEU	CA-CB-CG	5.56	128.10	115.30
2	M	193	LEU	CA-CB-CG	5.53	128.02	115.30
3	N	1290	LEU	CA-CB-CG	5.53	128.01	115.30
3	D	238	PRO	N-CA-CB	5.48	109.88	103.30
3	D	554	LEU	CA-CB-CG	5.44	127.81	115.30
2	M	244	PRO	CA-N-CD	-5.42	103.91	111.50
3	N	1201	CYS	CA-CB-SG	-5.36	104.34	114.00
2	C	853	LEU	CA-CB-CG	5.34	127.58	115.30
3	D	73	CYS	CA-CB-SG	5.32	123.58	114.00
3	N	1068	LEU	CA-CB-CG	-5.29	103.12	115.30
2	C	269	LEU	CA-CB-CG	5.27	127.42	115.30
3	N	171	LEU	CA-CB-CG	5.26	127.40	115.30
3	N	238	PRO	N-CA-CB	5.22	109.57	103.30
3	N	1209	LEU	N-CA-C	-5.18	97.02	111.00
3	N	705	ALA	C-N-CD	5.17	139.25	128.40
3	D	226	PRO	N-CA-CB	5.16	109.49	103.30
3	D	248	PRO	N-CA-CB	5.14	109.47	103.30
3	D	1209	LEU	N-CA-C	-5.11	97.21	111.00
3	N	710	ARG	NE-CZ-NH2	-5.10	117.75	120.30
3	N	373	PRO	N-CA-CB	5.09	109.41	103.30
2	C	559	LEU	CA-CB-CG	5.09	127.00	115.30
3	D	171	LEU	CA-CB-CG	5.08	126.99	115.30
3	N	136	ASP	C-N-CD	5.08	139.07	128.40
3	N	226	PRO	N-CA-CB	5.07	109.38	103.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	211	0
1	B	1806	0	1861	191	0
1	K	1806	0	1861	196	0
1	L	1806	0	1861	183	0
2	C	8828	0	8933	1013	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	8828	0	8933	1065	0
3	D	10797	0	10873	1260	0
3	N	10797	0	10873	1227	0
4	E	769	0	775	104	0
4	O	769	0	775	96	0
5	F	2770	0	2844	327	0
5	P	2770	0	2844	363	0
6	A	29	0	0	0	0
6	B	22	0	0	0	0
6	C	92	0	0	0	0
6	D	150	0	0	0	0
6	E	17	0	0	0	0
6	F	49	0	0	0	0
6	M	1	0	0	0	0
6	N	2	0	0	0	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	N	72	0	22	9	0
9	A	296	0	0	67	0
9	B	307	0	0	66	0
9	C	1308	0	0	281	0
9	D	1745	0	0	322	0
9	E	160	0	0	37	0
9	F	619	0	0	99	0
9	K	316	0	0	72	0
9	L	341	0	0	64	0
9	M	1401	0	0	325	0
9	N	1794	0	0	330	0
9	O	203	0	0	33	0
9	P	541	0	0	96	0
All	All	63021	0	54316	5952	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 55.

All (5952) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:VAL:HB	2:C:38:LYS:HG3	1.28	1.11
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.33	1.10
2:M:857:ASP:HB2	2:M:978:ARG:HG2	1.34	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:9100:G4P:H57	8:N:9100:G4P:H8	1.14	1.09
3:N:148:GLU:HB3	3:N:151:GLN:HB2	1.35	1.08
2:C:328:LEU:HD13	2:C:433:THR:HB	1.37	1.07
3:D:95:LEU:HD11	3:D:517:VAL:HG23	1.34	1.05
5:P:88:ILE:HD13	5:P:193:ARG:HB2	1.40	1.04
5:P:278:LEU:HB3	5:P:286:PRO:HG2	1.38	1.03
3:D:1101:VAL:HG22	3:D:1428:ALA:HB2	1.39	1.01
3:N:908:LYS:HB2	3:N:1027:GLY:HA3	1.41	1.01
3:N:172:PRO:HB3	3:N:178:LEU:HB3	1.43	1.01
2:C:577:PRO:HA	2:C:671:ASN:HD21	1.24	1.00
2:M:829:GLN:HE21	2:M:831:ARG:HD3	1.24	1.00
2:M:892:LEU:HD23	2:M:918:LEU:HD11	1.41	1.00
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.42	0.99
3:D:984:THR:HG22	3:D:987:GLU:HG3	1.44	0.99
2:M:546:LEU:HD12	2:M:565:GLN:HE22	1.26	0.99
3:D:422:ALA:HB3	3:D:427:VAL:HG22	1.42	0.98
3:D:1209:LEU:HD12	3:D:1210:SER:H	1.29	0.98
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.43	0.98
3:D:197:SER:HB3	3:D:203:ALA:HB3	1.47	0.97
3:D:637:LEU:HD21	3:D:642:CYS:HA	1.48	0.96
3:D:489:ARG:HG3	3:D:493:ARG:HH12	1.29	0.95
3:D:1432:LYS:HD2	3:D:1433:SER:H	1.28	0.95
4:O:40:LEU:HD21	4:O:67:GLU:HA	1.46	0.95
3:N:715:ALA:HB3	3:N:764:LEU:HA	1.48	0.95
2:C:627:ARG:HE	2:C:627:ARG:H	1.05	0.94
3:D:1389:LEU:HG	3:D:1390:LEU:HD23	1.48	0.94
2:M:601:GLY:HA2	2:M:616:GLU:HG2	1.48	0.94
2:C:110:GLU:HG2	2:C:369:PRO:HB3	1.47	0.94
3:N:18:ILE:HG23	3:N:518:PRO:HG3	1.48	0.94
5:P:371:LEU:HD22	5:P:375:LEU:HD22	1.47	0.94
3:D:1468:LEU:HD22	3:D:1470:ARG:HB2	1.50	0.94
5:F:278:LEU:HB3	5:F:286:PRO:HG2	1.48	0.94
3:D:1388:ARG:H	3:D:1388:ARG:HD2	1.29	0.93
3:D:1304:LYS:H	3:D:1304:LYS:HD3	1.33	0.93
2:M:777:ILE:HG23	5:P:409:LYS:HB2	1.50	0.93
3:N:1101:VAL:HG22	3:N:1428:ALA:HB2	1.51	0.93
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.51	0.92
2:M:34:VAL:HB	2:M:38:LYS:HG3	1.49	0.92
3:D:787:LEU:HD21	3:D:947:ILE:HD11	1.49	0.92
3:N:424:GLY:HA2	3:N:436:GLU:HA	1.52	0.92
2:C:64:LEU:HD22	2:C:359:MET:HG3	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:710:ILE:HD11	2:C:758:ARG:HE	1.33	0.91
3:D:424:GLY:HA2	3:D:436:GLU:HA	1.51	0.91
3:D:489:ARG:HE	3:D:493:ARG:HH22	1.18	0.91
2:M:95:TYR:HD2	2:M:114:PHE:HB3	1.37	0.91
3:N:32:ILE:HD12	3:N:527:MET:HG2	1.53	0.91
3:N:98:PRO:HG3	3:N:515:GLU:HB3	1.52	0.90
2:M:1109:VAL:HG11	3:N:5:VAL:HG22	1.52	0.90
2:M:331:ARG:HH12	2:M:427:VAL:HG13	1.37	0.90
2:C:952:LEU:HD12	2:C:969:GLN:HE22	1.34	0.90
3:N:1137:ARG:H	3:N:1137:ARG:HD2	1.35	0.89
2:C:945:ARG:HB2	2:C:945:ARG:HH11	1.36	0.89
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.54	0.89
2:C:711:GLU:HG2	2:C:822:VAL:HG12	1.53	0.89
3:D:87:ARG:HG3	3:D:88:TYR:H	1.38	0.89
3:D:154:THR:HB	9:D:3232:HOH:O	1.72	0.89
2:C:405:ARG:HH21	2:C:566:THR:HG21	1.34	0.89
2:M:952:LEU:HD12	2:M:969:GLN:HE22	1.38	0.89
3:N:1109:GLU:HG2	3:N:1201:CYS:HA	1.55	0.89
2:C:405:ARG:HH12	2:C:409:ARG:HH21	1.21	0.88
2:M:578:VAL:HG11	2:M:991:GLN:HB3	1.56	0.88
2:M:853:LEU:HD23	2:M:858:MET:HB3	1.52	0.88
2:C:207:LEU:HD22	2:C:221:LEU:HD21	1.56	0.88
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.53	0.88
3:N:191:LEU:HB3	3:N:195:VAL:HG21	1.56	0.88
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.39	0.88
2:C:938:LYS:HB3	2:C:939:ARG:HH21	1.39	0.88
9:K:4396:HOH:O	2:M:978:ARG:HA	1.74	0.87
1:L:57:TYR:HB3	1:L:141:GLU:HG3	1.55	0.87
3:N:133:ILE:HG21	3:N:454:ALA:HB1	1.55	0.87
3:D:191:LEU:HD12	3:D:211:VAL:HG21	1.56	0.87
3:N:65:ARG:HB2	5:P:375:LEU:HA	1.54	0.87
2:C:941:VAL:HA	2:C:944:LEU:HD12	1.54	0.87
3:N:1481:VAL:HG11	4:O:18:ARG:HA	1.56	0.86
2:M:148:PHE:HB3	2:M:313:LEU:HD22	1.57	0.86
2:M:690:ILE:HB	2:M:852:ILE:HD13	1.56	0.86
5:F:160:ASP:HA	5:F:163:LEU:HD12	1.55	0.86
5:P:252:ALA:HB1	5:P:265:VAL:HG21	1.58	0.86
3:N:646:LYS:HA	3:N:720:LEU:HD22	1.55	0.86
3:N:98:PRO:HG2	3:N:462:GLN:HE22	1.38	0.86
5:P:135:ILE:HD11	5:P:178:ARG:HD3	1.58	0.85
2:C:841:ASN:HD21	2:C:845:ASN:H	1.23	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:157:ARG:HD2	2:C:314:THR:HG22	1.58	0.85
3:D:119:SER:HB2	3:D:123:LEU:H	1.41	0.85
2:M:442:GLU:HG2	2:M:454:SER:HB2	1.58	0.85
3:D:127:LEU:HD21	3:D:461:ILE:HD11	1.57	0.85
3:N:172:PRO:HG3	3:N:178:LEU:HD22	1.59	0.85
3:D:44:LEU:HB2	9:D:9962:HOH:O	1.77	0.85
3:N:1389:LEU:H	3:N:1389:LEU:HD23	1.40	0.85
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.57	0.85
3:N:177:ALA:HB1	3:N:199:LEU:HD22	1.58	0.85
3:N:1090:ASP:HB3	3:N:1093:TYR:HB2	1.57	0.85
3:D:177:ALA:HB1	3:D:199:LEU:HD22	1.57	0.84
8:N:9100:G4P:H5 <sup>7</sup>	8:N:9100:G4P:C8	2.04	0.84
2:M:1097:LEU:H	2:M:1097:LEU:HD22	1.42	0.84
3:D:906:GLN:HB3	3:D:911:LEU:HD11	1.57	0.84
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.59	0.84
3:D:171:LEU:HD22	3:D:390:PRO:HG3	1.59	0.84
3:N:67:ARG:HD3	5:P:375:LEU:HD11	1.58	0.84
2:M:939:ARG:HD3	2:M:982:PRO:HD3	1.60	0.84
3:N:422:ALA:HB3	3:N:427:VAL:HG22	1.60	0.84
3:D:679:ARG:HH12	3:D:681:ARG:HD2	1.44	0.83
3:D:85:VAL:HB	3:D:89:ARG:HE	1.44	0.83
2:M:536:PRO:HB3	2:M:906:PHE:HD1	1.39	0.83
2:M:265:ARG:HA	9:M:9500:HOH:O	1.78	0.83
1:L:87:VAL:HG21	1:L:144:VAL:HG11	1.61	0.83
3:N:119:SER:H	3:N:123:LEU:HD22	1.43	0.83
2:C:1109:VAL:HG11	3:D:5:VAL:HG22	1.61	0.83
1:L:206:THR:HG22	1:L:209:GLU:HB2	1.61	0.83
2:M:136:ILE:HA	9:M:9466:HOH:O	1.79	0.82
3:N:1146:GLY:HA3	3:N:1207:TYR:HB2	1.61	0.82
2:C:1097:LEU:HD22	2:C:1097:LEU:H	1.41	0.82
5:P:142:ARG:HB3	5:P:142:ARG:HH11	1.42	0.82
3:D:890:VAL:HG13	3:D:926:LYS:HD3	1.60	0.82
1:B:87:VAL:HG21	1:B:144:VAL:HG11	1.59	0.82
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.62	0.82
3:D:6:ARG:HB3	3:D:6:ARG:NH1	1.95	0.82
2:M:266:ARG:HD3	2:M:288:ARG:HH12	1.44	0.82
2:M:498:GLN:HG3	2:M:516:ARG:HH21	1.44	0.81
2:M:841:ASN:HD21	2:M:845:ASN:H	1.23	0.81
4:E:76:GLY:HA3	4:E:79:LEU:HD13	1.62	0.81
2:M:650:ARG:H	2:M:650:ARG:HE	1.25	0.81
3:N:141:ILE:HD13	3:N:450:TYR:H	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLN:HE22	2:C:934:PHE:HB2	1.44	0.81
2:C:238:LEU:HA	2:C:241:LEU:HD12	1.63	0.81
3:D:212:ARG:HB2	3:D:445:ARG:HH22	1.45	0.81
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.61	0.81
2:M:89:THR:HG23	2:M:129:ILE:HA	1.62	0.81
3:N:175:VAL:HG12	9:N:2205:HOH:O	1.80	0.81
3:N:423:ASP:HB2	5:P:178:ARG:HD2	1.62	0.81
5:F:291:ILE:HG21	5:F:304:VAL:HG11	1.60	0.81
3:N:187:LYS:HE2	3:N:213:VAL:HG12	1.61	0.81
3:N:422:ALA:HB1	5:P:178:ARG:NH1	1.96	0.81
3:N:984:THR:HG22	3:N:987:GLU:HG3	1.62	0.81
2:C:89:THR:HG23	2:C:129:ILE:HA	1.59	0.81
2:C:139:GLN:HE22	2:C:415:PRO:HD2	1.45	0.81
2:C:244:PRO:HD2	2:C:245:GLY:H	1.42	0.81
1:K:112:ARG:HG2	9:K:1330:HOH:O	1.80	0.81
3:N:1045:MET:HG2	3:N:1073:SER:HA	1.61	0.81
2:C:442:GLU:HG2	2:C:454:SER:HB2	1.62	0.81
2:C:1054:THR:HA	9:C:9720:HOH:O	1.80	0.81
4:E:9:LEU:HB3	4:E:19:LEU:HD21	1.63	0.81
3:N:565:ILE:H	3:N:565:ILE:HD12	1.45	0.81
3:D:780:LYS:HD3	3:D:912:LYS:HD3	1.61	0.81
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.61	0.81
3:N:119:SER:HB2	3:N:123:LEU:HB2	1.61	0.81
3:N:800:LYS:HG2	3:N:829:VAL:HG12	1.62	0.81
2:C:704:HIS:HB3	2:C:829:GLN:HE21	1.45	0.81
3:N:414:ARG:HD3	9:N:9486:HOH:O	1.81	0.80
3:N:116:LEU:HB3	3:N:118:LEU:HD13	1.63	0.80
3:D:187:LYS:HE2	3:D:213:VAL:HG12	1.61	0.80
3:D:704:ARG:HD2	3:D:705:ALA:H	1.47	0.80
3:N:928:ALA:HA	3:N:931:LEU:HD12	1.64	0.80
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.61	0.80
2:C:971:LYS:HA	2:C:988:VAL:HA	1.62	0.80
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.61	0.80
3:N:558:LEU:HD13	5:P:145:PRO:HB3	1.64	0.80
2:M:238:LEU:HD23	2:M:241:LEU:HD12	1.64	0.80
3:N:899:LEU:HB2	3:N:917:GLN:HG2	1.61	0.80
3:D:1481:VAL:HG11	4:E:18:ARG:HA	1.63	0.80
3:N:906:GLN:HB3	3:N:911:LEU:HD11	1.64	0.80
5:P:406:ARG:HA	5:P:409:LYS:HG2	1.61	0.80
3:D:210:ARG:HD2	3:D:398:ALA:HB3	1.64	0.80
2:M:192:PRO:HB2	2:M:195:LEU:HD13	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:690:ILE:HB	2:C:852:ILE:HD13	1.64	0.80
3:N:422:ALA:HB1	5:P:178:ARG:HH12	1.46	0.80
2:M:340:MET:HA	9:M:2031:HOH:O	1.82	0.79
2:C:857:ASP:HB2	2:C:978:ARG:HG2	1.63	0.79
1:B:132:LEU:HD11	1:B:138:LEU:HD12	1.64	0.79
3:N:654:LYS:HD3	3:N:674:ARG:HH12	1.45	0.79
3:D:87:ARG:HG3	3:D:88:TYR:N	1.97	0.79
3:D:87:ARG:O	3:D:521:PRO:HB3	1.82	0.79
1:L:58:ILE:HB	1:L:61:VAL:HB	1.63	0.79
2:M:331:ARG:HB2	9:M:9297:HOH:O	1.81	0.79
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.63	0.79
2:M:650:ARG:HG2	2:M:653:ASP:HB2	1.65	0.79
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.62	0.79
3:N:87:ARG:O	3:N:521:PRO:HB3	1.83	0.79
2:C:290:LEU:H	2:C:290:LEU:HD13	1.47	0.79
3:D:427:VAL:HG23	9:D:2135:HOH:O	1.83	0.79
5:F:266:GLU:HA	5:F:269:ASN:HD22	1.47	0.79
3:N:87:ARG:HA	9:N:9625:HOH:O	1.83	0.79
2:C:601:GLY:HA2	2:C:616:GLU:HG2	1.65	0.79
8:N:9100:G4P:H8	8:N:9100:G4P:C5'	2.08	0.79
2:C:93:PRO:HA	9:C:9603:HOH:O	1.83	0.78
1:L:80:LEU:HD13	3:N:842:VAL:HG12	1.65	0.78
2:M:134:ARG:HA	9:M:9211:HOH:O	1.82	0.78
2:C:755:LEU:HD12	2:C:825:VAL:HG11	1.64	0.78
5:F:312:GLN:HB2	9:F:2094:HOH:O	1.84	0.78
3:N:135:LEU:HD11	3:N:452:ILE:HD11	1.64	0.78
2:C:325:ILE:HD12	2:C:325:ILE:H	1.47	0.78
2:M:693:GLU:HA	2:M:696:LYS:HG3	1.65	0.78
2:C:24:GLU:HB3	2:C:28:ARG:HH12	1.48	0.78
2:C:333:ILE:HG22	2:C:465:GLY:HA2	1.65	0.78
2:C:694:LEU:HD11	2:C:868:ASP:HB3	1.65	0.78
3:D:591:VAL:HG11	3:D:597:ASP:HA	1.66	0.78
2:M:987:ILE:HG23	3:N:948:THR:HG21	1.65	0.78
2:C:42:VAL:HG12	2:C:43:GLY:H	1.48	0.78
3:D:759:ALA:HA	3:D:763:MET:HE2	1.66	0.78
3:D:1328:GLY:HA3	9:D:2287:HOH:O	1.84	0.78
5:F:164:LYS:HA	5:F:171:LYS:NZ	1.98	0.78
2:M:650:ARG:H	2:M:650:ARG:NE	1.81	0.78
3:D:775:GLY:HA3	3:D:1145:TYR:HE1	1.49	0.78
2:M:164:PRO:HA	2:M:266:ARG:HH22	1.47	0.78
2:C:66:LEU:HB2	9:C:2120:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.66	0.78
3:D:90:MET:HG2	3:D:521:PRO:HD3	1.65	0.78
2:M:314:THR:HG22	9:M:2325:HOH:O	1.84	0.78
3:D:978:TYR:HA	9:D:2242:HOH:O	1.83	0.77
3:D:972:LEU:HG	3:D:976:GLN:HE22	1.47	0.77
1:K:34:VAL:HG21	9:M:9419:HOH:O	1.84	0.77
2:M:675:ALA:HA	2:M:989:VAL:HG12	1.64	0.77
3:N:434:ARG:HB2	3:N:447:VAL:HG22	1.66	0.77
1:B:58:ILE:HB	1:B:61:VAL:HB	1.66	0.77
3:D:553:ARG:HH21	5:F:215:GLU:HG2	1.48	0.77
5:F:214:GLN:HA	5:F:217:ASN:HD22	1.48	0.77
1:K:195:LEU:HG	9:K:1736:HOH:O	1.84	0.77
3:D:191:LEU:HB3	3:D:195:VAL:HG21	1.65	0.77
3:D:907:GLU:HA	9:D:9566:HOH:O	1.83	0.77
2:M:42:VAL:HG12	2:M:43:GLY:H	1.49	0.77
2:M:66:LEU:HD13	2:M:100:LEU:HB3	1.64	0.77
2:C:715:THR:HG22	2:C:717:LEU:H	1.47	0.77
3:D:1109:GLU:HG2	3:D:1201:CYS:HA	1.67	0.77
3:D:98:PRO:HG3	3:D:515:GLU:HB3	1.67	0.77
3:D:1388:ARG:N	3:D:1388:ARG:HH11	1.83	0.77
3:N:637:LEU:HD21	3:N:642:CYS:HA	1.67	0.77
4:O:48:MET:HB2	4:O:54:LEU:HB2	1.67	0.77
3:D:500:ARG:NH2	3:D:1388:ARG:HE	1.83	0.77
2:M:164:PRO:HA	2:M:266:ARG:HH12	1.49	0.77
2:M:971:LYS:HA	2:M:988:VAL:HA	1.65	0.77
1:K:53:VAL:HG12	1:K:167:VAL:HG21	1.67	0.77
1:K:136:GLY:HA3	9:K:1268:HOH:O	1.85	0.77
3:N:119:SER:HB2	3:N:123:LEU:H	1.49	0.77
5:P:130:VAL:HG21	5:P:159:ILE:HG21	1.67	0.77
2:C:575:GLN:H	2:C:667:ALA:HB1	1.49	0.76
2:C:838:LYS:HG3	2:C:997:LEU:HB2	1.65	0.76
3:N:783:ARG:NH1	3:N:1029:ARG:HG2	2.00	0.76
3:D:928:ALA:HA	3:D:931:LEU:HD12	1.67	0.76
5:F:394:ARG:HA	5:F:397:ILE:HD12	1.65	0.76
2:M:197:LEU:HB3	2:M:202:TYR:HB2	1.67	0.76
2:C:689:VAL:HG21	9:C:9624:HOH:O	1.86	0.76
3:D:562:ALA:HB1	3:D:567:ILE:HD11	1.66	0.76
3:D:777:PRO:HA	9:D:9581:HOH:O	1.85	0.76
3:D:583:ASP:OD1	3:D:604:THR:HB	1.84	0.76
5:F:287:THR:HG23	5:F:289:GLU:HB2	1.68	0.76
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:495:THR:HG23	2:C:517:ARG:HE	1.50	0.76
2:M:5:ARG:HB3	2:M:902:ILE:HB	1.68	0.76
8:N:9101:G4P:C8	8:N:9101:G4P:H5''	2.15	0.76
3:D:1376:MET:HE3	3:D:1421:LEU:HB2	1.67	0.76
3:D:1197:ARG:HD2	3:D:1396:GLU:HB2	1.68	0.76
3:N:41:ARG:HB2	9:N:2916:HOH:O	1.86	0.76
2:C:627:ARG:H	2:C:627:ARG:NE	1.83	0.76
1:K:58:ILE:HB	1:K:61:VAL:HB	1.67	0.76
1:L:76:VAL:HB	3:N:872:ARG:HH22	1.51	0.75
3:N:1194:CYS:HA	9:N:9487:HOH:O	1.86	0.75
5:P:321:ILE:HD11	5:P:329:TYR:HB2	1.67	0.75
1:B:27:PRO:HG2	1:B:186:LEU:HD12	1.66	0.75
5:F:88:ILE:HD13	5:F:193:ARG:HB2	1.66	0.75
1:K:214:ALA:HA	1:K:217:ILE:HD12	1.68	0.75
2:M:598:GLU:O	2:M:651:LYS:HG3	1.86	0.75
2:M:1005:MET:HG3	3:N:629:SER:HB2	1.68	0.75
1:A:67:THR:HA	9:A:9794:HOH:O	1.86	0.75
1:B:13:VAL:HA	9:B:9669:HOH:O	1.86	0.75
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.69	0.75
2:M:100:LEU:HD21	2:M:368:THR:HA	1.67	0.75
3:N:1381:VAL:HB	3:N:1389:LEU:O	1.86	0.75
5:P:416:ARG:HD2	5:P:419:ARG:HB2	1.67	0.75
3:D:1104:GLU:HA	3:D:1461:GLY:HA2	1.69	0.75
2:M:478:VAL:HG13	2:M:506:ASN:HB3	1.67	0.75
2:M:571:LEU:HD23	2:M:700:TYR:HA	1.68	0.75
9:N:9282:HOH:O	4:O:17:TYR:HB3	1.86	0.75
2:C:89:THR:HA	2:C:129:ILE:O	1.86	0.75
3:D:699:VAL:HG22	3:D:756:GLN:HE22	1.50	0.75
3:D:868:TYR:HD1	3:D:869:MET:H	1.31	0.75
3:D:1137:ARG:H	3:D:1137:ARG:HD2	1.52	0.75
4:E:28:GLN:HB3	9:E:9553:HOH:O	1.87	0.75
2:M:442:GLU:HB3	9:M:9245:HOH:O	1.87	0.75
2:M:724:ARG:HB2	2:M:740:GLU:HA	1.69	0.75
2:M:786:LYS:HD2	9:M:9396:HOH:O	1.85	0.75
2:C:500:ASN:HA	9:C:9718:HOH:O	1.86	0.75
2:M:1013:TYR:HE2	5:P:341:PRO:HD2	1.51	0.75
3:N:794:GLN:NE2	3:N:795:VAL:H	1.85	0.75
3:N:1217:ILE:HD12	3:N:1217:ILE:H	1.50	0.75
1:L:27:PRO:HG2	1:L:186:LEU:HD12	1.68	0.75
2:M:338:GLU:HA	2:M:341:THR:HG22	1.68	0.74
2:M:711:GLU:HG2	2:M:822:VAL:HG12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:181:VAL:HB	9:C:9674:HOH:O	1.86	0.74
3:N:133:ILE:HD13	3:N:454:ALA:HB1	1.69	0.74
2:C:737:LEU:HB3	9:C:9568:HOH:O	1.86	0.74
2:M:838:LYS:HG3	2:M:997:LEU:HB2	1.70	0.74
5:P:394:ARG:HA	5:P:397:ILE:HD12	1.67	0.74
3:D:99:ALA:HA	3:D:575:GLN:HE22	1.52	0.74
2:M:324:ASP:HB3	2:M:327:HIS:HD2	1.51	0.74
5:P:393:THR:HG22	5:P:394:ARG:H	1.51	0.74
2:C:1016:ILE:HD12	5:F:317:LEU:HD21	1.67	0.74
4:E:48:MET:HB2	4:E:54:LEU:HB2	1.70	0.74
2:M:965:GLU:HA	2:M:968:LEU:HD12	1.69	0.74
3:N:152:LEU:HD23	3:N:152:LEU:H	1.51	0.74
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.68	0.74
1:K:56:VAL:HG13	1:K:142:VAL:HG12	1.70	0.74
2:C:753:ASP:HA	9:D:9567:HOH:O	1.88	0.74
5:F:393:THR:HG22	5:F:394:ARG:H	1.52	0.74
1:K:42:ARG:NH1	2:M:857:ASP:HB3	2.02	0.74
1:A:58:ILE:HB	1:A:61:VAL:HB	1.69	0.74
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.69	0.74
3:D:658:LEU:HA	3:D:661:MET:HE3	1.70	0.74
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.70	0.74
1:L:94:LEU:HD21	1:L:119:ASP:HB2	1.68	0.74
2:M:328:LEU:HD12	9:M:9297:HOH:O	1.87	0.74
2:M:585:GLU:HB2	9:M:9626:HOH:O	1.88	0.74
3:N:197:SER:HB3	3:N:203:ALA:HB3	1.70	0.74
2:M:734:LEU:HD13	2:M:737:LEU:HD13	1.69	0.74
3:N:1382:THR:HG21	3:N:1418:LYS:HE3	1.70	0.73
3:N:1402:ALA:HB1	9:N:9626:HOH:O	1.88	0.73
9:C:9690:HOH:O	3:D:1064:GLY:HA2	1.87	0.73
3:D:756:GLN:HE21	3:D:760:ARG:HD2	1.51	0.73
2:M:110:GLU:HG2	2:M:369:PRO:HG3	1.68	0.73
3:N:191:LEU:HD13	3:N:195:VAL:HG11	1.70	0.73
3:N:890:VAL:HA	9:N:9430:HOH:O	1.88	0.73
3:N:1116:ASN:ND2	3:N:1193:THR:HB	2.03	0.73
2:C:724:ARG:HB2	2:C:740:GLU:HA	1.68	0.73
2:C:948:GLU:HA	9:C:2299:HOH:O	1.87	0.73
2:M:580:MET:HB2	9:M:9244:HOH:O	1.87	0.73
3:N:455:ARG:HH22	5:P:140:ARG:HB3	1.53	0.73
1:K:87:VAL:HG21	1:K:144:VAL:HG11	1.69	0.73
2:M:336:VAL:HA	2:M:339:LEU:HD12	1.68	0.73
2:C:1058:ASP:OD2	2:C:1083:GLU:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:534:ARG:HA	9:F:2094:HOH:O	1.88	0.73
2:M:89:THR:HA	2:M:129:ILE:O	1.88	0.73
2:M:325:ILE:HB	9:M:9421:HOH:O	1.88	0.73
2:M:395:LYS:HG2	2:M:397:GLU:HG2	1.71	0.73
2:M:546:LEU:HD12	2:M:565:GLN:NE2	2.01	0.73
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.51	0.73
2:M:568:ALA:HB1	2:M:668:LEU:HB3	1.69	0.73
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.71	0.73
3:N:441:ARG:HB3	3:N:443:VAL:HG23	1.69	0.73
3:D:1252:ILE:HG22	3:D:1253:THR:H	1.53	0.73
2:M:94:LEU:HA	9:M:9263:HOH:O	1.86	0.73
2:M:968:LEU:HB3	9:M:9311:HOH:O	1.88	0.73
5:F:164:LYS:HA	5:F:171:LYS:HZ3	1.54	0.73
3:N:52:PRO:HG2	9:N:9465:HOH:O	1.88	0.73
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.71	0.73
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.69	0.73
3:D:1496:GLU:HG3	3:D:1500:LYS:HE3	1.71	0.73
1:K:42:ARG:HH12	2:M:857:ASP:HB3	1.52	0.73
1:L:120:VAL:HG23	9:L:3068:HOH:O	1.89	0.73
3:N:630:VAL:HA	3:N:744:GLN:HG2	1.71	0.73
5:P:287:THR:HG23	5:P:289:GLU:HB2	1.70	0.73
3:D:1166:LEU:HD23	3:D:1166:LEU:H	1.53	0.73
2:M:492:ASP:HA	2:M:518:LYS:HB3	1.70	0.73
3:N:195:VAL:HB	3:N:205:TYR:HB2	1.69	0.73
3:D:675:ARG:O	3:D:678:GLU:HG2	1.88	0.72
4:E:6:ILE:HA	4:E:9:LEU:HD12	1.71	0.72
2:M:136:ILE:HG21	2:M:336:VAL:HG13	1.71	0.72
4:O:8:LYS:HG3	9:O:1143:HOH:O	1.89	0.72
1:A:166:PRO:HB3	9:A:9709:HOH:O	1.89	0.72
1:A:214:ALA:HA	1:A:217:ILE:HD12	1.68	0.72
2:C:118:ILE:H	2:C:118:ILE:HD13	1.53	0.72
2:C:150:PRO:HA	2:C:158:TYR:HB3	1.71	0.72
3:D:534:ARG:HH21	5:F:315:VAL:HG21	1.54	0.72
1:L:9:PRO:HB3	1:L:25:LEU:HG	1.71	0.72
2:M:176:VAL:HG22	2:M:182:VAL:HG13	1.70	0.72
2:C:1102:LEU:HB3	9:C:9776:HOH:O	1.89	0.72
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.70	0.72
1:L:89:PHE:HB3	1:L:94:LEU:HD13	1.71	0.72
3:N:1310:ARG:HE	3:N:1327:ARG:HB3	1.53	0.72
3:N:1314:LYS:HZ1	3:N:1317:ASP:HB2	1.54	0.72
4:O:87:LYS:HE2	4:O:91:ARG:HH21	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.71	0.72
3:D:1063:GLU:HG2	3:D:1064:GLY:H	1.54	0.72
3:D:1254:GLN:HB2	9:D:2152:HOH:O	1.88	0.72
3:D:1378:TYR:O	3:D:1420:LEU:HB3	1.90	0.72
1:L:204:SER:HA	9:L:2931:HOH:O	1.89	0.72
3:N:1118:ILE:HD11	3:N:1346:ARG:HE	1.53	0.72
3:N:1166:LEU:H	3:N:1166:LEU:HD23	1.54	0.72
2:C:1013:TYR:HB2	5:F:335:ASP:OD2	1.90	0.72
3:D:31:THR:HA	9:D:9962:HOH:O	1.88	0.72
3:D:475:LYS:HA	3:D:478:LEU:HD12	1.70	0.72
3:D:838:ARG:HH12	3:D:863:VAL:HG12	1.53	0.72
5:F:273:ARG:HA	5:F:276:ARG:HH11	1.54	0.72
5:F:416:ARG:HD2	5:F:419:ARG:HB2	1.71	0.72
1:B:23:PHE:HA	9:B:9669:HOH:O	1.89	0.72
3:D:54:LYS:HD3	3:D:55:ASP:H	1.54	0.72
3:N:1495:ILE:HA	9:N:9438:HOH:O	1.87	0.72
1:L:225:PHE:HA	9:L:2122:HOH:O	1.90	0.72
3:N:1314:LYS:NZ	3:N:1317:ASP:HB2	2.04	0.72
3:D:118:LEU:HB3	3:D:123:LEU:HD22	1.72	0.72
3:D:615:ARG:O	3:D:619:LEU:HB2	1.90	0.72
3:D:834:THR:OG1	3:D:838:ARG:HB3	1.89	0.72
3:D:601:ARG:HH12	3:D:613:ARG:HH21	1.38	0.71
2:M:324:ASP:HA	9:M:2460:HOH:O	1.90	0.71
3:N:705:ALA:HB3	3:N:706:PRO:HD3	1.69	0.71
3:D:699:VAL:HG22	3:D:756:GLN:NE2	2.06	0.71
3:N:692:GLU:HG2	3:N:720:LEU:HD12	1.71	0.71
2:C:689:VAL:CG2	2:C:870:ILE:HB	2.20	0.71
2:C:777:ILE:HG12	9:C:2212:HOH:O	1.89	0.71
1:B:123:MET:HG2	9:B:9676:HOH:O	1.90	0.71
1:K:94:LEU:HD21	1:K:119:ASP:HB2	1.71	0.71
1:K:117:VAL:HG22	9:K:4167:HOH:O	1.88	0.71
2:M:144:PRO:HA	2:M:163:ILE:HG23	1.73	0.71
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.55	0.71
2:C:197:LEU:HB3	2:C:202:TYR:HB2	1.72	0.71
3:N:162:ARG:HA	3:N:449:SER:HB3	1.71	0.71
5:P:131:VAL:HG13	5:P:178:ARG:HG2	1.72	0.71
2:C:371:LYS:O	2:C:372:LEU:HD12	1.91	0.71
3:D:1346:ARG:HA	3:D:1346:ARG:HE	1.54	0.71
1:L:176:ARG:HH12	3:N:884:ARG:NE	1.89	0.71
3:N:1127:GLU:HB3	9:N:9298:HOH:O	1.90	0.71
3:N:1330:ILE:HA	9:N:9632:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:309:LYS:HA	5:F:312:GLN:OE1	1.91	0.71
2:M:584:GLU:HG2	9:M:9244:HOH:O	1.90	0.71
2:M:1115:LEU:HD23	3:N:85:VAL:HA	1.73	0.71
2:C:536:PRO:HD2	2:C:537:LYS:NZ	2.06	0.71
3:D:658:LEU:HD11	3:D:674:ARG:HH11	1.54	0.71
1:L:167:VAL:HG22	9:L:2964:HOH:O	1.90	0.71
2:M:218:VAL:HG22	2:M:221:LEU:HD23	1.71	0.71
5:P:156:VAL:HA	5:P:159:ILE:HD12	1.72	0.71
2:M:184:MET:HG3	2:M:193:LEU:HD23	1.72	0.71
2:M:468:ARG:HB3	9:M:9590:HOH:O	1.90	0.71
2:M:621:VAL:HB	9:M:9858:HOH:O	1.91	0.71
2:M:882:LEU:HD12	3:N:1061:PHE:HB3	1.73	0.71
3:N:662:GLU:HB2	9:N:9379:HOH:O	1.89	0.71
3:N:810:GLU:O	3:N:813:LEU:HG	1.91	0.71
3:N:827:ILE:HA	9:N:9636:HOH:O	1.89	0.71
1:A:158:ILE:HG12	9:A:9709:HOH:O	1.90	0.70
2:C:259:GLY:HA3	9:C:2199:HOH:O	1.91	0.70
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.71	0.70
2:C:889:HIS:HE1	3:D:951:ILE:H	1.38	0.70
3:D:486:ARG:HH21	3:D:489:ARG:NE	1.88	0.70
1:L:41:ARG:HH11	1:L:177:VAL:HB	1.56	0.70
2:M:101:ILE:HG22	2:M:102:HIS:H	1.56	0.70
2:M:328:LEU:HD23	2:M:437:ARG:HD3	1.73	0.70
2:C:957:LYS:HB3	9:C:9884:HOH:O	1.90	0.70
2:M:176:VAL:HG13	2:M:182:VAL:HG22	1.73	0.70
2:M:603:VAL:HG21	2:M:643:VAL:HG11	1.73	0.70
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	1.71	0.70
3:N:64:LYS:HB2	5:P:376:ILE:O	1.91	0.70
2:C:86:LYS:HG3	2:C:813:VAL:HG12	1.72	0.70
2:C:874:LEU:HB2	9:C:2136:HOH:O	1.91	0.70
3:D:1432:LYS:CD	3:D:1433:SER:H	2.01	0.70
3:D:1462:LEU:HD23	9:D:3112:HOH:O	1.89	0.70
2:M:290:LEU:HD12	2:M:302:VAL:HG11	1.72	0.70
2:M:413:LEU:H	2:M:413:LEU:HD12	1.56	0.70
2:C:285:LEU:HD21	2:C:289:THR:HA	1.73	0.70
2:C:336:VAL:HB	9:C:9899:HOH:O	1.91	0.70
3:N:507:ASN:HA	9:N:9943:HOH:O	1.91	0.70
3:N:1373:ARG:HG2	3:N:1374:GLN:NE2	2.06	0.70
3:N:1410:GLU:HA	9:N:9265:HOH:O	1.91	0.70
2:C:13:ILE:HD12	9:C:9856:HOH:O	1.91	0.70
2:C:385:PHE:O	2:C:389:SER:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1115:LEU:HD23	3:D:85:VAL:HG12	1.74	0.70
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.74	0.70
3:D:815:ALA:HB3	9:D:9733:HOH:O	1.92	0.70
1:L:56:VAL:HG13	1:L:142:VAL:HG12	1.74	0.70
2:M:710:ILE:HB	2:M:790:LEU:HD13	1.73	0.70
1:A:146:ARG:HG2	9:A:9574:HOH:O	1.91	0.70
1:B:133:GLU:HG3	1:B:134:GLU:H	1.56	0.70
2:C:473:ARG:HE	2:C:531:PHE:HE1	1.39	0.70
3:N:709:HIS:HA	3:N:1227:GLN:HG2	1.73	0.70
1:K:91:ASN:HA	9:K:1224:HOH:O	1.91	0.70
2:M:1119:ARG:HA	2:M:1119:ARG:HE	1.57	0.70
5:P:184:ARG:HG2	5:P:188:ILE:HD11	1.74	0.70
2:C:861:LEU:HD23	2:C:863:ASP:H	1.57	0.70
3:D:119:SER:CB	3:D:123:LEU:HB2	2.22	0.70
4:E:32:ARG:HD3	9:E:9553:HOH:O	1.91	0.70
2:M:130:ASN:HA	9:M:2315:HOH:O	1.91	0.70
2:M:707:ARG:HD2	9:M:9630:HOH:O	1.91	0.70
1:A:219:ARG:HH12	1:B:219:ARG:HG2	1.57	0.70
2:C:405:ARG:NH1	2:C:409:ARG:HH21	1.90	0.70
2:C:689:VAL:HG23	2:C:870:ILE:HB	1.73	0.70
1:L:151:VAL:HB	1:L:169:ALA:HB3	1.74	0.70
5:F:135:ILE:HD11	5:F:178:ARG:HD2	1.73	0.70
3:N:131:LYS:HA	3:N:456:MET:HG3	1.72	0.70
1:A:42:ARG:NH1	2:C:857:ASP:HB3	2.06	0.69
1:B:80:LEU:HG	3:D:844:ALA:HB2	1.72	0.69
2:C:69:LEU:HB2	2:C:97:ARG:HB2	1.72	0.69
2:M:282:GLY:HA2	2:M:308:ARG:NH2	2.07	0.69
2:M:288:ARG:HH11	2:M:288:ARG:HG3	1.55	0.69
2:M:776:SER:HA	2:M:780:GLU:HB3	1.73	0.69
1:A:22:GLU:HB3	9:A:9573:HOH:O	1.92	0.69
2:C:197:LEU:HD13	2:C:207:LEU:HD21	1.74	0.69
3:D:710:ARG:HG2	3:D:710:ARG:HH11	1.56	0.69
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	1.72	0.69
5:F:270:LYS:HB3	5:F:295:MET:SD	2.31	0.69
1:L:62:LEU:HD12	9:L:6647:HOH:O	1.91	0.69
2:M:412:ALA:HA	9:M:9312:HOH:O	1.91	0.69
3:N:957:PRO:HG2	3:N:1007:VAL:HG12	1.73	0.69
3:N:1157:GLY:HA3	9:N:9424:HOH:O	1.92	0.69
2:C:776:SER:HA	2:C:780:GLU:HB3	1.72	0.69
3:D:537:THR:HG22	9:F:9559:HOH:O	1.91	0.69
2:M:39:ARG:HA	2:M:39:ARG:NE	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:284:ARG:HG2	2:M:285:LEU:H	1.54	0.69
2:M:777:ILE:O	5:P:409:LYS:HD2	1.92	0.69
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.73	0.69
2:C:969:GLN:HB3	9:C:9615:HOH:O	1.91	0.69
3:D:957:PRO:HG2	3:D:1007:VAL:HA	1.75	0.69
4:E:40:LEU:HD13	4:E:45:ARG:HD2	1.74	0.69
2:M:579:VAL:HG11	2:M:887:GLU:HG3	1.73	0.69
3:N:711:LEU:HD11	9:N:9759:HOH:O	1.92	0.69
1:A:222:LEU:HD12	1:B:215:VAL:HB	1.74	0.69
2:C:430:VAL:CG1	3:D:1075:HIS:HA	2.23	0.69
3:D:119:SER:H	3:D:123:LEU:HD13	1.56	0.69
5:F:79:ASP:HB3	5:F:80:PRO:HD3	1.73	0.69
5:F:366:ALA:HB2	9:F:2032:HOH:O	1.91	0.69
2:C:557:ARG:NH1	2:C:879:ARG:HE	1.90	0.69
2:C:710:ILE:HD11	2:C:758:ARG:NE	2.07	0.69
2:C:1111:ILE:HG13	2:C:1112:PHE:H	1.57	0.69
3:D:838:ARG:HA	9:D:9613:HOH:O	1.92	0.69
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.73	0.69
2:M:803:THR:HG22	2:M:825:VAL:HG13	1.75	0.69
2:C:436:GLY:HA2	2:C:538:GLN:O	1.92	0.69
3:D:156:GLU:HB2	9:D:3232:HOH:O	1.93	0.69
3:D:994:GLN:HB2	9:D:2834:HOH:O	1.93	0.69
1:L:112:ARG:HD2	9:L:1944:HOH:O	1.92	0.69
2:M:833:LEU:HD11	2:M:849:VAL:HG21	1.75	0.69
2:M:979:THR:HG23	2:M:981:GLU:H	1.55	0.69
5:P:337:HIS:HA	9:P:2159:HOH:O	1.92	0.69
2:C:102:HIS:HE1	2:C:367:LEU:HD21	1.56	0.69
2:C:148:PHE:HZ	2:C:281:LEU:HD13	1.56	0.69
3:D:549:ASN:HB3	9:D:2045:HOH:O	1.92	0.69
2:M:336:VAL:HG21	9:M:9234:HOH:O	1.93	0.69
2:M:436:GLY:HA2	2:M:538:GLN:O	1.93	0.69
2:C:1052:MET:HE3	2:C:1056:LYS:HD3	1.74	0.69
4:E:51:LEU:HG	4:E:53:GLY:H	1.58	0.69
2:M:89:THR:O	2:M:91:GLN:HG3	1.93	0.69
3:N:127:LEU:HD21	3:N:461:ILE:HD11	1.74	0.69
3:N:192:ALA:O	3:N:195:VAL:HG23	1.93	0.69
3:N:447:VAL:HG11	9:N:2028:HOH:O	1.93	0.69
4:O:70:THR:HG22	9:O:1901:HOH:O	1.93	0.69
1:A:53:VAL:HG12	1:A:167:VAL:HG21	1.72	0.69
1:B:151:VAL:HB	1:B:169:ALA:HB3	1.75	0.69
3:D:116:LEU:HB3	3:D:118:LEU:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:179:VAL:HG22	3:D:389:GLU:HG3	1.75	0.69
5:F:388:ALA:HB3	9:F:9936:HOH:O	1.92	0.69
1:K:86:VAL:HG12	1:K:124:ASN:ND2	2.08	0.69
2:M:3:ILE:HG21	9:M:2484:HOH:O	1.93	0.69
3:N:1326:THR:HG22	3:N:1327:ARG:H	1.57	0.69
2:M:328:LEU:HD13	2:M:433:THR:OG1	1.92	0.68
3:N:119:SER:OG	3:N:123:LEU:HD13	1.94	0.68
3:N:194:GLY:HA2	3:N:206:ARG:HD2	1.76	0.68
1:A:9:PRO:HB3	1:A:25:LEU:HG	1.75	0.68
3:D:162:ARG:NH2	3:D:434:ARG:HH21	1.90	0.68
3:D:194:GLY:HA2	3:D:206:ARG:HD2	1.74	0.68
3:D:798:GLU:HG2	3:D:799:LYS:H	1.57	0.68
3:N:1118:ILE:HD11	3:N:1346:ARG:NE	2.08	0.68
1:A:117:VAL:HG12	9:A:9774:HOH:O	1.94	0.68
2:C:237:ARG:HG2	9:C:2116:HOH:O	1.94	0.68
2:M:511:GLU:O	2:M:526:PRO:HD3	1.94	0.68
3:N:216:VAL:HA	9:N:2353:HOH:O	1.91	0.68
3:N:477:LEU:HD21	3:N:495:ARG:HE	1.56	0.68
2:C:751:PRO:HB2	3:D:680:GLN:HG3	1.74	0.68
5:F:76:SER:HB3	9:F:9637:HOH:O	1.92	0.68
3:N:1239:ARG:HB2	9:N:2464:HOH:O	1.92	0.68
1:B:64:GLU:HA	1:B:165:ILE:HD13	1.75	0.68
2:M:437:ARG:NH2	2:M:488:ALA:HA	2.08	0.68
3:N:141:ILE:H	3:N:141:ILE:HD12	1.58	0.68
3:N:161:LEU:HD21	3:N:452:ILE:HD13	1.75	0.68
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.76	0.68
3:D:73:CYS:HB3	3:D:76:CYS:O	1.93	0.68
3:D:411:THR:HG21	9:D:9778:HOH:O	1.94	0.68
3:N:796:ARG:HH21	3:N:828:LYS:HE2	1.58	0.68
3:N:1435:LEU:HG	3:N:1467:ILE:HD12	1.76	0.68
2:C:492:ASP:HA	2:C:518:LYS:HB3	1.74	0.68
2:C:1014:SER:HB3	9:C:9664:HOH:O	1.92	0.68
3:D:173:PRO:HD3	3:D:178:LEU:HD12	1.75	0.68
3:D:935:LYS:HB3	3:D:935:LYS:HZ2	1.57	0.68
3:D:1077:ALA:HB2	9:D:9673:HOH:O	1.93	0.68
1:K:86:VAL:HG12	1:K:124:ASN:HD22	1.59	0.68
3:N:90:MET:HG2	3:N:521:PRO:HD3	1.75	0.68
5:P:273:ARG:HG3	9:P:1952:HOH:O	1.93	0.68
2:C:24:GLU:HB3	2:C:28:ARG:NH1	2.09	0.68
2:C:577:PRO:HA	2:C:671:ASN:ND2	2.02	0.68
3:D:804:LEU:HD21	3:D:829:VAL:HG21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:876:SER:O	3:D:880:ILE:HG12	1.93	0.68
3:D:914:LEU:HA	9:D:2987:HOH:O	1.94	0.68
3:N:119:SER:HB3	9:N:9548:HOH:O	1.94	0.68
3:N:1277:ILE:HD12	9:N:9684:HOH:O	1.94	0.68
3:D:481:MET:HG3	3:D:493:ARG:HG2	1.75	0.68
3:D:976:GLN:HA	9:D:9904:HOH:O	1.94	0.68
2:M:164:PRO:CA	2:M:266:ARG:HH22	2.07	0.68
1:B:208:LEU:HD23	9:B:9568:HOH:O	1.94	0.68
2:C:760:SER:O	2:C:785:VAL:HG22	1.94	0.68
2:C:952:LEU:HD12	2:C:969:GLN:NE2	2.07	0.68
3:D:1401:GLU:HB3	9:D:9816:HOH:O	1.93	0.68
1:K:71:VAL:HA	9:K:1208:HOH:O	1.93	0.68
9:K:5477:HOH:O	2:M:605:LYS:HA	1.93	0.68
4:O:70:THR:HG21	9:O:2018:HOH:O	1.94	0.68
3:D:1335:LEU:HD23	3:D:1344:VAL:HA	1.76	0.67
2:M:284:ARG:HG2	2:M:285:LEU:N	2.09	0.67
5:P:132:ARG:O	5:P:136:LEU:HG	1.94	0.67
2:C:12:VAL:HG22	2:C:13:ILE:HG23	1.76	0.67
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.75	0.67
2:C:358:ARG:HH21	2:C:373:VAL:N	1.91	0.67
3:D:68:PHE:HB3	9:D:9610:HOH:O	1.94	0.67
3:D:629:SER:HB3	3:D:726:ILE:HD11	1.77	0.67
3:D:730:PRO:HA	3:D:733:CYS:SG	2.35	0.67
3:D:785:ILE:HG12	3:D:935:LYS:HA	1.73	0.67
5:F:77:THR:O	5:F:81:VAL:HG23	1.94	0.67
3:N:399:ARG:HG3	9:N:2124:HOH:O	1.94	0.67
5:P:373:LYS:HG2	9:P:2070:HOH:O	1.94	0.67
1:A:151:VAL:HB	1:A:169:ALA:HB3	1.76	0.67
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.75	0.67
3:D:488:ARG:H	3:D:488:ARG:NE	1.92	0.67
3:N:167:GLU:HA	9:N:9499:HOH:O	1.95	0.67
3:N:1438:ALA:O	3:N:1443:THR:HG22	1.94	0.67
1:B:41:ARG:HH11	1:B:177:VAL:HB	1.58	0.67
2:C:31:GLN:NE2	2:C:40:GLU:HB2	2.09	0.67
2:C:54:ILE:HG21	9:C:2671:HOH:O	1.94	0.67
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.77	0.67
5:F:321:ILE:HD11	5:F:329:TYR:HB2	1.75	0.67
2:M:183:SER:HB3	2:M:190:LYS:HD3	1.76	0.67
2:M:716:LYS:HA	2:M:716:LYS:HE3	1.75	0.67
3:N:1121:PRO:HD3	3:N:1346:ARG:NH2	2.09	0.67
5:P:163:LEU:HD22	5:P:174:LEU:HG	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1049:LEU:HD22	3:D:1472:ILE:HD11	1.77	0.67
3:D:1131:SER:O	3:D:1133:ARG:HG3	1.95	0.67
2:M:52:PHE:HB3	9:M:9629:HOH:O	1.95	0.67
3:N:481:MET:HE1	3:N:493:ARG:HE	1.60	0.67
2:C:23:VAL:HG12	9:C:2056:HOH:O	1.95	0.67
2:C:266:ARG:HD3	2:C:288:ARG:HE	1.57	0.67
2:C:841:ASN:HD21	2:C:845:ASN:N	1.93	0.67
2:C:1019:GLN:HG2	9:C:9664:HOH:O	1.95	0.67
3:D:576:GLU:HG3	9:F:9597:HOH:O	1.94	0.67
3:D:699:VAL:HG12	3:D:717:GLN:HG2	1.77	0.67
3:D:1395:LEU:HB2	9:D:2424:HOH:O	1.93	0.67
1:K:222:LEU:HD12	1:L:215:VAL:HB	1.75	0.67
2:M:50:GLU:HG2	2:M:265:ARG:NH1	2.09	0.67
2:M:339:LEU:HG	9:M:9771:HOH:O	1.95	0.67
2:M:1005:MET:HE3	3:N:645:PRO:HG2	1.75	0.67
2:C:612:VAL:HG22	2:C:622:GLU:HA	1.77	0.67
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.75	0.67
5:F:218:GLN:HA	5:F:221:ILE:HD12	1.75	0.67
5:F:234:LYS:HD3	5:F:236:SER:HB2	1.77	0.67
1:L:132:LEU:HB3	9:L:1114:HOH:O	1.95	0.67
2:M:64:LEU:HD22	2:M:359:MET:HG3	1.76	0.67
3:N:1381:VAL:HG23	9:N:9527:HOH:O	1.95	0.67
1:A:66:SER:HA	9:A:9605:HOH:O	1.94	0.67
1:K:12:THR:HG23	1:K:24:VAL:HB	1.76	0.67
1:L:77:GLU:HB3	9:L:1341:HOH:O	1.95	0.67
2:M:266:ARG:HD3	2:M:288:ARG:NH1	2.10	0.67
2:M:290:LEU:HB3	2:M:302:VAL:HG11	1.77	0.67
1:A:11:PHE:HB2	9:A:9706:HOH:O	1.94	0.67
1:A:41:ARG:HH11	1:A:177:VAL:HB	1.59	0.67
1:B:132:LEU:HB3	9:B:9733:HOH:O	1.94	0.67
2:C:300:ASP:OD2	2:C:303:PHE:HB2	1.94	0.67
2:C:673:LEU:HD22	2:C:867:VAL:HA	1.76	0.67
3:D:28:LYS:HD2	3:D:41:ARG:HD2	1.76	0.67
1:K:102:LYS:HG3	9:K:2209:HOH:O	1.95	0.67
2:M:269:LEU:HA	2:M:288:ARG:HD2	1.77	0.67
2:M:312:ALA:HB1	2:M:318:PRO:HG2	1.76	0.67
2:M:1090:LYS:HE2	3:N:88:TYR:O	1.95	0.67
3:N:699:VAL:H	3:N:756:GLN:NE2	1.93	0.67
3:N:1336:LEU:HD22	3:N:1421:LEU:HB2	1.77	0.67
5:P:102:LEU:O	5:P:106:VAL:HG23	1.95	0.67
1:B:9:PRO:HB3	1:B:25:LEU:HG	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:TYR:HE1	2:C:338:GLU:HG3	1.60	0.66
2:C:405:ARG:HD3	2:C:543:ASN:CG	2.16	0.66
1:L:86:VAL:HG12	1:L:124:ASN:ND2	2.10	0.66
2:M:397:GLU:HG3	2:M:633:GLN:HE22	1.60	0.66
2:M:489:THR:HA	9:M:9368:HOH:O	1.94	0.66
2:M:841:ASN:HD21	2:M:845:ASN:N	1.93	0.66
3:N:1313:VAL:HA	9:N:9426:HOH:O	1.94	0.66
5:P:358:LEU:HD11	5:P:370:LYS:HD2	1.77	0.66
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.60	0.66
3:D:633:VAL:HG22	3:D:635:PRO:HD3	1.76	0.66
1:L:26:GLU:HB3	1:L:194:LYS:HG3	1.76	0.66
2:M:16:PRO:HB2	2:M:460:ARG:HD3	1.78	0.66
2:M:490:GLU:HG2	2:M:494:TYR:HE1	1.59	0.66
2:M:759:THR:HB	2:M:785:VAL:HG11	1.77	0.66
2:M:1054:THR:HG21	2:M:1079:PRO:CB	2.25	0.66
3:N:145:VAL:HG22	3:N:146:PRO:HD2	1.77	0.66
3:N:1301:LYS:HG2	9:N:2064:HOH:O	1.96	0.66
1:A:2:LEU:HA	1:A:6:LEU:HD22	1.77	0.66
1:B:46:SER:O	1:B:148:VAL:HB	1.95	0.66
2:C:428:ARG:HH21	2:C:451:LEU:HD11	1.59	0.66
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.77	0.66
3:D:178:LEU:HG	3:D:200:ASP:H	1.61	0.66
1:K:97:VAL:HG23	9:K:1044:HOH:O	1.95	0.66
3:N:197:SER:HB2	3:N:205:TYR:CE1	2.30	0.66
1:A:185:ARG:HD2	9:A:9581:HOH:O	1.95	0.66
2:C:527:GLU:HG3	9:C:2408:HOH:O	1.95	0.66
3:D:168:THR:HB	3:D:393:ILE:HD12	1.78	0.66
3:D:1314:LYS:HG2	9:D:2456:HOH:O	1.94	0.66
4:E:46:PRO:HD3	4:E:66:LYS:HG2	1.77	0.66
1:L:186:LEU:HB2	9:L:1608:HOH:O	1.96	0.66
3:N:481:MET:CE	3:N:493:ARG:HE	2.08	0.66
3:N:537:THR:C	5:P:317:LEU:HB2	2.15	0.66
2:C:130:ASN:HA	9:C:9898:HOH:O	1.94	0.66
2:C:783:ARG:HG2	2:C:785:VAL:HB	1.78	0.66
3:D:684:LYS:HE2	9:D:9654:HOH:O	1.94	0.66
5:F:128:ARG:HD2	9:F:9581:HOH:O	1.96	0.66
2:M:162:ILE:HD12	2:M:172:ILE:HB	1.77	0.66
3:N:95:LEU:HD12	3:N:515:GLU:HA	1.77	0.66
3:N:825:ALA:HB1	9:N:9618:HOH:O	1.95	0.66
3:N:1242:HIS:CE1	3:N:1266:ARG:HH11	2.13	0.66
5:P:302:LYS:HB3	9:P:3098:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ARG:HH12	1:B:139:ASN:HB3	1.61	0.66
2:C:780:GLU:HG3	2:C:781:LYS:H	1.61	0.66
5:F:113:ILE:HG23	5:F:127:ILE:HB	1.76	0.66
5:P:140:ARG:HG3	9:P:2295:HOH:O	1.95	0.66
2:C:250:ARG:NH2	2:C:254:VAL:HB	2.11	0.66
3:D:97:THR:HG22	9:D:9686:HOH:O	1.96	0.66
9:D:2753:HOH:O	5:F:171:LYS:HG2	1.94	0.66
3:N:899:LEU:HD23	3:N:917:GLN:HB3	1.78	0.66
3:N:1393:GLN:HB2	3:N:1398:TRP:HE1	1.61	0.66
5:P:158:GLU:HA	5:P:161:GLN:HE21	1.61	0.66
2:C:338:GLU:HA	2:C:341:THR:HG22	1.77	0.66
3:D:1265:ALA:HB1	9:D:9823:HOH:O	1.96	0.66
2:M:129:ILE:HD13	9:M:9309:HOH:O	1.94	0.66
3:N:39:PRO:HB3	3:N:45:PHE:O	1.95	0.66
3:N:1196:THR:HA	9:N:9588:HOH:O	1.96	0.66
3:N:1501:GLU:HB3	9:N:9522:HOH:O	1.96	0.66
5:P:170:HIS:HA	5:P:173:TYR:HD1	1.61	0.66
2:C:66:LEU:HD13	2:C:100:LEU:HB3	1.78	0.66
2:C:176:VAL:HG12	2:C:182:VAL:HG22	1.77	0.66
2:M:394:PHE:HA	9:M:9211:HOH:O	1.96	0.66
3:N:984:THR:H	3:N:987:GLU:CD	1.99	0.66
1:A:102:LYS:HG2	9:A:9611:HOH:O	1.95	0.65
2:C:814:GLU:HG3	9:C:9712:HOH:O	1.95	0.65
2:C:1008:ARG:CZ	2:C:1020:PRO:HB3	2.26	0.65
5:F:155:THR:HA	9:F:9647:HOH:O	1.96	0.65
2:M:73:LEU:HB3	9:M:9468:HOH:O	1.97	0.65
2:M:451:LEU:HA	9:M:9532:HOH:O	1.97	0.65
2:M:905:ILE:HG12	9:M:9307:HOH:O	1.96	0.65
2:M:1018:GLN:HE21	2:M:1063:ARG:HH22	1.43	0.65
3:N:1311:LEU:HD23	3:N:1311:LEU:H	1.59	0.65
1:B:39:PRO:O	1:B:43:ILE:HG12	1.95	0.65
2:C:336:VAL:HG12	9:C:2001:HOH:O	1.96	0.65
2:C:534:VAL:H	2:C:538:GLN:HE22	1.44	0.65
2:C:611:ILE:HG12	9:C:9584:HOH:O	1.95	0.65
3:D:422:ALA:HB3	3:D:427:VAL:CG2	2.22	0.65
3:D:475:LYS:HD3	3:D:478:LEU:HD12	1.79	0.65
3:D:646:LYS:HA	3:D:720:LEU:HD23	1.77	0.65
3:D:1326:THR:HG22	3:D:1327:ARG:H	1.62	0.65
2:M:230:ARG:NE	2:M:237:ARG:HH22	1.94	0.65
2:M:744:ARG:HG3	2:M:747:ALA:HB2	1.77	0.65
2:M:829:GLN:NE2	2:M:831:ARG:HD3	2.06	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:150:THR:HG23	5:P:155:THR:HG21	1.79	0.65
1:A:50:GLY:HA3	1:A:173:PRO:HG3	1.78	0.65
3:D:32:ILE:HD12	3:D:527:MET:HG2	1.76	0.65
3:D:1459:LEU:HD12	3:D:1470:ARG:HH11	1.61	0.65
4:E:88:GLU:HA	9:E:9574:HOH:O	1.95	0.65
1:K:38:ASN:HB3	1:K:39:PRO:HD3	1.78	0.65
1:A:44:LEU:HD23	1:A:48:ILE:HD11	1.79	0.65
1:B:44:LEU:HD23	1:B:48:ILE:HD11	1.77	0.65
2:C:1115:LEU:H	2:C:1115:LEU:HD12	1.62	0.65
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.79	0.65
4:E:25:LYS:HA	4:E:28:GLN:CD	2.16	0.65
1:K:224:TYR:HB3	1:L:9:PRO:HB2	1.78	0.65
1:L:86:VAL:HG12	1:L:124:ASN:HD22	1.62	0.65
2:M:21:ILE:H	2:M:21:ILE:HD12	1.61	0.65
2:M:282:GLY:HA2	2:M:308:ARG:HH21	1.61	0.65
2:M:338:GLU:HB3	9:M:9771:HOH:O	1.96	0.65
3:N:191:LEU:HD12	3:N:211:VAL:HG21	1.79	0.65
3:N:212:ARG:HA	9:N:9240:HOH:O	1.96	0.65
1:A:59:GLU:HG3	1:A:60:ASP:H	1.61	0.65
3:D:1129:THR:HG23	3:D:1130:ARG:H	1.59	0.65
3:D:1404:ASN:ND2	3:D:1408:ILE:HD12	2.10	0.65
1:K:57:TYR:HE1	1:K:163:ASN:HB2	1.62	0.65
3:N:9:ARG:HD3	3:N:1456:LYS:HG2	1.79	0.65
3:N:175:VAL:HG13	3:N:217:LYS:CB	2.27	0.65
3:N:781:PRO:HG2	3:N:911:LEU:HD23	1.79	0.65
1:A:56:VAL:HG13	1:A:142:VAL:HG12	1.78	0.65
3:D:998:GLU:HA	9:D:2729:HOH:O	1.97	0.65
2:M:734:LEU:HA	2:M:737:LEU:HD13	1.79	0.65
3:N:128:TYR:HE2	3:N:458:ALA:HA	1.62	0.65
3:N:907:GLU:HA	9:N:9335:HOH:O	1.96	0.65
1:K:221:HIS:HA	1:K:224:TYR:CE2	2.31	0.65
2:M:39:ARG:HA	2:M:39:ARG:HE	1.62	0.65
2:M:1040:LEU:HG	9:M:9264:HOH:O	1.97	0.65
3:N:11:ALA:HB1	3:N:507:ASN:OD1	1.97	0.65
4:O:31:LEU:HD21	4:O:60:ALA:HB2	1.78	0.65
5:P:412:GLU:OE1	5:P:418:LEU:HD13	1.97	0.65
2:C:184:MET:HE3	2:C:186:VAL:HG13	1.79	0.65
2:C:230:ARG:HG3	9:C:9673:HOH:O	1.96	0.65
2:C:838:LYS:HD2	2:C:846:LYS:NZ	2.11	0.65
3:D:1388:ARG:HD2	3:D:1388:ARG:N	2.08	0.65
2:M:875:GLY:HA3	9:M:9227:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1239:ARG:HA	9:N:9644:HOH:O	1.96	0.65
5:F:291:ILE:HG23	5:F:304:VAL:HG21	1.77	0.65
1:L:75:VAL:HB	9:L:2024:HOH:O	1.97	0.65
2:M:627:ARG:HG3	2:M:628:PHE:H	1.61	0.65
3:N:470:LEU:HD22	3:N:499:VAL:HG13	1.78	0.65
3:N:1181:GLY:HA3	9:N:9860:HOH:O	1.95	0.65
3:N:1459:LEU:HD12	3:N:1470:ARG:NH1	2.12	0.65
5:P:261:PRO:HG3	9:P:4201:HOH:O	1.97	0.65
1:A:86:VAL:HG12	1:A:124:ASN:ND2	2.11	0.65
2:C:103:LYS:HE2	2:C:103:LYS:HA	1.79	0.65
3:D:1042:ARG:O	3:D:1057:VAL:HB	1.96	0.65
3:D:1102:THR:HG22	3:D:1222:GLY:HA2	1.78	0.65
2:M:266:ARG:HG2	9:M:9612:HOH:O	1.95	0.65
2:M:380:ALA:HB1	9:M:2219:HOH:O	1.97	0.65
2:M:1000:MET:SD	2:M:1001:VAL:HG22	2.37	0.65
3:N:52:PRO:HG3	3:N:80:VAL:HG23	1.78	0.65
1:A:206:THR:HG22	1:A:209:GLU:H	1.62	0.64
3:D:162:ARG:HH22	3:D:434:ARG:HH21	1.43	0.64
2:M:17:PRO:HB2	2:M:20:GLU:HB2	1.77	0.64
2:M:143:SER:HB2	2:M:276:LYS:HE2	1.79	0.64
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.78	0.64
3:N:126:VAL:HG13	3:N:132:TYR:HB2	1.79	0.64
3:N:484:PRO:O	3:N:489:ARG:HD2	1.97	0.64
3:N:800:LYS:HG3	3:N:830:ALA:HB3	1.79	0.64
3:N:1310:ARG:NE	3:N:1327:ARG:HB3	2.13	0.64
2:C:580:MET:O	2:C:902:ILE:HA	1.98	0.64
2:C:759:THR:HG22	9:C:9784:HOH:O	1.98	0.64
3:D:440:VAL:HA	9:D:2195:HOH:O	1.97	0.64
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.78	0.64
1:K:64:GLU:HG3	1:K:165:ILE:HD12	1.79	0.64
3:N:984:THR:HG22	3:N:987:GLU:CG	2.27	0.64
3:N:1432:LYS:NZ	3:N:1460:ILE:HB	2.12	0.64
5:P:130:VAL:HG13	5:P:156:VAL:HG23	1.78	0.64
1:A:193:ASP:HA	9:C:9642:HOH:O	1.95	0.64
1:B:100:LEU:HD12	1:B:115:LEU:HD21	1.79	0.64
2:C:946:ARG:HD2	2:C:984:GLU:HB2	1.77	0.64
3:D:1189:ARG:HG2	9:D:9851:HOH:O	1.96	0.64
1:K:72:LYS:NZ	2:M:644:VAL:HA	2.10	0.64
2:M:150:PRO:HA	2:M:158:TYR:HB3	1.79	0.64
2:M:232:GLU:HA	9:M:9931:HOH:O	1.98	0.64
2:M:462:ASP:HB2	9:M:9913:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:983:LEU:HB2	9:N:9836:HOH:O	1.96	0.64
3:N:1034:GLN:HA	3:N:1037:GLN:HE21	1.63	0.64
3:D:660:LYS:HA	3:D:663:GLU:HG3	1.79	0.64
2:M:1020:PRO:O	3:N:622:ARG:HD2	1.97	0.64
2:M:1098:ASP:HB2	3:N:21:TRP:HZ2	1.62	0.64
3:N:601:ARG:HB2	5:P:318:GLU:OE1	1.97	0.64
3:N:1095:THR:O	3:N:1099:VAL:HG23	1.97	0.64
5:P:185:GLN:HA	5:P:188:ILE:HD12	1.80	0.64
1:A:88:ARG:HG3	1:A:204:SER:O	1.98	0.64
2:C:1054:THR:HG21	2:C:1079:PRO:CB	2.20	0.64
5:F:286:PRO:HA	9:F:9596:HOH:O	1.97	0.64
1:K:41:ARG:HH11	1:K:177:VAL:HB	1.62	0.64
1:K:48:ILE:HG22	1:K:173:PRO:HD2	1.79	0.64
1:L:220:GLU:HG3	9:L:3319:HOH:O	1.96	0.64
2:M:760:SER:HA	9:M:9228:HOH:O	1.97	0.64
3:N:71:LYS:HD2	3:N:71:LYS:N	2.12	0.64
3:N:466:LYS:HD2	3:N:510:GLU:HG2	1.78	0.64
3:N:984:THR:HG23	3:N:986:ARG:H	1.63	0.64
1:A:153:ALA:HA	1:A:156:HIS:NE2	2.12	0.64
2:C:739:GLU:HG2	9:C:9982:HOH:O	1.96	0.64
2:C:862:PRO:HG3	2:C:975:TYR:HE1	1.63	0.64
3:D:806:PHE:O	3:D:808:THR:N	2.31	0.64
2:M:575:GLN:HB3	2:M:670:GLN:HA	1.80	0.64
2:M:943:VAL:HG13	2:M:985:GLY:H	1.62	0.64
2:M:1018:GLN:HG3	2:M:1060:ILE:HD11	1.78	0.64
3:N:794:GLN:HE21	3:N:795:VAL:N	1.95	0.64
1:B:86:VAL:HG12	1:B:124:ASN:ND2	2.12	0.64
2:C:606:VAL:HA	9:C:9584:HOH:O	1.95	0.64
2:C:831:ARG:NH2	2:C:999:HIS:HB2	2.12	0.64
3:D:513:ILE:HA	9:D:9584:HOH:O	1.96	0.64
3:D:631:ILE:HG21	3:D:745:MET:HG3	1.80	0.64
4:O:47:LYS:HA	4:O:54:LEU:HB3	1.80	0.64
1:B:162:ILE:HG23	1:B:163:ASN:ND2	2.11	0.64
2:C:403:SER:O	2:C:407:LYS:HD3	1.98	0.64
2:C:1114:GLY:HA2	9:C:2283:HOH:O	1.96	0.64
3:D:24:GLY:HA3	3:D:49:ILE:HG12	1.79	0.64
3:D:860:LEU:O	3:D:877:PRO:HD2	1.97	0.64
3:D:873:LEU:HD12	3:D:873:LEU:H	1.63	0.64
3:D:1058:ARG:HH11	3:D:1058:ARG:HG3	1.63	0.64
3:D:1279:GLY:O	3:D:1318:TYR:HA	1.98	0.64
3:D:1503:VAL:HG12	9:D:9672:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:401:GLU:O	5:F:405:LEU:HB2	1.97	0.64
1:K:59:GLU:HG3	1:K:60:ASP:H	1.63	0.64
1:L:39:PRO:O	1:L:43:ILE:HG12	1.97	0.64
2:M:159:ILE:HA	9:M:2059:HOH:O	1.96	0.64
3:N:64:LYS:NZ	5:P:377:ASP:HA	2.12	0.64
3:N:65:ARG:HB2	5:P:375:LEU:CA	2.28	0.64
3:N:161:LEU:O	3:N:449:SER:HB2	1.98	0.64
3:N:468:LEU:HB3	9:N:9474:HOH:O	1.98	0.64
5:P:271:LEU:HD22	5:P:291:ILE:HD11	1.80	0.64
2:C:17:PRO:HB2	2:C:20:GLU:HB2	1.80	0.64
2:C:110:GLU:H	2:C:368:THR:HG21	1.63	0.64
3:D:135:LEU:HD21	3:D:452:ILE:HG13	1.80	0.64
3:D:141:ILE:HD13	3:D:450:TYR:H	1.63	0.64
1:L:100:LEU:HD12	1:L:115:LEU:HD21	1.80	0.64
2:M:721:ARG:NH2	2:M:783:ARG:HH21	1.96	0.64
3:N:925:GLU:HB3	9:O:6558:HOH:O	1.98	0.64
9:C:9880:HOH:O	3:D:656:PHE:HA	1.97	0.64
3:D:6:ARG:HB3	3:D:6:ARG:HH11	1.61	0.64
3:D:694:VAL:HA	9:D:2200:HOH:O	1.97	0.64
5:F:132:ARG:NH2	5:F:184:ARG:HH12	1.96	0.64
1:L:44:LEU:HD23	1:L:48:ILE:HD11	1.79	0.64
3:N:794:GLN:NE2	3:N:795:VAL:N	2.47	0.64
3:N:834:THR:HG22	3:N:838:ARG:HE	1.62	0.64
3:N:850:LEU:H	3:N:850:LEU:HD12	1.62	0.64
1:B:112:ARG:HD2	9:B:9726:HOH:O	1.97	0.63
2:C:133:ASP:HB2	2:C:632:ASN:HD21	1.62	0.63
2:M:31:GLN:HB3	2:M:71:TYR:OH	1.98	0.63
2:M:325:ILE:O	2:M:331:ARG:HG3	1.97	0.63
3:N:462:GLN:HG3	3:N:513:ILE:HD13	1.79	0.63
3:N:1031:ASN:HB3	3:N:1034:GLN:CD	2.18	0.63
2:C:139:GLN:HA	2:C:411:SER:O	1.97	0.63
2:C:399:ASN:ND2	2:C:568:ALA:HB3	2.13	0.63
3:D:12:LEU:HD11	3:D:512:MET:HG2	1.77	0.63
3:D:149:LYS:H	3:D:149:LYS:HD3	1.61	0.63
3:D:690:ALA:HA	9:D:9783:HOH:O	1.97	0.63
3:N:798:GLU:HG2	3:N:799:LYS:H	1.62	0.63
5:P:184:ARG:O	5:P:188:ILE:HG13	1.99	0.63
5:P:291:ILE:HG21	5:P:304:VAL:HG11	1.78	0.63
2:C:47:ALA:HB3	9:C:9646:HOH:O	1.97	0.63
1:K:25:LEU:HD11	9:L:4548:HOH:O	1.97	0.63
1:K:42:ARG:HA	9:K:1228:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:84:ARG:NH1	2:M:128:ILE:HG12	2.13	0.63
2:M:603:VAL:HG21	2:M:643:VAL:CG1	2.28	0.63
2:M:721:ARG:HG2	9:M:9669:HOH:O	1.98	0.63
2:M:1020:PRO:HD2	3:N:622:ARG:HB2	1.79	0.63
2:M:1059:ASP:HA	9:M:9233:HOH:O	1.98	0.63
3:N:704:ARG:HG2	9:N:9545:HOH:O	1.98	0.63
3:N:820:GLU:HB2	3:N:836:VAL:HG11	1.80	0.63
1:A:18:ARG:HD3	1:A:123:MET:HE3	1.81	0.63
1:A:39:PRO:O	1:A:43:ILE:HG12	1.98	0.63
1:A:73:GLU:HG2	9:A:9656:HOH:O	1.97	0.63
1:A:74:ASP:HA	9:A:9794:HOH:O	1.99	0.63
2:C:823:VAL:HG13	9:C:9907:HOH:O	1.98	0.63
1:K:180:GLN:HB3	9:K:1076:HOH:O	1.97	0.63
2:M:404:LEU:HD23	2:M:587:VAL:HG13	1.80	0.63
5:P:94:LEU:HD13	5:P:96:LEU:H	1.62	0.63
5:P:266:GLU:HB2	5:P:270:LYS:NZ	2.12	0.63
1:A:42:ARG:HG2	1:A:42:ARG:HH11	1.64	0.63
1:A:170:VAL:HG21	9:A:9702:HOH:O	1.98	0.63
3:D:777:PRO:HB2	3:D:912:LYS:HD2	1.80	0.63
3:D:1004:THR:OG1	3:D:1036:ARG:HD3	1.98	0.63
3:D:1269:LYS:HD2	9:D:2737:HOH:O	1.98	0.63
1:L:152:PRO:HD2	1:L:155:LYS:HD3	1.80	0.63
1:L:185:ARG:NH1	3:N:692:GLU:HG3	2.13	0.63
2:M:331:ARG:NH1	2:M:427:VAL:HG13	2.12	0.63
2:M:493:ARG:HG3	9:M:9314:HOH:O	1.97	0.63
2:M:1007:ALA:HB2	9:M:9335:HOH:O	1.98	0.63
2:M:1016:ILE:HD12	3:N:526:PRO:HG2	1.80	0.63
3:N:9:ARG:HH12	3:N:11:ALA:HB2	1.63	0.63
3:N:172:PRO:HD2	3:N:389:GLU:O	1.98	0.63
3:N:429:SER:HG	3:N:432:TYR:HD2	1.46	0.63
3:N:1432:LYS:HZ3	3:N:1460:ILE:HB	1.63	0.63
5:P:291:ILE:HD13	5:P:304:VAL:HG13	1.79	0.63
1:B:203:GLY:HA2	9:B:9589:HOH:O	1.99	0.63
2:C:731:GLU:HG3	9:C:9837:HOH:O	1.97	0.63
2:C:987:ILE:HG23	9:C:9757:HOH:O	1.98	0.63
2:C:1024:LYS:HB2	9:C:9932:HOH:O	1.97	0.63
3:D:708:LEU:HD13	3:D:1231:GLU:HA	1.79	0.63
1:L:107:LYS:HD2	9:L:8983:HOH:O	1.98	0.63
2:M:164:PRO:HA	2:M:266:ARG:NH1	2.13	0.63
2:M:953:VAL:HG13	2:M:966:LEU:HD13	1.80	0.63
3:N:399:ARG:HB3	3:N:402:PRO:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:440:VAL:HG23	9:N:9421:HOH:O	1.98	0.63
3:N:1373:ARG:HG2	3:N:1374:GLN:HE21	1.63	0.63
1:A:18:ARG:O	1:A:207:PRO:HD3	1.99	0.63
1:A:104:GLU:HG3	9:A:9611:HOH:O	1.99	0.63
2:C:511:GLU:O	2:C:526:PRO:HD3	1.98	0.63
2:C:1016:ILE:HD13	2:C:1016:ILE:H	1.63	0.63
3:D:1394:VAL:HB	3:D:1397:LYS:HB2	1.80	0.63
5:F:113:ILE:HA	5:F:116:LEU:HD12	1.81	0.63
5:F:278:LEU:CB	5:F:286:PRO:HG2	2.24	0.63
1:K:178:ALA:HB3	1:K:198:ARG:HG3	1.80	0.63
2:M:502:PRO:HB2	2:M:509:ALA:HB3	1.79	0.63
2:M:528:GLU:HA	9:M:9431:HOH:O	1.99	0.63
3:N:107:ASP:HA	9:N:9514:HOH:O	1.99	0.63
3:N:441:ARG:HG2	9:N:9718:HOH:O	1.98	0.63
3:N:1175:ILE:O	3:N:1179:GLU:HG3	1.97	0.63
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.64	0.63
3:D:1215:VAL:HB	9:D:9841:HOH:O	1.99	0.63
2:M:129:ILE:HG22	2:M:130:ASN:N	2.14	0.63
2:M:164:PRO:HA	2:M:266:ARG:NH2	2.12	0.63
2:M:328:LEU:HA	9:M:9297:HOH:O	1.98	0.63
2:M:567:GLN:HB3	2:M:997:LEU:HD22	1.80	0.63
2:M:1057:SER:HB2	3:N:622:ARG:O	1.99	0.63
5:P:163:LEU:HD13	5:P:174:LEU:HD21	1.81	0.63
3:D:86:ARG:O	3:D:522:PRO:HD2	1.99	0.63
3:D:574:LEU:O	3:D:578:VAL:HG23	1.99	0.63
3:D:1150:ALA:O	3:D:1151:ARG:HD3	1.99	0.63
5:F:220:LEU:HD12	5:F:243:ILE:HD11	1.81	0.63
1:L:212:ASN:HB2	9:L:1267:HOH:O	1.98	0.63
2:M:129:ILE:HD11	9:M:9705:HOH:O	1.98	0.63
3:N:65:ARG:CB	5:P:375:LEU:HA	2.26	0.63
3:N:545:ARG:HD2	9:P:1680:HOH:O	1.98	0.63
3:N:598:ARG:HG2	3:N:598:ARG:HH11	1.63	0.63
3:N:806:PHE:O	3:N:808:THR:N	2.32	0.63
4:O:94:PRO:HG2	9:O:6584:HOH:O	1.97	0.63
5:P:402:ASN:HA	9:P:3207:HOH:O	1.99	0.63
2:C:1085:PHE:CD2	3:D:1468:LEU:HA	2.33	0.62
3:D:966:GLU:HA	3:D:969:ARG:NH1	2.14	0.62
3:D:1052:THR:HG23	9:D:2494:HOH:O	1.99	0.62
3:D:1209:LEU:HG	3:D:1211:MET:SD	2.39	0.62
5:F:231:ARG:HB3	5:F:233:PHE:CE2	2.34	0.62
1:K:14:ARG:HB3	9:K:1738:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1104:GLU:HB2	9:M:2124:HOH:O	1.99	0.62
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.33	0.62
3:D:521:PRO:HB2	3:D:524:LEU:HD12	1.80	0.62
3:D:984:THR:HG22	3:D:987:GLU:CG	2.27	0.62
3:D:988:ARG:HD2	9:D:9919:HOH:O	1.99	0.62
3:D:1068:LEU:HG	3:D:1072:ILE:HG12	1.80	0.62
3:D:1440:PHE:HB2	3:D:1442:ASN:ND2	2.15	0.62
4:E:74:VAL:HG12	4:E:79:LEU:HD21	1.80	0.62
1:K:39:PRO:O	1:K:43:ILE:HG12	1.99	0.62
1:K:100:LEU:HD12	1:K:115:LEU:HD21	1.81	0.62
1:L:88:ARG:HB2	9:L:1335:HOH:O	1.97	0.62
2:M:437:ARG:CZ	2:M:488:ALA:HA	2.28	0.62
2:M:966:LEU:HD11	2:M:986:PRO:HG2	1.80	0.62
3:N:1332:PRO:HD2	9:N:2721:HOH:O	1.98	0.62
3:N:1428:ALA:O	3:N:1431:THR:HG23	1.99	0.62
5:P:151:LEU:HB2	5:P:155:THR:OG1	1.99	0.62
5:P:361:LEU:HB3	9:P:1329:HOH:O	1.98	0.62
1:B:176:ARG:HB2	9:B:9702:HOH:O	1.99	0.62
3:D:810:GLU:O	3:D:813:LEU:HG	2.00	0.62
2:M:614:ARG:HG3	9:M:9292:HOH:O	2.00	0.62
2:M:1049:LEU:O	2:M:1053:LEU:HD23	1.99	0.62
3:N:103:TRP:HZ2	3:N:604:THR:HG23	1.63	0.62
3:N:871:LYS:HE2	3:N:873:LEU:HD21	1.79	0.62
3:N:890:VAL:HG13	3:N:926:LYS:HD3	1.81	0.62
1:A:78:ILE:HA	9:A:9585:HOH:O	1.99	0.62
2:C:752:GLY:H	2:C:792:VAL:HB	1.64	0.62
3:D:563:PRO:HG3	5:F:188:ILE:HG21	1.80	0.62
3:D:604:THR:HA	3:D:607:LEU:HD12	1.81	0.62
3:D:616:GLN:O	3:D:619:LEU:HB3	1.99	0.62
3:D:1390:LEU:HA	9:D:9843:HOH:O	1.99	0.62
3:N:607:LEU:HD23	9:N:2546:HOH:O	1.99	0.62
3:N:1279:GLY:O	3:N:1318:TYR:HA	2.00	0.62
3:D:434:ARG:HB2	3:D:447:VAL:HG13	1.81	0.62
3:D:551:ASN:HA	9:D:9809:HOH:O	1.99	0.62
3:D:972:LEU:HB2	9:D:2563:HOH:O	2.00	0.62
3:D:999:THR:HA	3:D:1002:LYS:HD2	1.82	0.62
3:D:1097:LYS:O	3:D:1101:VAL:HG23	1.99	0.62
2:M:586:ARG:NH1	2:M:586:ARG:HB3	2.13	0.62
3:N:137:PRO:HD2	3:N:453:ASP:CB	2.29	0.62
3:N:146:PRO:HA	9:N:9595:HOH:O	1.99	0.62
3:N:684:LYS:HB3	3:N:686:GLU:OE2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.63	0.62
1:B:52:ALA:HB3	9:B:9602:HOH:O	1.98	0.62
1:B:56:VAL:HG13	1:B:142:VAL:HG12	1.82	0.62
2:C:516:ARG:CZ	3:D:1068:LEU:HD22	2.29	0.62
3:D:220:ARG:HA	9:D:9675:HOH:O	1.99	0.62
3:D:1262:LEU:HD23	3:D:1352:ILE:HG12	1.80	0.62
1:K:226:SER:O	1:K:228:PRO:HD3	1.98	0.62
1:L:108:GLU:HB2	9:L:1445:HOH:O	2.00	0.62
2:M:254:VAL:HG13	2:M:258:TYR:HE1	1.64	0.62
2:M:719:PRO:HB3	9:M:9756:HOH:O	1.98	0.62
3:N:1034:GLN:HA	3:N:1037:GLN:NE2	2.14	0.62
3:N:1273:VAL:HG22	3:N:1326:THR:OG1	1.99	0.62
3:N:1421:LEU:HA	9:N:9377:HOH:O	1.98	0.62
8:N:9101:G4P:H5 <sup>7</sup>	8:N:9101:G4P:H8	1.80	0.62
1:A:180:GLN:NE2	2:C:934:PHE:HB2	2.14	0.62
2:C:195:LEU:O	2:C:199:VAL:HG23	1.98	0.62
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.14	0.62
3:D:631:ILE:HG12	3:D:743:ASP:O	1.99	0.62
3:D:1396:GLU:O	3:D:1400:VAL:HG23	2.00	0.62
2:M:304:LEU:HB3	2:M:305:PRO:HD3	1.82	0.62
3:N:1012:GLU:HG2	3:N:1021:TYR:OH	1.99	0.62
3:N:1394:VAL:HG13	9:N:2001:HOH:O	1.99	0.62
9:N:9288:HOH:O	4:O:54:LEU:HD11	2.00	0.62
1:B:20:TYR:HB3	9:B:9603:HOH:O	1.99	0.62
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.82	0.62
1:B:206:THR:HG22	1:B:209:GLU:H	1.64	0.62
2:C:442:GLU:HG2	2:C:454:SER:CB	2.28	0.62
2:C:1067:TYR:CG	5:F:341:PRO:HB3	2.34	0.62
5:F:158:GLU:HA	5:F:161:GLN:CD	2.19	0.62
2:M:492:ASP:HB2	9:M:9314:HOH:O	1.99	0.62
2:M:758:ARG:HG3	9:M:9349:HOH:O	2.00	0.62
3:N:1040:GLY:O	3:N:1060:SER:HB3	2.00	0.62
3:N:1271:LYS:HG3	9:N:9632:HOH:O	2.00	0.62
1:A:86:VAL:HG12	1:A:124:ASN:HD22	1.65	0.62
1:B:59:GLU:HG3	1:B:60:ASP:H	1.64	0.62
2:C:773:LEU:O	2:C:777:ILE:HG13	2.00	0.62
2:C:911:GLU:O	2:C:915:LYS:HG2	1.98	0.62
2:C:958:THR:HG22	9:C:2770:HOH:O	1.99	0.62
3:D:464:LEU:HA	9:D:9601:HOH:O	2.00	0.62
3:D:1378:TYR:OH	3:D:1431:THR:HG22	1.99	0.62
1:L:224:TYR:HB2	9:L:4548:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:225:SER:HB2	9:M:2105:HOH:O	2.00	0.62
2:M:497:ALA:HA	2:M:515:ALA:HA	1.82	0.62
2:M:536:PRO:HB3	2:M:906:PHE:CD1	2.29	0.62
3:N:1046:GLN:OE1	3:N:1079:LYS:HD3	1.99	0.62
5:P:166:LEU:HD13	5:P:170:HIS:HB2	1.82	0.62
5:P:195:VAL:HG11	5:P:217:ASN:OD1	2.00	0.62
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.82	0.62
2:C:186:VAL:HG23	2:C:187:ASN:H	1.64	0.62
2:C:497:ALA:HA	2:C:515:ALA:HA	1.81	0.62
2:C:793:PRO:HB3	9:C:9926:HOH:O	1.99	0.62
3:D:502:PHE:CE2	3:D:1452:ILE:HG23	2.34	0.62
3:D:701:LEU:O	3:D:747:VAL:HG23	2.00	0.62
3:D:1046:GLN:HB3	3:D:1052:THR:HG22	1.81	0.62
3:D:1243:THR:HB	3:D:1253:THR:HB	1.80	0.62
3:N:1042:ARG:O	3:N:1057:VAL:HB	2.00	0.62
1:B:64:GLU:HG3	1:B:165:ILE:HG21	1.80	0.61
2:C:189:ARG:HB3	9:C:9840:HOH:O	1.99	0.61
2:C:430:VAL:HG13	3:D:1075:HIS:HA	1.82	0.61
3:D:148:GLU:HG3	9:D:3099:HOH:O	1.99	0.61
3:D:152:LEU:HD23	3:D:152:LEU:H	1.64	0.61
3:D:434:ARG:HB2	3:D:447:VAL:HG22	1.80	0.61
3:D:484:PRO:O	3:D:489:ARG:HD2	2.00	0.61
2:M:610:ARG:HB2	9:M:9214:HOH:O	2.00	0.61
2:M:911:GLU:HB3	2:M:912:PRO:HD3	1.82	0.61
3:N:130:SER:HA	3:N:572:ARG:NH1	2.14	0.61
3:N:884:ARG:HD3	3:N:888:GLU:OE2	1.99	0.61
4:O:54:LEU:O	4:O:54:LEU:HD23	2.00	0.61
1:A:197:LEU:HD23	1:A:197:LEU:H	1.66	0.61
1:B:30:ARG:HD3	9:B:9697:HOH:O	2.00	0.61
1:B:117:VAL:HG21	9:B:9656:HOH:O	1.98	0.61
2:C:207:LEU:O	2:C:211:LEU:HB3	2.00	0.61
2:C:376:ARG:HB2	2:C:377:PRO:HD3	1.81	0.61
3:D:1273:VAL:HG22	3:D:1326:THR:OG1	2.00	0.61
5:F:85:LEU:HD12	9:F:9829:HOH:O	2.00	0.61
1:L:38:ASN:HB3	1:L:39:PRO:HD3	1.81	0.61
2:M:220:GLY:HA3	9:M:9787:HOH:O	1.99	0.61
2:M:952:LEU:HD12	2:M:969:GLN:NE2	2.11	0.61
3:N:421:LEU:HD12	3:N:435:VAL:HG11	1.81	0.61
2:C:28:ARG:HG3	9:C:2013:HOH:O	2.01	0.61
2:C:305:PRO:HA	2:C:308:ARG:HB3	1.82	0.61
2:C:327:HIS:HB3	2:C:330:ASN:HD22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:909:ALA:HB1	2:C:914:ILE:HD11	1.83	0.61
3:D:39:PRO:HB3	3:D:45:PHE:O	2.00	0.61
3:D:211:VAL:HG13	3:D:393:ILE:HA	1.83	0.61
5:F:394:ARG:HD3	9:F:2104:HOH:O	1.99	0.61
1:L:73:GLU:HB3	9:L:1341:HOH:O	1.98	0.61
2:M:611:ILE:HD11	2:M:641:PRO:HG3	1.81	0.61
2:M:961:GLU:HG2	9:M:2341:HOH:O	2.00	0.61
1:A:42:ARG:HD3	1:B:35:THR:HG23	1.83	0.61
2:C:176:VAL:HG12	2:C:182:VAL:HG13	1.81	0.61
3:D:664:LYS:HG2	9:D:2544:HOH:O	2.00	0.61
3:D:1310:ARG:HD2	9:D:2631:HOH:O	2.00	0.61
3:D:1438:ALA:O	3:D:1443:THR:HG22	2.00	0.61
1:K:18:ARG:O	1:K:207:PRO:HD3	2.00	0.61
2:M:1054:THR:HG23	2:M:1059:ASP:HB2	1.81	0.61
3:N:87:ARG:HD3	3:N:523:ASP:OD2	2.00	0.61
3:N:434:ARG:HG3	9:N:9455:HOH:O	2.00	0.61
4:O:40:LEU:HB3	9:O:2072:HOH:O	2.00	0.61
1:A:9:PRO:HD2	1:B:224:TYR:CD1	2.35	0.61
1:A:36:LEU:O	1:A:39:PRO:HD2	2.01	0.61
3:D:191:LEU:HD13	3:D:195:VAL:HG11	1.83	0.61
3:D:1197:ARG:HH12	3:D:1377:LYS:HB2	1.66	0.61
5:F:271:LEU:HD23	5:F:295:MET:HG3	1.82	0.61
1:L:20:TYR:OH	1:L:198:ARG:HD2	1.99	0.61
2:M:9:ILE:HG12	2:M:907:ASP:OD2	2.00	0.61
2:M:141:HIS:O	2:M:331:ARG:HA	2.00	0.61
2:M:412:ALA:HB1	2:M:419:THR:HG21	1.81	0.61
2:M:1013:TYR:CE2	5:P:341:PRO:HD2	2.34	0.61
2:M:1098:ASP:HB2	3:N:21:TRP:CZ2	2.35	0.61
3:N:568:ARG:HA	3:N:571:LYS:HE3	1.82	0.61
3:N:1403:LEU:HA	9:N:9392:HOH:O	2.00	0.61
5:P:308:LEU:O	5:P:312:GLN:HG3	2.01	0.61
1:B:128:HIS:HB3	9:B:9670:HOH:O	2.00	0.61
2:C:794:PRO:HB3	9:C:2362:HOH:O	1.99	0.61
3:D:3:LYS:HD3	3:D:3:LYS:H	1.65	0.61
3:D:895:VAL:O	3:D:899:LEU:HD12	2.01	0.61
1:L:66:SER:HA	9:L:6317:HOH:O	1.99	0.61
2:M:496:ILE:HG12	2:M:531:PHE:HB2	1.82	0.61
3:N:2:LYS:HB2	9:N:9489:HOH:O	2.00	0.61
3:N:81:THR:HB	3:N:85:VAL:CG2	2.31	0.61
3:N:991:GLN:HA	9:N:9221:HOH:O	2.00	0.61
5:P:148:LYS:HA	9:P:1661:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:353:GLU:HG2	5:P:417:LYS:HB3	1.81	0.61
1:A:96:THR:HG21	9:A:9575:HOH:O	2.00	0.61
2:C:413:LEU:H	2:C:413:LEU:HD12	1.66	0.61
2:C:1069:ALA:O	2:C:1074:GLU:HG2	2.01	0.61
3:D:580:ALA:HA	3:D:584:ASN:OD1	2.00	0.61
5:F:308:LEU:O	5:F:312:GLN:HG2	2.01	0.61
2:M:195:LEU:HB3	2:M:238:LEU:HD21	1.81	0.61
3:N:211:VAL:HG13	3:N:393:ILE:HA	1.81	0.61
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.82	0.61
3:N:1389:LEU:H	3:N:1389:LEU:CD2	2.12	0.61
5:P:94:LEU:HD12	5:P:97:GLU:N	2.15	0.61
1:A:30:ARG:HH22	1:B:155:LYS:NZ	1.98	0.61
1:A:223:THR:HB	9:A:9644:HOH:O	2.00	0.61
1:A:227:ASN:H	1:A:227:ASN:HD22	1.48	0.61
2:C:479:VAL:HG21	2:C:503:LEU:HD11	1.83	0.61
2:C:958:THR:HG23	2:C:961:GLU:HB2	1.82	0.61
5:F:192:LEU:O	5:F:196:VAL:HG23	2.01	0.61
1:K:17:GLY:HA3	9:K:3120:HOH:O	2.00	0.61
2:M:87:ASP:HB3	9:M:9773:HOH:O	2.00	0.61
2:M:189:ARG:HH21	2:M:243:ARG:NH2	1.98	0.61
2:M:910:LYS:HB3	9:M:9220:HOH:O	2.01	0.61
3:N:1109:GLU:HG2	3:N:1201:CYS:CA	2.30	0.61
3:N:1342:GLU:HB2	9:N:2770:HOH:O	1.99	0.61
2:C:21:ILE:H	2:C:21:ILE:HD12	1.66	0.61
2:C:762:LYS:HE2	2:C:771:GLU:OE1	2.01	0.61
2:C:1049:LEU:O	2:C:1053:LEU:HD23	2.00	0.61
3:D:1115:THR:HB	9:D:2390:HOH:O	2.01	0.61
5:P:122:LEU:HG	5:P:126:LEU:HD23	1.83	0.61
1:B:7:LYS:NZ	1:B:7:LYS:HB3	2.16	0.61
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.82	0.61
3:D:14:SER:HB2	3:D:17:LYS:HG3	1.83	0.61
3:D:172:PRO:HD2	3:D:389:GLU:O	2.00	0.61
3:D:957:PRO:CG	3:D:1007:VAL:HA	2.31	0.61
5:F:370:LYS:HE3	5:F:371:LEU:HG	1.83	0.61
2:M:647:GLN:HA	9:M:9256:HOH:O	2.00	0.61
3:N:836:VAL:HG13	9:N:9636:HOH:O	2.01	0.61
5:P:297:PRO:HA	9:P:7238:HOH:O	2.01	0.61
5:P:372:ARG:HB3	9:P:2070:HOH:O	2.00	0.61
5:P:393:THR:HG22	5:P:394:ARG:N	2.16	0.61
1:A:70:GLY:HA2	1:A:133:GLU:HG2	1.83	0.60
2:C:507:ARG:HB2	2:C:507:ARG:HH11	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:724:ARG:HG3	9:C:9568:HOH:O	2.01	0.60
2:C:1034:GLU:HG2	9:C:9872:HOH:O	2.01	0.60
3:D:86:ARG:NH1	3:D:522:PRO:HB2	2.16	0.60
2:M:96:ALA:HB2	9:M:9250:HOH:O	2.00	0.60
2:M:439:CYS:HB2	2:M:541:SER:HB3	1.82	0.60
2:M:721:ARG:HH21	2:M:783:ARG:HH21	1.48	0.60
3:N:743:ASP:HA	9:N:9297:HOH:O	2.00	0.60
3:D:1044:LEU:HA	9:D:2083:HOH:O	2.00	0.60
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.01	0.60
5:F:191:ASN:HA	9:F:9560:HOH:O	2.00	0.60
2:M:730:SER:O	2:M:734:LEU:HD23	2.01	0.60
2:M:881:ASN:HD22	2:M:881:ASN:H	1.47	0.60
1:B:86:VAL:HG12	1:B:124:ASN:HD22	1.66	0.60
2:C:18:LEU:H	2:C:18:LEU:HD12	1.67	0.60
2:C:328:LEU:HD11	2:C:434:HIS:CD2	2.36	0.60
2:C:893:ALA:HB1	9:C:9860:HOH:O	1.99	0.60
2:C:1115:LEU:HD22	3:D:88:TYR:HD1	1.65	0.60
3:D:806:PHE:CE1	3:D:813:LEU:HB3	2.36	0.60
5:F:398:ARG:HG2	5:F:402:ASN:HD22	1.66	0.60
2:M:71:TYR:HB2	9:M:9393:HOH:O	2.01	0.60
2:M:479:VAL:HG21	2:M:503:LEU:HD11	1.83	0.60
2:M:1004:LYS:HE3	2:M:1027:PHE:HE1	1.66	0.60
2:M:1101:THR:HB	3:N:5:VAL:HG13	1.82	0.60
3:N:860:LEU:HB2	3:N:861:GLN:NE2	2.16	0.60
1:A:227:ASN:HD22	1:A:227:ASN:N	2.00	0.60
2:C:432:ARG:HH11	2:C:432:ARG:HG3	1.66	0.60
2:C:838:LYS:HB3	2:C:848:VAL:HG22	1.82	0.60
2:C:949:LYS:HD2	3:D:796:ARG:HH21	1.67	0.60
2:C:1087:VAL:HG12	2:C:1091:GLU:OE1	2.01	0.60
3:D:17:LYS:HG2	9:D:2736:HOH:O	2.02	0.60
3:D:864:VAL:HG12	3:D:865:THR:H	1.66	0.60
2:M:707:ARG:HG2	9:M:9461:HOH:O	2.02	0.60
3:N:98:PRO:HG2	3:N:462:GLN:NE2	2.15	0.60
3:N:838:ARG:HB3	9:N:9286:HOH:O	2.00	0.60
3:N:1258:ARG:CZ	3:N:1262:LEU:HD11	2.30	0.60
5:P:142:ARG:HB3	5:P:142:ARG:NH1	2.16	0.60
5:P:225:GLU:HB3	5:P:226:LYS:HZ2	1.65	0.60
1:A:227:ASN:H	1:A:227:ASN:ND2	2.00	0.60
1:B:67:THR:HA	9:B:9649:HOH:O	2.02	0.60
2:C:15:LEU:HD22	9:C:9604:HOH:O	2.01	0.60
3:D:119:SER:HB2	3:D:123:LEU:N	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:754:PHE:HE2	3:D:1476:THR:HG21	1.66	0.60
3:D:1109:GLU:OE1	3:D:1201:CYS:HB2	2.01	0.60
3:D:1406:ARG:HA	9:D:9597:HOH:O	2.01	0.60
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.82	0.60
1:K:44:LEU:HD23	1:K:48:ILE:HD11	1.83	0.60
1:L:123:MET:HG3	9:L:2931:HOH:O	2.02	0.60
1:L:162:ILE:HG12	9:L:4752:HOH:O	2.00	0.60
1:L:226:SER:O	1:L:228:PRO:HD3	2.02	0.60
3:N:177:ALA:HA	3:N:199:LEU:HD13	1.83	0.60
3:N:490:ALA:HA	9:N:9668:HOH:O	1.99	0.60
5:P:198:ILE:HA	9:P:8888:HOH:O	2.01	0.60
1:A:134:GLU:HB3	9:A:9569:HOH:O	2.01	0.60
1:B:73:GLU:HA	9:B:9614:HOH:O	2.01	0.60
2:C:833:LEU:HD11	2:C:849:VAL:HG21	1.84	0.60
3:D:493:ARG:CD	3:D:1390:LEU:HD21	2.31	0.60
3:D:500:ARG:HH22	3:D:1388:ARG:HE	1.50	0.60
3:D:536:ALA:HA	5:F:315:VAL:O	2.01	0.60
3:D:719:VAL:O	3:D:721:VAL:HG13	2.01	0.60
1:K:211:LEU:O	1:K:215:VAL:HG13	2.01	0.60
2:M:69:LEU:HD12	2:M:97:ARG:HB3	1.83	0.60
2:M:203:ASP:O	2:M:207:LEU:HB2	2.01	0.60
2:M:234:ALA:HB1	9:M:9363:HOH:O	2.01	0.60
2:M:1096:ALA:O	3:N:13:ALA:HB2	2.01	0.60
3:N:123:LEU:HD11	3:N:152:LEU:HD22	1.84	0.60
3:N:858:VAL:HA	9:N:9450:HOH:O	1.99	0.60
3:N:1258:ARG:HG2	3:N:1262:LEU:HD13	1.82	0.60
1:A:23:PHE:HE1	1:A:208:LEU:HD22	1.67	0.60
2:C:204:GLN:HB3	2:C:222:MET:HG2	1.83	0.60
2:C:208:ALA:HB3	9:C:9874:HOH:O	2.01	0.60
3:D:598:ARG:HB2	9:D:3283:HOH:O	2.00	0.60
3:D:658:LEU:HD11	3:D:674:ARG:NH1	2.16	0.60
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.01	0.60
5:F:234:LYS:HB2	9:F:9575:HOH:O	2.01	0.60
1:K:110:LYS:HD3	9:K:1727:HOH:O	2.01	0.60
2:M:221:LEU:HG	9:M:9323:HOH:O	2.02	0.60
3:N:9:ARG:NH1	3:N:11:ALA:HB2	2.15	0.60
3:N:486:ARG:HH21	3:N:489:ARG:NE	2.00	0.60
3:N:728:LEU:HD22	3:N:745:MET:SD	2.42	0.60
3:N:817:GLU:O	3:N:821:VAL:HG23	2.01	0.60
3:N:902:LEU:HD11	9:N:2304:HOH:O	2.00	0.60
3:N:1290:LEU:HD22	9:N:9440:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1301:LYS:HD2	9:N:9307:HOH:O	2.00	0.60
2:C:218:VAL:HG11	9:C:9905:HOH:O	2.01	0.60
2:C:722:ILE:HG21	2:C:821:GLU:OE1	2.02	0.60
2:C:881:ASN:H	2:C:881:ASN:HD22	1.47	0.60
2:C:1002:GLU:HG3	3:D:744:GLN:HE22	1.66	0.60
2:C:1106:ASP:HA	9:C:9776:HOH:O	2.00	0.60
3:D:208:PRO:HB2	3:D:395:VAL:HG13	1.82	0.60
3:D:625:TYR:O	3:D:749:VAL:HG23	2.01	0.60
3:D:1314:LYS:HA	9:D:2549:HOH:O	2.00	0.60
5:F:138:SER:O	5:F:141:VAL:HG12	2.01	0.60
5:F:369:LEU:HD23	9:F:2056:HOH:O	2.01	0.60
3:N:633:VAL:HG22	3:N:635:PRO:HD3	1.83	0.60
3:N:1277:ILE:HG22	3:N:1278:ASP:N	2.17	0.60
5:P:93:LEU:HG	5:P:190:ALA:CB	2.32	0.60
5:P:363:GLU:O	5:P:367:MET:HG2	2.02	0.60
1:B:94:LEU:HD11	1:B:119:ASP:HB2	1.82	0.60
3:D:462:GLN:HG2	3:D:466:LYS:HE3	1.82	0.60
3:D:998:GLU:O	3:D:1002:LYS:HG3	2.01	0.60
2:M:295:ASP:HB2	9:M:2030:HOH:O	2.01	0.60
2:M:370:ALA:HB1	5:P:280:GLN:HB2	1.83	0.60
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.41	0.60
3:D:240:GLU:HA	9:D:3064:HOH:O	2.00	0.60
3:D:616:GLN:HB2	5:F:326:ASP:HB2	1.84	0.60
3:D:1415:VAL:HG21	9:D:9816:HOH:O	2.01	0.60
5:F:92:PRO:HB2	9:F:9606:HOH:O	2.02	0.60
5:F:102:LEU:HB2	5:F:187:LEU:HD12	1.84	0.60
1:L:73:GLU:HG3	1:L:130:ALA:HA	1.84	0.60
2:M:480:THR:HG22	2:M:482:GLU:H	1.66	0.60
2:M:660:ALA:HB1	2:M:667:ALA:O	2.02	0.60
2:M:946:ARG:HD2	2:M:984:GLU:HB2	1.83	0.60
3:N:654:LYS:HD3	3:N:674:ARG:NH1	2.16	0.60
3:N:698:LYS:HG3	4:O:59:ASN:HD21	1.67	0.60
5:P:160:ASP:HA	5:P:163:LEU:HD12	1.83	0.60
5:P:367:MET:HB3	5:P:370:LYS:NZ	2.17	0.60
1:A:100:LEU:HD12	1:A:115:LEU:HD21	1.83	0.59
1:B:191:ASP:HB2	9:B:9697:HOH:O	2.02	0.59
2:C:1013:TYR:HB3	2:C:1018:GLN:HE21	1.66	0.59
3:D:131:LYS:HA	3:D:456:MET:HG3	1.84	0.59
3:D:565:ILE:HG21	5:F:84:TYR:HB3	1.84	0.59
3:D:1100:ASP:HB3	3:D:1440:PHE:HZ	1.66	0.59
4:E:47:LYS:HD3	9:E:9670:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:98:PRO:O	3:N:458:ALA:HB3	2.02	0.59
3:N:1394:VAL:HB	3:N:1397:LYS:HD2	1.84	0.59
4:O:40:LEU:HB2	4:O:45:ARG:NE	2.17	0.59
5:P:361:LEU:HD11	5:P:408:LEU:HD13	1.84	0.59
1:A:219:ARG:NH1	1:B:219:ARG:HG2	2.18	0.59
2:C:69:LEU:HB3	9:C:9789:HOH:O	2.01	0.59
2:C:405:ARG:HH22	2:C:409:ARG:NH2	1.99	0.59
2:C:453:THR:HA	9:C:9566:HOH:O	2.02	0.59
3:D:119:SER:H	3:D:123:LEU:CD1	2.15	0.59
3:D:195:VAL:HB	3:D:205:TYR:HB2	1.84	0.59
3:D:592:THR:HG21	9:D:9883:HOH:O	2.00	0.59
3:D:1380:GLU:HG2	9:D:9843:HOH:O	2.02	0.59
2:M:172:ILE:HG12	2:M:186:VAL:HG12	1.84	0.59
2:M:266:ARG:CD	2:M:288:ARG:HH12	2.14	0.59
2:M:874:LEU:HD13	3:N:783:ARG:HB3	1.84	0.59
3:N:116:LEU:HD11	3:N:465:LEU:HG	1.84	0.59
3:N:1149:LEU:HD11	3:N:1160:LEU:HB3	1.84	0.59
2:C:585:GLU:HB3	2:C:589:ARG:HH22	1.66	0.59
3:D:488:ARG:HB3	3:D:488:ARG:NH1	2.18	0.59
5:F:415:THR:O	5:F:417:LYS:HG3	2.01	0.59
2:M:499:ALA:HA	2:M:532:MET:HE3	1.85	0.59
3:N:574:LEU:O	3:N:578:VAL:HG23	2.02	0.59
5:P:323:ASP:O	5:P:325:LYS:HG2	2.02	0.59
1:K:72:LYS:HZ1	2:M:644:VAL:HA	1.68	0.59
2:M:19:THR:HG21	2:M:124:ASP:O	2.02	0.59
2:M:579:VAL:CG1	2:M:887:GLU:HG3	2.32	0.59
2:M:606:VAL:CG2	2:M:645:VAL:HG22	2.32	0.59
3:N:9:ARG:HD3	3:N:1456:LYS:CG	2.32	0.59
3:N:9:ARG:HG3	3:N:1455:LYS:O	2.03	0.59
3:N:473:LEU:HD13	9:N:9510:HOH:O	2.02	0.59
3:N:1189:ARG:NH1	3:N:1189:ARG:HB3	2.16	0.59
1:A:226:SER:O	1:A:228:PRO:HD3	2.01	0.59
2:C:31:GLN:HB3	9:C:2301:HOH:O	2.02	0.59
2:C:266:ARG:HB3	9:C:9842:HOH:O	2.01	0.59
2:C:728:HIS:HB3	2:C:729:LEU:HD22	1.84	0.59
2:C:787:ASP:HA	9:C:9784:HOH:O	2.01	0.59
2:C:814:GLU:HA	9:C:9961:HOH:O	2.01	0.59
2:C:921:ALA:HA	9:C:2761:HOH:O	2.02	0.59
3:D:487:ALA:HB3	3:D:488:ARG:HE	1.66	0.59
3:D:1097:LYS:HB3	9:D:9630:HOH:O	2.03	0.59
4:E:23:VAL:HG21	9:E:9593:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:260:LEU:HA	2:M:291:ALA:HB2	1.84	0.59
2:M:507:ARG:HG3	9:M:9830:HOH:O	2.02	0.59
2:M:1054:THR:HG22	2:M:1055:LEU:N	2.17	0.59
2:M:1055:LEU:HD22	2:M:1066:ALA:HB2	1.84	0.59
3:N:84:ILE:HG22	9:N:9289:HOH:O	2.03	0.59
3:N:598:ARG:HG2	3:N:598:ARG:NH1	2.17	0.59
3:N:1003:VAL:O	3:N:1007:VAL:HG13	2.01	0.59
1:A:92:PRO:HA	9:A:9625:HOH:O	2.02	0.59
2:C:145:GLY:H	2:C:163:ILE:HG23	1.67	0.59
2:C:165:LEU:HD22	2:C:418:LEU:HD11	1.84	0.59
3:D:171:LEU:HD13	3:D:389:GLU:C	2.23	0.59
3:D:496:LEU:HG	3:D:500:ARG:HG2	1.85	0.59
3:D:781:PRO:HG2	3:D:911:LEU:HD23	1.83	0.59
1:K:2:LEU:HA	1:K:6:LEU:HD22	1.84	0.59
1:L:59:GLU:HG3	1:L:60:ASP:H	1.67	0.59
3:N:131:LYS:HB3	3:N:568:ARG:HG2	1.83	0.59
3:N:1379:VAL:HG11	3:N:1395:LEU:HD23	1.84	0.59
2:C:660:ALA:HB1	2:C:667:ALA:O	2.03	0.59
3:D:132:TYR:HA	9:D:9996:HOH:O	2.01	0.59
3:D:800:LYS:HE2	3:D:830:ALA:HB3	1.84	0.59
3:D:1489:GLN:HB2	9:D:9922:HOH:O	2.02	0.59
1:K:192:LEU:HG	9:K:2051:HOH:O	2.01	0.59
1:K:212:ASN:O	1:K:215:VAL:HG22	2.03	0.59
2:M:63:GLY:HA3	2:M:103:LYS:HG2	1.85	0.59
2:M:369:PRO:HA	9:M:9861:HOH:O	2.03	0.59
2:M:569:VAL:HG12	2:M:996:LYS:O	2.03	0.59
3:N:662:GLU:OE2	3:N:669:ASN:HA	2.03	0.59
3:N:1014:ASN:HB3	9:N:9749:HOH:O	2.02	0.59
3:N:1114:THR:CG2	3:N:1195:GLN:HB2	2.32	0.59
5:P:181:GLU:O	5:P:184:ARG:HB3	2.01	0.59
5:P:316:SER:OG	5:P:318:GLU:HG3	2.02	0.59
1:B:102:LYS:HD3	9:B:9822:HOH:O	2.03	0.59
2:C:35:PRO:HD2	2:C:38:LYS:HE2	1.83	0.59
2:C:184:MET:CE	2:C:186:VAL:HG13	2.32	0.59
2:C:710:ILE:CD1	2:C:758:ARG:HE	2.12	0.59
2:C:761:PHE:HB3	9:C:9910:HOH:O	2.01	0.59
9:C:2004:HOH:O	4:E:31:LEU:HD23	2.03	0.59
5:F:282:LEU:HD12	5:F:284:ARG:HB2	1.84	0.59
2:M:230:ARG:HE	2:M:237:ARG:HH22	1.48	0.59
2:M:386:PHE:HA	9:M:9269:HOH:O	2.01	0.59
2:M:691:SER:HB2	2:M:858:MET:SD	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:769:PRO:HA	9:M:9896:HOH:O	2.02	0.59
2:M:927:GLY:HA2	2:M:930:LYS:NZ	2.18	0.59
3:N:39:PRO:HB3	3:N:45:PHE:C	2.23	0.59
3:N:550:ARG:HH11	3:N:550:ARG:HG3	1.68	0.59
3:N:1102:THR:HG22	3:N:1222:GLY:HA2	1.82	0.59
3:N:1114:THR:HB	3:N:1195:GLN:OE1	2.02	0.59
1:B:42:ARG:HG2	1:B:42:ARG:HH11	1.67	0.59
2:C:328:LEU:HB2	2:C:433:THR:CG2	2.32	0.59
2:C:386:PHE:HA	9:C:9782:HOH:O	2.02	0.59
3:D:770:LEU:HD11	3:D:919:PHE:CE2	2.38	0.59
1:L:20:TYR:HE2	1:L:198:ARG:HB3	1.67	0.59
2:M:12:VAL:HG13	2:M:13:ILE:HG12	1.85	0.59
2:M:1001:VAL:HG23	9:M:9493:HOH:O	2.02	0.59
2:M:1033:GLY:O	2:M:1037:VAL:HG23	2.03	0.59
3:N:475:LYS:HA	3:N:478:LEU:HD12	1.85	0.59
3:N:1101:VAL:HG21	3:N:1424:VAL:HG22	1.84	0.59
5:P:113:ILE:HG23	5:P:127:ILE:HB	1.84	0.59
1:B:212:ASN:O	1:B:215:VAL:HG22	2.03	0.59
2:C:328:LEU:HD22	2:C:433:THR:O	2.03	0.59
3:D:1440:PHE:HB2	3:D:1442:ASN:HD21	1.66	0.59
3:D:1459:LEU:HB3	3:D:1465:ASN:HD22	1.67	0.59
2:M:144:PRO:O	2:M:276:LYS:HD3	2.03	0.59
2:M:837:ASP:HA	9:M:9267:HOH:O	2.03	0.59
3:N:19:ARG:HG3	9:N:9537:HOH:O	2.02	0.59
3:N:605:ASP:HA	3:N:610:LYS:HG3	1.85	0.59
3:N:703:ASN:ND2	3:N:713:ILE:HG12	2.18	0.59
3:N:1374:GLN:OE1	3:N:1377:LYS:HD3	2.02	0.59
3:D:565:ILE:H	3:D:565:ILE:HD12	1.68	0.58
5:F:132:ARG:HH21	5:F:184:ARG:HH12	1.51	0.58
3:N:499:VAL:O	3:N:503:LEU:HB2	2.03	0.58
3:N:887:ALA:HA	9:N:9628:HOH:O	2.03	0.58
3:N:1096:ARG:NH1	3:N:1096:ARG:HB2	2.17	0.58
3:N:1435:LEU:HD23	3:N:1464:GLU:HB2	1.85	0.58
2:C:44:ILE:HG13	2:C:344:PHE:CE2	2.38	0.58
2:C:964:LYS:HE3	9:C:2189:HOH:O	2.02	0.58
9:C:9643:HOH:O	3:D:532:GLY:HA2	2.03	0.58
3:D:430:ASP:HB2	9:D:2014:HOH:O	2.03	0.58
2:M:374:ASN:O	2:M:377:PRO:HD2	2.03	0.58
2:M:420:ARG:HD2	2:M:420:ARG:H	1.68	0.58
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.85	0.58
2:M:537:LYS:HA	2:M:545:ASN:ND2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:119:SER:HB2	3:N:123:LEU:N	2.17	0.58
3:N:957:PRO:HB3	3:N:1010:ASN:HD22	1.68	0.58
3:N:1364:HIS:CE1	3:N:1366:LYS:HG3	2.37	0.58
4:O:54:LEU:HD12	9:O:3002:HOH:O	2.02	0.58
5:P:93:LEU:HD22	5:P:98:GLU:HB3	1.85	0.58
1:A:178:ALA:HB2	2:C:864:GLY:H	1.66	0.58
2:C:225:SER:O	2:C:229:MET:HG2	2.04	0.58
2:C:1074:GLU:HA	9:C:2004:HOH:O	2.02	0.58
3:D:104:PHE:CD2	3:D:1448:THR:HG23	2.38	0.58
3:D:126:VAL:HG12	3:D:132:TYR:HB2	1.84	0.58
3:D:489:ARG:NE	3:D:493:ARG:HH22	1.95	0.58
3:D:1152:GLU:HG2	3:D:1159:ARG:HH21	1.67	0.58
2:M:258:TYR:HB3	9:M:2121:HOH:O	2.02	0.58
2:M:909:ALA:HB1	2:M:914:ILE:HD11	1.85	0.58
3:N:197:SER:CB	3:N:203:ALA:HB3	2.33	0.58
3:N:896:ALA:HB2	9:N:9628:HOH:O	2.03	0.58
5:P:371:LEU:HB2	9:P:5682:HOH:O	2.02	0.58
2:C:412:ALA:HB1	2:C:419:THR:HG21	1.86	0.58
2:C:551:GLU:OE1	2:C:906:PHE:HA	2.03	0.58
2:C:578:VAL:HG23	2:C:579:VAL:HG12	1.86	0.58
2:C:1103:ASP:CG	2:C:1104:GLU:H	2.06	0.58
3:D:122:GLU:HB3	9:D:9684:HOH:O	2.03	0.58
3:D:702:LEU:HD13	3:D:716:PHE:CD1	2.38	0.58
3:D:1131:SER:HB2	9:D:2660:HOH:O	2.02	0.58
3:D:1209:LEU:HD12	3:D:1210:SER:N	2.10	0.58
3:D:1282:ARG:NH1	3:D:1282:ARG:HB3	2.17	0.58
3:D:1341:PRO:HA	3:D:1344:VAL:HG23	1.85	0.58
3:D:1390:LEU:HD23	3:D:1390:LEU:H	1.68	0.58
1:K:26:GLU:HB3	1:K:194:LYS:HG3	1.85	0.58
1:K:89:PHE:HB3	1:K:94:LEU:HD13	1.85	0.58
1:K:229:GLN:HG2	9:K:3118:HOH:O	2.02	0.58
9:K:2958:HOH:O	2:M:830:LYS:HD2	2.03	0.58
2:M:3:ILE:HA	2:M:900:ARG:O	2.04	0.58
2:M:537:LYS:HA	2:M:545:ASN:HD21	1.68	0.58
2:M:954:THR:HG22	9:M:2147:HOH:O	2.03	0.58
3:N:432:TYR:HA	3:N:448:GLU:O	2.03	0.58
3:N:464:LEU:O	3:N:468:LEU:HG	2.03	0.58
3:N:794:GLN:HG2	3:N:905:PRO:HB3	1.85	0.58
3:N:820:GLU:HA	3:N:825:ALA:O	2.03	0.58
4:O:48:MET:HG2	4:O:49:GLN:H	1.67	0.58
5:P:209:PHE:HA	5:P:212:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:339:PRO:HB3	5:P:343:ASP:HB2	1.84	0.58
2:C:95:TYR:HD2	2:C:114:PHE:HB3	1.67	0.58
2:C:810:ASP:HB3	2:C:813:VAL:HG22	1.84	0.58
2:C:1021:LEU:HD22	5:F:331:ASP:O	2.02	0.58
3:D:378:ILE:HA	9:D:2848:HOH:O	2.02	0.58
3:D:799:LYS:HG2	3:D:826:PRO:CG	2.34	0.58
3:D:1389:LEU:HG	3:D:1390:LEU:H	1.69	0.58
3:D:1433:SER:HB2	3:D:1457:ASP:OD2	2.04	0.58
1:L:12:THR:OG1	1:L:24:VAL:HB	2.03	0.58
3:N:65:ARG:CG	3:N:66:GLN:H	2.16	0.58
3:N:441:ARG:HB3	3:N:443:VAL:CG2	2.33	0.58
3:N:481:MET:O	3:N:489:ARG:HB2	2.03	0.58
5:P:371:LEU:HB3	9:P:1119:HOH:O	2.02	0.58
1:A:89:PHE:HB3	1:A:94:LEU:HD13	1.85	0.58
2:C:402:SER:HA	2:C:566:THR:HG23	1.86	0.58
2:C:627:ARG:HD2	9:C:9630:HOH:O	2.02	0.58
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.86	0.58
2:C:756:VAL:HG21	2:C:823:VAL:HG11	1.85	0.58
2:C:1066:ALA:O	2:C:1070:ILE:HG13	2.03	0.58
3:D:32:ILE:HA	9:D:2671:HOH:O	2.04	0.58
3:D:481:MET:O	3:D:489:ARG:HB2	2.02	0.58
3:D:761:ILE:HD12	4:E:20:THR:HG23	1.84	0.58
1:K:191:ASP:HA	9:K:2079:HOH:O	2.03	0.58
2:M:24:GLU:HB3	9:M:9330:HOH:O	2.03	0.58
2:M:431:HIS:HB3	2:M:434:HIS:CD2	2.38	0.58
3:N:699:VAL:HG21	3:N:760:ARG:HB3	1.85	0.58
4:O:50:THR:HA	9:O:2107:HOH:O	2.03	0.58
1:A:113:ASP:HB3	9:A:9594:HOH:O	2.02	0.58
3:D:205:TYR:HE2	3:D:211:VAL:HG11	1.69	0.58
3:D:1264:GLU:HG3	9:D:9596:HOH:O	2.02	0.58
5:F:369:LEU:HA	9:F:2056:HOH:O	2.03	0.58
1:K:110:LYS:HB2	9:K:1330:HOH:O	2.04	0.58
1:K:217:ILE:HA	9:K:3364:HOH:O	2.02	0.58
2:M:148:PHE:CB	2:M:313:LEU:HD22	2.32	0.58
2:M:250:ARG:HE	2:M:253:ALA:HB3	1.66	0.58
2:M:1093:GLN:HE22	2:M:1098:ASP:HA	1.69	0.58
3:N:462:GLN:HA	3:N:513:ILE:HD13	1.86	0.58
3:N:539:ASP:HB2	5:P:318:GLU:OE2	2.03	0.58
3:N:580:ALA:HA	3:N:584:ASN:OD1	2.03	0.58
3:N:774:SER:HB3	3:N:1362:LYS:O	2.03	0.58
3:N:1049:SER:HA	9:N:9571:HOH:O	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1116:ASN:CG	3:N:1193:THR:HB	2.23	0.58
4:O:8:LYS:O	4:O:12:MET:HG3	2.04	0.58
2:C:129:ILE:HG22	2:C:130:ASN:N	2.18	0.58
4:E:47:LYS:HA	4:E:54:LEU:HB3	1.85	0.58
4:E:63:TRP:O	4:E:67:GLU:HG3	2.04	0.58
2:M:897:LEU:HD11	2:M:920:GLN:HG3	1.86	0.58
3:N:710:ARG:HD2	9:N:9333:HOH:O	2.03	0.58
3:N:1493:LYS:HB2	9:N:2722:HOH:O	2.03	0.58
5:P:291:ILE:HG23	5:P:304:VAL:HG21	1.86	0.58
1:A:229:GLN:HB2	9:A:9707:HOH:O	2.02	0.58
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.38	0.58
2:C:250:ARG:HH21	2:C:254:VAL:H	1.52	0.58
2:C:526:PRO:HB2	9:C:2408:HOH:O	2.03	0.58
3:D:445:ARG:HG2	3:D:445:ARG:HH11	1.69	0.58
3:D:456:MET:HG2	3:D:568:ARG:HH11	1.69	0.58
4:E:40:LEU:HB2	4:E:45:ARG:NE	2.19	0.58
5:F:265:VAL:HB	9:F:9892:HOH:O	2.04	0.58
2:M:290:LEU:HB3	2:M:302:VAL:CG1	2.33	0.58
2:M:853:LEU:HB3	2:M:858:MET:HE3	1.85	0.58
3:N:92:HIS:HA	3:N:519:VAL:HG23	1.85	0.58
3:N:149:LYS:HB2	9:N:9232:HOH:O	2.03	0.58
3:N:891:GLU:HB3	9:N:9355:HOH:O	2.04	0.58
4:O:58:PRO:HB2	9:O:4249:HOH:O	2.04	0.58
5:P:156:VAL:HG21	9:P:2305:HOH:O	2.03	0.58
5:P:234:LYS:HG2	9:P:1255:HOH:O	2.02	0.58
1:A:18:ARG:HH22	1:A:88:ARG:HH21	1.51	0.58
2:C:807:ARG:HD3	2:C:808:ARG:O	2.03	0.58
2:C:943:VAL:HG13	2:C:985:GLY:H	1.68	0.58
3:D:28:LYS:HD2	3:D:41:ARG:HH11	1.68	0.58
4:E:44:GLU:O	4:E:45:ARG:HD3	2.04	0.58
4:E:60:ALA:O	4:E:63:TRP:HB2	2.04	0.58
5:F:208:SER:HA	9:F:9649:HOH:O	2.03	0.58
2:M:244:PRO:HD2	2:M:245:GLY:H	1.68	0.58
2:M:554:ASP:HB2	2:M:880:MET:HB2	1.85	0.58
3:N:137:PRO:HD2	3:N:453:ASP:HB3	1.86	0.58
3:N:559:ALA:HA	9:N:9528:HOH:O	2.03	0.58
3:N:692:GLU:OE1	3:N:720:LEU:HB2	2.04	0.58
3:N:707:THR:HA	9:N:2395:HOH:O	2.04	0.58
3:D:434:ARG:HB3	9:D:9861:HOH:O	2.02	0.57
3:D:1240:THR:HG22	9:D:2840:HOH:O	2.03	0.57
9:D:2101:HOH:O	4:E:48:MET:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:132:LEU:HD11	1:L:138:LEU:HD13	1.85	0.57
2:M:371:LYS:O	2:M:372:LEU:HD12	2.04	0.57
2:M:481:ASP:HA	9:M:9383:HOH:O	2.04	0.57
2:M:564:MET:SD	2:M:846:LYS:HE2	2.44	0.57
2:M:683:ASN:HA	2:M:687:ALA:HB3	1.86	0.57
2:M:791:ARG:HB3	9:M:9305:HOH:O	2.03	0.57
3:N:1404:ASN:HB3	9:N:9535:HOH:O	2.04	0.57
3:N:1487:VAL:HG12	3:N:1488:ASP:N	2.19	0.57
9:N:9746:HOH:O	5:P:141:VAL:HG21	2.03	0.57
2:C:213:ALA:HB3	9:C:2338:HOH:O	2.04	0.57
2:C:1021:LEU:HG	2:C:1022:GLY:N	2.18	0.57
3:D:131:LYS:HE2	3:D:568:ARG:HG2	1.86	0.57
3:D:183:GLU:HA	3:D:186:VAL:HG12	1.86	0.57
3:D:489:ARG:HG3	3:D:493:ARG:NH1	2.11	0.57
3:D:996:TRP:CE2	3:D:1056:PRO:HG3	2.39	0.57
3:D:1321:ALA:O	3:D:1339:LYS:HD3	2.03	0.57
5:F:148:LYS:HA	9:F:9564:HOH:O	2.03	0.57
2:M:107:LEU:HD12	9:M:9281:HOH:O	2.03	0.57
2:M:142:ARG:HA	9:M:9253:HOH:O	2.04	0.57
3:N:430:ASP:HB2	3:N:432:TYR:CZ	2.39	0.57
3:N:1025:GLN:HB2	9:N:2440:HOH:O	2.04	0.57
3:N:1209:LEU:HD21	4:O:16:LYS:HD2	1.85	0.57
1:B:18:ARG:O	1:B:207:PRO:HD3	2.04	0.57
2:C:4:LYS:HD2	9:C:2407:HOH:O	2.05	0.57
3:D:28:LYS:HB2	9:D:9655:HOH:O	2.04	0.57
4:E:51:LEU:HD12	4:E:52:GLU:N	2.19	0.57
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.36	0.57
2:M:1093:GLN:HE22	2:M:1099:VAL:H	1.52	0.57
3:N:426:LYS:HB3	5:P:134:LYS:O	2.03	0.57
3:N:539:ASP:HB2	5:P:318:GLU:CD	2.24	0.57
3:N:875:THR:HG22	3:N:879:ARG:HG3	1.86	0.57
3:N:1412:LYS:O	3:N:1414:PRO:HD3	2.03	0.57
5:P:406:ARG:HG3	9:P:3208:HOH:O	2.03	0.57
2:C:332:ARG:HD2	2:C:464:LEU:HG	1.86	0.57
3:D:591:VAL:CG1	3:D:597:ASP:HA	2.33	0.57
5:F:82:ARG:O	5:F:86:HIS:HB2	2.03	0.57
5:F:416:ARG:HD2	5:F:419:ARG:CB	2.34	0.57
1:K:92:PRO:HD3	9:K:1224:HOH:O	2.05	0.57
1:L:152:PRO:HD2	1:L:155:LYS:CD	2.33	0.57
2:M:212:GLY:HA3	2:M:218:VAL:HG23	1.87	0.57
3:N:394:LEU:HA	9:N:9499:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:551:ASN:O	3:N:555:LYS:HG3	2.04	0.57
3:N:996:TRP:CD2	3:N:1056:PRO:HG2	2.39	0.57
3:N:1195:GLN:HA	9:N:2116:HOH:O	2.04	0.57
3:N:1324:PRO:HA	9:N:9374:HOH:O	2.02	0.57
5:P:118:GLU:HB3	9:P:7908:HOH:O	2.04	0.57
2:C:20:GLU:HG2	2:C:24:GLU:HG2	1.86	0.57
2:C:70:GLU:HA	9:C:9597:HOH:O	2.03	0.57
2:C:1025:ALA:HA	9:C:9926:HOH:O	2.04	0.57
3:D:467:GLU:HB2	9:D:9601:HOH:O	2.05	0.57
3:D:813:LEU:O	3:D:817:GLU:HB2	2.03	0.57
3:D:1239:ARG:HB2	9:D:3207:HOH:O	2.04	0.57
3:D:1490:LYS:HG3	9:D:9922:HOH:O	2.04	0.57
4:E:41:GLU:H	4:E:42:PRO:HD2	1.70	0.57
5:F:269:ASN:O	5:F:273:ARG:HG3	2.04	0.57
2:M:144:PRO:HB2	9:M:9612:HOH:O	2.04	0.57
2:M:549:PHE:CD2	2:M:886:LEU:HB3	2.39	0.57
2:M:984:GLU:HG2	3:N:944:THR:O	2.04	0.57
3:N:36:THR:HG22	3:N:38:LYS:HG3	1.87	0.57
3:N:65:ARG:HD3	3:N:66:GLN:H	1.70	0.57
3:N:957:PRO:HG3	3:N:1007:VAL:HA	1.85	0.57
3:N:1198:TYR:OH	3:N:1397:LYS:HE3	2.05	0.57
5:P:79:ASP:O	5:P:83:GLN:HG3	2.04	0.57
5:P:290:GLU:HG3	9:P:1848:HOH:O	2.05	0.57
1:A:212:ASN:O	1:A:215:VAL:HG22	2.05	0.57
2:C:683:ASN:HA	2:C:687:ALA:HB3	1.86	0.57
2:C:785:VAL:HG23	9:C:2281:HOH:O	2.04	0.57
4:E:36:LYS:HD3	9:E:9576:HOH:O	2.04	0.57
4:E:54:LEU:HG	4:E:58:PRO:HD2	1.86	0.57
5:F:205:ARG:HG3	5:F:251:ILE:HD13	1.86	0.57
5:F:300:ASP:HA	9:F:9948:HOH:O	2.03	0.57
1:K:112:ARG:HD2	9:K:3292:HOH:O	2.03	0.57
1:L:156:HIS:HD2	1:L:158:ILE:HG12	1.69	0.57
2:M:545:ASN:O	2:M:905:ILE:HD11	2.03	0.57
2:M:642:ARG:HB3	9:M:9448:HOH:O	2.04	0.57
2:M:964:LYS:O	2:M:968:LEU:HG	2.04	0.57
3:N:119:SER:CB	3:N:123:LEU:HB2	2.33	0.57
3:N:925:GLU:HG2	9:O:1095:HOH:O	2.03	0.57
5:P:152:ASP:HB2	5:P:153:PRO:HD3	1.87	0.57
1:A:10:VAL:HG21	9:A:9712:HOH:O	2.04	0.57
1:B:81:ASN:HB2	9:B:9809:HOH:O	2.03	0.57
2:C:677:MET:SD	2:C:987:ILE:HD13	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:194:GLY:H	3:D:206:ARG:HA	1.69	0.57
3:D:999:THR:O	3:D:1002:LYS:HB2	2.05	0.57
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.40	0.57
3:D:1435:LEU:HB2	3:D:1457:ASP:OD2	2.04	0.57
5:F:366:ALA:O	5:F:370:LYS:HB3	2.04	0.57
1:K:62:LEU:HD11	9:K:8889:HOH:O	2.04	0.57
2:M:165:LEU:HD21	2:M:334:ARG:NH2	2.20	0.57
2:M:524:VAL:HG22	2:M:525:SER:H	1.70	0.57
2:M:645:VAL:HG23	9:M:9422:HOH:O	2.05	0.57
3:N:95:LEU:HD12	3:N:515:GLU:CA	2.34	0.57
3:N:434:ARG:HB2	3:N:447:VAL:CG2	2.33	0.57
3:N:1164:ARG:HA	9:N:9915:HOH:O	2.04	0.57
3:N:1250:ALA:HB3	9:N:9357:HOH:O	2.04	0.57
5:P:416:ARG:HD2	5:P:419:ARG:CB	2.33	0.57
2:C:64:LEU:HD13	2:C:359:MET:SD	2.45	0.57
2:C:145:GLY:HA3	9:C:2144:HOH:O	2.04	0.57
2:C:163:ILE:HB	9:C:9761:HOH:O	2.05	0.57
2:C:203:ASP:O	2:C:207:LEU:HB2	2.03	0.57
2:C:417:GLY:O	2:C:418:LEU:HD13	2.05	0.57
2:C:495:THR:CG2	2:C:517:ARG:HE	2.15	0.57
2:C:538:GLN:HB2	9:C:2365:HOH:O	2.04	0.57
3:D:83:SER:HA	9:D:9574:HOH:O	2.05	0.57
3:D:642:CYS:SG	3:D:716:PHE:HB2	2.44	0.57
3:D:966:GLU:HG2	3:D:970:LYS:HE2	1.87	0.57
3:D:1119:SER:HB3	3:D:1185:GLU:HB3	1.85	0.57
3:D:1429:LEU:HG	9:D:2007:HOH:O	2.04	0.57
4:E:15:SER:HB2	9:E:9581:HOH:O	2.05	0.57
5:F:288:TYR:HD2	5:F:304:VAL:HB	1.70	0.57
2:M:194:VAL:HG12	9:M:9819:HOH:O	2.04	0.57
2:M:244:PRO:HG2	2:M:246:ASP:OD2	2.04	0.57
2:M:564:MET:HG2	2:M:840:ALA:HB3	1.86	0.57
2:M:758:ARG:HB3	2:M:789:SER:HA	1.85	0.57
3:N:179:VAL:HG21	9:N:2712:HOH:O	2.04	0.57
3:N:191:LEU:CB	3:N:195:VAL:HG21	2.30	0.57
3:N:431:VAL:HG13	9:N:9967:HOH:O	2.05	0.57
3:N:659:LYS:HG3	9:N:9809:HOH:O	2.02	0.57
3:N:701:LEU:HD21	3:N:763:MET:HE3	1.87	0.57
3:N:1133:ARG:HD2	9:N:9227:HOH:O	2.04	0.57
3:N:1396:GLU:O	3:N:1400:VAL:HG23	2.04	0.57
3:N:1495:ILE:HD11	4:O:84:ARG:HE	1.69	0.57
1:A:211:LEU:O	1:A:215:VAL:HG13	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:ILE:HG13	2:C:907:ASP:OD2	2.05	0.57
2:C:13:ILE:HD13	2:C:483:VAL:HG21	1.87	0.57
2:C:208:ALA:HA	2:C:218:VAL:CG2	2.35	0.57
3:D:32:ILE:O	5:F:258:ILE:HG23	2.03	0.57
3:D:396:VAL:HG22	3:D:447:VAL:HB	1.87	0.57
3:D:421:LEU:HD12	3:D:435:VAL:HG11	1.86	0.57
3:D:871:LYS:HG3	3:D:873:LEU:HG	1.87	0.57
3:D:1094:LEU:HB3	9:D:2067:HOH:O	2.05	0.57
1:K:62:LEU:H	1:K:62:LEU:HD12	1.70	0.57
1:K:202:ASP:HA	9:K:1200:HOH:O	2.05	0.57
2:M:66:LEU:HD11	2:M:98:LEU:HD22	1.87	0.57
2:M:152:PRO:HA	9:M:2090:HOH:O	2.04	0.57
3:N:25:GLU:HB3	9:N:9871:HOH:O	2.03	0.57
3:N:584:ASN:H	3:N:602:SER:CB	2.18	0.57
3:N:704:ARG:NH1	3:N:743:ASP:HB3	2.19	0.57
5:P:194:LEU:HD22	9:P:1975:HOH:O	2.05	0.57
5:P:250:ALA:HB2	9:P:3340:HOH:O	2.04	0.57
2:C:10:ARG:HG3	9:C:2815:HOH:O	2.04	0.57
2:C:65:VAL:O	2:C:101:ILE:HG12	2.05	0.57
2:C:278:GLU:HG2	2:C:283:ILE:O	2.05	0.57
2:C:807:ARG:HG2	9:C:9967:HOH:O	2.05	0.57
3:D:117:ASP:HB2	3:D:495:ARG:NH2	2.19	0.57
3:D:192:ALA:O	3:D:195:VAL:HG23	2.04	0.57
3:D:799:LYS:HG2	3:D:826:PRO:HG2	1.86	0.57
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.87	0.57
5:F:153:PRO:HB3	9:F:2137:HOH:O	2.05	0.57
5:F:316:SER:OG	5:F:318:GLU:HG3	2.04	0.57
2:M:226:VAL:HG12	9:M:2432:HOH:O	2.05	0.57
2:M:516:ARG:NE	3:N:1068:LEU:HD13	2.20	0.57
2:M:737:LEU:HD11	2:M:754:ILE:HB	1.85	0.57
2:M:1000:MET:HE3	2:M:1002:GLU:HB3	1.87	0.57
3:N:1031:ASN:HB3	3:N:1034:GLN:NE2	2.20	0.57
3:N:1096:ARG:HB2	3:N:1096:ARG:HH11	1.69	0.57
4:O:41:GLU:HB3	9:O:4432:HOH:O	2.04	0.57
5:P:74:LYS:HB2	9:P:2234:HOH:O	2.04	0.57
2:C:250:ARG:HD3	9:C:9820:HOH:O	2.05	0.56
2:C:446:GLY:O	2:C:449:ILE:HG13	2.05	0.56
3:D:834:THR:HB	3:D:838:ARG:HE	1.70	0.56
3:D:1364:HIS:NE2	3:D:1366:LYS:HE3	2.20	0.56
3:D:1390:LEU:HB2	9:D:2140:HOH:O	2.03	0.56
3:D:1503:VAL:HG11	9:D:2031:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:183:SER:CB	2:M:190:LYS:HD3	2.34	0.56
2:M:367:LEU:O	2:M:372:LEU:HD13	2.05	0.56
2:M:545:ASN:ND2	2:M:905:ILE:HG13	2.19	0.56
2:M:612:VAL:HG22	2:M:622:GLU:HA	1.87	0.56
2:M:1085:PHE:O	2:M:1088:LEU:HB3	2.05	0.56
5:P:252:ALA:CB	5:P:265:VAL:HG21	2.30	0.56
5:P:347:GLN:HB3	9:P:5652:HOH:O	2.04	0.56
5:P:368:VAL:HA	9:P:5682:HOH:O	2.03	0.56
1:A:141:GLU:HG3	9:A:9798:HOH:O	2.05	0.56
2:C:1009:SER:HB2	3:D:651:GLU:O	2.05	0.56
3:D:116:LEU:HD23	3:D:468:LEU:HD11	1.86	0.56
5:F:406:ARG:HA	5:F:409:LYS:HG2	1.85	0.56
1:L:83:LYS:HE2	1:L:167:VAL:HG12	1.86	0.56
2:M:490:GLU:HG2	2:M:494:TYR:CE1	2.40	0.56
3:N:423:ASP:OD2	5:P:174:LEU:HD22	2.05	0.56
4:O:32:ARG:HH11	4:O:32:ARG:HB2	1.70	0.56
4:O:44:GLU:O	4:O:45:ARG:HD3	2.04	0.56
1:A:9:PRO:HD2	1:B:224:TYR:CE1	2.40	0.56
1:A:119:ASP:HB3	9:A:9566:HOH:O	2.05	0.56
1:B:153:ALA:HA	1:B:156:HIS:CE1	2.40	0.56
1:B:162:ILE:HD13	9:B:9631:HOH:O	2.05	0.56
2:C:183:SER:OG	2:C:190:LYS:HD3	2.05	0.56
2:C:349:ALA:O	2:C:353:ARG:HG3	2.05	0.56
2:C:420:ARG:HD2	9:C:2422:HOH:O	2.05	0.56
2:C:866:PRO:HD2	9:C:9657:HOH:O	2.05	0.56
9:C:9888:HOH:O	3:D:651:GLU:HB3	2.05	0.56
3:D:186:VAL:HG21	3:D:213:VAL:HB	1.87	0.56
3:D:190:GLU:CD	3:D:190:GLU:H	2.09	0.56
3:D:573:MET:SD	5:F:210:LEU:HB3	2.46	0.56
3:D:701:LEU:C	3:D:702:LEU:HD12	2.25	0.56
3:D:1127:GLU:HB3	9:D:9585:HOH:O	2.04	0.56
5:F:228:GLU:HA	9:F:9639:HOH:O	2.04	0.56
5:F:406:ARG:HG2	5:F:409:LYS:HD3	1.86	0.56
1:L:188:GLN:HA	9:L:1637:HOH:O	2.05	0.56
2:M:2:GLU:HA	9:M:9520:HOH:O	2.05	0.56
2:M:160:ALA:HB3	2:M:174:LEU:HB2	1.88	0.56
2:M:233:GLU:HG3	9:M:2295:HOH:O	2.04	0.56
2:M:588:VAL:HG21	2:M:664:GLY:O	2.04	0.56
2:M:673:LEU:HB2	9:M:9318:HOH:O	2.04	0.56
2:M:734:LEU:O	2:M:737:LEU:HB2	2.06	0.56
2:M:1016:ILE:CD1	3:N:526:PRO:HG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:194:GLY:H	3:N:206:ARG:HA	1.70	0.56
3:N:379:ALA:HB2	9:N:2337:HOH:O	2.05	0.56
3:N:601:ARG:HH11	3:N:605:ASP:HB3	1.70	0.56
3:N:807:ALA:HB1	9:N:9607:HOH:O	2.06	0.56
3:N:955:VAL:O	3:N:1039:CYS:HB3	2.06	0.56
3:N:984:THR:HG22	3:N:987:GLU:H	1.69	0.56
3:N:1197:ARG:HB2	3:N:1396:GLU:OE2	2.04	0.56
3:N:1203:LYS:HD3	9:N:9886:HOH:O	2.04	0.56
3:N:1348:LEU:O	3:N:1352:ILE:HG13	2.05	0.56
3:N:1369:GLU:HB3	9:N:9676:HOH:O	2.06	0.56
5:P:262:VAL:HG23	9:P:3231:HOH:O	2.05	0.56
5:P:287:THR:HG22	5:P:290:GLU:OE1	2.05	0.56
1:A:49:PRO:HA	1:A:148:VAL:HG22	1.86	0.56
2:C:185:LYS:HD3	2:C:190:LYS:HE2	1.86	0.56
2:C:374:ASN:O	2:C:377:PRO:HD2	2.06	0.56
2:C:804:VAL:HG11	9:C:2137:HOH:O	2.05	0.56
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.87	0.56
2:C:1108:PRO:HG3	9:C:9868:HOH:O	2.05	0.56
3:D:820:GLU:HA	3:D:825:ALA:O	2.04	0.56
3:D:957:PRO:HG2	3:D:1007:VAL:HG12	1.86	0.56
3:D:1332:PRO:HB2	9:D:9823:HOH:O	2.04	0.56
3:D:1432:LYS:HD2	3:D:1433:SER:N	2.11	0.56
4:E:46:PRO:HD2	9:E:9659:HOH:O	2.04	0.56
1:K:151:VAL:HB	1:K:169:ALA:HB3	1.86	0.56
2:M:723:THR:C	2:M:725:ASP:H	2.09	0.56
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.86	0.56
3:N:631:ILE:HG12	3:N:743:ASP:O	2.05	0.56
1:A:123:MET:C	1:A:125:PRO:HD3	2.25	0.56
2:C:859:PRO:O	2:C:867:VAL:HG22	2.05	0.56
2:C:861:LEU:HD23	2:C:862:PRO:N	2.21	0.56
3:D:141:ILE:H	3:D:141:ILE:HD12	1.69	0.56
3:D:168:THR:CB	3:D:393:ILE:HD12	2.36	0.56
3:D:1437:ALA:O	3:D:1446:VAL:HG21	2.05	0.56
5:F:80:PRO:HG2	9:F:9637:HOH:O	2.04	0.56
5:F:413:SER:HA	5:F:416:ARG:CZ	2.36	0.56
3:N:12:LEU:HD23	3:N:13:ALA:H	1.70	0.56
3:N:148:GLU:HA	9:N:9837:HOH:O	2.04	0.56
3:N:169:TYR:N	3:N:170:PRO:HD3	2.20	0.56
3:N:169:TYR:HA	3:N:392:SER:HA	1.87	0.56
3:N:172:PRO:HA	3:N:178:LEU:HD13	1.88	0.56
3:N:221:ALA:HA	9:N:9249:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:681:ARG:NH1	3:N:681:ARG:HB2	2.20	0.56
3:N:834:THR:HA	3:N:838:ARG:HH21	1.70	0.56
3:N:999:THR:O	3:N:1002:LYS:HB2	2.06	0.56
3:N:1038:LEU:O	3:N:1060:SER:HB2	2.05	0.56
5:P:160:ASP:O	5:P:163:LEU:HB2	2.05	0.56
1:A:188:GLN:HG3	1:A:189:ARG:H	1.71	0.56
2:C:260:LEU:HA	2:C:291:ALA:HB2	1.87	0.56
3:D:30:GLU:HB3	3:D:40:GLU:HB3	1.87	0.56
3:D:64:LYS:HD3	9:F:9603:HOH:O	2.04	0.56
3:D:447:VAL:HG22	9:D:9908:HOH:O	2.05	0.56
3:D:893:GLU:HB2	9:D:2572:HOH:O	2.06	0.56
3:D:1087:ARG:NH1	3:D:1234:THR:HA	2.21	0.56
5:F:92:PRO:HB3	9:F:9758:HOH:O	2.05	0.56
1:K:70:GLY:HA2	1:K:133:GLU:HG2	1.87	0.56
1:L:18:ARG:O	1:L:207:PRO:HD3	2.06	0.56
2:M:292:ARG:HB2	2:M:299:LYS:HZ2	1.71	0.56
2:M:696:LYS:HA	9:M:9221:HOH:O	2.06	0.56
2:M:710:ILE:HB	2:M:790:LEU:HD22	1.86	0.56
3:N:430:ASP:HB2	3:N:432:TYR:CE2	2.41	0.56
2:C:101:ILE:HG22	2:C:102:HIS:H	1.71	0.56
2:C:367:LEU:O	2:C:372:LEU:HD13	2.06	0.56
3:D:136:ASP:CB	3:D:137:PRO:HD3	2.36	0.56
3:D:828:LYS:HD3	3:D:828:LYS:N	2.20	0.56
3:D:1018:ASN:O	3:D:1022:VAL:HG23	2.06	0.56
3:D:1381:VAL:HB	3:D:1389:LEU:O	2.05	0.56
4:E:44:GLU:HA	9:E:9565:HOH:O	2.04	0.56
5:F:102:LEU:O	5:F:106:VAL:HG23	2.06	0.56
5:F:163:LEU:HB3	5:F:174:LEU:HG	1.87	0.56
1:K:63:HIS:HA	9:K:1147:HOH:O	2.06	0.56
2:M:36:PRO:HG2	2:M:70:GLU:HB3	1.88	0.56
2:M:643:VAL:HG13	2:M:647:GLN:OE1	2.05	0.56
2:M:654:LEU:HD21	2:M:663:ASN:ND2	2.21	0.56
2:M:760:SER:O	2:M:785:VAL:HG22	2.05	0.56
2:M:889:HIS:NE2	2:M:970:GLY:HA3	2.21	0.56
3:N:86:ARG:O	3:N:522:PRO:HD2	2.06	0.56
3:N:877:PRO:O	3:N:880:ILE:HG22	2.05	0.56
3:N:1433:SER:HB2	3:N:1457:ASP:OD2	2.06	0.56
5:P:120:THR:HB	5:P:122:LEU:HB2	1.88	0.56
5:P:135:ILE:HD11	5:P:178:ARG:HB3	1.88	0.56
5:P:267:THR:HG23	5:P:299:TRP:HH2	1.70	0.56
1:A:224:TYR:CD1	1:B:9:PRO:HD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:PHE:HB3	1:B:94:LEU:HD13	1.88	0.56
2:C:95:TYR:CD2	2:C:114:PHE:HB3	2.41	0.56
2:C:208:ALA:HA	2:C:218:VAL:HG21	1.87	0.56
3:D:118:LEU:O	3:D:120:ALA:N	2.39	0.56
3:D:123:LEU:HA	9:D:2113:HOH:O	2.06	0.56
3:D:131:LYS:HB3	3:D:568:ARG:HG2	1.87	0.56
3:D:1137:ARG:H	3:D:1137:ARG:CD	2.18	0.56
3:D:1379:VAL:HG22	9:D:2424:HOH:O	2.05	0.56
1:K:73:GLU:HG3	1:K:130:ALA:HA	1.88	0.56
2:M:56:GLU:HB3	9:M:9316:HOH:O	2.06	0.56
2:M:117:HIS:HB2	9:M:9333:HOH:O	2.05	0.56
2:M:237:ARG:HG2	9:M:9833:HOH:O	2.05	0.56
2:M:674:VAL:HG12	2:M:990:GLY:O	2.06	0.56
3:N:553:ARG:HA	3:N:556:LYS:HD3	1.86	0.56
3:N:1045:MET:CG	3:N:1073:SER:HA	2.33	0.56
4:O:7:ASP:HB2	9:O:4398:HOH:O	2.05	0.56
1:A:11:PHE:CD1	1:B:225:PHE:HA	2.40	0.56
2:C:44:ILE:HA	9:C:9646:HOH:O	2.05	0.56
2:C:47:ALA:HA	9:C:9778:HOH:O	2.05	0.56
2:C:63:GLY:HA3	2:C:103:LYS:HG2	1.88	0.56
2:C:244:PRO:CD	2:C:245:GLY:H	2.16	0.56
3:D:36:THR:C	3:D:38:LYS:H	2.09	0.56
3:D:1277:ILE:HG22	3:D:1278:ASP:N	2.21	0.56
4:E:48:MET:HG2	4:E:49:GLN:H	1.70	0.56
2:M:14:PRO:HA	9:M:9656:HOH:O	2.06	0.56
2:M:261:ILE:HG22	2:M:262:ALA:H	1.71	0.56
2:M:573:ARG:HB3	2:M:670:GLN:NE2	2.20	0.56
3:N:208:PRO:HB2	3:N:395:VAL:HG13	1.87	0.56
3:N:1294:VAL:HB	9:N:9684:HOH:O	2.04	0.56
5:P:141:VAL:HB	9:P:2295:HOH:O	2.06	0.56
5:P:151:LEU:HB3	9:P:4293:HOH:O	2.05	0.56
5:P:205:ARG:HG3	5:P:251:ILE:HD13	1.87	0.56
1:A:206:THR:CG2	1:A:209:GLU:HG3	2.36	0.56
2:C:99:GLN:HB3	2:C:109:LYS:HG3	1.87	0.56
2:C:247:PRO:HD2	9:C:9820:HOH:O	2.06	0.56
2:C:734:LEU:O	2:C:737:LEU:HB2	2.06	0.56
2:C:742:VAL:HG21	9:C:9683:HOH:O	2.06	0.56
3:D:432:TYR:HB3	3:D:448:GLU:HA	1.88	0.56
3:D:496:LEU:HD11	3:D:500:ARG:HE	1.70	0.56
3:D:728:LEU:HD22	3:D:745:MET:SD	2.45	0.56
3:D:1150:ALA:HA	9:D:9851:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1314:LYS:HD3	3:D:1314:LYS:N	2.21	0.56
3:D:1412:LYS:O	3:D:1414:PRO:HD3	2.06	0.56
5:F:287:THR:HG22	5:F:290:GLU:OE1	2.06	0.56
1:K:41:ARG:HG3	1:K:177:VAL:HB	1.88	0.56
1:K:88:ARG:NH1	1:K:90:LEU:HD23	2.21	0.56
1:K:192:LEU:HD21	9:K:1294:HOH:O	2.06	0.56
2:M:770:GLU:HB3	5:P:350:LEU:HD21	1.88	0.56
2:M:881:ASN:H	2:M:881:ASN:ND2	2.03	0.56
3:N:186:VAL:HG21	3:N:213:VAL:HB	1.87	0.56
3:N:709:HIS:CD2	3:N:1231:GLU:HG3	2.41	0.56
3:N:1462:LEU:HD21	3:N:1474:ALA:HB2	1.88	0.56
5:P:124:PRO:HB3	9:P:1676:HOH:O	2.06	0.56
2:C:831:ARG:HA	9:C:9680:HOH:O	2.06	0.55
3:D:12:LEU:HD21	3:D:104:PHE:HE1	1.71	0.55
3:D:207:PHE:HA	9:D:3106:HOH:O	2.05	0.55
3:D:1065:LEU:HD12	3:D:1069:GLU:HB3	1.88	0.55
1:L:123:MET:C	1:L:125:PRO:HD3	2.26	0.55
2:M:398:THR:HA	2:M:633:GLN:HG3	1.88	0.55
3:N:22:SER:HA	3:N:90:MET:O	2.06	0.55
3:N:133:ILE:HG21	3:N:454:ALA:CB	2.32	0.55
3:N:183:GLU:HA	3:N:186:VAL:HG12	1.87	0.55
3:N:390:PRO:HG2	5:P:98:GLU:OE1	2.06	0.55
4:O:32:ARG:HB2	4:O:32:ARG:NH1	2.20	0.55
4:O:47:LYS:N	4:O:54:LEU:HD22	2.22	0.55
5:P:80:PRO:HA	5:P:83:GLN:HB2	1.87	0.55
1:A:115:LEU:HB3	9:A:9587:HOH:O	2.06	0.55
2:C:536:PRO:HD2	2:C:537:LYS:HZ3	1.71	0.55
2:C:890:LEU:HD13	2:C:914:ILE:HG13	1.88	0.55
3:D:400:VAL:HA	3:D:442:ASN:O	2.06	0.55
2:M:369:PRO:HB3	9:M:2382:HOH:O	2.07	0.55
2:M:492:ASP:HB3	2:M:518:LYS:HD2	1.87	0.55
2:M:918:LEU:HD23	2:M:968:LEU:HA	1.88	0.55
3:N:456:MET:SD	3:N:568:ARG:HD3	2.46	0.55
3:N:1029:ARG:CZ	8:N:9101:G4P:O2D	2.54	0.55
5:P:197:SER:HB2	9:P:5517:HOH:O	2.06	0.55
1:B:170:VAL:HG22	9:B:9562:HOH:O	2.05	0.55
2:C:614:ARG:HD2	9:C:2802:HOH:O	2.07	0.55
3:D:1473:PRO:HB2	9:D:3112:HOH:O	2.05	0.55
4:E:45:ARG:HB3	4:E:46:PRO:HD2	1.89	0.55
5:F:361:LEU:HD21	5:F:408:LEU:HD12	1.88	0.55
1:K:42:ARG:HG2	1:K:42:ARG:HH11	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:177:VAL:HG13	1:L:197:LEU:HD21	1.88	0.55
2:M:191:PHE:HA	9:M:9556:HOH:O	2.06	0.55
2:M:482:GLU:HB3	9:M:9208:HOH:O	2.06	0.55
2:M:553:ASP:HA	2:M:881:ASN:HA	1.88	0.55
2:M:670:GLN:HE22	2:M:699:PHE:HA	1.71	0.55
2:M:768:THR:HG22	2:M:771:GLU:H	1.72	0.55
3:N:166:GLN:HB3	3:N:395:VAL:HG21	1.87	0.55
3:N:477:LEU:HD23	9:N:2072:HOH:O	2.06	0.55
3:N:703:ASN:HD22	3:N:713:ILE:HG12	1.71	0.55
3:N:964:LEU:HG	9:N:9387:HOH:O	2.06	0.55
3:N:1008:PHE:O	3:N:1012:GLU:HG3	2.06	0.55
3:N:1372:VAL:HA	3:N:1375:MET:CE	2.36	0.55
3:N:1390:LEU:HD22	9:N:9553:HOH:O	2.06	0.55
3:N:1434:TRP:CZ3	3:N:1457:ASP:HB2	2.41	0.55
9:N:2002:HOH:O	5:P:315:VAL:HG11	2.06	0.55
1:A:223:THR:HG22	9:A:9752:HOH:O	2.05	0.55
1:B:175:ARG:O	3:D:851:LEU:HD21	2.07	0.55
2:C:139:GLN:NE2	2:C:415:PRO:HD2	2.17	0.55
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.87	0.55
2:C:503:LEU:HD12	2:C:507:ARG:O	2.06	0.55
2:C:949:LYS:HD2	3:D:796:ARG:NH2	2.21	0.55
3:D:423:ASP:OD2	5:F:174:LEU:HD22	2.07	0.55
3:D:644:LEU:HG	3:D:718:PRO:HB3	1.89	0.55
3:D:908:LYS:HB3	3:D:1027:GLY:CA	2.27	0.55
5:F:115:LYS:HE3	9:F:9566:HOH:O	2.07	0.55
9:K:1228:HOH:O	2:M:856:GLU:HB3	2.06	0.55
2:M:250:ARG:HE	2:M:253:ALA:CB	2.19	0.55
3:N:625:TYR:O	3:N:749:VAL:HG23	2.07	0.55
3:N:996:TRP:CE2	3:N:1056:PRO:HG2	2.41	0.55
3:N:1119:SER:HB2	3:N:1185:GLU:HB3	1.87	0.55
3:N:1137:ARG:HA	9:N:9839:HOH:O	2.06	0.55
5:P:81:VAL:HG23	9:P:1606:HOH:O	2.04	0.55
5:P:161:GLN:HG2	9:P:1559:HOH:O	2.06	0.55
1:B:48:ILE:HG22	1:B:173:PRO:HD2	1.87	0.55
2:C:57:GLU:O	2:C:62:GLY:HA3	2.06	0.55
3:D:141:ILE:HG23	9:D:9965:HOH:O	2.06	0.55
3:D:165:LYS:O	3:D:165:LYS:HD3	2.06	0.55
3:D:775:GLY:HA3	3:D:1145:TYR:CE1	2.37	0.55
4:E:90:GLU:HB2	9:E:9648:HOH:O	2.05	0.55
5:F:93:LEU:HD22	5:F:98:GLU:HB3	1.89	0.55
5:F:166:LEU:O	5:F:171:LYS:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:280:GLN:HG2	5:F:281:GLU:HG3	1.89	0.55
5:F:320:PRO:O	5:F:321:ILE:HD13	2.07	0.55
2:M:3:ILE:HG22	9:M:9511:HOH:O	2.05	0.55
2:M:841:ASN:HD22	2:M:841:ASN:H	1.55	0.55
3:N:36:THR:C	3:N:38:LYS:H	2.09	0.55
3:N:613:ARG:HD2	9:N:2236:HOH:O	2.06	0.55
3:N:1449:GLU:O	3:N:1452:ILE:HG22	2.07	0.55
3:N:1497:GLU:O	3:N:1501:GLU:HG3	2.07	0.55
5:P:85:LEU:HD13	9:P:5383:HOH:O	2.05	0.55
2:C:328:LEU:HD21	2:C:434:HIS:HD2	1.71	0.55
2:C:333:ILE:HD13	2:C:467:ILE:HD11	1.87	0.55
3:D:539:ASP:HA	9:D:2979:HOH:O	2.06	0.55
3:D:570:GLU:HB2	5:F:214:GLN:NE2	2.21	0.55
3:D:1341:PRO:O	3:D:1344:VAL:HG23	2.07	0.55
5:F:143:HIS:HB3	9:F:9613:HOH:O	2.05	0.55
1:K:49:PRO:HA	1:K:148:VAL:HG12	1.89	0.55
1:K:86:VAL:HG13	1:K:123:MET:HB2	1.89	0.55
2:M:516:ARG:NH1	3:N:1068:LEU:HD22	2.21	0.55
2:M:524:VAL:CG2	2:M:528:GLU:HB2	2.36	0.55
3:N:108:VAL:HB	3:N:109:PRO:HD3	1.88	0.55
1:B:99:LEU:HA	9:B:9656:HOH:O	2.06	0.55
2:C:227:PHE:HB3	9:C:2116:HOH:O	2.07	0.55
2:C:254:VAL:HG22	2:C:258:TYR:CE1	2.42	0.55
2:C:290:LEU:HB3	9:C:9841:HOH:O	2.05	0.55
2:C:577:PRO:HG3	2:C:993:PHE:CZ	2.42	0.55
3:D:39:PRO:HB3	3:D:45:PHE:C	2.26	0.55
3:D:92:HIS:HA	3:D:519:VAL:HG23	1.87	0.55
3:D:93:ILE:HG22	9:D:2002:HOH:O	2.07	0.55
3:D:126:VAL:HG11	9:D:2381:HOH:O	2.05	0.55
3:D:138:LYS:HG3	9:D:2920:HOH:O	2.05	0.55
3:D:485:SER:HB2	9:D:3145:HOH:O	2.05	0.55
3:D:710:ARG:HG3	3:D:711:LEU:HD22	1.89	0.55
3:D:1118:ILE:HD11	3:D:1192:LEU:HB2	1.89	0.55
3:D:1389:LEU:HD23	3:D:1389:LEU:H	1.72	0.55
5:F:278:LEU:HB3	5:F:286:PRO:CG	2.31	0.55
1:L:214:ALA:HA	1:L:217:ILE:HD12	1.88	0.55
2:M:218:VAL:HG13	9:M:9323:HOH:O	2.07	0.55
2:M:226:VAL:HG21	9:M:2143:HOH:O	2.05	0.55
2:M:275:TYR:O	2:M:279:GLU:HG2	2.05	0.55
2:M:417:GLY:O	2:M:418:LEU:HD13	2.06	0.55
2:M:777:ILE:HG13	5:P:405:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:810:ASP:HB3	2:M:813:VAL:HG22	1.89	0.55
2:M:816:LYS:HB2	2:M:819:VAL:HG21	1.87	0.55
2:M:1043:TYR:CE2	3:N:763:MET:HA	2.42	0.55
2:M:1111:ILE:HG13	2:M:1112:PHE:H	1.72	0.55
3:N:758:GLU:HB3	4:O:20:THR:HG21	1.88	0.55
4:O:31:LEU:HD21	4:O:60:ALA:CB	2.36	0.55
4:O:42:PRO:HD2	9:O:4230:HOH:O	2.05	0.55
5:P:363:GLU:HG2	5:P:364:ARG:N	2.22	0.55
1:B:7:LYS:O	1:B:7:LYS:HD2	2.07	0.55
2:C:367:LEU:HA	2:C:371:LYS:HB2	1.89	0.55
2:C:444:PRO:HA	9:C:9645:HOH:O	2.06	0.55
2:C:492:ASP:HB2	9:C:2376:HOH:O	2.06	0.55
3:D:645:PRO:HA	3:D:721:VAL:O	2.07	0.55
1:K:158:ILE:HB	9:K:2046:HOH:O	2.05	0.55
2:M:57:GLU:O	2:M:62:GLY:HA3	2.06	0.55
3:N:36:THR:HG22	9:N:9685:HOH:O	2.06	0.55
3:N:141:ILE:HG21	9:N:9453:HOH:O	2.06	0.55
3:N:149:LYS:HD3	3:N:149:LYS:H	1.71	0.55
3:N:787:LEU:HD21	3:N:947:ILE:HD13	1.88	0.55
3:N:1243:THR:HB	3:N:1253:THR:HB	1.88	0.55
1:A:104:GLU:HB2	9:A:9584:HOH:O	2.06	0.55
2:C:1038:TRP:NE1	3:D:1099:VAL:HG11	2.21	0.55
3:D:543:LEU:HA	3:D:546:ARG:HG2	1.89	0.55
3:D:1101:VAL:HG11	3:D:1427:SER:HB3	1.88	0.55
3:D:1192:LEU:HD22	3:D:1345:GLU:OE2	2.06	0.55
3:D:1365:ASP:O	3:D:1369:GLU:HG3	2.07	0.55
3:D:1468:LEU:HD21	9:D:2087:HOH:O	2.07	0.55
5:F:136:LEU:HD11	5:F:141:VAL:HG21	1.89	0.55
5:F:153:PRO:HG2	5:F:154:LYS:H	1.71	0.55
1:K:27:PRO:HB2	9:K:1056:HOH:O	2.06	0.55
1:K:42:ARG:HD2	9:K:4396:HOH:O	2.07	0.55
1:L:48:ILE:HG22	1:L:173:PRO:HD2	1.88	0.55
2:M:323:ASP:HA	9:M:9235:HOH:O	2.06	0.55
2:M:720:GLU:HG2	9:M:9228:HOH:O	2.07	0.55
3:N:107:ASP:OD2	3:N:109:PRO:HD2	2.07	0.55
3:N:1496:GLU:HB2	9:N:9255:HOH:O	2.05	0.55
5:P:170:HIS:HA	5:P:173:TYR:CD1	2.41	0.55
5:P:196:VAL:O	5:P:200:LYS:HB2	2.07	0.55
1:A:178:ALA:CB	2:C:864:GLY:H	2.20	0.55
1:B:23:PHE:CZ	1:B:208:LEU:HD22	2.42	0.55
2:C:405:ARG:HD3	2:C:543:ASN:ND2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:589:ARG:HD3	2:C:596:TYR:CE2	2.41	0.55
2:C:755:LEU:CD1	2:C:825:VAL:HG11	2.34	0.55
3:D:53:ILE:HG22	9:D:2190:HOH:O	2.07	0.55
3:D:554:LEU:HG	9:D:9809:HOH:O	2.06	0.55
3:D:812:ALA:HA	9:D:9733:HOH:O	2.06	0.55
3:D:1442:ASN:HB3	9:D:3067:HOH:O	2.06	0.55
4:E:84:ARG:HD2	4:E:87:LYS:HD3	1.89	0.55
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.87	0.55
1:K:60:ASP:HB3	9:K:4731:HOH:O	2.06	0.55
1:K:146:ARG:HG3	9:K:1164:HOH:O	2.06	0.55
1:L:41:ARG:NH1	1:L:177:VAL:HB	2.21	0.55
2:M:534:VAL:H	2:M:538:GLN:HE22	1.55	0.55
2:M:614:ARG:HD3	9:M:9224:HOH:O	2.05	0.55
2:M:944:LEU:O	2:M:947:ALA:HB3	2.07	0.55
2:M:1105:LYS:HG2	9:M:9543:HOH:O	2.07	0.55
3:D:133:ILE:HG12	9:D:9996:HOH:O	2.06	0.54
3:D:729:HIS:CE1	3:D:731:LEU:HG	2.42	0.54
3:D:1487:VAL:HG23	4:E:74:VAL:O	2.07	0.54
1:K:9:PRO:HD2	1:L:224:TYR:CD1	2.41	0.54
1:K:76:VAL:HA	1:K:79:ILE:HG12	1.89	0.54
2:M:567:GLN:HE22	2:M:838:LYS:NZ	2.05	0.54
3:N:177:ALA:CA	3:N:199:LEU:HD13	2.38	0.54
3:N:596:SER:HA	9:N:2771:HOH:O	2.08	0.54
3:N:1119:SER:HA	3:N:1186:VAL:O	2.07	0.54
3:N:1124:GLN:CD	3:N:1135:ARG:HA	2.28	0.54
5:P:125:ASP:O	5:P:129:GLU:HG2	2.07	0.54
1:B:135:GLY:HA3	9:B:9591:HOH:O	2.08	0.54
2:C:111:ASP:HA	9:C:2107:HOH:O	2.06	0.54
3:D:462:GLN:HA	3:D:513:ILE:CD1	2.37	0.54
3:D:470:LEU:HB2	3:D:503:LEU:HD21	1.89	0.54
3:D:487:ALA:HB1	3:D:488:ARG:HH21	1.71	0.54
3:D:1468:LEU:O	3:D:1468:LEU:HD23	2.07	0.54
3:D:1481:VAL:CG1	4:E:18:ARG:HA	2.34	0.54
4:E:57:ASP:H	4:E:58:PRO:HD3	1.73	0.54
5:F:93:LEU:HG	5:F:190:ALA:CB	2.37	0.54
5:F:302:LYS:HA	9:F:9730:HOH:O	2.06	0.54
5:F:371:LEU:HD11	9:F:9735:HOH:O	2.07	0.54
2:M:108:ILE:HG12	9:M:2211:HOH:O	2.06	0.54
2:M:376:ARG:HB3	2:M:377:PRO:HD3	1.88	0.54
3:N:648:MET:HG2	3:N:652:LEU:HD23	1.88	0.54
5:P:323:ASP:HB3	9:P:4379:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:897:LEU:HD11	2:C:920:GLN:HG3	1.89	0.54
2:C:1013:TYR:HB3	9:C:2050:HOH:O	2.06	0.54
2:C:1081:VAL:HB	2:C:1086:ARG:NE	2.22	0.54
3:D:19:ARG:HA	9:D:2218:HOH:O	2.07	0.54
3:D:146:PRO:HG2	9:D:9704:HOH:O	2.07	0.54
3:D:197:SER:CB	3:D:203:ALA:HB3	2.30	0.54
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.37	0.54
3:D:1014:ASN:O	3:D:1016:PRO:HD3	2.07	0.54
4:E:56:ASP:HB2	9:E:9649:HOH:O	2.07	0.54
5:F:181:GLU:O	5:F:184:ARG:HB3	2.08	0.54
5:F:262:VAL:HG23	9:F:9614:HOH:O	2.07	0.54
2:M:719:PRO:HD3	9:M:2003:HOH:O	2.07	0.54
2:M:1051:GLU:C	2:M:1056:LYS:HD2	2.28	0.54
2:M:1057:SER:OG	3:N:621:LYS:HE2	2.07	0.54
3:N:704:ARG:HD2	3:N:705:ALA:H	1.71	0.54
5:P:166:LEU:O	5:P:171:LYS:HB2	2.07	0.54
1:A:7:LYS:NZ	1:A:186:LEU:HD23	2.22	0.54
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.88	0.54
1:A:62:LEU:HD12	1:A:62:LEU:H	1.71	0.54
1:B:137:ARG:NH1	1:B:139:ASN:HB3	2.21	0.54
2:C:165:LEU:HD13	9:C:2088:HOH:O	2.06	0.54
3:D:41:ARG:HG3	9:D:9655:HOH:O	2.05	0.54
3:D:214:GLU:HB2	3:D:390:PRO:HD2	1.90	0.54
3:D:816:HIS:HA	9:D:3219:HOH:O	2.07	0.54
3:D:1169:ASP:HB2	9:D:2059:HOH:O	2.07	0.54
3:D:1449:GLU:HB2	9:D:9628:HOH:O	2.07	0.54
1:K:206:THR:HG22	1:K:209:GLU:HG3	1.88	0.54
2:M:159:ILE:HB	9:M:9671:HOH:O	2.06	0.54
2:M:532:MET:HE1	9:M:9849:HOH:O	2.06	0.54
1:A:186:LEU:HB2	9:A:9592:HOH:O	2.07	0.54
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.89	0.54
2:C:328:LEU:CD1	2:C:433:THR:HB	2.26	0.54
2:C:455:LEU:HD13	2:C:456:ALA:O	2.07	0.54
2:C:598:GLU:O	2:C:651:LYS:HG3	2.07	0.54
2:C:640:ARG:HD3	2:C:642:ARG:NH2	2.22	0.54
2:C:666:LEU:HD12	2:C:667:ALA:H	1.73	0.54
2:C:1015:LEU:HB3	2:C:1016:ILE:HD13	1.88	0.54
1:K:18:ARG:NH2	1:K:88:ARG:HH21	2.05	0.54
9:K:6214:HOH:O	1:L:229:GLN:HB3	2.06	0.54
2:M:72:ARG:HB3	9:M:9754:HOH:O	2.07	0.54
2:M:159:ILE:HG21	2:M:175:GLU:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:286:SER:HB3	2:M:299:LYS:HE2	1.89	0.54
2:M:649:VAL:HA	2:M:650:ARG:NH2	2.22	0.54
2:M:1089:VAL:O	2:M:1093:GLN:HG2	2.07	0.54
3:N:101:HIS:O	3:N:105:VAL:HG23	2.07	0.54
3:N:400:VAL:HG23	9:N:2141:HOH:O	2.07	0.54
3:N:634:GLY:O	3:N:637:LEU:HB3	2.07	0.54
3:N:638:LYS:HE2	9:N:2726:HOH:O	2.08	0.54
3:N:693:GLU:HA	9:N:9838:HOH:O	2.05	0.54
3:N:814:ALA:HB2	9:N:9382:HOH:O	2.08	0.54
3:N:838:ARG:HD2	3:N:874:GLU:OE2	2.08	0.54
5:P:367:MET:HB3	5:P:370:LYS:HZ2	1.72	0.54
1:A:41:ARG:HG3	1:A:177:VAL:HB	1.88	0.54
2:C:53:PRO:HA	9:C:9804:HOH:O	2.07	0.54
3:D:608:SER:O	3:D:614:PHE:HB2	2.08	0.54
3:D:1033:GLN:HB3	3:D:1036:ARG:HH21	1.73	0.54
3:D:1209:LEU:CD2	3:D:1216:SER:H	2.21	0.54
5:F:314:PRO:HD3	9:F:9825:HOH:O	2.07	0.54
5:F:364:ARG:HB3	5:F:364:ARG:HH11	1.72	0.54
1:K:189:ARG:HD2	9:K:1183:HOH:O	2.08	0.54
1:L:9:PRO:HD3	9:L:3141:HOH:O	2.07	0.54
3:N:100:ALA:H	3:N:575:GLN:HE22	1.54	0.54
1:B:94:LEU:HD21	1:B:119:ASP:OD1	2.08	0.54
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.90	0.54
3:D:669:ASN:HD21	3:D:671:LYS:HB2	1.72	0.54
3:D:1397:LYS:HG3	9:D:2561:HOH:O	2.08	0.54
4:E:47:LYS:N	4:E:54:LEU:HD22	2.23	0.54
5:F:153:PRO:HB2	9:F:9865:HOH:O	2.07	0.54
1:L:80:LEU:CD1	3:N:842:VAL:HG12	2.35	0.54
1:L:143:ARG:HE	1:L:158:ILE:HG21	1.72	0.54
2:M:2:GLU:HB3	9:M:2027:HOH:O	2.07	0.54
2:M:34:VAL:HG22	9:M:9591:HOH:O	2.07	0.54
2:M:495:THR:HA	9:M:9319:HOH:O	2.08	0.54
3:N:138:LYS:H	3:N:138:LYS:HD2	1.73	0.54
3:N:246:PRO:HA	9:N:2931:HOH:O	2.06	0.54
3:N:690:ALA:O	3:N:694:VAL:HG23	2.08	0.54
3:N:1122:LEU:HD11	3:N:1186:VAL:HG23	1.90	0.54
3:N:1408:ILE:HB	9:N:9535:HOH:O	2.07	0.54
4:O:60:ALA:O	4:O:63:TRP:HB2	2.08	0.54
1:A:88:ARG:HB2	1:A:204:SER:HA	1.90	0.54
1:B:41:ARG:NH1	1:B:177:VAL:HB	2.22	0.54
1:B:107:LYS:HB3	9:B:9616:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:THR:HG23	9:C:9938:HOH:O	2.07	0.54
2:C:1054:THR:HG23	2:C:1059:ASP:HB2	1.90	0.54
3:D:441:ARG:HB3	3:D:443:VAL:CG2	2.37	0.54
3:D:637:LEU:HD11	3:D:642:CYS:N	2.22	0.54
3:D:761:ILE:HD11	4:E:23:VAL:HG11	1.89	0.54
4:E:69:LEU:HD11	9:E:9579:HOH:O	2.07	0.54
5:F:156:VAL:HA	5:F:159:ILE:HD12	1.89	0.54
2:M:208:ALA:HB2	9:M:9323:HOH:O	2.08	0.54
2:M:266:ARG:HB3	9:M:9251:HOH:O	2.06	0.54
2:M:279:GLU:HG3	2:M:280:LYS:HG3	1.89	0.54
2:M:383:ARG:HG3	9:M:9744:HOH:O	2.07	0.54
2:M:469:THR:N	9:M:9590:HOH:O	2.40	0.54
9:M:9528:HOH:O	5:P:280:GLN:HA	2.07	0.54
3:N:149:LYS:HD3	3:N:149:LYS:N	2.23	0.54
4:O:14:ASP:HA	9:O:5443:HOH:O	2.08	0.54
1:B:74:ASP:HA	9:B:9649:HOH:O	2.07	0.54
1:B:86:VAL:HG13	1:B:123:MET:HB2	1.89	0.54
2:C:45:GLN:HG2	9:C:9991:HOH:O	2.07	0.54
2:C:405:ARG:HH12	2:C:409:ARG:NH2	2.00	0.54
2:C:798:GLY:H	2:C:827:VAL:CG1	2.20	0.54
2:C:1014:SER:HB2	5:F:331:ASP:HA	1.90	0.54
3:D:404:GLU:HB3	3:D:414:ARG:NE	2.23	0.54
3:D:474:GLU:HG3	3:D:500:ARG:HE	1.72	0.54
3:D:906:GLN:HB3	3:D:911:LEU:CD1	2.32	0.54
3:D:1119:SER:HA	3:D:1186:VAL:O	2.08	0.54
3:D:1258:ARG:HG2	3:D:1262:LEU:HD13	1.89	0.54
3:D:1312:LEU:HA	9:D:3003:HOH:O	2.08	0.54
5:F:89:GLY:HA3	9:F:9884:HOH:O	2.08	0.54
1:L:2:LEU:HD13	1:L:3:ASP:OD1	2.08	0.54
2:M:346:VAL:O	2:M:350:ARG:HG3	2.08	0.54
2:M:425:PHE:HB3	9:N:9251:HOH:O	2.07	0.54
2:M:1093:GLN:NE2	2:M:1099:VAL:H	2.06	0.54
3:N:537:THR:O	5:P:317:LEU:HB2	2.08	0.54
1:A:119:ASP:HA	9:A:9646:HOH:O	2.07	0.54
1:B:73:GLU:HG3	1:B:130:ALA:HA	1.90	0.54
2:C:305:PRO:O	2:C:308:ARG:HB3	2.07	0.54
2:C:714:ASP:OD2	2:C:719:PRO:HG3	2.08	0.54
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.89	0.54
2:C:878:SER:HA	3:D:1034:GLN:OE1	2.07	0.54
3:D:62:LYS:HG3	9:D:2359:HOH:O	2.07	0.54
3:D:141:ILE:HG12	3:D:449:SER:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1462:LEU:HD21	3:D:1474:ALA:HB2	1.89	0.54
5:F:140:ARG:HA	9:F:9613:HOH:O	2.08	0.54
5:F:158:GLU:O	5:F:161:GLN:HB2	2.07	0.54
2:M:320:HIS:HA	9:M:9779:HOH:O	2.08	0.54
2:M:448:ASN:HB2	2:M:452:ILE:HD11	1.89	0.54
2:M:637:LEU:HD23	2:M:659:PRO:HG2	1.89	0.54
3:N:523:ASP:N	9:N:9625:HOH:O	2.41	0.54
3:N:644:LEU:HD12	3:N:645:PRO:N	2.23	0.54
5:P:270:LYS:HD2	9:P:8061:HOH:O	2.08	0.54
1:A:86:VAL:HG13	1:A:123:MET:HB2	1.90	0.53
2:C:356:ARG:HA	9:C:2205:HOH:O	2.07	0.53
2:C:535:SER:OG	2:C:537:LYS:HE2	2.08	0.53
2:C:944:LEU:O	2:C:947:ALA:HB3	2.08	0.53
2:C:1019:GLN:HE21	3:D:621:LYS:HG3	1.73	0.53
3:D:207:PHE:HB3	3:D:208:PRO:HD2	1.89	0.53
3:D:546:ARG:O	3:D:550:ARG:HG2	2.08	0.53
3:D:935:LYS:HB3	3:D:935:LYS:NZ	2.23	0.53
3:D:1136:LYS:HE3	3:D:1139:ASP:OD2	2.08	0.53
3:D:1262:LEU:HD23	3:D:1352:ILE:CG1	2.38	0.53
1:K:27:PRO:HG2	1:K:186:LEU:HD22	1.90	0.53
1:L:86:VAL:HG13	1:L:123:MET:HB2	1.89	0.53
2:M:50:GLU:HB3	9:M:9948:HOH:O	2.07	0.53
2:M:266:ARG:HB2	2:M:288:ARG:NH1	2.23	0.53
2:M:916:GLU:HA	9:M:9478:HOH:O	2.07	0.53
9:M:9380:HOH:O	5:P:279:GLN:HG2	2.09	0.53
3:N:190:GLU:CD	3:N:190:GLU:H	2.11	0.53
3:N:1262:LEU:HD23	3:N:1352:ILE:CG1	2.38	0.53
3:N:1281:VAL:HG21	3:N:1313:VAL:HG21	1.90	0.53
5:P:222:ARG:HD3	9:P:1708:HOH:O	2.08	0.53
5:P:291:ILE:HD13	5:P:304:VAL:CG1	2.38	0.53
9:A:9633:HOH:O	2:C:607:ASP:HA	2.08	0.53
2:C:31:GLN:HG3	2:C:40:GLU:O	2.08	0.53
2:C:84:ARG:HH12	2:C:128:ILE:HD13	1.73	0.53
2:C:408:ARG:NH1	2:C:542:VAL:HG13	2.23	0.53
3:D:720:LEU:H	3:D:720:LEU:HD12	1.71	0.53
3:D:1009:LYS:HE3	9:D:2148:HOH:O	2.09	0.53
5:F:277:GLN:O	5:F:280:GLN:HB3	2.07	0.53
1:K:109:VAL:HG23	1:K:132:LEU:HD13	1.90	0.53
2:M:148:PHE:HB3	2:M:313:LEU:CD2	2.36	0.53
2:M:173:ASP:HB2	2:M:185:LYS:HE3	1.89	0.53
2:M:244:PRO:HB3	9:M:9820:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:253:ALA:O	2:M:256:TYR:HB2	2.08	0.53
2:M:368:THR:HB	2:M:369:PRO:HD3	1.90	0.53
2:M:572:ILE:HD11	2:M:698:ASP:HB3	1.90	0.53
3:N:96:ALA:HB3	3:N:554:LEU:HG	1.90	0.53
3:N:99:ALA:HB1	3:N:575:GLN:NE2	2.23	0.53
3:N:389:GLU:HG3	9:N:2712:HOH:O	2.08	0.53
3:N:1063:GLU:HG3	3:N:1064:GLY:H	1.72	0.53
3:N:1066:THR:HG23	3:N:1069:GLU:OE1	2.08	0.53
2:C:239:PHE:CE1	2:C:246:ASP:HB3	2.44	0.53
2:C:571:LEU:HD13	2:C:670:GLN:OE1	2.08	0.53
3:D:71:LYS:HB2	9:D:9610:HOH:O	2.08	0.53
3:D:1109:GLU:HA	9:D:2056:HOH:O	2.09	0.53
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.89	0.53
5:F:292:ALA:HA	5:F:299:TRP:HB3	1.90	0.53
2:M:95:TYR:CD2	2:M:114:PHE:HB3	2.29	0.53
3:N:147:VAL:HB	9:N:2267:HOH:O	2.07	0.53
3:N:397:LYS:HG2	9:N:2124:HOH:O	2.07	0.53
3:N:486:ARG:O	3:N:489:ARG:HG2	2.08	0.53
3:N:1023:MET:O	3:N:1028:ALA:HB3	2.07	0.53
3:N:1301:LYS:HA	9:N:9307:HOH:O	2.08	0.53
9:N:9959:HOH:O	5:P:375:LEU:HD13	2.08	0.53
5:P:81:VAL:HG13	9:P:4331:HOH:O	2.07	0.53
5:P:169:GLU:H	5:P:169:GLU:CD	2.11	0.53
1:A:44:LEU:HD22	9:A:9579:HOH:O	2.08	0.53
1:B:123:MET:C	1:B:125:PRO:HD3	2.28	0.53
2:C:36:PRO:HB3	9:C:9597:HOH:O	2.08	0.53
2:C:878:SER:HB2	3:D:1029:ARG:HD2	1.89	0.53
2:C:897:LEU:HD22	9:C:9860:HOH:O	2.08	0.53
3:D:421:LEU:HG	9:D:2049:HOH:O	2.08	0.53
3:D:470:LEU:HD11	3:D:509:PRO:HG3	1.90	0.53
3:D:1253:THR:HG23	3:D:1258:ARG:HH11	1.72	0.53
5:F:160:ASP:O	5:F:163:LEU:HB2	2.09	0.53
5:F:403:LYS:HD3	9:F:9572:HOH:O	2.08	0.53
2:M:571:LEU:HD21	2:M:700:TYR:CD2	2.44	0.53
2:M:722:ILE:HG23	2:M:722:ILE:O	2.08	0.53
3:N:221:ALA:HB2	9:N:2049:HOH:O	2.08	0.53
3:N:464:LEU:HA	9:N:2397:HOH:O	2.09	0.53
3:N:637:LEU:HD12	3:N:641:GLN:HG3	1.89	0.53
3:N:1459:LEU:HD12	3:N:1470:ARG:HH11	1.74	0.53
2:C:141:HIS:HB2	2:C:418:LEU:HD12	1.90	0.53
2:C:165:LEU:HA	2:C:166:PRO:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:TYR:CE1	2:C:338:GLU:HG3	2.43	0.53
2:C:432:ARG:HG3	2:C:432:ARG:NH1	2.23	0.53
2:C:721:ARG:HE	2:C:783:ARG:NH2	2.06	0.53
2:C:861:LEU:HG	2:C:862:PRO:HD2	1.89	0.53
3:D:7:LYS:HE2	9:D:2085:HOH:O	2.09	0.53
3:D:243:ALA:HB2	9:D:2875:HOH:O	2.09	0.53
3:D:584:ASN:H	3:D:602:SER:CB	2.21	0.53
3:D:961:LYS:HD2	9:D:9896:HOH:O	2.08	0.53
3:D:1364:HIS:ND1	3:D:1366:LYS:HG3	2.23	0.53
1:K:9:PRO:HB3	1:K:25:LEU:HG	1.91	0.53
1:L:97:VAL:HG23	9:L:7067:HOH:O	2.08	0.53
1:L:184:THR:HG22	1:L:192:LEU:O	2.07	0.53
2:M:9:ILE:HG12	2:M:907:ASP:CG	2.28	0.53
2:M:12:VAL:HG12	2:M:534:VAL:HG13	1.91	0.53
2:M:594:ALA:HB1	2:M:656:ALA:O	2.09	0.53
3:N:429:SER:HA	9:N:2866:HOH:O	2.09	0.53
3:N:819:GLY:O	3:N:822:ALA:HB3	2.08	0.53
3:N:854:ALA:HB2	9:N:9448:HOH:O	2.07	0.53
3:N:1246:VAL:HG22	9:N:2507:HOH:O	2.08	0.53
1:A:213:GLN:O	1:A:217:ILE:HG13	2.08	0.53
2:C:18:LEU:HD23	2:C:542:VAL:HG11	1.90	0.53
2:C:84:ARG:HA	9:C:9908:HOH:O	2.08	0.53
2:C:759:THR:HG21	2:C:783:ARG:NH1	2.23	0.53
2:C:1057:SER:OG	3:D:621:LYS:HG2	2.09	0.53
3:D:412:GLY:O	3:D:421:LEU:HB3	2.09	0.53
3:D:601:ARG:HH22	3:D:613:ARG:NE	2.06	0.53
3:D:676:MET:CE	3:D:684:LYS:H	2.22	0.53
3:D:1173:LEU:HD22	9:D:9959:HOH:O	2.08	0.53
2:M:141:HIS:HE1	2:M:332:ARG:HD3	1.74	0.53
2:M:379:GLU:O	2:M:383:ARG:HB2	2.08	0.53
2:M:536:PRO:CG	2:M:906:PHE:HB2	2.39	0.53
2:M:1005:MET:HE1	3:N:648:MET:HB2	1.91	0.53
2:M:1052:MET:SD	2:M:1056:LYS:HD3	2.48	0.53
3:N:1472:ILE:O	3:N:1477:GLY:HA3	2.08	0.53
1:B:206:THR:HB	1:B:209:GLU:OE2	2.09	0.53
2:C:136:ILE:CG2	2:C:336:VAL:HG13	2.39	0.53
2:C:200:LEU:HD13	2:C:300:ASP:CG	2.28	0.53
2:C:874:LEU:HD11	3:D:784:ASP:HA	1.91	0.53
2:C:929:ARG:HH11	2:C:929:ARG:HG3	1.73	0.53
2:C:1067:TYR:O	2:C:1071:ILE:HG12	2.08	0.53
2:C:1102:LEU:HD11	3:D:9:ARG:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:138:LYS:HA	9:D:2798:HOH:O	2.09	0.53
3:D:489:ARG:HE	3:D:493:ARG:NH2	1.97	0.53
3:D:984:THR:HG23	3:D:986:ARG:H	1.73	0.53
3:D:1264:GLU:HG2	9:D:9600:HOH:O	2.07	0.53
3:D:1384:PRO:HB3	9:D:2732:HOH:O	2.09	0.53
4:E:15:SER:HA	9:E:9559:HOH:O	2.08	0.53
5:F:172:ARG:O	5:F:176:ILE:HG13	2.09	0.53
2:M:280:LYS:HG2	9:M:2041:HOH:O	2.09	0.53
2:M:777:ILE:HG23	5:P:409:LYS:CB	2.31	0.53
2:M:1056:LYS:HE2	9:M:9265:HOH:O	2.09	0.53
3:N:637:LEU:HD11	3:N:642:CYS:N	2.24	0.53
3:N:728:LEU:HD12	3:N:729:HIS:H	1.74	0.53
3:N:907:GLU:OE1	3:N:909:ASN:HB2	2.09	0.53
5:P:76:SER:HB2	9:P:1916:HOH:O	2.08	0.53
1:A:10:VAL:HG12	1:A:12:THR:HG23	1.90	0.53
1:A:27:PRO:HB2	9:A:9811:HOH:O	2.08	0.53
1:B:23:PHE:HE1	1:B:208:LEU:HD13	1.74	0.53
1:B:175:ARG:HB2	1:B:200:TRP:HB3	1.91	0.53
2:C:26:TYR:CE2	2:C:30:LEU:HD21	2.43	0.53
2:C:137:VAL:HG21	2:C:393:GLN:HE22	1.73	0.53
2:C:976:ASP:HA	9:C:9567:HOH:O	2.09	0.53
2:C:1034:GLU:HG3	2:C:1035:MET:N	2.24	0.53
2:C:1065:ALA:HB1	2:C:1077:PRO:HG2	1.90	0.53
3:D:487:ALA:CB	3:D:488:ARG:HH21	2.22	0.53
3:D:564:GLU:HB3	9:D:9582:HOH:O	2.08	0.53
3:D:865:THR:HG22	3:D:874:GLU:HG2	1.91	0.53
3:D:1231:GLU:HG3	3:D:1232:PRO:N	2.23	0.53
5:F:132:ARG:HH21	5:F:184:ARG:NH1	2.06	0.53
5:F:144:ILE:HB	5:F:145:PRO:HD3	1.90	0.53
5:F:420:ASP:HA	9:F:9593:HOH:O	2.08	0.53
2:M:225:SER:HB2	2:M:229:MET:HE2	1.91	0.53
3:N:112:ILE:HG22	3:N:512:MET:SD	2.49	0.53
3:N:484:PRO:HB3	9:N:9533:HOH:O	2.09	0.53
3:N:1304:LYS:H	3:N:1304:LYS:HD3	1.74	0.53
3:N:1383:ASP:HB3	3:N:1416:ALA:H	1.74	0.53
4:O:27:ALA:O	4:O:31:LEU:HG	2.09	0.53
5:P:234:LYS:HB2	9:P:4664:HOH:O	2.07	0.53
1:B:153:ALA:HA	1:B:156:HIS:NE2	2.24	0.53
1:B:176:ARG:HG3	1:B:200:TRP:CE3	2.44	0.53
1:B:182:GLU:O	1:B:194:LYS:HB3	2.09	0.53
2:C:64:LEU:HD11	9:C:2120:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:193:LEU:HD13	2:C:193:LEU:O	2.09	0.53
2:C:423:ALA:HA	9:C:2245:HOH:O	2.09	0.53
2:C:455:LEU:HD13	2:C:459:ALA:HB3	1.91	0.53
2:C:485:TYR:HD2	9:C:9588:HOH:O	1.90	0.53
2:C:876:VAL:H	2:C:877:PRO:HD2	1.74	0.53
2:C:1092:LEU:CD1	2:C:1099:VAL:HG21	2.39	0.53
2:C:1111:ILE:HG13	2:C:1112:PHE:N	2.22	0.53
3:D:432:TYR:HA	3:D:448:GLU:O	2.08	0.53
3:D:462:GLN:HG3	3:D:513:ILE:HD13	1.91	0.53
3:D:994:GLN:O	3:D:998:GLU:HG3	2.08	0.53
3:D:1003:VAL:O	3:D:1007:VAL:HG13	2.08	0.53
5:F:157:GLU:HA	9:F:2058:HOH:O	2.08	0.53
1:K:96:THR:OG1	1:K:143:ARG:HD2	2.09	0.53
1:K:123:MET:C	1:K:125:PRO:HD3	2.29	0.53
1:L:87:VAL:HG23	9:L:1617:HOH:O	2.09	0.53
1:L:182:GLU:HA	9:N:9281:HOH:O	2.09	0.53
2:M:139:GLN:O	2:M:333:ILE:HA	2.08	0.53
2:M:142:ARG:HD3	9:M:2230:HOH:O	2.09	0.53
2:M:150:PRO:HB2	9:M:9278:HOH:O	2.07	0.53
2:M:473:ARG:HB3	9:M:9208:HOH:O	2.09	0.53
2:M:713:ARG:O	2:M:720:GLU:HG3	2.09	0.53
2:M:904:PRO:HG2	9:M:9888:HOH:O	2.08	0.53
3:N:118:LEU:O	3:N:120:ALA:N	2.41	0.53
3:N:608:SER:O	3:N:614:PHE:HB2	2.09	0.53
3:N:814:ALA:O	3:N:818:ARG:HG3	2.09	0.53
3:N:1350:GLU:O	3:N:1354:LYS:HG2	2.09	0.53
4:O:41:GLU:HG2	9:O:1576:HOH:O	2.09	0.53
5:P:266:GLU:HG3	9:P:8061:HOH:O	2.08	0.53
2:C:41:ASN:HD22	2:C:41:ASN:H	1.56	0.53
2:C:478:VAL:HG13	2:C:506:ASN:HB3	1.91	0.53
2:C:751:PRO:HA	2:C:792:VAL:HB	1.89	0.53
2:C:897:LEU:HB3	2:C:899:GLN:HG2	1.91	0.53
3:D:804:LEU:HD12	3:D:831:GLY:HA3	1.90	0.53
3:D:1102:THR:HG22	3:D:1222:GLY:CA	2.38	0.53
3:D:1197:ARG:HD2	3:D:1396:GLU:CB	2.36	0.53
3:D:1337:GLU:HA	9:D:9894:HOH:O	2.09	0.53
3:D:1383:ASP:HB3	3:D:1416:ALA:H	1.73	0.53
3:D:1495:ILE:HD12	3:D:1498:ALA:HB3	1.90	0.53
5:F:119:ILE:HD13	5:F:170:HIS:CG	2.44	0.53
1:L:136:GLY:HA3	9:L:1193:HOH:O	2.07	0.53
2:M:290:LEU:H	2:M:290:LEU:HD13	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:663:ASN:HB2	9:M:9366:HOH:O	2.08	0.53
2:M:695:LEU:HD21	2:M:833:LEU:HB3	1.91	0.53
2:M:841:ASN:HD22	2:M:841:ASN:N	2.06	0.53
3:N:89:ARG:O	3:N:521:PRO:HG3	2.09	0.53
3:N:187:LYS:HD3	9:N:9419:HOH:O	2.09	0.53
3:N:502:PHE:CE1	3:N:509:PRO:HB3	2.44	0.53
3:N:1018:ASN:O	3:N:1022:VAL:HG23	2.09	0.53
3:N:1320:GLU:H	3:N:1323:GLN:NE2	2.06	0.53
5:P:393:THR:CG2	5:P:394:ARG:H	2.22	0.53
1:B:2:LEU:HD12	1:B:3:ASP:N	2.24	0.52
1:B:5:LYS:HG3	9:B:9765:HOH:O	2.08	0.52
1:B:178:ALA:C	1:B:198:ARG:HH21	2.12	0.52
2:C:100:LEU:HD23	2:C:368:THR:HA	1.90	0.52
2:C:114:PHE:HE2	5:F:283:GLY:HA3	1.73	0.52
2:C:205:GLU:HB3	9:C:2115:HOH:O	2.09	0.52
2:C:1039:ALA:HB3	3:D:713:ILE:HD12	1.90	0.52
3:D:98:PRO:O	3:D:458:ALA:HB3	2.08	0.52
3:D:591:VAL:HG12	3:D:592:THR:O	2.09	0.52
3:D:1020:LEU:HA	3:D:1023:MET:HE2	1.90	0.52
3:D:1446:VAL:HG22	9:D:9970:HOH:O	2.09	0.52
5:F:315:VAL:HG12	5:F:316:SER:N	2.24	0.52
5:F:376:ILE:HD13	9:F:2134:HOH:O	2.07	0.52
1:K:227:ASN:HD22	1:K:227:ASN:H	1.56	0.52
2:M:69:LEU:HB2	2:M:97:ARG:HB2	1.91	0.52
2:M:186:VAL:HG23	2:M:187:ASN:H	1.73	0.52
2:M:443:THR:HB	2:M:453:THR:HG22	1.91	0.52
2:M:637:LEU:HB2	9:M:9559:HOH:O	2.09	0.52
2:M:722:ILE:HG22	9:M:9639:HOH:O	2.09	0.52
2:M:1012:PRO:HD2	2:M:1021:LEU:O	2.09	0.52
1:A:73:GLU:HG3	1:A:130:ALA:HA	1.90	0.52
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.91	0.52
1:B:90:LEU:HB3	9:B:9609:HOH:O	2.09	0.52
2:C:805:ARG:HA	9:C:9907:HOH:O	2.10	0.52
3:D:634:GLY:O	3:D:637:LEU:HB3	2.08	0.52
3:D:819:GLY:O	3:D:822:ALA:HB3	2.09	0.52
3:D:1173:LEU:HB3	9:D:9959:HOH:O	2.08	0.52
3:D:1232:PRO:HB2	3:D:1356:TYR:HE2	1.74	0.52
1:L:165:ILE:HD12	1:L:165:ILE:O	2.09	0.52
1:L:212:ASN:O	1:L:215:VAL:HG22	2.09	0.52
2:M:267:TYR:CE1	2:M:338:GLU:HG3	2.44	0.52
2:M:289:THR:O	2:M:291:ALA:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:602:GLU:HG2	2:M:603:VAL:N	2.24	0.52
2:M:1009:SER:HB2	3:N:651:GLU:O	2.09	0.52
5:P:367:MET:HA	5:P:370:LYS:HD3	1.92	0.52
2:C:243:ARG:O	2:C:243:ARG:HD2	2.09	0.52
2:C:752:GLY:N	2:C:792:VAL:HB	2.25	0.52
2:C:1001:VAL:HG13	9:C:9609:HOH:O	2.10	0.52
3:D:439:LEU:HB3	9:D:2486:HOH:O	2.10	0.52
3:D:1496:GLU:O	3:D:1500:LYS:HG3	2.09	0.52
5:F:112:ALA:O	5:F:116:LEU:HG	2.10	0.52
5:F:264:MET:O	5:F:268:ILE:HG13	2.09	0.52
5:F:323:ASP:O	5:F:325:LYS:HG3	2.10	0.52
5:F:357:ALA:O	5:F:361:LEU:HD23	2.09	0.52
1:K:36:LEU:O	1:K:39:PRO:HD2	2.09	0.52
1:K:154:GLU:HA	9:M:9690:HOH:O	2.09	0.52
2:M:165:LEU:HA	2:M:166:PRO:O	2.10	0.52
2:M:185:LYS:HD2	9:M:9853:HOH:O	2.08	0.52
2:M:343:GLN:HG2	2:M:385:PHE:HB2	1.91	0.52
2:M:402:SER:HA	2:M:566:THR:HG23	1.92	0.52
2:M:774:LEU:O	2:M:777:ILE:HB	2.09	0.52
2:M:1101:THR:HB	3:N:5:VAL:CG1	2.39	0.52
3:N:792:ILE:HG23	3:N:793:THR:HG23	1.89	0.52
3:N:1014:ASN:O	3:N:1016:PRO:HD3	2.09	0.52
3:N:1075:HIS:HA	9:N:9472:HOH:O	2.09	0.52
3:N:1490:LYS:HE3	9:O:1697:HOH:O	2.10	0.52
4:O:48:MET:CB	4:O:54:LEU:HB2	2.39	0.52
4:O:50:THR:HG22	9:O:1369:HOH:O	2.10	0.52
4:O:57:ASP:H	4:O:58:PRO:HD3	1.75	0.52
1:B:45:LEU:HD21	1:B:177:VAL:HG23	1.90	0.52
2:C:294:GLU:HB2	9:C:2038:HOH:O	2.09	0.52
2:C:965:GLU:HA	9:C:2351:HOH:O	2.09	0.52
3:D:208:PRO:HB2	3:D:395:VAL:HG22	1.91	0.52
3:D:228:ALA:HA	9:D:9867:HOH:O	2.10	0.52
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.92	0.52
3:D:690:ALA:O	3:D:694:VAL:HG23	2.10	0.52
3:D:972:LEU:HG	3:D:976:GLN:NE2	2.19	0.52
3:D:1165:TYR:OH	3:D:1203:LYS:HD3	2.09	0.52
4:E:83:ASP:HA	9:E:9560:HOH:O	2.09	0.52
1:L:97:VAL:HG11	1:L:120:VAL:HG21	1.90	0.52
1:L:143:ARG:NE	1:L:158:ILE:HG21	2.24	0.52
2:M:17:PRO:HD3	9:M:9857:HOH:O	2.08	0.52
2:M:237:ARG:HG3	9:M:9694:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:987:ILE:CG2	3:N:948:THR:HG21	2.39	0.52
2:M:1014:SER:HA	5:P:334:PRO:HA	1.92	0.52
3:N:431:VAL:HG21	9:N:9483:HOH:O	2.08	0.52
3:N:704:ARG:CD	3:N:705:ALA:H	2.21	0.52
3:N:890:VAL:HG11	3:N:922:LEU:HD13	1.91	0.52
3:N:899:LEU:HD13	3:N:900:ILE:HG23	1.90	0.52
3:N:1378:TYR:HD1	3:N:1422:MET:SD	2.32	0.52
3:N:1437:ALA:O	3:N:1446:VAL:HG21	2.08	0.52
3:N:1440:PHE:HB3	3:N:1442:ASN:ND2	2.24	0.52
5:P:392:VAL:HG13	9:P:6344:HOH:O	2.09	0.52
1:B:97:VAL:HG11	1:B:120:VAL:HG21	1.90	0.52
2:C:136:ILE:HD13	2:C:392:SER:HB2	1.92	0.52
2:C:266:ARG:HB2	2:C:288:ARG:HE	1.75	0.52
2:C:435:TYR:O	2:C:437:ARG:HG3	2.09	0.52
2:C:682:TYR:HA	3:D:635:PRO:HG2	1.91	0.52
3:D:8:VAL:HG12	3:D:1434:TRP:HH2	1.74	0.52
3:D:169:TYR:HA	3:D:392:SER:HA	1.91	0.52
3:D:817:GLU:O	3:D:821:VAL:HG23	2.09	0.52
3:D:970:LYS:HD2	9:D:2768:HOH:O	2.09	0.52
3:D:1393:GLN:HB2	3:D:1398:TRP:HE1	1.75	0.52
3:D:1394:VAL:HB	3:D:1397:LYS:HD2	1.90	0.52
5:F:96:LEU:HB2	9:F:9854:HOH:O	2.09	0.52
1:L:184:THR:O	1:L:192:LEU:HB2	2.09	0.52
2:M:599:GLU:HG2	9:M:9329:HOH:O	2.09	0.52
2:M:651:LYS:HB3	9:M:9725:HOH:O	2.09	0.52
2:M:1018:GLN:NE2	2:M:1063:ARG:HH22	2.08	0.52
9:M:9280:HOH:O	3:N:952:ASP:HB3	2.09	0.52
3:N:518:PRO:HB3	9:N:9475:HOH:O	2.09	0.52
3:N:828:LYS:HE3	9:N:9267:HOH:O	2.09	0.52
3:N:1277:ILE:HD11	9:N:2604:HOH:O	2.08	0.52
3:N:1284:GLU:HB3	9:N:2710:HOH:O	2.08	0.52
5:P:123:ASP:HB3	5:P:125:ASP:OD1	2.09	0.52
5:P:295:MET:HB3	5:P:299:TRP:CD1	2.44	0.52
2:C:267:TYR:HA	9:C:9947:HOH:O	2.08	0.52
2:C:594:ALA:HB1	2:C:656:ALA:O	2.09	0.52
2:C:1007:ALA:HB2	3:D:648:MET:HG3	1.90	0.52
3:D:498:VAL:HG13	9:D:2123:HOH:O	2.10	0.52
3:D:643:GLY:HA3	3:D:727:GLN:HG3	1.92	0.52
3:D:1410:GLU:HA	9:D:9597:HOH:O	2.08	0.52
5:F:376:ILE:HD12	9:F:2054:HOH:O	2.10	0.52
5:F:398:ARG:HG2	5:F:402:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:42:ARG:NH1	9:K:1228:HOH:O	2.41	0.52
2:M:200:LEU:HD13	2:M:300:ASP:OD2	2.10	0.52
2:M:725:ASP:HB3	2:M:783:ARG:NH1	2.25	0.52
3:N:583:ASP:HA	3:N:602:SER:OG	2.09	0.52
3:N:1393:GLN:HB2	3:N:1398:TRP:NE1	2.24	0.52
4:O:40:LEU:HD12	4:O:40:LEU:O	2.09	0.52
4:O:51:LEU:C	4:O:53:GLY:H	2.12	0.52
5:P:364:ARG:HB3	5:P:365:GLU:OE1	2.10	0.52
1:A:125:PRO:HB2	9:A:9597:HOH:O	2.10	0.52
1:B:20:TYR:HE2	1:B:198:ARG:HB3	1.74	0.52
1:B:184:THR:O	1:B:192:LEU:HB2	2.10	0.52
2:C:597:ALA:HA	9:C:9658:HOH:O	2.10	0.52
2:C:838:LYS:HD2	2:C:846:LYS:HZ1	1.75	0.52
2:C:1008:ARG:HD2	2:C:1028:GLY:C	2.30	0.52
2:C:1015:LEU:HD12	5:F:333:ILE:HG21	1.92	0.52
2:C:1056:LYS:HB3	3:D:624:ASP:H	1.74	0.52
3:D:480:GLU:O	3:D:484:PRO:HD2	2.10	0.52
3:D:1478:SER:HA	9:D:9950:HOH:O	2.10	0.52
9:D:9641:HOH:O	5:F:375:LEU:HD11	2.08	0.52
1:L:125:PRO:HD2	9:L:2226:HOH:O	2.09	0.52
2:M:383:ARG:HG2	9:M:9403:HOH:O	2.09	0.52
2:M:589:ARG:HD3	2:M:596:TYR:CE2	2.45	0.52
2:M:1054:THR:HG23	2:M:1059:ASP:CB	2.39	0.52
3:N:493:ARG:O	3:N:497:GLU:HG3	2.10	0.52
3:N:601:ARG:HB2	5:P:318:GLU:CD	2.30	0.52
3:N:785:ILE:HG12	3:N:935:LYS:HA	1.92	0.52
3:N:1433:SER:HB2	3:N:1457:ASP:CG	2.30	0.52
3:N:1465:ASN:HD21	3:N:1470:ARG:CZ	2.23	0.52
8:N:9101:G4P:H4'	9:N:9248:HOH:O	2.10	0.52
5:P:203:THR:HG22	9:P:4204:HOH:O	2.09	0.52
1:A:14:ARG:HG2	9:A:9563:HOH:O	2.09	0.52
1:A:50:GLY:CA	1:A:173:PRO:HG3	2.39	0.52
1:A:176:ARG:HD2	9:A:9580:HOH:O	2.10	0.52
2:C:216:GLU:HG2	2:C:217:LEU:HD23	1.91	0.52
2:C:534:VAL:N	2:C:538:GLN:HE22	2.08	0.52
3:D:152:LEU:HD23	3:D:152:LEU:N	2.25	0.52
3:D:191:LEU:CB	3:D:195:VAL:HG21	2.37	0.52
3:D:431:VAL:HG11	9:D:9858:HOH:O	2.10	0.52
3:D:507:ASN:HA	9:D:9571:HOH:O	2.08	0.52
5:F:259:ARG:HG2	5:F:259:ARG:HH11	1.74	0.52
2:M:129:ILE:HG22	2:M:130:ASN:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:727:PRO:HG3	2:M:783:ARG:NH1	2.25	0.52
2:M:771:GLU:HB2	9:M:9677:HOH:O	2.09	0.52
2:M:949:LYS:NZ	3:N:796:ARG:HH22	2.08	0.52
3:N:119:SER:HB2	3:N:123:LEU:CB	2.35	0.52
3:N:436:GLU:HB2	3:N:445:ARG:HB2	1.91	0.52
3:N:524:LEU:C	3:N:526:PRO:HD3	2.30	0.52
3:N:657:LEU:HD13	3:N:691:LEU:HA	1.91	0.52
3:N:875:THR:HG21	3:N:902:LEU:HD12	1.92	0.52
5:P:395:GLU:O	5:P:399:GLN:HB2	2.09	0.52
1:A:153:ALA:HB3	9:A:9823:HOH:O	2.09	0.52
2:C:224:GLU:OE1	2:C:226:VAL:HB	2.09	0.52
2:C:242:LEU:HA	9:C:9763:HOH:O	2.08	0.52
2:C:620:LEU:HA	9:C:9918:HOH:O	2.08	0.52
2:C:841:ASN:C	2:C:841:ASN:HD22	2.12	0.52
3:D:1104:GLU:OE2	3:D:1432:LYS:HE2	2.10	0.52
3:D:1132:LEU:HB2	9:D:2139:HOH:O	2.10	0.52
5:F:135:ILE:CD1	5:F:178:ARG:HD2	2.39	0.52
5:F:270:LYS:HE2	9:F:2083:HOH:O	2.09	0.52
1:L:12:THR:HB	9:L:8156:HOH:O	2.08	0.52
1:L:42:ARG:HG2	1:L:42:ARG:HH11	1.74	0.52
2:M:690:ILE:HG12	2:M:849:VAL:HG13	1.91	0.52
9:M:9265:HOH:O	3:N:751:LEU:HG	2.10	0.52
3:N:141:ILE:HB	9:N:9513:HOH:O	2.09	0.52
3:N:215:TYR:O	3:N:389:GLU:HB3	2.10	0.52
3:N:909:ASN:HA	3:N:912:LYS:HZ2	1.74	0.52
3:N:1403:LEU:HD23	9:N:9392:HOH:O	2.10	0.52
5:P:270:LYS:HD3	9:P:5561:HOH:O	2.09	0.52
1:A:51:THR:HG23	9:A:9681:HOH:O	2.08	0.52
1:A:61:VAL:HA	9:A:9599:HOH:O	2.08	0.52
2:C:420:ARG:HD3	9:C:9964:HOH:O	2.09	0.52
2:C:606:VAL:HG21	2:C:645:VAL:HG22	1.91	0.52
2:C:791:ARG:HB2	9:C:2241:HOH:O	2.09	0.52
2:C:866:PRO:HD2	9:C:2231:HOH:O	2.09	0.52
3:D:804:LEU:HD12	3:D:804:LEU:O	2.10	0.52
5:F:185:GLN:HA	5:F:188:ILE:HD12	1.92	0.52
1:L:194:LYS:HG2	9:L:1718:HOH:O	2.10	0.52
2:M:55:GLU:HG3	9:M:2409:HOH:O	2.09	0.52
2:M:206:THR:O	2:M:210:GLU:HB2	2.09	0.52
2:M:352:ALA:HA	2:M:355:VAL:HG12	1.92	0.52
2:M:604:ALA:HB3	2:M:612:VAL:O	2.10	0.52
2:M:786:LYS:HA	9:M:9432:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:9336:HOH:O	5:P:342:VAL:HA	2.09	0.52
3:N:136:ASP:HB3	3:N:137:PRO:HD3	1.92	0.52
3:N:414:ARG:HG2	9:N:9972:HOH:O	2.10	0.52
3:N:459:GLU:O	3:N:463:GLN:HG2	2.09	0.52
3:N:1258:ARG:NH2	3:N:1262:LEU:HD11	2.25	0.52
4:O:33:HIS:CG	4:O:89:MET:HG2	2.45	0.52
5:P:214:GLN:O	5:P:217:ASN:HB2	2.10	0.52
1:A:177:VAL:O	2:C:864:GLY:HA2	2.09	0.51
1:B:160:ASP:HB2	9:B:9744:HOH:O	2.10	0.51
2:C:166:PRO:HD2	9:C:9681:HOH:O	2.09	0.51
2:C:250:ARG:HG2	9:C:9691:HOH:O	2.10	0.51
2:C:503:LEU:HD23	9:C:2771:HOH:O	2.09	0.51
3:D:422:ALA:H	3:D:427:VAL:HG11	1.75	0.51
3:D:623:VAL:HG12	3:D:625:TYR:H	1.75	0.51
3:D:1127:GLU:HB2	9:D:9997:HOH:O	2.09	0.51
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.91	0.51
1:K:189:ARG:HD3	9:K:2051:HOH:O	2.10	0.51
1:L:175:ARG:HB2	1:L:200:TRP:HB3	1.91	0.51
2:M:284:ARG:HD3	9:M:2023:HOH:O	2.10	0.51
2:M:755:LEU:HD11	2:M:792:VAL:HA	1.92	0.51
3:N:65:ARG:CG	5:P:375:LEU:HD12	2.40	0.51
3:N:692:GLU:CG	3:N:720:LEU:HD12	2.40	0.51
3:N:971:LEU:O	3:N:975:GLU:HG2	2.09	0.51
3:N:1120:VAL:HB	3:N:1144:LEU:HD21	1.92	0.51
5:P:158:GLU:HA	5:P:161:GLN:NE2	2.25	0.51
5:P:340:SER:O	5:P:342:VAL:N	2.43	0.51
1:B:101:LEU:HA	9:B:9586:HOH:O	2.09	0.51
1:B:126:ASP:HA	9:B:9726:HOH:O	2.09	0.51
2:C:99:GLN:HA	9:C:2465:HOH:O	2.08	0.51
2:C:166:PRO:HG2	9:C:9694:HOH:O	2.09	0.51
2:C:773:LEU:HD23	2:C:774:LEU:N	2.24	0.51
2:C:1017:THR:HG23	9:C:9664:HOH:O	2.09	0.51
2:C:1096:ALA:O	3:D:13:ALA:HB2	2.10	0.51
3:D:56:TYR:O	3:D:80:VAL:HG11	2.10	0.51
3:D:609:GLY:CA	3:D:613:ARG:HB3	2.40	0.51
4:E:51:LEU:HG	4:E:53:GLY:N	2.26	0.51
5:F:110:MET:O	5:F:114:LYS:HG3	2.10	0.51
1:K:29:GLU:HB2	9:K:2006:HOH:O	2.10	0.51
2:M:200:LEU:HD13	2:M:300:ASP:CG	2.31	0.51
2:M:735:ARG:HD2	9:M:2232:HOH:O	2.10	0.51
2:M:756:VAL:O	2:M:789:SER:HB3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:98:PRO:CG	3:N:462:GLN:HE22	2.17	0.51
3:N:197:SER:HB2	3:N:205:TYR:HE1	1.72	0.51
3:N:475:LYS:O	3:N:478:LEU:HB2	2.10	0.51
3:N:732:VAL:HG11	3:N:765:SER:OG	2.10	0.51
3:N:853:VAL:HG13	3:N:858:VAL:O	2.09	0.51
3:N:1038:LEU:HA	3:N:1061:PHE:HB2	1.92	0.51
3:N:1137:ARG:H	3:N:1137:ARG:CD	2.13	0.51
9:N:9482:HOH:O	5:P:132:ARG:HD3	2.10	0.51
2:C:252:LYS:HE3	9:C:2326:HOH:O	2.10	0.51
2:C:288:ARG:HG3	2:C:289:THR:N	2.26	0.51
2:C:384:GLU:HA	2:C:388:ARG:HH21	1.75	0.51
2:C:603:VAL:HG21	2:C:643:VAL:HG11	1.93	0.51
2:C:1033:GLY:O	2:C:1037:VAL:HG23	2.09	0.51
3:D:881:LEU:HD11	3:D:884:ARG:NH2	2.25	0.51
3:D:1336:LEU:HD13	3:D:1344:VAL:HG21	1.92	0.51
5:F:144:ILE:HG23	9:F:9661:HOH:O	2.11	0.51
5:F:393:THR:HA	9:F:9726:HOH:O	2.09	0.51
1:K:155:LYS:HE3	9:K:2316:HOH:O	2.09	0.51
2:M:164:PRO:HB3	9:M:9286:HOH:O	2.09	0.51
2:M:230:ARG:NH1	9:M:9242:HOH:O	2.43	0.51
2:M:312:ALA:HB1	2:M:318:PRO:CG	2.39	0.51
2:M:444:PRO:HD2	2:M:452:ILE:HG13	1.92	0.51
2:M:597:ALA:HB1	9:M:9609:HOH:O	2.09	0.51
2:M:798:GLY:H	2:M:827:VAL:CG1	2.23	0.51
3:N:679:ARG:HG2	3:N:681:ARG:HD3	1.92	0.51
3:N:984:THR:CG2	3:N:987:GLU:H	2.23	0.51
1:B:194:LYS:HG2	9:B:9628:HOH:O	2.11	0.51
2:C:1069:ALA:HA	2:C:1074:GLU:OE1	2.10	0.51
2:C:1101:THR:HG22	3:D:8:VAL:HG22	1.91	0.51
9:C:9793:HOH:O	3:D:90:MET:HB2	2.10	0.51
3:D:116:LEU:CD2	3:D:468:LEU:HD11	2.40	0.51
3:D:699:VAL:CG1	3:D:717:GLN:HG2	2.41	0.51
3:D:889:ALA:O	3:D:929:ARG:HD2	2.11	0.51
3:D:984:THR:CG2	3:D:987:GLU:H	2.24	0.51
3:D:1309:ALA:HA	9:D:9716:HOH:O	2.11	0.51
3:D:1411:GLY:O	3:D:1413:THR:HG23	2.10	0.51
3:D:1472:ILE:O	3:D:1477:GLY:HA3	2.11	0.51
4:E:90:GLU:HG3	9:E:9578:HOH:O	2.10	0.51
5:F:140:ARG:HG3	5:F:141:VAL:N	2.26	0.51
1:L:91:ASN:O	1:L:94:LEU:HD12	2.10	0.51
2:M:120:LEU:O	2:M:127:PHE:HD1	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:140:ILE:HG22	2:M:331:ARG:HB3	1.93	0.51
3:N:550:ARG:HG3	3:N:550:ARG:NH1	2.23	0.51
3:N:602:SER:HB3	9:N:9292:HOH:O	2.11	0.51
3:N:768:ASN:HB3	9:N:9759:HOH:O	2.11	0.51
3:N:1244:GLY:HA3	9:N:9415:HOH:O	2.11	0.51
3:N:1412:LYS:O	3:N:1412:LYS:HG3	2.10	0.51
5:P:139:ALA:HB1	5:P:152:ASP:HB3	1.92	0.51
5:P:392:VAL:HG12	5:P:396:ARG:HB2	1.92	0.51
2:C:54:ILE:HG23	2:C:54:ILE:O	2.10	0.51
2:C:218:VAL:O	2:C:221:LEU:HB3	2.11	0.51
2:C:1014:SER:CB	5:F:331:ASP:HA	2.40	0.51
9:C:9824:HOH:O	5:F:373:LYS:HB3	2.09	0.51
3:D:28:LYS:HD2	3:D:41:ARG:CD	2.41	0.51
3:D:402:PRO:HB3	9:D:9656:HOH:O	2.09	0.51
3:D:486:ARG:HA	3:D:486:ARG:HE	1.76	0.51
3:D:609:GLY:HA2	3:D:613:ARG:HB3	1.92	0.51
3:D:699:VAL:N	3:D:756:GLN:HE22	2.09	0.51
3:D:1013:GLU:HG3	9:D:9868:HOH:O	2.10	0.51
3:D:1497:GLU:O	3:D:1501:GLU:HG3	2.10	0.51
5:F:273:ARG:HA	5:F:276:ARG:NH1	2.23	0.51
5:F:314:PRO:HB2	9:F:9559:HOH:O	2.09	0.51
1:K:42:ARG:NH1	9:K:4396:HOH:O	2.43	0.51
1:K:123:MET:HB3	9:K:1711:HOH:O	2.09	0.51
2:M:260:LEU:HA	2:M:291:ALA:CB	2.39	0.51
2:M:279:GLU:HG3	2:M:280:LYS:N	2.26	0.51
2:M:524:VAL:HG22	2:M:525:SER:N	2.26	0.51
2:M:697:ARG:HG3	9:M:9636:HOH:O	2.09	0.51
2:M:824:ARG:HD3	9:M:9630:HOH:O	2.11	0.51
9:M:2120:HOH:O	4:O:32:ARG:HA	2.09	0.51
3:N:101:HIS:HD2	3:N:582:LEU:HD13	1.75	0.51
3:N:1047:LYS:HA	3:N:1053:PHE:CE1	2.46	0.51
5:P:134:LYS:HG3	5:P:178:ARG:NH2	2.25	0.51
5:P:366:ALA:O	5:P:370:LYS:HB3	2.10	0.51
1:A:45:LEU:HD21	9:A:9583:HOH:O	2.11	0.51
1:A:146:ARG:HG3	9:A:9567:HOH:O	2.11	0.51
1:B:6:LEU:C	1:B:8:ALA:H	2.14	0.51
1:B:129:ILE:HG23	9:B:9809:HOH:O	2.10	0.51
2:C:182:VAL:HG12	9:C:9945:HOH:O	2.11	0.51
2:C:283:ILE:HG22	9:C:2143:HOH:O	2.11	0.51
2:C:476:GLY:C	2:C:478:VAL:H	2.14	0.51
2:C:857:ASP:HB2	2:C:978:ARG:CG	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:861:LEU:HD23	2:C:863:ASP:N	2.26	0.51
3:D:10:ILE:HG13	3:D:1434:TRP:CZ2	2.46	0.51
3:D:1264:GLU:O	3:D:1266:ARG:HG3	2.10	0.51
5:F:126:LEU:O	5:F:130:VAL:HG23	2.11	0.51
1:L:206:THR:CG2	1:L:209:GLU:H	2.23	0.51
2:M:455:LEU:HD13	2:M:456:ALA:O	2.10	0.51
2:M:651:LYS:HE3	9:M:9350:HOH:O	2.10	0.51
2:M:674:VAL:HG23	2:M:869:VAL:O	2.11	0.51
2:M:1045:ALA:HA	3:N:758:GLU:OE1	2.11	0.51
2:M:1108:PRO:HD2	9:M:2092:HOH:O	2.10	0.51
3:N:30:GLU:HB3	3:N:40:GLU:HB3	1.92	0.51
3:N:186:VAL:HG11	3:N:213:VAL:HB	1.93	0.51
3:N:893:GLU:HA	9:N:9628:HOH:O	2.10	0.51
3:N:1368:ILE:O	3:N:1372:VAL:HG23	2.10	0.51
5:P:404:ALA:HB2	9:P:7921:HOH:O	2.09	0.51
1:B:51:THR:HA	1:B:171:PHE:HD1	1.76	0.51
2:C:276:LYS:HD3	9:C:2144:HOH:O	2.10	0.51
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.93	0.51
2:C:1088:LEU:O	2:C:1091:GLU:HB2	2.11	0.51
3:D:162:ARG:HG3	3:D:163:TYR:N	2.26	0.51
3:D:171:LEU:HG	9:D:3222:HOH:O	2.11	0.51
3:D:493:ARG:HD2	3:D:1390:LEU:HD21	1.92	0.51
3:D:581:LEU:HD23	3:D:581:LEU:H	1.75	0.51
3:D:770:LEU:HA	9:D:9581:HOH:O	2.11	0.51
3:D:809:PRO:O	3:D:812:ALA:HB3	2.11	0.51
3:D:853:VAL:HG13	3:D:858:VAL:O	2.11	0.51
5:F:209:PHE:CE2	5:F:213:ILE:HD11	2.46	0.51
2:M:603:VAL:O	2:M:646:GLY:HA2	2.11	0.51
3:N:67:ARG:CD	5:P:375:LEU:HD11	2.36	0.51
3:N:474:GLU:O	3:N:478:LEU:HG	2.10	0.51
3:N:1044:LEU:HD21	3:N:1056:PRO:HG3	1.92	0.51
3:N:1087:ARG:NE	3:N:1238:MET:HB2	2.26	0.51
3:N:1240:THR:O	3:N:1257:PRO:HB3	2.10	0.51
2:C:578:VAL:HG11	2:C:991:GLN:HB3	1.92	0.51
2:C:583:LEU:O	2:C:587:VAL:HG23	2.10	0.51
3:D:174:GLY:HA3	9:D:9734:HOH:O	2.09	0.51
3:D:783:ARG:NH1	3:D:1029:ARG:HD3	2.26	0.51
5:F:194:LEU:HB2	9:F:9560:HOH:O	2.09	0.51
1:K:111:ALA:HB3	1:K:124:ASN:O	2.10	0.51
1:L:79:ILE:HA	1:L:82:LEU:HD12	1.93	0.51
2:M:195:LEU:O	2:M:199:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:205:GLU:HA	2:M:209:ARG:NH2	2.25	0.51
2:M:309:TYR:HA	2:M:312:ALA:HB3	1.93	0.51
2:M:331:ARG:HG2	9:M:9957:HOH:O	2.10	0.51
3:N:701:LEU:O	3:N:747:VAL:HG23	2.10	0.51
3:N:800:LYS:HG2	3:N:829:VAL:CG1	2.37	0.51
3:N:906:GLN:HB3	3:N:911:LEU:CD1	2.38	0.51
3:N:1262:LEU:HD23	3:N:1352:ILE:HG12	1.92	0.51
3:N:1432:LYS:HG3	3:N:1433:SER:H	1.76	0.51
1:A:145:ASP:HB3	9:A:9570:HOH:O	2.10	0.51
2:C:694:LEU:CD1	2:C:868:ASP:HB3	2.38	0.51
2:C:1021:LEU:HD12	3:D:622:ARG:HH12	1.75	0.51
3:D:8:VAL:HG12	3:D:1434:TRP:CH2	2.45	0.51
3:D:141:ILE:HD13	3:D:450:TYR:N	2.26	0.51
3:D:1196:THR:HA	9:D:9591:HOH:O	2.10	0.51
3:D:1212:ALA:HB1	9:D:2669:HOH:O	2.10	0.51
5:F:305:GLU:HG2	5:F:309:LYS:HE3	1.93	0.51
1:K:119:ASP:HB3	9:K:1333:HOH:O	2.10	0.51
1:K:166:PRO:HA	9:K:2046:HOH:O	2.10	0.51
2:M:140:ILE:HA	2:M:332:ARG:O	2.11	0.51
2:M:266:ARG:H	2:M:288:ARG:NH1	2.09	0.51
2:M:431:HIS:CD2	2:M:433:THR:H	2.29	0.51
2:M:897:LEU:HB3	2:M:899:GLN:HG2	1.93	0.51
2:M:901:TYR:CE2	2:M:917:LEU:HD13	2.46	0.51
2:M:911:GLU:O	2:M:915:LYS:HG2	2.10	0.51
3:N:32:ILE:O	5:P:258:ILE:HG23	2.11	0.51
3:N:179:VAL:HG13	9:N:2353:HOH:O	2.10	0.51
3:N:422:ALA:HB3	3:N:427:VAL:CG2	2.37	0.51
4:O:87:LYS:HB2	9:O:2278:HOH:O	2.11	0.51
5:P:260:ILE:HG12	5:P:264:MET:HB2	1.92	0.51
5:P:350:LEU:HD12	5:P:422:LEU:HD13	1.92	0.51
1:A:23:PHE:O	1:A:196:THR:HA	2.10	0.51
1:B:227:ASN:HB2	9:B:9778:HOH:O	2.11	0.51
2:C:70:GLU:HB3	9:C:9688:HOH:O	2.11	0.51
2:C:121:MET:HA	2:C:127:PHE:CD2	2.45	0.51
2:C:339:LEU:HD13	2:C:391:LEU:HD21	1.93	0.51
2:C:670:GLN:HE22	2:C:699:PHE:HA	1.76	0.51
2:C:723:THR:C	2:C:725:ASP:H	2.14	0.51
3:D:80:VAL:HA	9:D:2231:HOH:O	2.11	0.51
3:D:770:LEU:HD21	3:D:919:PHE:CE1	2.46	0.51
3:D:1264:GLU:HG2	9:D:2050:HOH:O	2.11	0.51
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1388:ARG:HB2	9:D:2873:HOH:O	2.11	0.51
1:K:175:ARG:HD3	9:K:2112:HOH:O	2.10	0.51
1:L:187:GLY:HA2	9:N:2058:HOH:O	2.10	0.51
2:M:70:GLU:OE1	2:M:97:ARG:HD3	2.10	0.51
2:M:368:THR:HG22	9:M:9372:HOH:O	2.11	0.51
2:M:694:LEU:HD23	2:M:697:ARG:HH21	1.75	0.51
9:M:9230:HOH:O	5:P:405:LEU:HG	2.11	0.51
4:O:72:ARG:HG3	9:O:1901:HOH:O	2.11	0.51
1:B:162:ILE:HD12	9:B:9818:HOH:O	2.11	0.50
2:C:61:LYS:HG3	9:C:2460:HOH:O	2.10	0.50
2:C:63:GLY:HA3	2:C:103:LYS:CG	2.41	0.50
2:C:118:ILE:H	2:C:118:ILE:CD1	2.23	0.50
2:C:283:ILE:HB	2:C:284:ARG:HD2	1.92	0.50
2:C:332:ARG:HG2	2:C:465:GLY:HA3	1.92	0.50
2:C:470:PRO:HG2	9:C:9634:HOH:O	2.11	0.50
3:D:626:SER:HB3	3:D:748:HIS:ND1	2.27	0.50
3:D:777:PRO:O	3:D:912:LYS:HE3	2.11	0.50
3:D:812:ALA:O	3:D:816:HIS:HB2	2.11	0.50
3:D:953:ASP:HA	9:D:9611:HOH:O	2.10	0.50
3:D:1313:VAL:HA	9:D:9855:HOH:O	2.11	0.50
3:D:1376:MET:SD	3:D:1421:LEU:HD13	2.51	0.50
4:E:70:THR:HA	9:E:9683:HOH:O	2.11	0.50
5:F:304:VAL:HG12	5:F:308:LEU:HD11	1.91	0.50
1:K:227:ASN:HD22	1:K:227:ASN:N	2.08	0.50
2:M:27:ARG:HH11	2:M:27:ARG:HG3	1.76	0.50
2:M:73:LEU:HG	9:M:9263:HOH:O	2.11	0.50
2:M:520:GLU:HG3	9:M:9551:HOH:O	2.11	0.50
2:M:928:LYS:HG3	2:M:932:GLU:HG3	1.92	0.50
3:N:9:ARG:HG2	3:N:9:ARG:HH11	1.74	0.50
3:N:156:GLU:HB3	9:N:9891:HOH:O	2.11	0.50
3:N:601:ARG:NE	3:N:613:ARG:HH21	2.09	0.50
3:N:645:PRO:HA	3:N:721:VAL:O	2.11	0.50
3:N:813:LEU:HD21	9:N:9724:HOH:O	2.09	0.50
3:N:1307:LYS:HG3	9:N:9927:HOH:O	2.11	0.50
3:N:1312:LEU:HD12	3:N:1326:THR:O	2.12	0.50
3:N:1481:VAL:CG1	4:O:18:ARG:HA	2.36	0.50
4:O:39:VAL:HB	4:O:72:ARG:HD3	1.93	0.50
5:P:128:ARG:NH1	5:P:128:ARG:HB2	2.26	0.50
1:A:18:ARG:HH22	1:A:88:ARG:NH2	2.09	0.50
1:A:18:ARG:NH2	1:A:88:ARG:HH21	2.07	0.50
1:A:152:PRO:HB3	9:C:9586:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HH22	2:C:932:GLU:CD	2.13	0.50
1:B:12:THR:OG1	1:B:24:VAL:HB	2.11	0.50
1:B:62:LEU:H	1:B:62:LEU:HD12	1.75	0.50
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.94	0.50
2:C:478:VAL:HA	2:C:506:ASN:O	2.11	0.50
2:C:545:ASN:O	2:C:905:ILE:HD11	2.11	0.50
2:C:1100:GLN:HB3	9:D:9712:HOH:O	2.09	0.50
3:D:550:ARG:HH11	3:D:550:ARG:HG3	1.76	0.50
3:D:596:SER:C	3:D:598:ARG:H	2.14	0.50
3:D:827:ILE:O	3:D:837:GLY:HA3	2.11	0.50
3:D:868:TYR:HB2	3:D:873:LEU:HD11	1.94	0.50
3:D:1346:ARG:HA	3:D:1346:ARG:NE	2.26	0.50
4:E:51:LEU:HD13	9:E:9663:HOH:O	2.10	0.50
5:F:93:LEU:HD21	5:F:102:LEU:HD11	1.92	0.50
5:F:271:LEU:HD22	5:F:291:ILE:HD11	1.93	0.50
1:K:23:PHE:O	1:K:196:THR:HA	2.11	0.50
1:L:26:GLU:CB	1:L:194:LYS:HG3	2.41	0.50
1:L:112:ARG:HG3	9:L:6646:HOH:O	2.11	0.50
2:M:182:VAL:HG23	9:M:9649:HOH:O	2.10	0.50
2:M:310:LEU:O	2:M:314:THR:HG23	2.11	0.50
2:M:945:ARG:O	2:M:948:GLU:HG3	2.11	0.50
3:N:760:ARG:HH21	4:O:3:GLU:CD	2.14	0.50
3:N:1063:GLU:HB3	9:N:2394:HOH:O	2.11	0.50
3:N:1128:VAL:HA	9:N:2136:HOH:O	2.10	0.50
3:N:1147:ARG:HB3	3:N:1188:VAL:HG21	1.93	0.50
3:N:1493:LYS:HD2	9:N:2553:HOH:O	2.11	0.50
5:P:140:ARG:HA	9:P:7056:HOH:O	2.10	0.50
1:A:143:ARG:HD3	1:A:158:ILE:HG21	1.93	0.50
1:A:186:LEU:HA	9:A:9786:HOH:O	2.11	0.50
2:C:55:GLU:HG2	9:C:2166:HOH:O	2.11	0.50
2:C:157:ARG:HH11	2:C:157:ARG:HG3	1.76	0.50
2:C:577:PRO:HG3	2:C:993:PHE:CE2	2.47	0.50
2:C:756:VAL:HG21	2:C:823:VAL:CG1	2.41	0.50
2:C:799:ILE:O	2:C:801:VAL:HG13	2.11	0.50
2:C:965:GLU:HG3	9:C:2351:HOH:O	2.11	0.50
3:D:58:CYS:SG	3:D:59:ALA:N	2.83	0.50
3:D:416:ALA:H	3:D:417:PRO:CD	2.25	0.50
3:D:566:ILE:HD11	5:F:192:LEU:CD2	2.41	0.50
3:D:838:ARG:CG	3:D:865:THR:HG23	2.41	0.50
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.11	0.50
3:D:1284:GLU:HB3	9:D:9836:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1362:LYS:HE3	9:D:9887:HOH:O	2.10	0.50
5:F:94:LEU:HB2	5:F:98:GLU:OE2	2.11	0.50
1:K:171:PHE:O	1:K:172:SER:C	2.50	0.50
1:L:2:LEU:HA	1:L:6:LEU:HD22	1.92	0.50
2:M:41:ASN:HD22	2:M:41:ASN:H	1.58	0.50
2:M:195:LEU:HA	9:M:9289:HOH:O	2.12	0.50
2:M:568:ALA:CB	2:M:668:LEU:HB3	2.40	0.50
2:M:952:LEU:CD1	2:M:969:GLN:HE22	2.19	0.50
2:M:969:GLN:HB3	9:M:9280:HOH:O	2.10	0.50
2:M:1083:GLU:N	9:M:9233:HOH:O	2.43	0.50
2:M:1087:VAL:HG12	2:M:1091:GLU:OE2	2.11	0.50
3:N:1104:GLU:HA	3:N:1461:GLY:HA2	1.93	0.50
3:N:1476:THR:HG23	4:O:21:VAL:CG2	2.41	0.50
5:P:167:PRO:HB2	5:P:169:GLU:OE1	2.11	0.50
5:P:396:ARG:HA	5:P:399:GLN:HE21	1.76	0.50
2:C:53:PRO:HG3	9:C:9996:HOH:O	2.10	0.50
2:C:108:ILE:HB	9:C:9838:HOH:O	2.12	0.50
2:C:259:GLY:HA2	2:C:290:LEU:O	2.10	0.50
2:C:345:ARG:HD3	9:C:9778:HOH:O	2.10	0.50
2:C:725:ASP:O	2:C:727:PRO:HD3	2.11	0.50
2:C:745:ILE:HG12	9:C:9595:HOH:O	2.11	0.50
2:C:1058:ASP:OD1	2:C:1084:SER:N	2.43	0.50
3:D:475:LYS:HD3	3:D:478:LEU:CD1	2.40	0.50
3:D:1128:VAL:HB	3:D:1131:SER:OG	2.12	0.50
1:L:180:GLN:HG2	9:L:1240:HOH:O	2.10	0.50
2:M:15:LEU:HD22	9:M:9656:HOH:O	2.12	0.50
2:M:31:GLN:HB2	9:M:9742:HOH:O	2.10	0.50
2:M:149:THR:HA	9:M:9241:HOH:O	2.11	0.50
2:M:431:HIS:HD2	2:M:433:THR:H	1.60	0.50
2:M:516:ARG:CZ	3:N:1068:LEU:HD22	2.41	0.50
2:M:678:PRO:O	3:N:943:THR:HG23	2.12	0.50
2:M:744:ARG:HA	9:M:9460:HOH:O	2.10	0.50
9:M:2444:HOH:O	3:N:744:GLN:HG3	2.12	0.50
3:N:596:SER:C	3:N:598:ARG:H	2.15	0.50
3:N:1127:GLU:HA	9:N:2957:HOH:O	2.10	0.50
5:P:93:LEU:HD12	5:P:191:ASN:HD21	1.76	0.50
1:A:46:SER:HA	9:A:9582:HOH:O	2.11	0.50
1:B:111:ALA:HB3	1:B:124:ASN:O	2.11	0.50
2:C:426:ASP:HA	2:C:429:ASP:OD2	2.12	0.50
2:C:479:VAL:HG22	2:C:506:ASN:O	2.12	0.50
3:D:22:SER:HA	3:D:90:MET:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:132:TYR:N	3:D:132:TYR:CD1	2.79	0.50
3:D:933:ALA:O	3:D:937:TYR:HD1	1.94	0.50
3:D:1109:GLU:HG2	3:D:1201:CYS:CA	2.37	0.50
2:M:28:ARG:HG2	2:M:28:ARG:HH11	1.76	0.50
2:M:202:TYR:CE1	2:M:304:LEU:HD22	2.45	0.50
2:M:428:ARG:HA	2:M:450:GLY:HA3	1.94	0.50
2:M:516:ARG:HB2	9:M:9549:HOH:O	2.11	0.50
2:M:728:HIS:O	2:M:729:LEU:HD22	2.12	0.50
3:N:13:ALA:HB1	3:N:18:ILE:HD11	1.94	0.50
3:N:17:LYS:HG3	9:N:9504:HOH:O	2.10	0.50
3:N:102:ILE:HD13	3:N:586:ARG:HB2	1.94	0.50
3:N:165:LYS:HE2	9:N:9671:HOH:O	2.12	0.50
3:N:427:VAL:CG2	3:N:435:VAL:HB	2.42	0.50
3:N:1121:PRO:HD3	3:N:1346:ARG:HH22	1.76	0.50
5:P:94:LEU:HD12	5:P:97:GLU:HB2	1.93	0.50
5:P:260:ILE:HD11	5:P:264:MET:HB3	1.94	0.50
5:P:367:MET:HB3	9:P:3256:HOH:O	2.10	0.50
1:A:41:ARG:NH1	1:A:177:VAL:HB	2.25	0.50
1:A:111:ALA:HB3	1:A:124:ASN:O	2.12	0.50
1:A:156:HIS:H	1:A:156:HIS:CD2	2.29	0.50
1:A:184:THR:O	1:A:192:LEU:HD12	2.11	0.50
1:B:60:ASP:HB2	9:B:9588:HOH:O	2.11	0.50
1:B:211:LEU:O	1:B:215:VAL:HG13	2.12	0.50
2:C:19:THR:HG21	2:C:124:ASP:O	2.11	0.50
2:C:266:ARG:HH11	2:C:266:ARG:HG3	1.77	0.50
2:C:514:VAL:HG22	9:C:9943:HOH:O	2.11	0.50
2:C:604:ALA:HB3	2:C:612:VAL:O	2.12	0.50
2:C:644:VAL:HB	9:C:2682:HOH:O	2.12	0.50
2:C:669:GLY:O	2:C:670:GLN:HG3	2.12	0.50
2:C:770:GLU:HG2	9:D:9612:HOH:O	2.11	0.50
2:C:958:THR:HB	9:C:9980:HOH:O	2.11	0.50
3:D:399:ARG:HB3	3:D:402:PRO:HG3	1.92	0.50
3:D:630:VAL:HG12	3:D:631:ILE:N	2.27	0.50
3:D:939:PHE:O	3:D:942:SER:HB3	2.12	0.50
3:D:1351:GLU:HA	3:D:1351:GLU:OE1	2.11	0.50
3:D:1409:ALA:HB2	9:D:2109:HOH:O	2.11	0.50
9:D:2101:HOH:O	4:E:48:MET:HG3	2.11	0.50
5:F:209:PHE:HA	5:F:212:LEU:HD12	1.93	0.50
5:F:392:VAL:HG13	9:F:9894:HOH:O	2.10	0.50
1:K:151:VAL:HG22	9:K:3152:HOH:O	2.11	0.50
2:M:264:PRO:HB2	2:M:289:THR:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:456:ALA:HA	2:M:541:SER:HA	1.93	0.50
2:M:478:VAL:HA	2:M:506:ASN:O	2.12	0.50
2:M:564:MET:HA	9:M:9338:HOH:O	2.11	0.50
2:M:769:PRO:HD2	9:M:9815:HOH:O	2.11	0.50
2:M:876:VAL:H	2:M:877:PRO:HD2	1.75	0.50
3:N:2:LYS:HG2	3:N:3:LYS:HZ2	1.76	0.50
3:N:65:ARG:CD	3:N:66:GLN:H	2.25	0.50
3:N:81:THR:HB	3:N:85:VAL:HG21	1.91	0.50
3:N:112:ILE:HD11	3:N:124:GLU:CD	2.32	0.50
3:N:136:ASP:CB	3:N:137:PRO:HD3	2.42	0.50
3:N:637:LEU:HD11	3:N:642:CYS:CA	2.41	0.50
3:N:714:GLN:HE22	3:N:732:VAL:HB	1.77	0.50
3:N:958:GLU:HB3	9:N:9999:HOH:O	2.10	0.50
3:N:1123:PHE:CE1	3:N:1134:LEU:HG	2.46	0.50
3:N:1124:GLN:OE1	3:N:1135:ARG:HA	2.12	0.50
3:N:1462:LEU:HD22	3:N:1472:ILE:HG23	1.94	0.50
1:A:115:LEU:HD12	1:A:115:LEU:O	2.11	0.50
1:A:182:GLU:O	1:A:194:LYS:HB3	2.11	0.50
1:B:90:LEU:HD23	1:B:91:ASN:HD22	1.77	0.50
1:B:195:LEU:HD12	1:B:196:THR:N	2.27	0.50
2:C:607:ASP:C	2:C:609:ASN:H	2.15	0.50
3:D:969:ARG:HA	9:D:2563:HOH:O	2.11	0.50
3:D:1319:VAL:HA	3:D:1323:GLN:OE1	2.12	0.50
5:F:340:SER:O	5:F:342:VAL:N	2.45	0.50
2:M:792:VAL:N	9:M:9305:HOH:O	2.44	0.50
2:M:875:GLY:O	2:M:879:ARG:HD3	2.12	0.50
3:N:73:CYS:HB3	3:N:76:CYS:O	2.11	0.50
3:N:827:ILE:HG23	9:N:9636:HOH:O	2.12	0.50
3:N:1103:HIS:HD2	3:N:1462:LEU:H	1.58	0.50
3:N:1106:VAL:HG21	3:N:1474:ALA:HB2	1.93	0.50
3:N:1129:THR:HG23	3:N:1130:ARG:H	1.77	0.50
3:N:1335:LEU:HD11	9:N:2029:HOH:O	2.11	0.50
3:N:1349:VAL:HG22	3:N:1372:VAL:HG21	1.94	0.50
3:N:1404:ASN:ND2	3:N:1408:ILE:HD12	2.27	0.50
2:C:289:THR:O	2:C:291:ALA:N	2.44	0.50
2:C:759:THR:HG21	2:C:783:ARG:CZ	2.42	0.50
3:D:115:LEU:CD1	3:D:499:VAL:HG22	2.42	0.50
3:D:563:PRO:HB3	9:F:9576:HOH:O	2.11	0.50
3:D:676:MET:HG3	9:D:9957:HOH:O	2.11	0.50
3:D:894:LYS:HA	9:D:2557:HOH:O	2.11	0.50
1:K:5:LYS:HZ1	1:L:224:TYR:HE1	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:36:LEU:O	1:L:39:PRO:HD2	2.12	0.50
2:M:110:GLU:HB3	9:M:9372:HOH:O	2.12	0.50
2:M:139:GLN:HB3	2:M:334:ARG:HB2	1.93	0.50
2:M:476:GLY:C	2:M:478:VAL:H	2.16	0.50
2:M:649:VAL:HA	2:M:650:ARG:HH21	1.77	0.50
3:N:104:PHE:CD2	3:N:1448:THR:HG23	2.47	0.50
3:N:486:ARG:HA	3:N:489:ARG:HD3	1.93	0.50
3:N:521:PRO:O	3:N:525:ARG:HG2	2.12	0.50
3:N:844:ALA:O	3:N:867:ARG:HB3	2.11	0.50
3:N:956:ILE:HG12	3:N:1039:CYS:O	2.11	0.50
3:N:1124:GLN:HB2	9:N:9329:HOH:O	2.12	0.50
5:P:147:LEU:H	5:P:147:LEU:HD12	1.77	0.50
5:P:278:LEU:HB3	5:P:286:PRO:CG	2.27	0.50
1:A:184:THR:HG23	1:A:192:LEU:HB2	1.93	0.50
2:C:45:GLN:HB2	2:C:71:TYR:CE2	2.47	0.50
2:C:260:LEU:HA	2:C:291:ALA:CB	2.41	0.50
2:C:747:ALA:O	2:C:800:VAL:HG23	2.12	0.50
3:D:6:ARG:HB3	3:D:6:ARG:CZ	2.42	0.50
3:D:959:GLU:HG3	3:D:1006:ALA:HB1	1.93	0.50
3:D:1101:VAL:HG21	3:D:1424:VAL:HG13	1.93	0.50
3:D:1362:LYS:HG3	9:D:2173:HOH:O	2.12	0.50
5:F:372:ARG:HB3	9:F:2056:HOH:O	2.12	0.50
1:K:7:LYS:NZ	1:K:27:PRO:HG2	2.27	0.50
2:M:64:LEU:HD13	9:M:9296:HOH:O	2.12	0.50
2:M:139:GLN:OE1	2:M:415:PRO:HD2	2.12	0.50
2:M:304:LEU:HB2	9:M:9883:HOH:O	2.11	0.50
2:M:390:GLN:HA	9:P:4407:HOH:O	2.10	0.50
3:N:129:PHE:O	3:N:572:ARG:HG3	2.11	0.50
3:N:519:VAL:HG13	3:N:544:TYR:CE1	2.47	0.50
3:N:599:PRO:HD2	9:N:9833:HOH:O	2.12	0.50
3:N:681:ARG:HB2	3:N:681:ARG:HH11	1.77	0.50
3:N:813:LEU:HD23	9:N:9996:HOH:O	2.10	0.50
5:P:215:GLU:O	5:P:218:GLN:HB3	2.11	0.50
5:P:261:PRO:HD3	9:P:8018:HOH:O	2.12	0.50
1:A:153:ALA:HA	1:A:156:HIS:CD2	2.47	0.49
1:B:189:ARG:HD2	9:B:9618:HOH:O	2.11	0.49
2:C:295:ASP:C	2:C:297:GLU:H	2.15	0.49
2:C:479:VAL:HG21	2:C:503:LEU:HD21	1.93	0.49
2:C:769:PRO:HA	9:C:9981:HOH:O	2.12	0.49
2:C:1059:ASP:HB2	9:C:9720:HOH:O	2.12	0.49
3:D:67:ARG:HA	3:D:67:ARG:HE	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:166:GLN:HB3	3:D:395:VAL:HG21	1.94	0.49
3:D:497:GLU:HB2	9:D:2123:HOH:O	2.11	0.49
3:D:864:VAL:HA	9:D:9613:HOH:O	2.11	0.49
3:D:1281:VAL:HG21	3:D:1313:VAL:HG21	1.92	0.49
5:F:158:GLU:HA	5:F:161:GLN:NE2	2.27	0.49
5:F:277:GLN:HA	9:F:9672:HOH:O	2.11	0.49
1:L:111:ALA:HB3	1:L:124:ASN:O	2.12	0.49
2:M:48:PHE:HA	9:M:9688:HOH:O	2.11	0.49
2:M:164:PRO:HD2	2:M:170:PRO:O	2.12	0.49
3:N:3:LYS:HA	9:N:2915:HOH:O	2.12	0.49
3:N:502:PHE:CD1	3:N:509:PRO:HB3	2.47	0.49
3:N:543:LEU:HD22	3:N:580:ALA:HB1	1.93	0.49
3:N:1079:LYS:HG3	3:N:1080:GLY:N	2.26	0.49
3:N:1378:TYR:OH	3:N:1431:THR:HA	2.12	0.49
4:O:45:ARG:HB3	4:O:46:PRO:HD2	1.92	0.49
5:P:119:ILE:HG12	9:P:2011:HOH:O	2.11	0.49
5:P:321:ILE:HD11	5:P:329:TYR:CB	2.39	0.49
5:P:393:THR:O	5:P:397:ILE:HG13	2.11	0.49
5:P:422:LEU:H	5:P:422:LEU:HD12	1.77	0.49
2:C:86:LYS:CG	2:C:813:VAL:HG12	2.39	0.49
2:C:148:PHE:CE1	2:C:281:LEU:HD22	2.47	0.49
2:C:350:ARG:HB3	9:C:2086:HOH:O	2.12	0.49
2:C:674:VAL:HG12	2:C:990:GLY:O	2.12	0.49
2:C:786:LYS:HG3	9:C:2781:HOH:O	2.11	0.49
3:D:127:LEU:HD12	3:D:457:GLY:H	1.77	0.49
3:D:169:TYR:N	3:D:170:PRO:HD3	2.27	0.49
3:D:217:LYS:HA	9:D:9649:HOH:O	2.13	0.49
3:D:405:ASP:OD1	3:D:407:VAL:HG23	2.13	0.49
3:D:474:GLU:O	3:D:478:LEU:HG	2.12	0.49
3:D:629:SER:HA	9:D:2061:HOH:O	2.12	0.49
3:D:1263:PHE:HA	3:D:1375:MET:HE2	1.93	0.49
3:D:1274:ILE:O	3:D:1274:ILE:HD12	2.13	0.49
4:E:41:GLU:CA	4:E:45:ARG:HG3	2.42	0.49
5:F:273:ARG:HD3	9:F:9638:HOH:O	2.12	0.49
1:L:145:ASP:HB3	9:L:7895:HOH:O	2.12	0.49
1:L:161:ARG:HB3	9:L:4752:HOH:O	2.12	0.49
2:M:346:VAL:HG12	2:M:350:ARG:HE	1.77	0.49
2:M:606:VAL:HG21	2:M:645:VAL:HG22	1.95	0.49
3:N:65:ARG:HB2	5:P:375:LEU:O	2.12	0.49
3:N:87:ARG:HG3	3:N:524:LEU:HG	1.93	0.49
3:N:180:LYS:HG3	9:N:9302:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:455:ARG:HH22	5:P:140:ARG:CB	2.25	0.49
3:N:507:ASN:HB2	9:N:9257:HOH:O	2.12	0.49
3:N:966:GLU:O	3:N:969:ARG:HG2	2.11	0.49
3:N:1189:ARG:HB3	3:N:1189:ARG:CZ	2.43	0.49
4:O:40:LEU:HD11	4:O:67:GLU:HG2	1.94	0.49
2:C:36:PRO:HG2	2:C:70:GLU:HB3	1.94	0.49
2:C:194:VAL:HG21	2:C:221:LEU:O	2.12	0.49
3:D:147:VAL:HA	9:D:9668:HOH:O	2.11	0.49
3:D:172:PRO:HB3	3:D:178:LEU:CB	2.42	0.49
4:E:24:ALA:O	4:E:28:GLN:HG3	2.12	0.49
5:F:125:ASP:HA	9:F:9581:HOH:O	2.12	0.49
5:F:160:ASP:HA	5:F:163:LEU:CD1	2.34	0.49
1:K:62:LEU:HD22	2:M:745:ILE:HB	1.94	0.49
1:K:229:GLN:HB2	9:K:5388:HOH:O	2.10	0.49
1:L:54:THR:HG21	1:L:143:ARG:NH2	2.26	0.49
1:L:76:VAL:HG23	9:L:2024:HOH:O	2.12	0.49
1:L:114:PHE:HB3	9:L:6216:HOH:O	2.11	0.49
2:M:246:ASP:HB3	9:M:9919:HOH:O	2.12	0.49
2:M:259:GLY:HA2	2:M:290:LEU:O	2.12	0.49
3:N:389:GLU:HG2	9:N:9256:HOH:O	2.11	0.49
3:N:704:ARG:HH12	3:N:743:ASP:CB	2.26	0.49
4:O:47:LYS:CA	4:O:54:LEU:HB3	2.42	0.49
5:P:172:ARG:O	5:P:176:ILE:HG13	2.11	0.49
5:P:278:LEU:HD13	5:P:290:GLU:HB3	1.95	0.49
5:P:357:ALA:HB1	5:P:408:LEU:HD11	1.94	0.49
5:P:373:LYS:HD3	5:P:378:GLY:C	2.32	0.49
1:A:30:ARG:HH22	1:B:155:LYS:HZ2	1.60	0.49
2:C:266:ARG:HB2	2:C:288:ARG:NE	2.27	0.49
2:C:394:PHE:HB3	9:C:9833:HOH:O	2.12	0.49
2:C:479:VAL:CG2	2:C:503:LEU:HD11	2.41	0.49
2:C:590:ASP:HA	9:C:9671:HOH:O	2.11	0.49
2:C:727:PRO:HG2	2:C:785:VAL:HG12	1.93	0.49
2:C:769:PRO:HB2	9:D:9612:HOH:O	2.12	0.49
2:C:919:ALA:HB2	9:C:9756:HOH:O	2.12	0.49
3:D:795:VAL:CG1	3:D:863:VAL:HG22	2.42	0.49
3:D:1274:ILE:HB	3:D:1322:GLY:HA2	1.94	0.49
3:D:1366:LYS:HA	3:D:1369:GLU:OE1	2.11	0.49
1:L:163:ASN:HA	9:L:5364:HOH:O	2.12	0.49
2:M:9:ILE:CD1	2:M:536:PRO:HD3	2.43	0.49
2:M:42:VAL:HG22	2:M:268:ASP:OD2	2.13	0.49
2:M:193:LEU:O	2:M:193:LEU:HD13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:452:ILE:HG12	9:M:9712:HOH:O	2.12	0.49
2:M:958:THR:HG23	2:M:961:GLU:HG3	1.93	0.49
3:N:165:LYS:HB2	3:N:395:VAL:HG11	1.93	0.49
3:N:558:LEU:HD13	5:P:145:PRO:CB	2.39	0.49
3:N:1092:GLY:O	3:N:1096:ARG:N	2.45	0.49
3:N:1110:ALA:HB1	9:N:9774:HOH:O	2.11	0.49
1:A:184:THR:HG22	1:A:192:LEU:O	2.12	0.49
2:C:627:ARG:HE	2:C:627:ARG:N	1.89	0.49
3:D:177:ALA:HA	3:D:199:LEU:HD13	1.94	0.49
3:D:427:VAL:CG2	3:D:435:VAL:HB	2.42	0.49
3:D:868:TYR:H	3:D:873:LEU:HD11	1.77	0.49
3:D:902:LEU:HD23	3:D:902:LEU:H	1.78	0.49
3:D:935:LYS:HZ3	3:D:936:TYR:N	2.10	0.49
3:D:1396:GLU:HA	3:D:1399:ASP:OD2	2.13	0.49
5:F:299:TRP:HD1	9:F:9664:HOH:O	1.95	0.49
1:K:91:ASN:O	1:K:94:LEU:HD12	2.13	0.49
1:L:109:VAL:HG23	1:L:132:LEU:HD13	1.94	0.49
2:M:98:LEU:O	2:M:109:LYS:HG3	2.13	0.49
2:M:313:LEU:HD12	9:M:2079:HOH:O	2.11	0.49
2:M:720:GLU:HB3	9:M:9349:HOH:O	2.11	0.49
3:N:9:ARG:HA	3:N:1455:LYS:O	2.12	0.49
3:N:112:ILE:HD11	3:N:124:GLU:HG2	1.93	0.49
3:N:131:LYS:HB2	3:N:456:MET:HE2	1.94	0.49
3:N:581:LEU:HD12	3:N:582:LEU:N	2.27	0.49
5:P:144:ILE:HB	5:P:145:PRO:HD3	1.95	0.49
2:C:28:ARG:HA	9:C:2297:HOH:O	2.12	0.49
2:C:40:GLU:HG2	9:C:2473:HOH:O	2.13	0.49
2:C:327:HIS:HB3	2:C:330:ASN:ND2	2.28	0.49
2:C:549:PHE:CD2	2:C:886:LEU:HB3	2.47	0.49
2:C:602:GLU:HB3	9:C:9979:HOH:O	2.12	0.49
2:C:1115:LEU:HD23	3:D:85:VAL:CG1	2.40	0.49
3:D:181:ASP:O	3:D:185:VAL:HG23	2.13	0.49
3:D:399:ARG:HB2	3:D:444:VAL:HG13	1.94	0.49
3:D:413:ASP:HA	9:D:2284:HOH:O	2.12	0.49
3:D:486:ARG:O	3:D:489:ARG:HG2	2.12	0.49
3:D:1303:TYR:HA	9:D:2028:HOH:O	2.13	0.49
3:D:1379:VAL:N	9:D:2424:HOH:O	2.44	0.49
3:D:1499:ARG:HA	9:D:2938:HOH:O	2.11	0.49
5:F:167:PRO:HB2	5:F:169:GLU:OE1	2.13	0.49
1:K:206:THR:CG2	1:K:209:GLU:H	2.24	0.49
1:L:45:LEU:HD21	1:L:177:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:332:ARG:HG2	2:M:333:ILE:N	2.27	0.49
2:M:644:VAL:HB	9:M:9422:HOH:O	2.12	0.49
2:M:777:ILE:HG22	2:M:778:PHE:HD1	1.76	0.49
2:M:897:LEU:HB3	2:M:899:GLN:NE2	2.28	0.49
3:N:135:LEU:HD13	3:N:147:VAL:HG12	1.94	0.49
3:N:401:TYR:N	3:N:402:PRO:HD3	2.28	0.49
3:N:1102:THR:HG22	3:N:1222:GLY:CA	2.42	0.49
5:P:163:LEU:HB3	5:P:174:LEU:HG	1.94	0.49
1:B:162:ILE:HB	9:B:9818:HOH:O	2.11	0.49
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.94	0.49
2:C:551:GLU:HG3	2:C:552:HIS:CD2	2.47	0.49
2:C:744:ARG:HA	9:C:9595:HOH:O	2.13	0.49
2:C:1035:MET:HB3	3:D:707:THR:HB	1.94	0.49
3:D:710:ARG:HG2	3:D:710:ARG:NH1	2.25	0.49
3:D:1159:ARG:HG3	3:D:1159:ARG:HH11	1.76	0.49
5:F:169:GLU:HA	9:F:9835:HOH:O	2.11	0.49
5:F:266:GLU:HA	5:F:269:ASN:ND2	2.24	0.49
1:K:184:THR:O	1:K:192:LEU:HB2	2.12	0.49
1:K:198:ARG:HD3	1:K:200:TRP:CH2	2.48	0.49
1:L:41:ARG:HG3	1:L:177:VAL:HB	1.94	0.49
2:M:82:GLU:HG3	9:M:9567:HOH:O	2.13	0.49
2:M:101:ILE:HG22	2:M:102:HIS:N	2.26	0.49
2:M:583:LEU:O	2:M:587:VAL:HG23	2.13	0.49
2:M:1028:GLY:HA2	9:M:9259:HOH:O	2.12	0.49
3:N:26:VAL:N	9:N:9259:HOH:O	2.44	0.49
3:N:153:LEU:HD22	9:N:2799:HOH:O	2.11	0.49
3:N:1147:ARG:O	3:N:1165:TYR:HA	2.12	0.49
3:N:1476:THR:HG23	4:O:21:VAL:HG22	1.94	0.49
1:A:26:GLU:HB3	1:A:194:LYS:HG3	1.95	0.49
2:C:689:VAL:HG21	2:C:870:ILE:HB	1.93	0.49
2:C:1102:LEU:HD11	9:D:9712:HOH:O	2.13	0.49
3:D:179:VAL:CG2	3:D:389:GLU:HG3	2.42	0.49
3:D:1023:MET:O	3:D:1028:ALA:HB3	2.12	0.49
3:D:1213:ARG:HB2	3:D:1214:PRO:CD	2.43	0.49
3:D:1310:ARG:HB3	9:D:9775:HOH:O	2.13	0.49
4:E:25:LYS:O	4:E:28:GLN:HB2	2.13	0.49
5:F:350:LEU:O	5:F:354:LEU:HG	2.13	0.49
5:F:395:GLU:O	5:F:399:GLN:HB2	2.12	0.49
1:K:11:PHE:HB2	9:K:3188:HOH:O	2.12	0.49
1:L:101:LEU:HA	9:L:1474:HOH:O	2.13	0.49
2:M:222:MET:HG3	9:M:2024:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:269:LEU:HD22	2:M:288:ARG:HB2	1.94	0.49
2:M:545:ASN:HB3	2:M:583:LEU:HD12	1.95	0.49
2:M:776:SER:HA	2:M:780:GLU:CB	2.41	0.49
3:N:412:GLY:O	3:N:421:LEU:HB3	2.12	0.49
3:N:657:LEU:HD22	3:N:691:LEU:HD13	1.93	0.49
3:N:947:ILE:O	3:N:947:ILE:HD12	2.12	0.49
3:N:957:PRO:CG	3:N:1007:VAL:HG12	2.39	0.49
3:N:968:ASP:O	3:N:971:LEU:HB3	2.12	0.49
3:N:1004:THR:O	3:N:1007:VAL:HG22	2.13	0.49
3:N:1448:THR:O	3:N:1451:ALA:HB3	2.13	0.49
9:N:2509:HOH:O	5:P:94:LEU:HD21	2.13	0.49
4:O:25:LYS:O	4:O:28:GLN:HB2	2.13	0.49
5:P:277:GLN:HG2	9:P:1413:HOH:O	2.12	0.49
5:P:320:PRO:HB3	9:P:5311:HOH:O	2.12	0.49
1:B:184:THR:HG22	1:B:192:LEU:O	2.11	0.49
1:B:195:LEU:HD12	1:B:196:THR:H	1.76	0.49
2:C:27:ARG:HH11	2:C:27:ARG:HG3	1.77	0.49
2:C:142:ARG:HG3	9:C:2425:HOH:O	2.11	0.49
2:C:446:GLY:HA3	9:C:9687:HOH:O	2.12	0.49
2:C:564:MET:HG2	2:C:840:ALA:HB3	1.95	0.49
2:C:1073:GLY:HA3	3:D:659:LYS:NZ	2.28	0.49
3:D:89:ARG:O	3:D:521:PRO:HG3	2.13	0.49
3:D:116:LEU:O	3:D:118:LEU:N	2.45	0.49
3:D:1012:GLU:HB3	9:D:9868:HOH:O	2.13	0.49
3:D:1047:LYS:HG2	3:D:1053:PHE:CE1	2.47	0.49
5:F:162:LYS:HE3	9:F:9869:HOH:O	2.13	0.49
1:K:182:GLU:O	1:K:194:LYS:HB3	2.12	0.49
1:L:132:LEU:HG	9:L:2881:HOH:O	2.12	0.49
2:M:42:VAL:HA	2:M:46:ALA:HB2	1.95	0.49
2:M:472:ARG:HE	2:M:532:MET:HE2	1.77	0.49
2:M:956:GLY:HA2	9:M:2324:HOH:O	2.12	0.49
3:N:168:THR:OG1	3:N:393:ILE:HB	2.11	0.49
3:N:1330:ILE:HG12	9:N:9950:HOH:O	2.13	0.49
3:N:1442:ASN:HD22	3:N:1442:ASN:H	1.60	0.49
4:O:63:TRP:O	4:O:67:GLU:HG3	2.13	0.49
5:P:76:SER:O	5:P:80:PRO:HD2	2.12	0.49
5:P:168:LYS:HG3	9:P:3066:HOH:O	2.12	0.49
1:A:45:LEU:HD21	1:A:177:VAL:HG23	1.93	0.49
1:A:94:LEU:HD21	1:A:119:ASP:HB2	1.94	0.49
1:B:48:ILE:HG23	9:B:9710:HOH:O	2.12	0.49
2:C:84:ARG:HH11	2:C:84:ARG:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:PRO:C	2:C:276:LYS:HZ2	2.16	0.49
2:C:595:LEU:CD1	2:C:639:GLN:HG2	2.43	0.49
3:D:186:VAL:HG11	3:D:213:VAL:HB	1.94	0.49
3:D:661:MET:CE	3:D:673:ALA:HB1	2.42	0.49
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.95	0.49
3:D:1247:ALA:HB1	9:D:2742:HOH:O	2.13	0.49
3:D:1348:LEU:O	3:D:1352:ILE:HG13	2.13	0.49
3:D:1465:ASN:OD1	3:D:1470:ARG:HB3	2.12	0.49
4:E:30:LEU:O	4:E:35:PHE:HA	2.12	0.49
5:F:152:ASP:HB2	5:F:153:PRO:HD3	1.94	0.49
5:F:419:ARG:HG2	5:F:419:ARG:HH11	1.76	0.49
1:L:62:LEU:HD12	1:L:62:LEU:H	1.78	0.49
2:M:288:ARG:HB3	9:M:9500:HOH:O	2.12	0.49
2:M:657:ASP:HB3	2:M:661:SER:OG	2.13	0.49
2:M:696:LYS:HA	9:M:9665:HOH:O	2.12	0.49
2:M:841:ASN:OD1	2:M:843:HIS:HB2	2.13	0.49
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.95	0.49
3:N:141:ILE:H	3:N:141:ILE:CD1	2.24	0.49
3:N:413:ASP:OD2	3:N:419:ASP:HA	2.13	0.49
3:N:1282:ARG:HG2	9:N:9906:HOH:O	2.12	0.49
3:N:1287:GLU:HA	9:N:9764:HOH:O	2.12	0.49
3:N:1437:ALA:HB2	9:N:9283:HOH:O	2.11	0.49
5:P:77:THR:O	5:P:80:PRO:HG2	2.13	0.49
5:P:198:ILE:HG12	5:P:244:ARG:HH12	1.78	0.49
5:P:375:LEU:HG	9:P:3218:HOH:O	2.13	0.49
1:A:34:VAL:HA	9:A:9604:HOH:O	2.12	0.48
1:B:162:ILE:HG13	9:B:9680:HOH:O	2.13	0.48
2:C:216:GLU:H	2:C:216:GLU:CD	2.16	0.48
3:D:145:VAL:HG21	9:D:9785:HOH:O	2.13	0.48
3:D:729:HIS:ND1	3:D:730:PRO:N	2.61	0.48
3:D:1148:VAL:HG11	3:D:1203:LYS:HD2	1.95	0.48
3:D:1304:LYS:HD3	3:D:1304:LYS:N	2.16	0.48
3:D:1336:LEU:HD13	3:D:1376:MET:HE1	1.95	0.48
1:K:186:LEU:HB2	1:K:192:LEU:CD1	2.43	0.48
2:M:100:LEU:HG	2:M:368:THR:HG23	1.94	0.48
2:M:144:PRO:HA	2:M:163:ILE:O	2.13	0.48
2:M:254:VAL:HG12	9:M:2026:HOH:O	2.12	0.48
2:M:534:VAL:H	2:M:538:GLN:NE2	2.11	0.48
2:M:570:PRO:HB3	2:M:660:ALA:HB2	1.94	0.48
2:M:575:GLN:HG2	2:M:671:ASN:ND2	2.27	0.48
3:N:806:PHE:CE1	3:N:813:LEU:HB3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1120:VAL:HA	3:N:1346:ARG:HH22	1.78	0.48
3:N:1282:ARG:HB2	3:N:1293:PHE:HB2	1.95	0.48
9:N:9359:HOH:O	4:O:50:THR:HG21	2.12	0.48
1:B:23:PHE:O	1:B:196:THR:HA	2.12	0.48
1:B:159:LYS:HE3	9:B:9720:HOH:O	2.14	0.48
2:C:164:PRO:HD2	2:C:170:PRO:O	2.13	0.48
2:C:266:ARG:O	2:C:288:ARG:HD3	2.13	0.48
2:C:428:ARG:HA	2:C:450:GLY:HA3	1.94	0.48
2:C:574:ALA:O	2:C:575:GLN:HB2	2.12	0.48
2:C:877:PRO:HB3	3:D:1020:LEU:CD1	2.43	0.48
3:D:169:TYR:CG	3:D:169:TYR:O	2.67	0.48
3:D:235:ALA:HB1	9:D:9573:HOH:O	2.13	0.48
3:D:873:LEU:HA	9:D:2884:HOH:O	2.12	0.48
4:E:8:LYS:HD3	9:E:9637:HOH:O	2.13	0.48
5:F:115:LYS:HD3	5:F:173:TYR:CE2	2.48	0.48
5:F:139:ALA:HB1	5:F:152:ASP:HB3	1.94	0.48
1:L:119:ASP:HB3	9:L:1485:HOH:O	2.12	0.48
1:L:229:GLN:HG2	9:L:6318:HOH:O	2.13	0.48
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.48	0.48
2:M:269:LEU:HB3	9:M:9569:HOH:O	2.13	0.48
2:M:446:GLY:O	2:M:449:ILE:HG13	2.12	0.48
2:M:736:ASP:HA	2:M:744:ARG:NH1	2.28	0.48
3:N:422:ALA:H	3:N:427:VAL:HG11	1.77	0.48
3:N:493:ARG:NH2	3:N:1389:LEU:HD11	2.28	0.48
3:N:704:ARG:HH12	3:N:743:ASP:CG	2.16	0.48
3:N:863:VAL:HG12	9:N:9938:HOH:O	2.12	0.48
3:N:983:LEU:HA	3:N:987:GLU:OE2	2.12	0.48
3:N:1049:SER:OG	3:N:1051:GLU:HG2	2.14	0.48
5:P:185:GLN:O	5:P:189:GLU:HG3	2.13	0.48
2:C:42:VAL:HG12	2:C:43:GLY:N	2.24	0.48
2:C:114:PHE:CE2	5:F:283:GLY:HA3	2.48	0.48
2:C:722:ILE:HG22	9:C:2273:HOH:O	2.13	0.48
9:C:2198:HOH:O	5:F:350:LEU:HD21	2.12	0.48
3:D:618:LEU:HD21	9:D:2041:HOH:O	2.14	0.48
3:D:649:ALA:CB	3:D:691:LEU:HD21	2.43	0.48
3:D:754:PHE:O	3:D:757:ALA:HB3	2.13	0.48
3:D:786:ILE:HD13	3:D:1027:GLY:HA3	1.94	0.48
5:F:300:ASP:HB2	9:F:9768:HOH:O	2.13	0.48
5:F:371:LEU:HA	5:F:375:LEU:HB2	1.95	0.48
1:K:65:PHE:HE1	2:M:799:ILE:HD11	1.78	0.48
2:M:189:ARG:HH21	2:M:243:ARG:CZ	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:261:ILE:CG2	2:M:262:ALA:H	2.26	0.48
2:M:343:GLN:HB2	9:M:2031:HOH:O	2.13	0.48
2:M:549:PHE:HB3	2:M:552:HIS:CD2	2.48	0.48
2:M:631:SER:HG	2:M:635:THR:N	2.11	0.48
2:M:1065:ALA:HB1	2:M:1077:PRO:HG2	1.96	0.48
3:N:55:ASP:HA	3:N:82:LYS:HG2	1.94	0.48
3:N:869:MET:HA	9:N:2163:HOH:O	2.14	0.48
3:N:959:GLU:HG3	3:N:1006:ALA:HB1	1.95	0.48
3:N:1087:ARG:HE	3:N:1238:MET:HB2	1.77	0.48
3:N:1147:ARG:HB3	3:N:1188:VAL:CG2	2.42	0.48
3:N:1276:GLU:HG3	3:N:1303:TYR:OH	2.13	0.48
1:B:1:MET:O	1:B:6:LEU:HD22	2.13	0.48
2:C:328:LEU:HB2	2:C:433:THR:HG21	1.95	0.48
2:C:572:ILE:HD11	2:C:698:ASP:HB3	1.94	0.48
2:C:807:ARG:HD2	9:C:2355:HOH:O	2.12	0.48
3:D:2:LYS:HB3	9:D:9972:HOH:O	2.12	0.48
3:D:882:PHE:HA	3:D:885:ILE:HD12	1.95	0.48
3:D:1058:ARG:HG3	3:D:1058:ARG:NH1	2.28	0.48
3:D:1117:TYR:HB3	9:D:9720:HOH:O	2.12	0.48
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.13	0.48
3:D:1463:LYS:HG2	9:D:2672:HOH:O	2.12	0.48
4:E:23:VAL:HG23	4:E:64:ALA:HB3	1.94	0.48
5:F:169:GLU:CD	5:F:169:GLU:H	2.15	0.48
2:M:48:PHE:CD2	2:M:52:PHE:HE2	2.31	0.48
2:M:52:PHE:HE1	2:M:98:LEU:HD21	1.78	0.48
2:M:226:VAL:HG13	2:M:227:PHE:CD2	2.48	0.48
2:M:722:ILE:HG21	2:M:821:GLU:OE2	2.13	0.48
2:M:753:ASP:HA	3:N:679:ARG:HD2	1.95	0.48
3:N:104:PHE:CE2	3:N:1448:THR:HG23	2.48	0.48
3:N:416:ALA:H	3:N:417:PRO:CD	2.26	0.48
3:N:557:LEU:HD11	9:P:1239:HOH:O	2.13	0.48
3:N:829:VAL:HB	9:N:9280:HOH:O	2.12	0.48
3:N:1058:ARG:HG2	9:N:9994:HOH:O	2.12	0.48
3:N:1382:THR:HA	9:N:9517:HOH:O	2.12	0.48
4:O:50:THR:HG23	9:O:1048:HOH:O	2.13	0.48
5:P:155:THR:O	5:P:159:ILE:HG13	2.14	0.48
5:P:288:TYR:H	5:P:288:TYR:HD1	1.60	0.48
2:C:204:GLN:HA	9:C:9805:HOH:O	2.12	0.48
2:C:803:THR:HG22	2:C:825:VAL:HG22	1.95	0.48
3:D:984:THR:HG22	3:D:987:GLU:H	1.79	0.48
3:D:1413:THR:HA	9:D:9958:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:14:ASP:HA	9:E:9592:HOH:O	2.13	0.48
5:F:271:LEU:HD21	5:F:299:TRP:CZ3	2.48	0.48
1:K:227:ASN:H	1:K:227:ASN:ND2	2.12	0.48
2:M:149:THR:HG22	9:M:9475:HOH:O	2.12	0.48
2:M:165:LEU:HD22	9:M:9925:HOH:O	2.13	0.48
2:M:381:ALA:HB1	9:M:9341:HOH:O	2.12	0.48
2:M:455:LEU:HD22	2:M:459:ALA:CB	2.44	0.48
2:M:551:GLU:CD	2:M:551:GLU:H	2.16	0.48
2:M:597:ALA:HA	9:M:9794:HOH:O	2.13	0.48
2:M:643:VAL:HG23	9:M:9275:HOH:O	2.12	0.48
3:N:64:LYS:HZ3	5:P:377:ASP:HA	1.78	0.48
3:N:200:ASP:HA	9:N:2149:HOH:O	2.13	0.48
3:N:561:GLY:HA3	9:N:9263:HOH:O	2.13	0.48
3:N:860:LEU:HB2	3:N:861:GLN:HE22	1.77	0.48
3:N:1147:ARG:HD2	3:N:1188:VAL:HG21	1.95	0.48
3:N:1440:PHE:O	3:N:1443:THR:HG23	2.13	0.48
4:O:45:ARG:HA	9:O:6351:HOH:O	2.13	0.48
5:P:94:LEU:HB3	5:P:98:GLU:HB2	1.95	0.48
5:P:147:LEU:HD13	9:P:1942:HOH:O	2.13	0.48
5:P:163:LEU:HD13	5:P:174:LEU:CD2	2.43	0.48
2:C:683:ASN:OD1	2:C:872:ASN:HB2	2.14	0.48
3:D:149:LYS:HB3	9:D:2253:HOH:O	2.13	0.48
3:D:177:ALA:C	3:D:199:LEU:HD13	2.32	0.48
3:D:218:LYS:N	9:D:9726:HOH:O	2.45	0.48
3:D:396:VAL:HG13	3:D:447:VAL:HA	1.96	0.48
3:D:500:ARG:NH2	3:D:1388:ARG:NE	2.57	0.48
3:D:845:ASN:O	3:D:848:GLU:HB2	2.14	0.48
3:D:1038:LEU:HA	3:D:1061:PHE:HB2	1.95	0.48
3:D:1188:VAL:HG11	9:D:9650:HOH:O	2.14	0.48
3:D:1314:LYS:HD3	3:D:1314:LYS:H	1.77	0.48
3:D:1354:LYS:HA	9:D:2684:HOH:O	2.13	0.48
3:D:1435:LEU:HG	3:D:1467:ILE:HD12	1.95	0.48
1:L:6:LEU:C	1:L:8:ALA:H	2.17	0.48
2:M:142:ARG:HB2	2:M:163:ILE:HD13	1.95	0.48
2:M:490:GLU:O	2:M:493:ARG:HB2	2.14	0.48
2:M:978:ARG:HH11	2:M:978:ARG:HG3	1.79	0.48
2:M:1067:TYR:HE1	3:N:655:PRO:HG3	1.77	0.48
3:N:2:LYS:HG2	3:N:3:LYS:NZ	2.28	0.48
3:N:500:ARG:HH11	3:N:500:ARG:HG3	1.78	0.48
3:N:549:ASN:ND2	5:P:254:GLN:NE2	2.62	0.48
3:N:861:GLN:CD	3:N:861:GLN:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:962:GLN:O	3:N:966:GLU:HG3	2.14	0.48
3:N:1047:LYS:HD2	3:N:1051:GLU:HG3	1.95	0.48
5:P:96:LEU:HD12	9:P:1515:HOH:O	2.12	0.48
1:A:65:PHE:CZ	2:C:830:LYS:HG3	2.49	0.48
1:A:143:ARG:CD	1:A:158:ILE:HG21	2.44	0.48
1:B:36:LEU:O	1:B:39:PRO:HD2	2.13	0.48
2:C:12:VAL:HA	9:C:2815:HOH:O	2.14	0.48
2:C:87:ASP:HB2	9:C:9712:HOH:O	2.13	0.48
2:C:244:PRO:HG2	2:C:246:ASP:OD1	2.13	0.48
2:C:341:THR:HG21	9:C:9696:HOH:O	2.13	0.48
2:C:404:LEU:HD12	2:C:407:LYS:HE2	1.95	0.48
3:D:562:ALA:HB1	3:D:567:ILE:CD1	2.39	0.48
3:D:699:VAL:H	3:D:756:GLN:HE22	1.62	0.48
3:D:800:LYS:HE2	3:D:830:ALA:CB	2.43	0.48
3:D:830:ALA:HB1	9:D:2375:HOH:O	2.14	0.48
3:D:864:VAL:HG12	3:D:865:THR:N	2.28	0.48
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.49	0.48
3:D:1114:THR:CG2	3:D:1195:GLN:HB2	2.44	0.48
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.96	0.48
3:D:1281:VAL:HG21	3:D:1313:VAL:CG2	2.44	0.48
4:E:40:LEU:HD12	4:E:40:LEU:O	2.13	0.48
5:F:236:SER:HA	9:F:9646:HOH:O	2.14	0.48
1:L:107:LYS:HB2	9:L:1363:HOH:O	2.14	0.48
1:L:182:GLU:HB2	9:L:8791:HOH:O	2.14	0.48
2:M:69:LEU:HB2	2:M:97:ARG:CB	2.44	0.48
2:M:295:ASP:C	2:M:297:GLU:H	2.16	0.48
2:M:300:ASP:OD2	2:M:303:PHE:HB2	2.13	0.48
2:M:333:ILE:HG22	2:M:465:GLY:HA2	1.95	0.48
2:M:334:ARG:HB3	9:M:9771:HOH:O	2.12	0.48
2:M:712:ALA:HB3	2:M:821:GLU:HG3	1.95	0.48
3:N:87:ARG:HD2	3:N:524:LEU:HD23	1.96	0.48
3:N:166:GLN:HB3	3:N:395:VAL:CG2	2.43	0.48
3:N:588:GLY:HA2	9:N:9647:HOH:O	2.13	0.48
3:N:630:VAL:HG12	3:N:631:ILE:N	2.27	0.48
3:N:1243:THR:O	3:N:1269:LYS:HG3	2.12	0.48
3:N:1333:HIS:O	3:N:1336:LEU:HB3	2.14	0.48
3:N:1425:THR:HG22	3:N:1429:LEU:HD22	1.96	0.48
3:N:1449:GLU:HG3	9:N:9417:HOH:O	2.13	0.48
5:P:148:LYS:HB2	5:P:148:LYS:NZ	2.28	0.48
1:A:127:LEU:HD12	1:A:128:HIS:N	2.29	0.48
2:C:443:THR:HG21	3:D:1078:ARG:HE	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:958:THR:HG23	2:C:961:GLU:H	1.78	0.48
3:D:54:LYS:HD3	3:D:55:ASP:OD1	2.14	0.48
3:D:162:ARG:CZ	3:D:162:ARG:HB2	2.43	0.48
3:D:162:ARG:HB3	9:D:9697:HOH:O	2.13	0.48
3:D:524:LEU:C	3:D:526:PRO:HD3	2.34	0.48
3:D:556:LYS:HB3	9:F:9588:HOH:O	2.12	0.48
3:D:702:LEU:O	3:D:713:ILE:HA	2.14	0.48
3:D:966:GLU:HG3	3:D:969:ARG:NH2	2.28	0.48
3:D:1263:PHE:O	3:D:1424:VAL:HG23	2.13	0.48
3:D:1372:VAL:O	3:D:1375:MET:HB2	2.13	0.48
5:F:393:THR:HG22	5:F:394:ARG:N	2.27	0.48
5:F:421:PHE:C	5:F:423:ASP:H	2.16	0.48
1:K:178:ALA:HB2	2:M:864:GLY:H	1.78	0.48
1:K:183:ASP:OD1	2:M:938:LYS:HE3	2.14	0.48
1:K:198:ARG:HD3	1:K:200:TRP:HH2	1.79	0.48
1:L:56:VAL:HB	1:L:165:ILE:HD11	1.94	0.48
2:M:334:ARG:HD2	9:M:9389:HOH:O	2.13	0.48
2:M:769:PRO:HD3	9:M:2572:HOH:O	2.13	0.48
2:M:929:ARG:NH2	9:M:2113:HOH:O	2.45	0.48
2:M:976:ASP:HB3	2:M:979:THR:HG22	1.94	0.48
3:N:202:VAL:HG11	9:N:9932:HOH:O	2.13	0.48
3:N:399:ARG:HB2	3:N:444:VAL:HG13	1.96	0.48
3:N:502:PHE:CE2	3:N:1452:ILE:HG13	2.49	0.48
3:N:813:LEU:HD12	3:N:814:ALA:N	2.29	0.48
3:N:959:GLU:HB2	3:N:963:TYR:CE2	2.49	0.48
3:N:1213:ARG:HB2	3:N:1214:PRO:CD	2.44	0.48
3:N:1376:MET:HB3	9:N:9377:HOH:O	2.13	0.48
5:P:158:GLU:HA	5:P:161:GLN:HG3	1.95	0.48
2:C:92:ALA:O	2:C:118:ILE:HD13	2.14	0.48
2:C:165:LEU:HD12	2:C:166:PRO:HA	1.95	0.48
2:C:309:TYR:HA	2:C:312:ALA:HB3	1.95	0.48
2:C:882:LEU:HD12	3:D:1061:PHE:HB3	1.95	0.48
2:C:1095:LEU:HD11	3:D:603:LEU:HB3	1.95	0.48
3:D:18:ILE:HD12	3:D:518:PRO:HG3	1.96	0.48
3:D:988:ARG:HB3	9:D:9919:HOH:O	2.14	0.48
3:D:1339:LYS:HD2	9:D:2575:HOH:O	2.14	0.48
5:F:80:PRO:HA	5:F:83:GLN:HB3	1.94	0.48
5:F:299:TRP:CD2	5:F:303:ARG:HD3	2.49	0.48
1:K:6:LEU:C	1:K:8:ALA:H	2.17	0.48
1:K:89:PHE:HZ	1:K:144:VAL:HG12	1.79	0.48
2:M:190:LYS:NZ	9:M:9816:HOH:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:983:ILE:HD12	2:M:987:ILE:HD12	1.94	0.48
2:M:1004:LYS:HE3	2:M:1027:PHE:CE1	2.48	0.48
3:N:137:PRO:HB2	9:N:9902:HOH:O	2.13	0.48
3:N:142:LEU:HA	9:N:9368:HOH:O	2.14	0.48
3:N:181:ASP:O	3:N:185:VAL:HG23	2.14	0.48
3:N:826:PRO:HD2	3:N:829:VAL:HG22	1.96	0.48
3:N:1046:GLN:N	9:N:9308:HOH:O	2.43	0.48
3:N:1478:SER:C	3:N:1480:PHE:N	2.67	0.48
5:P:416:ARG:NH1	5:P:419:ARG:HD3	2.29	0.48
9:A:9662:HOH:O	2:C:645:VAL:HG21	2.14	0.48
1:B:47:SER:O	1:B:49:PRO:N	2.47	0.48
1:B:220:GLU:HB3	9:B:9783:HOH:O	2.14	0.48
2:C:68:PHE:HZ	2:C:71:TYR:HD2	1.61	0.48
2:C:369:PRO:HG2	2:C:370:ALA:H	1.78	0.48
2:C:751:PRO:HA	2:C:792:VAL:CG1	2.44	0.48
2:C:1072:LYS:HE2	9:C:2855:HOH:O	2.14	0.48
2:C:1081:VAL:HB	2:C:1086:ARG:HE	1.79	0.48
9:C:9793:HOH:O	3:D:21:TRP:HB3	2.13	0.48
3:D:179:VAL:HG21	9:D:9579:HOH:O	2.13	0.48
3:D:957:PRO:HG2	3:D:1007:VAL:CA	2.42	0.48
4:E:81:PRO:HA	9:E:9589:HOH:O	2.14	0.48
5:F:260:ILE:HD11	5:F:264:MET:HB3	1.96	0.48
1:L:156:HIS:CD2	1:L:158:ILE:HG12	2.49	0.48
2:M:292:ARG:HB2	2:M:299:LYS:NZ	2.28	0.48
2:M:892:LEU:HD21	2:M:967:PHE:CE1	2.48	0.48
3:N:584:ASN:H	3:N:602:SER:HB3	1.79	0.48
3:N:834:THR:HG22	3:N:838:ARG:NE	2.28	0.48
3:N:1156:LEU:HD23	3:N:1182:GLU:OE1	2.13	0.48
3:N:1168:MET:HE2	9:N:9270:HOH:O	2.14	0.48
3:N:1380:GLU:HG2	3:N:1381:VAL:N	2.28	0.48
3:N:1415:VAL:HG23	9:N:9894:HOH:O	2.14	0.48
2:C:13:ILE:HD13	2:C:483:VAL:HG11	1.95	0.47
2:C:56:GLU:HG2	9:C:2542:HOH:O	2.13	0.47
2:C:130:ASN:HB3	9:C:9665:HOH:O	2.12	0.47
2:C:762:LYS:HD3	2:C:771:GLU:OE2	2.13	0.47
2:C:1115:LEU:HD22	3:D:88:TYR:CD1	2.47	0.47
3:D:62:LYS:HD3	9:D:2796:HOH:O	2.13	0.47
3:D:86:ARG:HG2	3:D:523:ASP:OD1	2.14	0.47
3:D:154:THR:HG22	9:D:9682:HOH:O	2.14	0.47
3:D:795:VAL:HG13	3:D:863:VAL:HG22	1.96	0.47
5:F:220:LEU:O	5:F:224:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:67:ASP:HA	9:M:9629:HOH:O	2.12	0.47
2:M:302:VAL:O	2:M:306:THR:HG23	2.14	0.47
2:M:397:GLU:H	2:M:633:GLN:HE22	1.62	0.47
2:M:859:PRO:O	2:M:867:VAL:HG22	2.14	0.47
2:M:1005:MET:HG2	9:M:9335:HOH:O	2.14	0.47
3:N:8:VAL:HG23	9:N:9608:HOH:O	2.13	0.47
3:N:71:LYS:HE3	9:N:2288:HOH:O	2.13	0.47
3:N:965:GLU:HB3	9:N:9892:HOH:O	2.14	0.47
3:N:984:THR:HG23	3:N:986:ARG:N	2.29	0.47
3:N:1147:ARG:NH2	9:N:9659:HOH:O	2.47	0.47
5:P:352:GLU:HG2	9:P:6518:HOH:O	2.14	0.47
5:P:400:ILE:HG12	9:P:1779:HOH:O	2.13	0.47
1:A:91:ASN:HA	9:A:9714:HOH:O	2.13	0.47
1:B:9:PRO:HB3	1:B:25:LEU:CG	2.44	0.47
2:C:18:LEU:HD12	2:C:18:LEU:N	2.28	0.47
2:C:91:GLN:HG2	2:C:119:PRO:HG3	1.96	0.47
3:D:119:SER:N	3:D:123:LEU:HD13	2.28	0.47
3:D:542:ASP:O	3:D:546:ARG:HG2	2.13	0.47
3:D:827:ILE:HG12	9:D:2351:HOH:O	2.14	0.47
3:D:1036:ARG:HG2	9:D:9667:HOH:O	2.15	0.47
3:D:1133:ARG:NH2	9:D:9997:HOH:O	2.47	0.47
3:D:1236:LEU:HD22	3:D:1355:VAL:HG12	1.96	0.47
3:D:1240:THR:O	3:D:1257:PRO:HB3	2.13	0.47
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.44	0.47
4:E:81:PRO:HD3	9:E:9619:HOH:O	2.13	0.47
4:E:96:GLU:HA	9:E:9628:HOH:O	2.12	0.47
5:F:270:LYS:HE3	9:F:9917:HOH:O	2.13	0.47
2:M:92:ALA:HB1	9:M:9468:HOH:O	2.13	0.47
2:M:141:HIS:HB2	2:M:418:LEU:HD12	1.94	0.47
2:M:324:ASP:HB3	2:M:327:HIS:CD2	2.40	0.47
2:M:503:LEU:HD12	2:M:505:GLY:O	2.14	0.47
2:M:644:VAL:HG22	2:M:647:GLN:NE2	2.29	0.47
2:M:679:PHE:CD1	2:M:870:ILE:HD13	2.48	0.47
2:M:879:ARG:HD2	2:M:879:ARG:H	1.78	0.47
3:N:12:LEU:HB2	9:N:9257:HOH:O	2.13	0.47
3:N:448:GLU:CD	3:N:448:GLU:N	2.67	0.47
3:N:496:LEU:HG	3:N:500:ARG:HG2	1.96	0.47
3:N:706:PRO:HG2	9:N:9369:HOH:O	2.13	0.47
3:N:907:GLU:O	3:N:911:LEU:HD13	2.13	0.47
3:N:920:LEU:HA	9:N:2152:HOH:O	2.13	0.47
3:N:1197:ARG:HD3	9:N:9581:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1311:LEU:H	3:N:1311:LEU:CD2	2.24	0.47
3:N:1435:LEU:HB2	9:N:9646:HOH:O	2.15	0.47
5:P:131:VAL:O	5:P:135:ILE:HG12	2.14	0.47
1:A:64:GLU:OE2	1:A:76:VAL:HG13	2.14	0.47
2:C:365:ASP:C	2:C:367:LEU:HD23	2.34	0.47
2:C:724:ARG:HD3	2:C:740:GLU:HA	1.96	0.47
2:C:831:ARG:HH21	2:C:999:HIS:HB2	1.78	0.47
3:D:488:ARG:HB3	3:D:488:ARG:CZ	2.44	0.47
3:D:523:ASP:HB3	9:D:2189:HOH:O	2.13	0.47
3:D:894:LYS:O	3:D:898:GLU:HG3	2.13	0.47
3:D:983:LEU:HA	3:D:987:GLU:OE2	2.14	0.47
3:D:1092:GLY:O	3:D:1096:ARG:N	2.42	0.47
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.44	0.47
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.15	0.47
3:D:1493:LYS:HD3	9:D:9925:HOH:O	2.14	0.47
1:L:96:THR:HB	1:L:145:ASP:OD2	2.13	0.47
2:M:506:ASN:HB2	9:M:9830:HOH:O	2.13	0.47
2:M:516:ARG:NH2	3:N:1068:LEU:HB2	2.28	0.47
2:M:926:PHE:O	2:M:929:ARG:HB2	2.14	0.47
3:N:76:CYS:HA	9:N:9585:HOH:O	2.14	0.47
3:N:441:ARG:HA	3:N:441:ARG:HE	1.79	0.47
3:N:799:LYS:HG2	9:N:9312:HOH:O	2.14	0.47
3:N:1191:PRO:HD3	3:N:1204:CYS:O	2.13	0.47
3:N:1253:THR:HG23	3:N:1258:ARG:HH11	1.79	0.47
5:P:257:THR:HB	5:P:314:PRO:HG3	1.97	0.47
1:A:140:MET:HA	9:A:9798:HOH:O	2.14	0.47
1:B:162:ILE:HG21	9:B:9631:HOH:O	2.14	0.47
2:C:34:VAL:HG22	9:C:9698:HOH:O	2.14	0.47
2:C:291:ALA:O	2:C:292:ARG:HB2	2.14	0.47
2:C:721:ARG:HD3	9:C:9781:HOH:O	2.14	0.47
2:C:971:LYS:NZ	9:C:9615:HOH:O	2.47	0.47
2:C:1105:LYS:O	2:C:1107:ASN:N	2.48	0.47
3:D:796:ARG:NH1	3:D:861:GLN:HB2	2.30	0.47
3:D:1044:LEU:HB2	9:D:2029:HOH:O	2.14	0.47
3:D:1307:LYS:HG2	9:D:2092:HOH:O	2.14	0.47
3:D:1379:VAL:HG11	3:D:1395:LEU:HD23	1.96	0.47
4:E:47:LYS:CA	4:E:54:LEU:HB3	2.45	0.47
4:E:51:LEU:C	4:E:53:GLY:H	2.16	0.47
5:F:104:ARG:HG3	5:F:229:TYR:OH	2.15	0.47
5:F:215:GLU:O	5:F:218:GLN:HB3	2.15	0.47
5:F:325:LYS:HB2	9:F:9915:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:173:PRO:HB2	1:K:205:VAL:HG22	1.96	0.47
1:L:8:ALA:HA	9:L:1271:HOH:O	2.14	0.47
1:L:23:PHE:O	1:L:196:THR:HA	2.13	0.47
1:L:115:LEU:HD12	1:L:115:LEU:O	2.14	0.47
1:L:169:ALA:HA	9:L:1542:HOH:O	2.15	0.47
1:L:201:THR:HG22	1:L:203:GLY:H	1.79	0.47
2:M:254:VAL:HG13	2:M:258:TYR:CE1	2.48	0.47
2:M:313:LEU:HD13	2:M:321:GLU:O	2.15	0.47
2:M:325:ILE:HG21	9:M:2230:HOH:O	2.15	0.47
2:M:607:ASP:C	2:M:609:ASN:H	2.17	0.47
2:M:965:GLU:HG2	9:M:9258:HOH:O	2.15	0.47
9:M:9660:HOH:O	3:N:20:SER:HA	2.13	0.47
3:N:74:GLU:HG2	9:N:2213:HOH:O	2.12	0.47
3:N:523:ASP:O	3:N:526:PRO:HG3	2.14	0.47
3:N:845:ASN:H	3:N:848:GLU:HG3	1.78	0.47
3:N:1360:GLY:HA3	9:N:9449:HOH:O	2.14	0.47
4:O:47:LYS:O	4:O:54:LEU:HD13	2.14	0.47
5:P:209:PHE:CZ	5:P:213:ILE:HD11	2.49	0.47
5:P:353:GLU:CG	5:P:417:LYS:HB3	2.44	0.47
1:A:88:ARG:HD2	1:A:123:MET:HE2	1.96	0.47
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.35	0.47
1:A:193:ASP:OD2	2:C:938:LYS:HD2	2.14	0.47
1:B:105:GLY:HA3	9:B:9797:HOH:O	2.14	0.47
1:B:206:THR:HG22	1:B:209:GLU:HG3	1.95	0.47
9:C:9757:HOH:O	3:D:948:THR:HG21	2.13	0.47
3:D:79:GLU:HG2	3:D:80:VAL:N	2.29	0.47
3:D:928:ALA:O	3:D:931:LEU:HB2	2.14	0.47
4:E:82:GLU:HG2	4:E:83:ASP:H	1.80	0.47
1:L:133:GLU:HG3	1:L:134:GLU:H	1.80	0.47
2:M:164:PRO:HA	2:M:266:ARG:CZ	2.44	0.47
2:M:164:PRO:CA	2:M:266:ARG:HH12	2.23	0.47
2:M:926:PHE:HE1	9:M:2113:HOH:O	1.97	0.47
3:N:136:ASP:CG	3:N:137:PRO:HD3	2.35	0.47
3:N:396:VAL:HG22	3:N:447:VAL:HB	1.97	0.47
3:N:704:ARG:HG2	9:N:9228:HOH:O	2.13	0.47
3:N:734:GLU:HB3	9:N:9236:HOH:O	2.14	0.47
3:N:809:PRO:O	3:N:812:ALA:HB3	2.15	0.47
3:N:969:ARG:HD3	9:N:9710:HOH:O	2.13	0.47
3:N:1046:GLN:HG2	9:N:9308:HOH:O	2.13	0.47
3:N:1086:LEU:HD22	9:N:9961:HOH:O	2.14	0.47
4:O:41:GLU:HB3	4:O:42:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLU:O	1:A:110:LYS:HG3	2.15	0.47
1:A:228:PRO:HG3	9:A:9640:HOH:O	2.14	0.47
2:C:507:ARG:HG2	2:C:508:ILE:O	2.14	0.47
2:C:551:GLU:HB3	2:C:906:PHE:CD2	2.49	0.47
2:C:728:HIS:C	2:C:729:LEU:HD22	2.35	0.47
3:D:809:PRO:HB2	3:D:812:ALA:HB2	1.97	0.47
3:D:1194:CYS:HB3	3:D:1373:ARG:NH2	2.29	0.47
3:D:1210:SER:HA	9:D:2674:HOH:O	2.13	0.47
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.96	0.47
3:D:1263:PHE:CE1	3:D:1352:ILE:HD13	2.50	0.47
3:D:1353:GLN:O	3:D:1357:ARG:HD2	2.14	0.47
3:D:1487:VAL:HG12	3:D:1488:ASP:H	1.78	0.47
2:M:91:GLN:HA	2:M:119:PRO:HA	1.95	0.47
2:M:298:PHE:HB2	9:M:2564:HOH:O	2.13	0.47
2:M:344:PHE:O	2:M:348:LEU:HD13	2.14	0.47
2:M:403:SER:C	2:M:407:LYS:HE2	2.35	0.47
2:M:444:PRO:HG2	2:M:452:ILE:CD1	2.45	0.47
2:M:910:LYS:HB2	9:M:2099:HOH:O	2.14	0.47
2:M:939:ARG:HD2	9:M:9308:HOH:O	2.14	0.47
3:N:62:LYS:HE2	9:N:2079:HOH:O	2.15	0.47
3:N:98:PRO:HG3	3:N:515:GLU:CB	2.37	0.47
3:N:123:LEU:HD11	3:N:152:LEU:CD2	2.45	0.47
3:N:463:GLN:HB3	9:N:9580:HOH:O	2.14	0.47
3:N:836:VAL:HG12	9:N:9618:HOH:O	2.14	0.47
3:N:1161:GLU:HG2	3:N:1164:ARG:HB2	1.95	0.47
3:N:1274:ILE:HB	3:N:1322:GLY:HA2	1.97	0.47
3:N:1396:GLU:HA	3:N:1399:ASP:OD2	2.14	0.47
4:O:30:LEU:O	4:O:35:PHE:HA	2.15	0.47
5:P:161:GLN:HA	5:P:164:LYS:HD2	1.96	0.47
5:P:402:ASN:O	5:P:406:ARG:HD2	2.15	0.47
1:A:74:ASP:O	1:A:78:ILE:HG13	2.15	0.47
1:A:176:ARG:HA	9:A:9583:HOH:O	2.14	0.47
1:B:41:ARG:HG3	1:B:177:VAL:HB	1.95	0.47
1:B:109:VAL:HG23	1:B:132:LEU:HD13	1.96	0.47
2:C:73:LEU:HD12	2:C:73:LEU:N	2.29	0.47
2:C:73:LEU:HD11	2:C:94:LEU:HD13	1.96	0.47
2:C:250:ARG:HH21	2:C:254:VAL:HB	1.79	0.47
2:C:253:ALA:O	2:C:256:TYR:HB2	2.15	0.47
2:C:334:ARG:HA	2:C:338:GLU:OE2	2.15	0.47
2:C:346:VAL:O	2:C:350:ARG:HG3	2.15	0.47
2:C:403:SER:C	2:C:407:LYS:HD3	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:408:ARG:HD2	2:C:542:VAL:CG2	2.44	0.47
2:C:458:TYR:O	2:C:460:ARG:HD2	2.14	0.47
2:C:524:VAL:HG22	2:C:528:GLU:HB2	1.96	0.47
2:C:536:PRO:HD2	2:C:537:LYS:HZ1	1.80	0.47
2:C:603:VAL:O	2:C:646:GLY:HA2	2.15	0.47
2:C:953:VAL:HB	2:C:962:GLN:CG	2.45	0.47
2:C:987:ILE:HD11	3:D:946:GLY:HA2	1.96	0.47
2:C:988:VAL:N	9:C:9757:HOH:O	2.46	0.47
2:C:1005:MET:SD	3:D:648:MET:HB2	2.55	0.47
2:C:1072:LYS:HD3	9:C:9670:HOH:O	2.14	0.47
3:D:50:PHE:HB3	3:D:522:PRO:HG2	1.97	0.47
3:D:60:CYS:SG	3:D:62:LYS:HG2	2.54	0.47
3:D:393:ILE:H	3:D:393:ILE:HG13	1.53	0.47
3:D:523:ASP:O	3:D:526:PRO:HG3	2.14	0.47
3:D:579:ASP:HB2	9:D:9699:HOH:O	2.14	0.47
3:D:613:ARG:HA	9:D:9688:HOH:O	2.15	0.47
3:D:646:LYS:HG3	3:D:647:ARG:N	2.29	0.47
3:D:804:LEU:HD21	3:D:829:VAL:CG2	2.42	0.47
3:D:838:ARG:HH12	3:D:863:VAL:CG1	2.27	0.47
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.49	0.47
3:D:893:GLU:O	3:D:896:ALA:HB3	2.15	0.47
3:D:1084:THR:HG23	9:D:2894:HOH:O	2.13	0.47
3:D:1109:GLU:CD	3:D:1202:GLN:H	2.18	0.47
3:D:1271:LYS:HD2	3:D:1334:GLN:OE1	2.14	0.47
5:F:209:PHE:O	5:F:213:ILE:HG13	2.14	0.47
5:F:226:LYS:HB2	9:F:9706:HOH:O	2.15	0.47
5:F:335:ASP:HB2	9:F:9582:HOH:O	2.15	0.47
1:K:48:ILE:HA	1:K:49:PRO:HD3	1.75	0.47
1:K:108:GLU:O	1:K:110:LYS:HG3	2.14	0.47
2:M:66:LEU:CD1	2:M:98:LEU:HD22	2.45	0.47
2:M:129:ILE:HG12	2:M:134:ARG:HD2	1.95	0.47
2:M:261:ILE:HG22	2:M:262:ALA:N	2.29	0.47
2:M:432:ARG:H	2:M:432:ARG:HD3	1.80	0.47
2:M:586:ARG:HB3	2:M:586:ARG:HH11	1.79	0.47
2:M:799:ILE:HD13	2:M:799:ILE:N	2.30	0.47
3:N:93:ILE:HG12	3:N:548:ILE:HD11	1.97	0.47
3:N:208:PRO:HB2	3:N:395:VAL:HG22	1.95	0.47
3:N:210:ARG:HB3	9:N:9661:HOH:O	2.15	0.47
3:N:400:VAL:HA	3:N:442:ASN:O	2.14	0.47
3:N:754:PHE:O	3:N:757:ALA:HB3	2.15	0.47
3:N:785:ILE:H	3:N:785:ILE:HD12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:840:LYS:HA	9:N:9609:HOH:O	2.14	0.47
3:N:998:GLU:O	3:N:1002:LYS:HG3	2.13	0.47
3:N:1182:GLU:HG3	9:N:9246:HOH:O	2.14	0.47
3:N:1189:ARG:HA	3:N:1189:ARG:HH11	1.80	0.47
3:N:1310:ARG:O	3:N:1327:ARG:HB2	2.15	0.47
3:N:1406:ARG:O	3:N:1406:ARG:HG2	2.15	0.47
4:O:54:LEU:HG	4:O:58:PRO:CG	2.45	0.47
5:P:182:ALA:O	5:P:185:GLN:HB2	2.14	0.47
5:P:257:THR:CB	5:P:314:PRO:HG3	2.45	0.47
5:P:288:TYR:HA	5:P:291:ILE:CG2	2.45	0.47
5:P:396:ARG:HD2	9:P:6184:HOH:O	2.14	0.47
5:P:405:LEU:HD23	9:P:3207:HOH:O	2.13	0.47
5:P:416:ARG:HH11	5:P:419:ARG:HB2	1.80	0.47
1:A:106:PRO:HG3	9:A:9569:HOH:O	2.15	0.47
1:B:192:LEU:HG	9:B:9584:HOH:O	2.15	0.47
2:C:651:LYS:HE3	9:C:2035:HOH:O	2.15	0.47
2:C:749:VAL:HA	9:C:9864:HOH:O	2.15	0.47
2:C:877:PRO:HD3	3:D:949:ILE:CD1	2.44	0.47
2:C:916:GLU:O	2:C:919:ALA:HB3	2.15	0.47
3:D:50:PHE:O	3:D:86:ARG:HA	2.14	0.47
3:D:102:ILE:HD12	3:D:579:ASP:HB3	1.96	0.47
3:D:447:VAL:HG23	9:D:9599:HOH:O	2.14	0.47
3:D:493:ARG:HD3	3:D:1390:LEU:HD21	1.97	0.47
3:D:644:LEU:HD12	3:D:644:LEU:O	2.15	0.47
3:D:959:GLU:HB2	3:D:963:TYR:CE1	2.49	0.47
3:D:1404:ASN:CG	3:D:1408:ILE:HD12	2.35	0.47
3:D:1448:THR:O	3:D:1451:ALA:HB3	2.15	0.47
4:E:48:MET:CB	4:E:54:LEU:HB2	2.39	0.47
5:F:245:GLN:HA	9:F:9828:HOH:O	2.13	0.47
5:F:276:ARG:HB3	9:F:9760:HOH:O	2.15	0.47
5:F:369:LEU:O	5:F:373:LYS:HB2	2.14	0.47
5:F:406:ARG:HA	5:F:409:LYS:CD	2.45	0.47
1:K:45:LEU:HD21	1:K:177:VAL:HG23	1.97	0.47
2:M:47:ALA:HA	2:M:50:GLU:OE2	2.14	0.47
2:M:257:VAL:C	2:M:259:GLY:H	2.18	0.47
2:M:283:ILE:HG12	9:M:9557:HOH:O	2.15	0.47
2:M:625:LEU:HB3	2:M:639:GLN:HB2	1.96	0.47
2:M:1074:GLU:HG3	9:M:2120:HOH:O	2.13	0.47
3:N:17:LYS:HG2	3:N:21:TRP:CE2	2.50	0.47
3:N:445:ARG:HH11	3:N:445:ARG:HG2	1.80	0.47
3:N:704:ARG:HD3	9:N:9228:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:795:VAL:CG1	3:N:863:VAL:HG13	2.44	0.47
3:N:1231:GLU:HB3	3:N:1232:PRO:HD3	1.97	0.47
4:O:9:LEU:HB3	4:O:19:LEU:HD21	1.96	0.47
5:P:284:ARG:HB3	9:P:4605:HOH:O	2.15	0.47
2:C:100:LEU:CD2	2:C:368:THR:HA	2.44	0.47
2:C:165:LEU:HD12	2:C:166:PRO:C	2.36	0.47
2:C:1016:ILE:HD13	2:C:1016:ILE:N	2.29	0.47
2:C:1039:ALA:CB	3:D:713:ILE:HD12	2.45	0.47
2:C:1085:PHE:O	2:C:1088:LEU:HB3	2.15	0.47
3:D:475:LYS:O	3:D:478:LEU:HB2	2.15	0.47
3:D:601:ARG:HH22	3:D:613:ARG:HE	1.63	0.47
3:D:1045:MET:HA	9:D:2022:HOH:O	2.14	0.47
3:D:1217:ILE:HD13	3:D:1480:PHE:CE2	2.49	0.47
5:F:397:ILE:HG21	9:F:9936:HOH:O	2.14	0.47
1:K:152:PRO:HD2	1:K:155:LYS:HB2	1.97	0.47
2:M:342:ASP:O	2:M:346:VAL:HG23	2.15	0.47
2:M:346:VAL:HG12	2:M:350:ARG:NE	2.29	0.47
2:M:701:THR:HG22	2:M:832:LYS:HA	1.97	0.47
2:M:782:ALA:HB1	9:M:9603:HOH:O	2.14	0.47
2:M:1038:TRP:HD1	2:M:1041:GLU:OE1	1.98	0.47
9:M:9896:HOH:O	5:P:373:LYS:HB3	2.14	0.47
3:N:607:LEU:HA	9:N:2546:HOH:O	2.15	0.47
3:N:974:ILE:HG12	3:N:991:GLN:HE21	1.79	0.47
3:N:1033:GLN:HA	9:N:2161:HOH:O	2.14	0.47
3:N:1074:SER:O	3:N:1077:ALA:HB3	2.15	0.47
3:N:1148:VAL:O	3:N:1189:ARG:HG2	2.15	0.47
5:P:191:ASN:HA	9:P:1478:HOH:O	2.15	0.47
1:A:6:LEU:C	1:A:8:ALA:H	2.18	0.47
2:C:253:ALA:HB3	9:C:2420:HOH:O	2.14	0.47
2:C:913:GLU:O	2:C:916:GLU:HB3	2.15	0.47
3:D:54:LYS:HA	5:F:337:HIS:HE1	1.80	0.47
3:D:445:ARG:HG2	3:D:445:ARG:NH1	2.30	0.47
3:D:676:MET:HE1	3:D:684:LYS:H	1.80	0.47
3:D:1194:CYS:SG	3:D:1200:VAL:HA	2.55	0.47
3:D:1339:LYS:HG2	3:D:1343:ALA:HB2	1.97	0.47
5:F:142:ARG:HA	9:F:9681:HOH:O	2.15	0.47
1:K:138:LEU:HB2	9:K:8021:HOH:O	2.15	0.47
1:K:184:THR:HG22	1:K:192:LEU:O	2.15	0.47
1:L:90:LEU:HD21	9:L:3389:HOH:O	2.15	0.47
2:M:152:PRO:HD2	9:M:9283:HOH:O	2.14	0.47
2:M:165:LEU:HD12	2:M:166:PRO:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:310:LEU:HD11	9:M:2059:HOH:O	2.15	0.47
2:M:676:ILE:CG2	2:M:988:VAL:HG13	2.44	0.47
2:M:871:LEU:HD12	2:M:872:ASN:O	2.14	0.47
2:M:1083:GLU:O	2:M:1087:VAL:HG23	2.15	0.47
3:N:1020:LEU:HA	3:N:1023:MET:HE2	1.97	0.47
3:N:1134:LEU:HB2	9:N:2308:HOH:O	2.15	0.47
5:P:99:GLU:OE1	5:P:235:PHE:HB3	2.15	0.47
1:B:173:PRO:HB2	1:B:205:VAL:HG22	1.98	0.46
2:C:41:ASN:H	2:C:41:ASN:ND2	2.12	0.46
2:C:89:THR:HG22	2:C:91:GLN:HG3	1.97	0.46
2:C:184:MET:HE1	2:C:186:VAL:N	2.30	0.46
2:C:942:GLU:HG3	9:C:9752:HOH:O	2.14	0.46
2:C:1052:MET:HG3	3:D:623:VAL:CG2	2.45	0.46
3:D:865:THR:HG22	9:D:9766:HOH:O	2.14	0.46
3:D:992:ILE:HA	9:D:2129:HOH:O	2.14	0.46
5:F:108:GLU:HG3	5:F:176:ILE:HG21	1.96	0.46
5:F:166:LEU:HD13	5:F:170:HIS:CB	2.44	0.46
1:K:54:THR:HG21	1:K:145:ASP:OD1	2.15	0.46
1:L:108:GLU:O	1:L:110:LYS:HG3	2.15	0.46
2:M:165:LEU:HD21	2:M:334:ARG:HH21	1.79	0.46
2:M:485:TYR:HD2	9:M:9411:HOH:O	1.97	0.46
2:M:600:ASP:HA	9:M:2442:HOH:O	2.14	0.46
3:N:566:ILE:CD1	5:P:217:ASN:HD22	2.28	0.46
3:N:686:GLU:HG2	9:N:2678:HOH:O	2.14	0.46
3:N:1052:THR:HG22	9:N:9337:HOH:O	2.15	0.46
3:N:1188:VAL:HG22	3:N:1189:ARG:O	2.15	0.46
3:N:1219:GLU:HG3	4:O:17:TYR:OH	2.15	0.46
3:N:1472:ILE:HG22	3:N:1474:ALA:H	1.80	0.46
4:O:39:VAL:HG12	9:O:1697:HOH:O	2.14	0.46
5:P:106:VAL:HA	9:P:1566:HOH:O	2.15	0.46
5:P:359:SER:HA	9:P:1489:HOH:O	2.15	0.46
1:A:50:GLY:N	9:A:9574:HOH:O	2.47	0.46
1:A:191:ASP:O	1:A:192:LEU:HD23	2.16	0.46
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.98	0.46
2:C:2:GLU:HG2	9:C:2528:HOH:O	2.16	0.46
2:C:6:PHE:CE1	2:C:909:ALA:HB2	2.51	0.46
2:C:217:LEU:HD23	9:C:9668:HOH:O	2.15	0.46
2:C:369:PRO:HG2	9:C:2433:HOH:O	2.15	0.46
2:C:517:ARG:HB2	9:C:9578:HOH:O	2.15	0.46
2:C:591:SER:HB2	9:C:9610:HOH:O	2.15	0.46
2:C:678:PRO:HG3	2:C:873:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:899:GLN:OE1	2:C:901:TYR:HE2	1.98	0.46
9:C:9869:HOH:O	3:D:1068:LEU:HD13	2.15	0.46
3:D:207:PHE:HB3	3:D:395:VAL:HG21	1.97	0.46
3:D:458:ALA:HB2	9:D:2106:HOH:O	2.15	0.46
3:D:539:ASP:HB3	3:D:600:LEU:HD12	1.97	0.46
3:D:542:ASP:HA	3:D:545:ARG:HE	1.80	0.46
3:D:702:LEU:HD13	3:D:716:PHE:HD1	1.81	0.46
3:D:754:PHE:CE2	3:D:1476:THR:HG21	2.49	0.46
3:D:1165:TYR:HB2	9:D:9690:HOH:O	2.15	0.46
4:E:76:GLY:N	4:E:79:LEU:HD22	2.29	0.46
5:F:287:THR:CG2	5:F:289:GLU:HB2	2.41	0.46
5:F:365:GLU:O	5:F:369:LEU:HD12	2.15	0.46
2:M:19:THR:HG22	2:M:23:VAL:HG23	1.97	0.46
2:M:151:ASP:HB2	2:M:157:ARG:O	2.15	0.46
2:M:278:GLU:HG3	2:M:283:ILE:O	2.16	0.46
2:M:405:ARG:HD2	2:M:442:GLU:OE2	2.15	0.46
3:N:36:THR:O	3:N:38:LYS:N	2.48	0.46
3:N:50:PHE:CB	3:N:522:PRO:HG2	2.46	0.46
3:N:711:LEU:C	3:N:713:ILE:H	2.19	0.46
4:O:39:VAL:HA	9:O:1697:HOH:O	2.15	0.46
5:P:166:LEU:HD22	5:P:170:HIS:HB2	1.98	0.46
5:P:192:LEU:HD22	9:P:4506:HOH:O	2.15	0.46
5:P:264:MET:O	5:P:268:ILE:HG13	2.16	0.46
5:P:315:VAL:HG12	5:P:316:SER:H	1.80	0.46
1:B:115:LEU:HD12	1:B:115:LEU:O	2.14	0.46
1:B:213:GLN:O	1:B:217:ILE:HG13	2.15	0.46
2:C:35:PRO:HD2	2:C:38:LYS:CE	2.46	0.46
2:C:91:GLN:HA	2:C:119:PRO:HA	1.96	0.46
2:C:230:ARG:HB2	2:C:233:GLU:HB3	1.97	0.46
2:C:246:ASP:HB2	9:C:2442:HOH:O	2.15	0.46
2:C:422:ARG:HD3	9:C:2680:HOH:O	2.16	0.46
2:C:657:ASP:OD1	2:C:661:SER:HB2	2.14	0.46
2:C:737:LEU:HD11	2:C:754:ILE:HG21	1.95	0.46
2:C:861:LEU:CD2	2:C:863:ASP:H	2.28	0.46
2:C:933:GLY:HA2	9:C:2021:HOH:O	2.16	0.46
2:C:1102:LEU:N	3:D:7:LYS:O	2.48	0.46
3:D:172:PRO:HB3	3:D:178:LEU:HB3	1.98	0.46
3:D:206:ARG:HA	3:D:206:ARG:HH11	1.80	0.46
3:D:462:GLN:HA	3:D:513:ILE:HD13	1.96	0.46
3:D:1074:SER:O	3:D:1077:ALA:HB3	2.15	0.46
5:F:147:LEU:HD23	9:F:9698:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:29:GLU:HB3	9:K:4304:HOH:O	2.14	0.46
1:K:162:ILE:HG13	1:K:163:ASN:ND2	2.30	0.46
2:M:127:PHE:O	2:M:133:ASP:HA	2.16	0.46
2:M:313:LEU:C	2:M:315:ALA:H	2.17	0.46
2:M:725:ASP:O	2:M:727:PRO:HD3	2.15	0.46
2:M:773:LEU:HD11	5:P:405:LEU:HD13	1.97	0.46
2:M:950:LEU:HD12	2:M:952:LEU:HD21	1.97	0.46
3:N:168:THR:OG1	3:N:393:ILE:HD12	2.15	0.46
3:N:408:GLU:HG2	9:N:9546:HOH:O	2.15	0.46
3:N:433:GLY:HA3	3:N:450:TYR:HA	1.96	0.46
3:N:686:GLU:HG3	9:N:2781:HOH:O	2.14	0.46
3:N:809:PRO:HB2	3:N:812:ALA:HB2	1.96	0.46
3:N:829:VAL:HG22	9:N:9736:HOH:O	2.15	0.46
3:N:1031:ASN:OD1	3:N:1033:GLN:HB2	2.15	0.46
3:N:1340:GLY:O	3:N:1344:VAL:HG23	2.15	0.46
5:P:109:GLY:HA3	9:P:1566:HOH:O	2.14	0.46
5:P:351:SER:HB2	9:P:6220:HOH:O	2.15	0.46
1:A:197:LEU:HD23	1:A:197:LEU:N	2.27	0.46
1:A:217:ILE:HB	9:A:9598:HOH:O	2.15	0.46
2:C:313:LEU:C	2:C:315:ALA:H	2.18	0.46
2:C:601:GLY:HA3	2:C:615:TYR:HA	1.98	0.46
2:C:922:PHE:HD2	9:C:2177:HOH:O	1.99	0.46
3:D:13:ALA:O	3:D:511:TRP:HB3	2.15	0.46
3:D:919:PHE:HA	3:D:927:THR:OG1	2.16	0.46
3:D:1209:LEU:HD13	3:D:1219:GLU:OE2	2.15	0.46
3:D:1277:ILE:CD1	3:D:1301:LYS:HB2	2.45	0.46
3:D:1379:VAL:O	3:D:1392:GLY:HA2	2.16	0.46
1:L:75:VAL:O	1:L:79:ILE:HG23	2.15	0.46
2:M:480:THR:HG22	2:M:482:GLU:N	2.30	0.46
2:M:546:LEU:HA	2:M:581:THR:OG1	2.15	0.46
2:M:560:MET:O	2:M:564:MET:HB2	2.15	0.46
2:M:1034:GLU:HA	2:M:1037:VAL:CG2	2.46	0.46
3:N:806:PHE:HE1	3:N:813:LEU:HB3	1.80	0.46
3:N:827:ILE:O	3:N:837:GLY:HA3	2.15	0.46
3:N:842:VAL:HG23	9:N:9393:HOH:O	2.14	0.46
3:N:1478:SER:C	3:N:1480:PHE:H	2.17	0.46
4:O:40:LEU:CG	4:O:67:GLU:HG2	2.45	0.46
4:O:41:GLU:H	4:O:42:PRO:HD2	1.80	0.46
4:O:41:GLU:CA	4:O:45:ARG:HG3	2.45	0.46
5:P:231:ARG:HA	9:P:2972:HOH:O	2.15	0.46
1:A:57:TYR:CE1	1:A:163:ASN:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:129:ILE:HD12	2:C:129:ILE:N	2.31	0.46
2:C:498:GLN:HG3	9:C:9570:HOH:O	2.16	0.46
2:C:524:VAL:HG22	2:C:525:SER:H	1.81	0.46
2:C:1036:GLU:HA	3:D:707:THR:HG21	1.97	0.46
2:C:1059:ASP:N	9:C:9720:HOH:O	2.49	0.46
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.20	0.46
3:D:431:VAL:HG12	9:D:2014:HOH:O	2.15	0.46
3:D:446:VAL:HG11	9:D:9698:HOH:O	2.15	0.46
3:D:523:ASP:OD1	3:D:523:ASP:N	2.47	0.46
3:D:534:ARG:HG3	9:D:2518:HOH:O	2.15	0.46
3:D:1351:GLU:O	3:D:1354:LYS:HB2	2.16	0.46
1:K:184:THR:O	1:K:192:LEU:HD12	2.15	0.46
2:M:19:THR:HG22	2:M:19:THR:O	2.15	0.46
2:M:504:GLU:HA	9:M:9395:HOH:O	2.16	0.46
2:M:544:THR:HA	2:M:562:SER:OG	2.15	0.46
2:M:564:MET:HG2	2:M:840:ALA:CB	2.46	0.46
2:M:841:ASN:ND2	2:M:845:ASN:N	2.64	0.46
3:N:65:ARG:HG2	5:P:375:LEU:HA	1.98	0.46
3:N:772:PRO:HG3	9:N:9333:HOH:O	2.15	0.46
3:N:1044:LEU:CD2	3:N:1056:PRO:HG3	2.46	0.46
3:N:1192:LEU:HD22	3:N:1345:GLU:OE2	2.14	0.46
4:O:86:GLN:O	4:O:90:GLU:HG3	2.15	0.46
5:P:416:ARG:HA	9:P:4146:HOH:O	2.15	0.46
2:C:89:THR:O	2:C:91:GLN:HG3	2.14	0.46
2:C:187:ASN:HB3	9:C:9640:HOH:O	2.15	0.46
2:C:250:ARG:HD2	9:C:9629:HOH:O	2.15	0.46
2:C:358:ARG:HB3	2:C:371:LYS:O	2.16	0.46
2:C:549:PHE:HB3	2:C:552:HIS:HD2	1.80	0.46
2:C:751:PRO:HB2	3:D:680:GLN:CG	2.44	0.46
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.97	0.46
3:D:550:ARG:HG3	3:D:550:ARG:NH1	2.30	0.46
3:D:687:VAL:O	3:D:690:ALA:HB3	2.15	0.46
3:D:704:ARG:CD	3:D:705:ALA:H	2.25	0.46
3:D:1051:GLU:HB3	9:D:2777:HOH:O	2.15	0.46
3:D:1472:ILE:HG22	3:D:1474:ALA:H	1.80	0.46
4:E:39:VAL:HA	9:E:9571:HOH:O	2.14	0.46
5:F:112:ALA:HA	5:F:173:TYR:HD2	1.80	0.46
1:K:115:LEU:HD12	1:K:115:LEU:O	2.15	0.46
1:L:134:GLU:HG2	9:L:6529:HOH:O	2.16	0.46
2:M:145:GLY:H	2:M:163:ILE:CG2	2.28	0.46
2:M:207:LEU:O	2:M:211:LEU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:288:ARG:HG3	2:M:288:ARG:NH1	2.26	0.46
2:M:578:VAL:HG21	2:M:991:GLN:O	2.16	0.46
2:M:630:ARG:HH11	2:M:630:ARG:HG3	1.80	0.46
3:N:414:ARG:HA	9:N:9486:HOH:O	2.16	0.46
3:N:570:GLU:HB2	5:P:214:GLN:NE2	2.30	0.46
3:N:1158:VAL:HG12	3:N:1159:ARG:N	2.31	0.46
3:N:1385:GLY:HA2	3:N:1413:THR:HG21	1.97	0.46
3:N:1442:ASN:HD22	3:N:1443:THR:N	2.13	0.46
4:O:13:VAL:HG11	4:O:19:LEU:HB2	1.98	0.46
5:P:94:LEU:HB3	5:P:98:GLU:H	1.81	0.46
5:P:349:LEU:HD23	9:P:2092:HOH:O	2.16	0.46
5:P:367:MET:HA	5:P:370:LYS:HG2	1.98	0.46
2:C:141:HIS:HE1	2:C:332:ARG:HE	1.62	0.46
2:C:148:PHE:HE1	2:C:281:LEU:HD22	1.80	0.46
2:C:464:LEU:HB3	9:C:2642:HOH:O	2.16	0.46
2:C:671:ASN:HD22	2:C:993:PHE:HD2	1.64	0.46
9:C:9607:HOH:O	3:D:18:ILE:HD11	2.14	0.46
3:D:32:ILE:HG13	3:D:45:PHE:HD2	1.80	0.46
3:D:166:GLN:HB3	3:D:395:VAL:CG2	2.46	0.46
3:D:202:VAL:O	3:D:204:LEU:HG	2.15	0.46
3:D:711:LEU:C	3:D:713:ILE:H	2.18	0.46
3:D:1294:VAL:HG13	9:D:2676:HOH:O	2.15	0.46
3:D:1354:LYS:HD3	9:D:2684:HOH:O	2.15	0.46
3:D:1384:PRO:HG3	3:D:1389:LEU:N	2.31	0.46
9:D:9992:HOH:O	5:F:168:LYS:HG2	2.15	0.46
5:F:267:THR:HA	5:F:270:LYS:HZ2	1.80	0.46
1:K:41:ARG:NH1	1:K:177:VAL:HB	2.29	0.46
1:L:83:LYS:HG2	9:L:4413:HOH:O	2.15	0.46
2:M:265:ARG:HD2	9:M:2426:HOH:O	2.15	0.46
2:M:281:LEU:HB2	2:M:309:TYR:CD1	2.51	0.46
2:M:564:MET:CE	2:M:846:LYS:HE2	2.45	0.46
2:M:586:ARG:HH12	2:M:590:ASP:CG	2.19	0.46
2:M:724:ARG:HB2	2:M:741:GLY:N	2.31	0.46
2:M:770:GLU:HA	2:M:770:GLU:OE2	2.15	0.46
2:M:1036:GLU:HG3	3:N:707:THR:OG1	2.15	0.46
2:M:1104:GLU:O	3:N:7:LYS:HE2	2.15	0.46
3:N:127:LEU:HD12	3:N:128:TYR:N	2.30	0.46
3:N:649:ALA:HB3	3:N:691:LEU:HD21	1.97	0.46
3:N:702:LEU:O	3:N:713:ILE:HA	2.15	0.46
3:N:770:LEU:HD23	3:N:777:PRO:HA	1.98	0.46
3:N:861:GLN:HB2	9:N:9290:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1236:LEU:HA	3:N:1359:GLN:OE1	2.16	0.46
4:O:94:PRO:HA	9:O:9005:HOH:O	2.15	0.46
1:B:95:GLN:HB3	9:B:9815:HOH:O	2.15	0.46
2:C:405:ARG:HH22	2:C:409:ARG:HH21	1.63	0.46
2:C:405:ARG:NH2	2:C:566:THR:HG21	2.17	0.46
2:C:455:LEU:HD22	2:C:459:ALA:CB	2.46	0.46
2:C:626:ARG:NH1	2:C:637:LEU:HD12	2.30	0.46
2:C:723:THR:HA	9:C:9700:HOH:O	2.15	0.46
2:C:756:VAL:CG2	2:C:823:VAL:HG11	2.45	0.46
2:C:774:LEU:HB2	9:C:2198:HOH:O	2.15	0.46
2:C:870:ILE:N	2:C:870:ILE:HD12	2.31	0.46
2:C:1059:ASP:OD1	2:C:1080:SER:HB2	2.16	0.46
2:C:1102:LEU:CD1	3:D:9:ARG:HG2	2.45	0.46
3:D:438:ASP:OD2	3:D:440:VAL:HB	2.16	0.46
3:D:633:VAL:HB	3:D:740:PHE:CE1	2.51	0.46
3:D:814:ALA:O	3:D:818:ARG:HG3	2.16	0.46
3:D:1026:SER:HB2	9:D:9566:HOH:O	2.15	0.46
3:D:1144:LEU:HD11	3:D:1186:VAL:HG21	1.96	0.46
4:E:51:LEU:HD22	9:E:9663:HOH:O	2.16	0.46
1:L:182:GLU:O	1:L:194:LYS:HB3	2.16	0.46
1:L:185:ARG:HH12	3:N:692:GLU:HG3	1.79	0.46
2:M:22:GLN:O	2:M:121:MET:HE1	2.16	0.46
2:M:585:GLU:O	2:M:588:VAL:HG22	2.16	0.46
2:M:713:ARG:HG2	2:M:713:ARG:HH11	1.81	0.46
2:M:749:VAL:HG23	2:M:749:VAL:O	2.15	0.46
2:M:1083:GLU:HG2	9:M:9233:HOH:O	2.16	0.46
3:N:65:ARG:HG2	5:P:374:GLY:O	2.15	0.46
3:N:687:VAL:O	3:N:690:ALA:HB3	2.15	0.46
3:N:756:GLN:O	3:N:760:ARG:HG2	2.15	0.46
5:P:87:GLU:O	5:P:91:VAL:HG23	2.16	0.46
5:P:93:LEU:CD2	5:P:98:GLU:HB3	2.46	0.46
1:B:201:THR:HG22	1:B:203:GLY:H	1.81	0.46
2:C:212:GLY:HA3	2:C:218:VAL:HG23	1.98	0.46
2:C:408:ARG:HD2	2:C:542:VAL:HG21	1.98	0.46
2:C:597:ALA:O	2:C:652:GLY:N	2.47	0.46
2:C:1000:MET:HB2	2:C:1002:GLU:HG2	1.97	0.46
3:D:104:PHE:HE2	3:D:1448:THR:HA	1.81	0.46
3:D:1293:PHE:HB3	9:D:9737:HOH:O	2.15	0.46
3:D:1376:MET:HG2	3:D:1421:LEU:HA	1.97	0.46
1:K:75:VAL:O	1:K:79:ILE:HG23	2.16	0.46
2:M:404:LEU:HA	2:M:407:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:613:VAL:HB	9:M:9426:HOH:O	2.14	0.46
2:M:946:ARG:HB2	9:M:9918:HOH:O	2.16	0.46
3:N:27:GLU:N	9:N:9304:HOH:O	2.49	0.46
3:N:186:VAL:HG13	3:N:187:LYS:N	2.31	0.46
3:N:187:LYS:HA	9:N:9419:HOH:O	2.16	0.46
3:N:395:VAL:O	3:N:395:VAL:HG12	2.16	0.46
3:N:657:LEU:O	3:N:661:MET:HG2	2.16	0.46
3:N:1076:GLY:HA2	3:N:1079:LYS:HG2	1.98	0.46
5:P:113:ILE:HG23	5:P:127:ILE:CG2	2.45	0.46
5:P:125:ASP:HB2	9:P:8230:HOH:O	2.16	0.46
5:P:220:LEU:O	5:P:224:VAL:HG23	2.16	0.46
1:A:209:GLU:O	1:A:213:GLN:HG3	2.16	0.46
1:B:19:GLU:HG3	9:B:9589:HOH:O	2.15	0.46
2:C:66:LEU:HD11	2:C:98:LEU:HD22	1.98	0.46
2:C:133:ASP:HB2	2:C:632:ASN:ND2	2.27	0.46
2:C:569:VAL:HG12	2:C:996:LYS:O	2.16	0.46
2:C:724:ARG:HB2	2:C:740:GLU:CA	2.42	0.46
2:C:768:THR:HG22	2:C:771:GLU:H	1.81	0.46
2:C:808:ARG:HD3	9:C:2330:HOH:O	2.15	0.46
2:C:887:GLU:OE1	2:C:992:MET:HA	2.15	0.46
3:D:154:THR:HG22	3:D:155:ASP:H	1.81	0.46
3:D:465:LEU:HD22	3:D:510:GLU:HA	1.98	0.46
3:D:493:ARG:O	3:D:497:GLU:HG2	2.16	0.46
3:D:508:ARG:HA	3:D:509:PRO:HD2	1.71	0.46
3:D:649:ALA:HB3	3:D:691:LEU:HD21	1.97	0.46
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	1.97	0.46
5:F:220:LEU:O	5:F:223:ALA:HB3	2.16	0.46
1:K:70:GLY:HA2	1:K:133:GLU:CG	2.46	0.46
2:M:115:LEU:O	2:M:115:LEU:HD12	2.16	0.46
2:M:207:LEU:HD22	2:M:221:LEU:CD2	2.46	0.46
2:M:839:LEU:HD11	2:M:849:VAL:HG22	1.98	0.46
2:M:1056:LYS:HB3	3:N:624:ASP:H	1.80	0.46
3:N:38:LYS:NZ	3:N:59:ALA:HB1	2.30	0.46
3:N:50:PHE:O	3:N:86:ARG:HA	2.15	0.46
3:N:138:LYS:HD3	9:N:9902:HOH:O	2.16	0.46
3:N:525:ARG:N	3:N:526:PRO:HD3	2.31	0.46
3:N:1232:PRO:HB3	3:N:1361:VAL:HG21	1.97	0.46
3:N:1281:VAL:HG23	3:N:1317:ASP:O	2.15	0.46
3:N:1393:GLN:CB	3:N:1398:TRP:HE1	2.28	0.46
3:N:1498:ALA:HB2	9:N:9438:HOH:O	2.16	0.46
5:P:394:ARG:HB3	9:P:6528:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.97	0.45
1:B:14:ARG:HA	9:B:9663:HOH:O	2.15	0.45
1:B:50:GLY:HA3	1:B:171:PHE:O	2.16	0.45
2:C:1:MET:SD	2:C:900:ARG:HD3	2.56	0.45
2:C:6:PHE:HA	2:C:8:ARG:HH21	1.80	0.45
2:C:157:ARG:HD2	2:C:314:THR:CG2	2.39	0.45
2:C:721:ARG:HA	9:C:2273:HOH:O	2.16	0.45
2:C:815:LEU:HD21	2:C:819:VAL:O	2.16	0.45
2:C:1097:LEU:H	2:C:1097:LEU:CD2	2.20	0.45
3:D:90:MET:HE3	3:D:520:LEU:HA	1.97	0.45
3:D:521:PRO:C	3:D:525:ARG:HH11	2.20	0.45
3:D:1097:LYS:HD2	9:D:9821:HOH:O	2.16	0.45
3:D:1122:LEU:HD12	3:D:1122:LEU:N	2.30	0.45
3:D:1283:ILE:HG22	3:D:1284:GLU:H	1.81	0.45
3:D:1375:MET:SD	3:D:1423:GLY:HA2	2.55	0.45
5:F:371:LEU:CD2	5:F:375:LEU:HD22	2.45	0.45
2:M:251:ASP:HB3	2:M:252:LYS:HD2	1.97	0.45
2:M:818:GLY:HA3	9:M:2517:HOH:O	2.16	0.45
2:M:1060:ILE:HG12	2:M:1063:ARG:NH2	2.30	0.45
3:N:651:GLU:HG2	9:N:2423:HOH:O	2.16	0.45
1:A:5:LYS:HA	1:A:5:LYS:HE3	1.97	0.45
2:C:17:PRO:O	2:C:20:GLU:HB3	2.17	0.45
2:C:24:GLU:HA	9:C:2056:HOH:O	2.15	0.45
2:C:208:ALA:HB1	2:C:218:VAL:HG11	1.97	0.45
2:C:585:GLU:HG2	2:C:665:PHE:CD2	2.51	0.45
2:C:768:THR:HG23	9:C:2074:HOH:O	2.16	0.45
2:C:945:ARG:HB3	9:C:2615:HOH:O	2.17	0.45
2:C:1058:ASP:CG	2:C:1084:SER:H	2.19	0.45
3:D:11:ALA:HB2	9:D:9902:HOH:O	2.14	0.45
3:D:125:GLN:HE22	3:D:587:ARG:HE	1.65	0.45
3:D:464:LEU:O	3:D:468:LEU:HG	2.16	0.45
3:D:776:GLU:HB3	3:D:912:LYS:HE2	1.98	0.45
3:D:1121:PRO:C	3:D:1122:LEU:HD12	2.36	0.45
3:D:1146:GLY:CA	3:D:1207:TYR:HB2	2.39	0.45
3:D:1147:ARG:O	3:D:1165:TYR:HA	2.16	0.45
3:D:1188:VAL:HG22	3:D:1189:ARG:O	2.15	0.45
5:F:173:TYR:HA	5:F:176:ILE:HD12	1.97	0.45
5:F:214:GLN:O	5:F:217:ASN:HB2	2.16	0.45
5:F:238:TYR:HB2	9:F:9643:HOH:O	2.16	0.45
5:F:309:LYS:HD3	9:F:9794:HOH:O	2.16	0.45
1:K:33:GLY:O	1:K:195:LEU:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:212:ASN:HD22	1:K:212:ASN:N	2.13	0.45
2:M:16:PRO:HB3	2:M:460:ARG:HH11	1.81	0.45
2:M:174:LEU:HB2	2:M:310:LEU:HD22	1.99	0.45
2:M:218:VAL:HG22	2:M:221:LEU:CD2	2.42	0.45
2:M:252:LYS:HE2	2:M:296:GLY:HA3	1.97	0.45
2:M:399:ASN:ND2	2:M:568:ALA:HB3	2.31	0.45
2:M:1034:GLU:HA	2:M:1037:VAL:HG23	1.98	0.45
3:N:166:GLN:HE21	3:N:167:GLU:C	2.19	0.45
3:N:445:ARG:H	3:N:445:ARG:HD2	1.79	0.45
3:N:468:LEU:HD12	9:N:9350:HOH:O	2.16	0.45
3:N:919:PHE:HA	3:N:927:THR:OG1	2.17	0.45
3:N:928:ALA:O	3:N:931:LEU:HB2	2.15	0.45
5:P:266:GLU:HB2	5:P:270:LYS:HZ2	1.80	0.45
5:P:289:GLU:O	5:P:293:GLU:HG3	2.17	0.45
2:C:21:ILE:HD12	2:C:21:ILE:N	2.30	0.45
2:C:685:GLU:HB3	9:C:2345:HOH:O	2.15	0.45
2:C:962:GLN:N	9:C:9884:HOH:O	2.49	0.45
3:D:84:ILE:HG13	3:D:85:VAL:N	2.31	0.45
3:D:148:GLU:HG2	9:D:9755:HOH:O	2.15	0.45
3:D:178:LEU:HD11	9:D:2532:HOH:O	2.15	0.45
3:D:577:ALA:O	3:D:580:ALA:HB3	2.17	0.45
3:D:1259:VAL:O	3:D:1263:PHE:HD1	1.99	0.45
5:F:356:LYS:HD3	9:F:9676:HOH:O	2.15	0.45
1:K:57:TYR:CE1	1:K:163:ASN:HB2	2.46	0.45
1:L:143:ARG:HB2	9:L:7130:HOH:O	2.15	0.45
2:M:194:VAL:HG13	2:M:221:LEU:HD12	1.97	0.45
2:M:424:GLY:O	2:M:428:ARG:HG3	2.17	0.45
2:M:545:ASN:HB2	9:M:9531:HOH:O	2.16	0.45
2:M:605:LYS:HD2	9:M:9417:HOH:O	2.16	0.45
2:M:627:ARG:HD2	9:M:9479:HOH:O	2.17	0.45
2:M:841:ASN:ND2	2:M:845:ASN:HB3	2.32	0.45
2:M:955:PRO:HG2	9:M:9748:HOH:O	2.15	0.45
3:N:154:THR:HG23	3:N:157:GLU:H	1.81	0.45
3:N:182:GLY:HA2	9:N:9237:HOH:O	2.15	0.45
3:N:479:GLU:HB3	9:N:9264:HOH:O	2.15	0.45
3:N:660:LYS:O	3:N:664:LYS:HG3	2.16	0.45
3:N:737:ASN:C	9:N:9228:HOH:O	2.54	0.45
5:P:366:ALA:HB2	9:P:1329:HOH:O	2.15	0.45
1:A:48:ILE:HA	1:A:49:PRO:HD3	1.79	0.45
1:A:89:PHE:HB2	9:A:9614:HOH:O	2.15	0.45
1:A:90:LEU:HA	9:A:9720:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HB2	1:A:200:TRP:CZ3	2.52	0.45
2:C:136:ILE:HD11	9:C:9782:HOH:O	2.15	0.45
2:C:288:ARG:HH11	2:C:288:ARG:HA	1.82	0.45
2:C:707:ARG:HG3	2:C:826:TYR:CZ	2.51	0.45
2:C:794:PRO:HD2	9:C:9926:HOH:O	2.16	0.45
3:D:660:LYS:O	3:D:663:GLU:HB2	2.16	0.45
3:D:699:VAL:HG21	3:D:760:ARG:HB3	1.98	0.45
3:D:710:ARG:HG3	3:D:711:LEU:N	2.31	0.45
3:D:1168:MET:HA	3:D:1168:MET:HE3	1.97	0.45
5:F:93:LEU:CD2	5:F:98:GLU:HB3	2.46	0.45
5:F:230:LYS:HA	9:F:9842:HOH:O	2.16	0.45
1:K:197:LEU:N	9:K:1736:HOH:O	2.48	0.45
2:M:42:VAL:HG12	2:M:43:GLY:N	2.26	0.45
2:M:59:LYS:HB3	9:M:9726:HOH:O	2.16	0.45
2:M:187:ASN:HB3	9:M:2286:HOH:O	2.16	0.45
2:M:273:GLY:HA2	9:M:9612:HOH:O	2.17	0.45
2:M:353:ARG:HA	9:M:9887:HOH:O	2.16	0.45
2:M:367:LEU:HA	2:M:371:LYS:HB2	1.98	0.45
2:M:492:ASP:CA	2:M:518:LYS:HB3	2.43	0.45
2:M:1076:VAL:HG22	3:N:752:SER:HB3	1.98	0.45
9:M:9246:HOH:O	5:P:345:ALA:HA	2.15	0.45
3:N:50:PHE:HB3	3:N:522:PRO:HG2	1.99	0.45
3:N:1283:ILE:HG22	3:N:1284:GLU:H	1.82	0.45
4:O:70:THR:HA	9:O:2214:HOH:O	2.16	0.45
4:O:82:GLU:HG3	9:O:2121:HOH:O	2.17	0.45
5:P:405:LEU:HG	9:P:3208:HOH:O	2.16	0.45
1:B:80:LEU:HD13	3:D:842:VAL:HG12	1.98	0.45
1:B:226:SER:O	1:B:228:PRO:HD3	2.16	0.45
2:C:204:GLN:HB2	9:C:2456:HOH:O	2.17	0.45
2:C:584:GLU:O	2:C:588:VAL:HG13	2.16	0.45
2:C:820:ARG:HA	9:C:2072:HOH:O	2.17	0.45
3:D:4:GLU:HG3	9:D:2516:HOH:O	2.15	0.45
3:D:500:ARG:HA	9:D:2025:HOH:O	2.16	0.45
3:D:684:LYS:O	3:D:687:VAL:HG23	2.17	0.45
3:D:1033:GLN:O	3:D:1036:ARG:HB3	2.16	0.45
3:D:1103:HIS:HA	3:D:1223:ILE:CD1	2.45	0.45
3:D:1343:ALA:HA	9:D:2807:HOH:O	2.15	0.45
3:D:1356:TYR:HD2	3:D:1361:VAL:HG11	1.82	0.45
3:D:1428:ALA:C	3:D:1430:SER:H	2.18	0.45
3:D:1493:LYS:HE2	9:D:9651:HOH:O	2.16	0.45
1:K:156:HIS:CD2	1:K:158:ILE:HG12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:16:PRO:O	2:M:18:LEU:HD12	2.15	0.45
2:M:183:SER:HA	2:M:190:LYS:HB2	1.99	0.45
2:M:292:ARG:CZ	2:M:299:LYS:HD3	2.47	0.45
2:M:502:PRO:HA	9:M:2305:HOH:O	2.16	0.45
2:M:612:VAL:HG22	2:M:622:GLU:HG3	1.99	0.45
2:M:727:PRO:HG3	2:M:783:ARG:CZ	2.47	0.45
2:M:1030:GLN:O	3:N:622:ARG:HA	2.17	0.45
2:M:1085:PHE:CE2	3:N:1468:LEU:HG	2.51	0.45
3:N:10:ILE:HG13	3:N:1434:TRP:CZ2	2.52	0.45
3:N:116:LEU:O	3:N:118:LEU:N	2.49	0.45
3:N:543:LEU:O	3:N:546:ARG:HB2	2.16	0.45
3:N:577:ALA:O	3:N:580:ALA:HB3	2.17	0.45
3:N:701:LEU:C	3:N:702:LEU:HD12	2.37	0.45
3:N:704:ARG:HH12	3:N:743:ASP:HB3	1.79	0.45
3:N:953:ASP:OD1	3:N:1019:PRO:HG2	2.17	0.45
3:N:1054:GLU:HB2	9:N:9784:HOH:O	2.17	0.45
3:N:1114:THR:HG22	3:N:1195:GLN:HB2	1.97	0.45
3:N:1176:LYS:O	3:N:1179:GLU:HB2	2.17	0.45
3:N:1299:PHE:HB2	9:N:2802:HOH:O	2.16	0.45
3:N:1409:ALA:HB2	9:N:9520:HOH:O	2.16	0.45
4:O:77:GLU:HB2	9:O:2132:HOH:O	2.15	0.45
5:P:133:ALA:HB1	9:P:2305:HOH:O	2.15	0.45
5:P:292:ALA:O	5:P:299:TRP:HB2	2.15	0.45
5:P:315:VAL:HG12	5:P:316:SER:N	2.31	0.45
1:A:20:TYR:HE2	1:A:198:ARG:HB3	1.81	0.45
2:C:164:PRO:HA	2:C:266:ARG:HH12	1.80	0.45
2:C:475:VAL:HA	9:C:9621:HOH:O	2.16	0.45
2:C:505:GLY:HA3	9:C:9589:HOH:O	2.17	0.45
2:C:580:MET:HB3	9:C:2049:HOH:O	2.16	0.45
2:C:1016:ILE:H	2:C:1016:ILE:CD1	2.20	0.45
2:C:1081:VAL:HB	2:C:1086:ARG:NH2	2.31	0.45
3:D:206:ARG:HB3	3:D:206:ARG:NH1	2.32	0.45
3:D:213:VAL:HA	9:D:2673:HOH:O	2.16	0.45
3:D:452:ILE:HG23	3:D:452:ILE:O	2.17	0.45
3:D:777:PRO:HD2	3:D:912:LYS:HE2	1.97	0.45
3:D:1103:HIS:HA	3:D:1223:ILE:HD12	1.99	0.45
3:D:1256:LEU:HB3	3:D:1257:PRO:HD3	1.98	0.45
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.97	0.45
5:F:160:ASP:OD2	5:F:163:LEU:HD12	2.16	0.45
1:L:153:ALA:HA	1:L:156:HIS:CE1	2.51	0.45
2:M:84:ARG:HH12	2:M:128:ILE:HG12	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:250:ARG:HD2	9:M:9919:HOH:O	2.17	0.45
2:M:799:ILE:HD13	2:M:799:ILE:H	1.81	0.45
2:M:892:LEU:HD13	2:M:989:VAL:O	2.16	0.45
3:N:572:ARG:O	3:N:575:GLN:HB3	2.17	0.45
3:N:988:ARG:HD2	3:N:992:ILE:CD1	2.46	0.45
3:N:1195:GLN:HG3	9:N:2116:HOH:O	2.17	0.45
3:N:1359:GLN:HE21	3:N:1359:GLN:HB3	1.49	0.45
3:N:1428:ALA:C	3:N:1430:SER:H	2.20	0.45
4:O:29:GLN:HB2	4:O:33:HIS:HD2	1.81	0.45
5:P:217:ASN:O	5:P:220:LEU:HB3	2.16	0.45
5:P:361:LEU:HD22	5:P:404:ALA:HB1	1.99	0.45
1:A:219:ARG:HG2	9:A:9621:HOH:O	2.17	0.45
1:B:207:PRO:HD2	9:B:9568:HOH:O	2.17	0.45
1:B:228:PRO:HG2	9:B:9723:HOH:O	2.15	0.45
2:C:151:ASP:OD1	2:C:152:PRO:HD2	2.17	0.45
2:C:202:TYR:CZ	2:C:304:LEU:HD22	2.51	0.45
2:C:262:ALA:HB2	9:C:2720:HOH:O	2.15	0.45
2:C:717:LEU:HD11	2:C:764:GLU:O	2.16	0.45
2:C:777:ILE:HG23	9:C:9997:HOH:O	2.16	0.45
2:C:1083:GLU:O	2:C:1087:VAL:HG23	2.16	0.45
2:C:1089:VAL:HG13	2:C:1099:VAL:HB	1.98	0.45
3:D:148:GLU:CD	3:D:148:GLU:N	2.70	0.45
3:D:196:VAL:HG13	3:D:202:VAL:HG13	1.98	0.45
3:D:441:ARG:O	3:D:443:VAL:N	2.44	0.45
3:D:586:ARG:HD2	9:D:2072:HOH:O	2.17	0.45
3:D:808:THR:HB	3:D:809:PRO:HD3	1.97	0.45
3:D:908:LYS:NZ	8:N:9100:G4P:O2D	2.49	0.45
3:D:1087:ARG:HD2	9:D:9624:HOH:O	2.17	0.45
3:D:1148:VAL:HG13	3:D:1163:GLY:O	2.15	0.45
3:D:1460:ILE:HA	9:D:2240:HOH:O	2.17	0.45
2:M:172:ILE:HA	2:M:185:LYS:O	2.16	0.45
2:M:288:ARG:NH1	2:M:289:THR:HG23	2.31	0.45
2:M:327:HIS:ND1	2:M:433:THR:HG21	2.32	0.45
2:M:395:LYS:HE3	2:M:407:LYS:HZ2	1.82	0.45
2:M:407:LYS:HG2	9:M:9254:HOH:O	2.15	0.45
2:M:501:THR:O	2:M:503:LEU:HD23	2.16	0.45
2:M:575:GLN:H	2:M:667:ALA:HB1	1.81	0.45
2:M:713:ARG:HD2	9:M:9901:HOH:O	2.17	0.45
2:M:1050:GLN:HG2	2:M:1079:PRO:HG2	1.99	0.45
2:M:1088:LEU:O	2:M:1091:GLU:HB2	2.17	0.45
3:N:179:VAL:HG11	9:N:2712:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:421:LEU:HD12	3:N:435:VAL:CG1	2.44	0.45
3:N:631:ILE:HG21	3:N:745:MET:HG3	1.97	0.45
3:N:813:LEU:O	3:N:817:GLU:HB2	2.15	0.45
3:N:964:LEU:O	3:N:968:ASP:HB2	2.17	0.45
3:N:1017:PHE:HZ	9:N:9258:HOH:O	1.98	0.45
3:N:1194:CYS:SG	3:N:1200:VAL:HA	2.57	0.45
3:N:1241:PHE:O	3:N:1257:PRO:HB3	2.17	0.45
3:N:1312:LEU:HG	3:N:1327:ARG:HG3	1.99	0.45
3:N:1433:SER:HB2	3:N:1457:ASP:OD1	2.17	0.45
5:P:166:LEU:HD13	5:P:170:HIS:CB	2.47	0.45
1:A:22:GLU:N	9:A:9810:HOH:O	2.49	0.45
1:A:53:VAL:HG21	1:A:82:LEU:HB3	1.99	0.45
1:B:13:VAL:HG11	1:B:208:LEU:HD21	1.99	0.45
1:B:34:VAL:HG11	2:C:978:ARG:HB3	1.98	0.45
2:C:958:THR:CG2	2:C:961:GLU:HB2	2.46	0.45
2:C:1047:HIS:CD2	3:D:1471:LEU:HD11	2.52	0.45
2:C:1081:VAL:HB	2:C:1086:ARG:CZ	2.47	0.45
3:D:175:VAL:HG11	9:D:9726:HOH:O	2.17	0.45
3:D:560:GLN:HG3	5:F:221:ILE:HG21	1.99	0.45
3:D:570:GLU:OE2	5:F:214:GLN:HG3	2.16	0.45
3:D:792:ILE:HD12	3:D:941:PHE:CE1	2.52	0.45
3:D:867:ARG:HG3	9:D:2678:HOH:O	2.16	0.45
3:D:972:LEU:CG	3:D:976:GLN:HE22	2.23	0.45
3:D:986:ARG:NH1	3:D:986:ARG:HB2	2.32	0.45
4:E:41:GLU:HB3	4:E:42:PRO:HD3	1.98	0.45
5:F:257:THR:C	5:F:258:ILE:HG13	2.37	0.45
5:F:376:ILE:HG22	9:F:9780:HOH:O	2.16	0.45
1:L:2:LEU:HD12	1:L:3:ASP:H	1.82	0.45
1:L:166:PRO:HB2	9:L:3282:HOH:O	2.16	0.45
1:L:176:ARG:HH12	3:N:884:ARG:CZ	2.29	0.45
2:M:20:GLU:O	2:M:24:GLU:HB2	2.16	0.45
2:M:404:LEU:CD2	2:M:587:VAL:HG13	2.47	0.45
2:M:709:GLU:CD	2:M:824:ARG:HG2	2.38	0.45
2:M:745:ILE:HG12	9:M:9460:HOH:O	2.17	0.45
2:M:1031:ARG:HB3	9:N:9740:HOH:O	2.16	0.45
3:N:177:ALA:C	3:N:199:LEU:HD13	2.37	0.45
3:N:448:GLU:CD	3:N:448:GLU:H	2.20	0.45
3:N:590:PRO:HD2	9:N:9686:HOH:O	2.16	0.45
3:N:701:LEU:O	3:N:702:LEU:HD12	2.16	0.45
3:N:792:ILE:O	3:N:878:GLY:HA3	2.17	0.45
3:N:824:ASN:O	3:N:826:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:957:PRO:CG	3:N:1007:VAL:HA	2.46	0.45
3:N:1390:LEU:HD13	9:N:9981:HOH:O	2.17	0.45
3:N:1425:THR:O	3:N:1429:LEU:HD13	2.17	0.45
4:O:40:LEU:HB2	4:O:45:ARG:CD	2.46	0.45
4:O:54:LEU:HG	4:O:58:PRO:HG2	1.99	0.45
5:P:171:LYS:HG2	5:P:175:HIS:CE1	2.52	0.45
1:A:41:ARG:HH1	1:A:41:ARG:HG3	1.82	0.45
1:A:109:VAL:HG23	1:A:132:LEU:HD13	1.98	0.45
1:B:68:ILE:HG23	9:B:9743:HOH:O	2.16	0.45
2:C:612:VAL:HG22	2:C:622:GLU:CA	2.46	0.45
2:C:672:VAL:HG23	2:C:868:ASP:OD2	2.17	0.45
2:C:676:ILE:HG22	2:C:988:VAL:O	2.17	0.45
2:C:838:LYS:HD2	2:C:846:LYS:HZ3	1.81	0.45
3:D:95:LEU:HA	9:D:2002:HOH:O	2.17	0.45
3:D:170:PRO:O	3:D:391:ALA:HB3	2.17	0.45
3:D:216:VAL:HG12	9:D:9564:HOH:O	2.17	0.45
3:D:561:GLY:HA2	9:D:9763:HOH:O	2.17	0.45
3:D:833:GLU:HB2	9:D:2078:HOH:O	2.16	0.45
3:D:1005:GLN:HB2	9:D:9713:HOH:O	2.16	0.45
3:D:1046:GLN:HB3	3:D:1052:THR:CG2	2.47	0.45
5:F:96:LEU:O	5:F:100:VAL:HG23	2.17	0.45
2:M:397:GLU:H	2:M:633:GLN:NE2	2.14	0.45
2:M:455:LEU:HD22	2:M:459:ALA:HB1	1.98	0.45
2:M:673:LEU:HD13	9:M:9318:HOH:O	2.16	0.45
3:N:469:ASP:OD1	3:N:471:GLU:HB2	2.17	0.45
3:N:693:GLU:HG3	4:O:48:MET:HE3	1.98	0.45
4:O:32:ARG:C	4:O:34:GLY:H	2.20	0.45
5:P:306:GLU:O	5:P:310:ILE:HG13	2.17	0.45
1:B:176:ARG:HB3	9:B:9633:HOH:O	2.16	0.45
2:C:404:LEU:HA	2:C:407:LYS:HZ3	1.81	0.45
2:C:650:ARG:HG3	9:C:9988:HOH:O	2.17	0.45
2:C:764:GLU:HG3	9:F:9714:HOH:O	2.16	0.45
2:C:881:ASN:H	2:C:881:ASN:ND2	2.14	0.45
2:C:1014:SER:OG	5:F:331:ASP:HA	2.17	0.45
3:D:161:LEU:O	3:D:449:SER:HB2	2.17	0.45
3:D:1141:GLU:O	3:D:1145:TYR:HB2	2.17	0.45
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.81	0.45
5:F:84:TYR:HD2	5:F:192:LEU:HD13	1.82	0.45
5:F:125:ASP:O	5:F:129:GLU:HG2	2.16	0.45
5:F:151:LEU:HB2	5:F:155:THR:OG1	2.17	0.45
1:K:57:TYR:CD2	1:K:161:ARG:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:35:PRO:HD2	2:M:38:LYS:HG2	1.99	0.45
2:M:742:VAL:HG12	2:M:743:VAL:N	2.32	0.45
2:M:955:PRO:HD3	9:M:9923:HOH:O	2.17	0.45
3:N:133:ILE:HD11	3:N:456:MET:HE3	1.99	0.45
3:N:161:LEU:HG	3:N:449:SER:OG	2.17	0.45
3:N:789:LEU:HD12	3:N:911:LEU:HD21	1.98	0.45
3:N:1000:THR:O	3:N:1003:VAL:HG22	2.17	0.45
3:N:1459:LEU:HB3	3:N:1465:ASN:HD22	1.82	0.45
5:P:77:THR:HA	9:P:1606:HOH:O	2.17	0.45
5:P:150:THR:HG23	5:P:155:THR:CG2	2.46	0.45
2:C:134:ARG:HG3	2:C:393:GLN:O	2.17	0.44
2:C:257:VAL:C	2:C:259:GLY:H	2.21	0.44
2:C:439:CYS:HB2	2:C:541:SER:HB3	1.99	0.44
2:C:895:TYR:HD1	2:C:991:GLN:HE21	1.64	0.44
3:D:12:LEU:HD21	3:D:104:PHE:CE1	2.52	0.44
3:D:35:ARG:HD3	9:D:2024:HOH:O	2.17	0.44
3:D:59:ALA:HB2	9:D:2190:HOH:O	2.17	0.44
3:D:416:ALA:HB3	3:D:417:PRO:HD3	1.99	0.44
3:D:421:LEU:HD12	3:D:435:VAL:CG1	2.47	0.44
3:D:441:ARG:HB3	3:D:443:VAL:HG23	1.98	0.44
3:D:844:ALA:O	3:D:867:ARG:HB3	2.17	0.44
3:D:956:ILE:HB	9:D:2735:HOH:O	2.18	0.44
5:F:153:PRO:CG	5:F:154:LYS:H	2.30	0.44
5:F:295:MET:HA	5:F:295:MET:HE2	1.99	0.44
1:L:49:PRO:HA	1:L:148:VAL:HG12	2.00	0.44
1:L:213:GLN:HG3	9:L:1267:HOH:O	2.17	0.44
2:M:276:LYS:HG3	9:M:9544:HOH:O	2.16	0.44
2:M:927:GLY:HA2	2:M:930:LYS:HZ2	1.81	0.44
3:N:829:VAL:HA	9:N:9979:HOH:O	2.17	0.44
3:N:903:ASP:HA	9:N:9960:HOH:O	2.17	0.44
3:N:1031:ASN:O	3:N:1034:GLN:HB2	2.17	0.44
9:N:9941:HOH:O	5:P:312:GLN:HB3	2.16	0.44
5:P:413:SER:HA	9:P:2117:HOH:O	2.16	0.44
1:A:181:VAL:HG12	9:C:9642:HOH:O	2.18	0.44
2:C:64:LEU:HD13	2:C:359:MET:CG	2.47	0.44
2:C:172:ILE:H	2:C:172:ILE:HD12	1.82	0.44
3:D:177:ALA:CA	3:D:199:LEU:HD13	2.46	0.44
3:D:191:LEU:HD22	3:D:195:VAL:HG11	1.99	0.44
3:D:699:VAL:HB	3:D:716:PHE:O	2.18	0.44
3:D:1149:LEU:HD11	3:D:1160:LEU:HB3	2.00	0.44
3:D:1260:ILE:HG21	9:D:2566:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:54:LEU:HG	4:E:58:PRO:CG	2.47	0.44
5:F:134:LYS:NZ	5:F:160:ASP:HB2	2.31	0.44
5:F:274:THR:O	5:F:278:LEU:HG	2.18	0.44
5:F:371:LEU:HD22	5:F:375:LEU:HD22	1.97	0.44
2:M:34:VAL:CB	2:M:38:LYS:HG3	2.33	0.44
2:M:64:LEU:HD22	2:M:359:MET:CG	2.43	0.44
2:M:301:GLU:HA	9:M:2582:HOH:O	2.17	0.44
2:M:302:VAL:HG13	2:M:303:PHE:N	2.32	0.44
2:M:759:THR:N	9:M:9349:HOH:O	2.44	0.44
2:M:906:PHE:CZ	3:N:1067:VAL:HA	2.52	0.44
2:M:1105:LYS:O	2:M:1107:ASN:N	2.50	0.44
3:N:42:ASP:HB2	9:N:9477:HOH:O	2.16	0.44
3:N:130:SER:HA	3:N:572:ARG:HH12	1.82	0.44
3:N:141:ILE:HD12	3:N:141:ILE:N	2.26	0.44
3:N:472:ALA:HA	9:N:9220:HOH:O	2.18	0.44
3:N:689:ASP:HB3	9:O:1346:HOH:O	2.17	0.44
3:N:724:GLN:HA	9:N:9508:HOH:O	2.17	0.44
3:N:893:GLU:O	3:N:896:ALA:HB3	2.17	0.44
3:N:1109:GLU:CG	3:N:1201:CYS:HA	2.38	0.44
5:P:287:THR:CG2	5:P:289:GLU:HB2	2.43	0.44
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.52	0.44
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.46	0.44
1:B:206:THR:CG2	1:B:209:GLU:H	2.29	0.44
2:C:65:VAL:HG12	2:C:67:ASP:OD1	2.16	0.44
2:C:147:TYR:HE2	2:C:330:ASN:OD1	1.99	0.44
2:C:327:HIS:HE2	2:C:492:ASP:CG	2.21	0.44
2:C:439:CYS:SG	2:C:540:PHE:HB3	2.57	0.44
2:C:492:ASP:HB3	2:C:518:LYS:HD3	1.99	0.44
2:C:742:VAL:HG12	2:C:743:VAL:N	2.31	0.44
2:C:798:GLY:H	2:C:827:VAL:HG11	1.81	0.44
3:D:186:VAL:HG13	3:D:187:LYS:N	2.32	0.44
3:D:789:LEU:HD22	3:D:882:PHE:CE1	2.52	0.44
3:D:881:LEU:HD11	3:D:884:ARG:HH21	1.81	0.44
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.16	0.44
3:D:1068:LEU:O	3:D:1069:GLU:C	2.55	0.44
3:D:1110:ALA:HB1	9:D:2073:HOH:O	2.17	0.44
3:D:1498:ALA:HA	9:E:9588:HOH:O	2.17	0.44
4:E:13:VAL:HG11	4:E:19:LEU:HB2	1.99	0.44
4:E:85:LEU:HA	9:E:9561:HOH:O	2.17	0.44
5:F:300:ASP:O	5:F:304:VAL:HG23	2.17	0.44
1:K:92:PRO:HB2	9:K:1355:HOH:O	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:2274:HOH:O	2:M:865:THR:HG22	2.16	0.44
1:L:132:LEU:HD22	9:L:4720:HOH:O	2.17	0.44
2:M:119:PRO:HB2	9:M:9763:HOH:O	2.16	0.44
2:M:224:GLU:HB3	2:M:227:PHE:CD1	2.52	0.44
2:M:436:GLY:O	2:M:469:THR:HB	2.17	0.44
2:M:918:LEU:HD12	2:M:918:LEU:HA	1.85	0.44
3:N:427:VAL:HG13	9:N:9378:HOH:O	2.16	0.44
3:N:452:ILE:HG21	9:N:9295:HOH:O	2.17	0.44
3:N:481:MET:SD	3:N:1388:ARG:HG2	2.57	0.44
3:N:549:ASN:ND2	5:P:254:GLN:HE21	2.16	0.44
3:N:712:GLY:HA3	9:N:2395:HOH:O	2.16	0.44
1:B:86:VAL:HG23	9:B:9660:HOH:O	2.17	0.44
1:B:169:ALA:HB1	1:B:171:PHE:CE2	2.52	0.44
2:C:127:PHE:O	2:C:133:ASP:HA	2.17	0.44
2:C:209:ARG:O	2:C:213:ALA:HB2	2.17	0.44
2:C:254:VAL:HG22	2:C:258:TYR:HE1	1.81	0.44
2:C:480:THR:HG22	2:C:482:GLU:H	1.83	0.44
2:C:516:ARG:NH1	3:D:1068:LEU:HD22	2.32	0.44
2:C:631:SER:HB3	2:C:637:LEU:HD22	2.00	0.44
2:C:816:LYS:O	2:C:819:VAL:HB	2.18	0.44
2:C:926:PHE:O	2:C:929:ARG:HB2	2.17	0.44
2:C:930:LYS:HD3	2:C:960:GLU:OE1	2.18	0.44
3:D:210:ARG:HG3	9:D:9645:HOH:O	2.17	0.44
3:D:422:ALA:O	3:D:427:VAL:HG21	2.18	0.44
3:D:450:TYR:HB3	9:D:2159:HOH:O	2.17	0.44
3:D:500:ARG:HH22	3:D:1388:ARG:NE	2.15	0.44
3:D:814:ALA:HB2	9:D:2210:HOH:O	2.17	0.44
3:D:1344:VAL:HG11	3:D:1421:LEU:HD22	2.00	0.44
5:F:291:ILE:HG23	5:F:292:ALA:N	2.32	0.44
1:K:12:THR:HG21	9:K:1709:HOH:O	2.16	0.44
1:K:133:GLU:N	9:K:1268:HOH:O	2.50	0.44
2:M:418:LEU:HB2	9:M:2268:HOH:O	2.16	0.44
2:M:928:LYS:HA	2:M:928:LYS:HE2	1.99	0.44
2:M:1015:LEU:HA	5:P:335:ASP:HB2	1.99	0.44
3:N:427:VAL:HB	3:N:435:VAL:CG2	2.48	0.44
3:N:500:ARG:HG3	3:N:500:ARG:NH1	2.33	0.44
3:N:864:VAL:HG12	3:N:865:THR:H	1.82	0.44
3:N:983:LEU:HD13	9:N:9836:HOH:O	2.17	0.44
5:P:113:ILE:HD12	9:P:4659:HOH:O	2.18	0.44
1:A:95:GLN:HB3	9:A:9602:HOH:O	2.17	0.44
9:A:9736:HOH:O	1:B:156:HIS:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ILE:HA	1:B:82:LEU:HD12	2.00	0.44
1:B:206:THR:HG22	1:B:209:GLU:CG	2.48	0.44
2:C:45:GLN:NE2	9:C:2296:HOH:O	2.49	0.44
2:C:188:LYS:C	2:C:188:LYS:HD3	2.37	0.44
2:C:321:GLU:HG3	9:C:2328:HOH:O	2.18	0.44
2:C:560:MET:O	2:C:564:MET:HB2	2.17	0.44
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.47	0.44
2:C:899:GLN:HA	9:C:2768:HOH:O	2.17	0.44
3:D:186:VAL:HG23	3:D:211:VAL:CG1	2.48	0.44
3:D:907:GLU:O	3:D:911:LEU:HD13	2.18	0.44
3:D:1341:PRO:HA	3:D:1344:VAL:CG2	2.46	0.44
3:D:1382:THR:O	3:D:1384:PRO:HD3	2.17	0.44
3:D:1393:GLN:HB3	9:D:9676:HOH:O	2.17	0.44
4:E:50:THR:HG23	9:E:9582:HOH:O	2.16	0.44
1:K:30:ARG:HH22	1:L:155:LYS:NZ	2.16	0.44
1:K:83:LYS:HD3	9:K:2976:HOH:O	2.18	0.44
1:L:113:ASP:HA	9:L:1552:HOH:O	2.18	0.44
2:M:8:ARG:HG3	9:M:9876:HOH:O	2.17	0.44
2:M:21:ILE:HD12	2:M:21:ILE:N	2.30	0.44
2:M:49:ARG:HB2	9:M:9976:HOH:O	2.17	0.44
2:M:432:ARG:HH11	2:M:432:ARG:HG3	1.82	0.44
2:M:479:VAL:CG2	2:M:503:LEU:HD11	2.47	0.44
2:M:598:GLU:N	9:M:9609:HOH:O	2.50	0.44
2:M:777:ILE:HG22	2:M:778:PHE:N	2.31	0.44
2:M:860:HIS:CE1	2:M:977:GLY:HA2	2.51	0.44
2:M:1008:ARG:HG2	2:M:1008:ARG:HH11	1.82	0.44
2:M:1067:TYR:CD2	5:P:345:ALA:HB2	2.53	0.44
2:M:1095:LEU:HD23	3:N:582:LEU:HD23	1.99	0.44
3:N:101:HIS:CD2	3:N:582:LEU:HD22	2.52	0.44
3:N:192:ALA:HB3	9:N:9235:HOH:O	2.18	0.44
3:N:513:ILE:H	3:N:513:ILE:HG13	1.65	0.44
3:N:619:LEU:O	3:N:619:LEU:HD23	2.18	0.44
3:N:767:HIS:C	3:N:768:ASN:HD22	2.20	0.44
3:N:796:ARG:NE	3:N:828:LYS:HZ3	2.15	0.44
3:N:808:THR:HB	3:N:809:PRO:HD3	1.98	0.44
3:N:1003:VAL:O	3:N:1006:ALA:HB3	2.18	0.44
3:N:1277:ILE:CG2	3:N:1278:ASP:N	2.80	0.44
1:B:10:VAL:HA	9:B:9606:HOH:O	2.17	0.44
2:C:811:PRO:HD2	2:C:813:VAL:HG13	1.99	0.44
3:D:87:ARG:HD2	3:D:88:TYR:CE2	2.53	0.44
3:D:470:LEU:HB3	3:D:503:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:835:SER:HB3	9:D:2297:HOH:O	2.16	0.44
4:E:23:VAL:HG11	9:E:9593:HOH:O	2.18	0.44
1:K:31:GLY:N	1:K:193:ASP:OD1	2.51	0.44
1:K:42:ARG:CZ	9:K:4396:HOH:O	2.65	0.44
1:K:189:ARG:HG2	1:K:190:THR:N	2.33	0.44
1:L:77:GLU:HG3	9:N:2080:HOH:O	2.18	0.44
2:M:31:GLN:HB3	2:M:31:GLN:HE21	1.50	0.44
2:M:492:ASP:HA	9:M:9579:HOH:O	2.18	0.44
2:M:563:ASN:HA	9:M:9240:HOH:O	2.16	0.44
2:M:676:ILE:HG22	2:M:988:VAL:O	2.17	0.44
2:M:799:ILE:O	2:M:801:VAL:HG13	2.17	0.44
2:M:860:HIS:HA	2:M:866:PRO:HA	1.99	0.44
2:M:893:ALA:O	2:M:897:LEU:HB2	2.16	0.44
2:M:1085:PHE:O	2:M:1089:VAL:HG23	2.17	0.44
3:N:38:LYS:HG3	9:N:9685:HOH:O	2.16	0.44
3:N:85:VAL:O	3:N:89:ARG:HG3	2.18	0.44
3:N:768:ASN:HD22	3:N:768:ASN:N	2.15	0.44
3:N:1417:TRP:HD1	9:N:9725:HOH:O	2.00	0.44
4:O:70:THR:HG22	4:O:71:GLY:H	1.83	0.44
5:P:266:GLU:HB2	5:P:270:LYS:HZ3	1.80	0.44
1:B:26:GLU:CB	1:B:194:LYS:HG3	2.48	0.44
2:C:584:GLU:HB2	2:C:666:LEU:H	1.83	0.44
2:C:607:ASP:HB2	2:C:610:ARG:H	1.81	0.44
2:C:639:GLN:HB3	2:C:656:ALA:HB1	2.00	0.44
2:C:1021:LEU:HD13	5:F:331:ASP:O	2.18	0.44
2:C:1067:TYR:CE1	2:C:1071:ILE:HD11	2.52	0.44
3:D:168:THR:HG22	3:D:170:PRO:HD3	2.00	0.44
3:D:563:PRO:HG3	5:F:188:ILE:CG2	2.47	0.44
3:D:986:ARG:HB2	3:D:986:ARG:HH11	1.83	0.44
3:D:1470:ARG:HG2	3:D:1471:LEU:N	2.32	0.44
4:E:91:ARG:CZ	9:E:9574:HOH:O	2.66	0.44
1:K:41:ARG:HH11	1:K:41:ARG:HG3	1.83	0.44
1:K:97:VAL:HG11	1:K:120:VAL:HG21	1.99	0.44
1:L:14:ARG:HH22	1:L:24:VAL:CG2	2.31	0.44
1:L:80:LEU:HD13	3:N:842:VAL:CG1	2.42	0.44
2:M:288:ARG:HH12	2:M:289:THR:HG23	1.82	0.44
2:M:338:GLU:HA	2:M:341:THR:CG2	2.44	0.44
2:M:545:ASN:HD21	2:M:905:ILE:HG13	1.82	0.44
3:N:12:LEU:CD2	3:N:13:ALA:H	2.30	0.44
3:N:18:ILE:HG21	3:N:516:ALA:O	2.17	0.44
3:N:138:LYS:H	3:N:138:LYS:CD	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:441:ARG:HD2	9:N:9328:HOH:O	2.18	0.44
3:N:895:VAL:O	3:N:899:LEU:HD12	2.17	0.44
3:N:994:GLN:HE21	3:N:998:GLU:CD	2.20	0.44
3:N:1162:GLU:HB3	9:N:9990:HOH:O	2.18	0.44
3:N:1384:PRO:HG3	3:N:1389:LEU:N	2.33	0.44
3:N:1487:VAL:CG1	3:N:1488:ASP:N	2.81	0.44
5:P:339:PRO:HA	9:P:1420:HOH:O	2.18	0.44
2:C:250:ARG:HD2	9:C:2643:HOH:O	2.17	0.44
2:C:456:ALA:HA	2:C:541:SER:HA	1.98	0.44
2:C:517:ARG:O	2:C:519:GLY:N	2.51	0.44
2:C:913:GLU:HB3	9:C:2225:HOH:O	2.17	0.44
2:C:1052:MET:HG3	3:D:623:VAL:HG21	1.98	0.44
3:D:36:THR:O	3:D:38:LYS:N	2.50	0.44
3:D:82:LYS:O	3:D:84:ILE:N	2.51	0.44
3:D:116:LEU:HB3	3:D:118:LEU:CD1	2.44	0.44
3:D:130:SER:CB	3:D:572:ARG:HH12	2.30	0.44
3:D:697:GLY:HA3	4:E:59:ASN:OD1	2.17	0.44
3:D:937:TYR:HA	3:D:940:THR:OG1	2.18	0.44
3:D:964:LEU:O	3:D:968:ASP:HB2	2.18	0.44
3:D:1044:LEU:N	9:D:2029:HOH:O	2.51	0.44
3:D:1101:VAL:CG1	3:D:1427:SER:HB3	2.46	0.44
4:E:51:LEU:HD21	9:E:9611:HOH:O	2.17	0.44
5:F:111:GLU:O	5:F:115:LYS:HG3	2.18	0.44
1:K:72:LYS:HZ1	2:M:644:VAL:HG12	1.82	0.44
1:L:176:ARG:HH22	3:N:884:ARG:HE	1.65	0.44
2:M:303:PHE:HZ	9:M:2121:HOH:O	2.00	0.44
2:M:872:ASN:OD1	2:M:874:LEU:N	2.47	0.44
2:M:1081:VAL:HB	2:M:1086:ARG:NE	2.32	0.44
3:N:70:GLY:C	3:N:71:LYS:HD2	2.38	0.44
3:N:196:VAL:HG13	3:N:202:VAL:CG1	2.47	0.44
3:N:396:VAL:HG13	3:N:447:VAL:HA	2.00	0.44
3:N:421:LEU:HD11	3:N:437:VAL:HG22	1.99	0.44
3:N:566:ILE:HG12	5:P:217:ASN:HD22	1.83	0.44
3:N:606:ILE:HG21	9:N:2854:HOH:O	2.18	0.44
3:N:1145:TYR:HA	9:N:2585:HOH:O	2.17	0.44
3:N:1192:LEU:N	9:N:9676:HOH:O	2.50	0.44
3:N:1397:LYS:HG2	9:N:2363:HOH:O	2.17	0.44
4:O:70:THR:HG22	4:O:71:GLY:N	2.33	0.44
2:C:129:ILE:HG22	2:C:130:ASN:H	1.83	0.44
2:C:167:LYS:C	2:C:169:GLY:H	2.21	0.44
2:C:365:ASP:O	2:C:367:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:440:PRO:HD2	9:C:2264:HOH:O	2.18	0.44
2:C:720:GLU:HA	2:C:759:THR:O	2.18	0.44
2:C:749:VAL:HG23	2:C:749:VAL:O	2.18	0.44
2:C:789:SER:HB2	9:C:9581:HOH:O	2.18	0.44
2:C:823:VAL:HG22	9:C:9907:HOH:O	2.18	0.44
2:C:896:PHE:HB2	9:C:2761:HOH:O	2.18	0.44
2:C:929:ARG:HG3	2:C:929:ARG:NH1	2.33	0.44
3:D:171:LEU:HD11	3:D:388:HIS:CB	2.48	0.44
3:D:395:VAL:O	3:D:395:VAL:HG12	2.18	0.44
3:D:953:ASP:OD1	3:D:1019:PRO:HG2	2.18	0.44
3:D:1036:ARG:NH1	9:D:9667:HOH:O	2.51	0.44
3:D:1197:ARG:HG3	3:D:1198:TYR:N	2.33	0.44
3:D:1244:GLY:HA3	9:D:2849:HOH:O	2.17	0.44
5:F:187:LEU:HD23	5:F:191:ASN:HD22	1.82	0.44
5:F:259:ARG:HG2	5:F:259:ARG:NH1	2.32	0.44
5:F:315:VAL:HG12	5:F:316:SER:H	1.83	0.44
5:F:353:GLU:HA	9:F:9676:HOH:O	2.17	0.44
1:K:227:ASN:HB2	9:K:1432:HOH:O	2.17	0.44
2:M:31:GLN:NE2	2:M:34:VAL:HG23	2.33	0.44
2:M:31:GLN:OE1	2:M:40:GLU:HB2	2.16	0.44
2:M:50:GLU:OE2	2:M:345:ARG:HD2	2.18	0.44
2:M:130:ASN:HB3	9:M:9773:HOH:O	2.18	0.44
2:M:272:ALA:HB1	9:M:9251:HOH:O	2.17	0.44
2:M:588:VAL:HG23	2:M:596:TYR:OH	2.18	0.44
2:M:747:ALA:HB1	9:M:9356:HOH:O	2.17	0.44
2:M:798:GLY:H	2:M:827:VAL:HG11	1.82	0.44
3:N:196:VAL:HG13	3:N:202:VAL:HG13	1.99	0.44
3:N:205:TYR:N	3:N:205:TYR:CD1	2.86	0.44
3:N:1147:ARG:HD2	3:N:1188:VAL:CG2	2.48	0.44
3:N:1281:VAL:HG21	3:N:1313:VAL:CG2	2.48	0.44
3:N:1459:LEU:HD13	3:N:1465:ASN:HA	1.99	0.44
5:P:361:LEU:HD21	5:P:408:LEU:HB2	1.99	0.44
1:A:85:LEU:HD12	1:A:124:ASN:HB3	2.00	0.43
1:B:85:LEU:HD12	1:B:124:ASN:HB3	2.00	0.43
2:C:610:ARG:HD2	9:C:9662:HOH:O	2.18	0.43
2:C:773:LEU:HA	9:C:9824:HOH:O	2.18	0.43
2:C:774:LEU:O	2:C:777:ILE:HB	2.18	0.43
2:C:781:LYS:HD2	9:C:9791:HOH:O	2.17	0.43
2:C:860:HIS:HA	2:C:866:PRO:HA	1.99	0.43
2:C:941:VAL:O	2:C:944:LEU:HB2	2.18	0.43
2:C:1101:THR:C	2:C:1102:LEU:HD12	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:34:TYR:CD1	3:D:35:ARG:N	2.86	0.43
3:D:154:THR:HG22	3:D:155:ASP:N	2.32	0.43
3:D:562:ALA:CB	3:D:567:ILE:HD11	2.40	0.43
3:D:653:PHE:CD1	3:D:653:PHE:N	2.86	0.43
3:D:767:HIS:C	3:D:768:ASN:HD22	2.22	0.43
3:D:966:GLU:HG3	9:D:2760:HOH:O	2.17	0.43
3:D:1136:LYS:HB2	3:D:1139:ASP:OD2	2.18	0.43
3:D:1314:LYS:HE2	9:D:3278:HOH:O	2.18	0.43
3:D:1394:VAL:CG2	3:D:1397:LYS:HD2	2.47	0.43
4:E:29:GLN:HG3	9:E:9594:HOH:O	2.18	0.43
5:F:113:ILE:HG23	5:F:127:ILE:CB	2.46	0.43
5:F:288:TYR:CE2	5:F:305:GLU:HA	2.52	0.43
2:M:192:PRO:HB3	2:M:194:VAL:HG23	1.99	0.43
2:M:286:SER:HB3	2:M:299:LYS:CE	2.47	0.43
2:M:292:ARG:HE	2:M:299:LYS:HZ2	1.65	0.43
2:M:520:GLU:HA	2:M:521:PRO:HD3	1.76	0.43
2:M:768:THR:HG23	9:M:9276:HOH:O	2.17	0.43
2:M:918:LEU:HD23	2:M:968:LEU:O	2.17	0.43
3:N:65:ARG:HD3	3:N:66:GLN:N	2.31	0.43
3:N:126:VAL:HG23	9:N:9692:HOH:O	2.18	0.43
3:N:142:LEU:HB3	9:N:9595:HOH:O	2.17	0.43
3:N:172:PRO:CG	3:N:178:LEU:HD22	2.40	0.43
3:N:729:HIS:CE1	3:N:935:LYS:HD3	2.52	0.43
3:N:984:THR:HB	3:N:987:GLU:OE1	2.18	0.43
3:N:1326:THR:HG21	9:N:2275:HOH:O	2.18	0.43
3:N:1412:LYS:C	3:N:1414:PRO:HD3	2.39	0.43
5:P:222:ARG:HD2	5:P:242:TRP:CE3	2.54	0.43
2:C:183:SER:HA	2:C:190:LYS:HB2	1.99	0.43
2:C:250:ARG:HH21	2:C:254:VAL:N	2.14	0.43
2:C:431:HIS:CD2	2:C:433:THR:H	2.36	0.43
2:C:614:ARG:HG3	9:C:9611:HOH:O	2.18	0.43
3:D:395:VAL:HB	9:D:9923:HOH:O	2.18	0.43
3:D:1063:GLU:HG2	3:D:1064:GLY:N	2.29	0.43
3:D:1209:LEU:HD11	4:E:16:LYS:NZ	2.33	0.43
3:D:1374:GLN:OE1	3:D:1377:LYS:HD3	2.18	0.43
3:D:1499:ARG:HB3	9:D:2661:HOH:O	2.18	0.43
4:E:70:THR:HG22	4:E:71:GLY:N	2.33	0.43
5:F:164:LYS:HD2	9:F:9652:HOH:O	2.18	0.43
5:F:207:LEU:HD12	5:F:212:LEU:CD2	2.48	0.43
5:F:404:ALA:O	5:F:408:LEU:HB2	2.19	0.43
1:K:11:PHE:HB2	9:L:2122:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:78:ILE:O	1:L:82:LEU:HG	2.18	0.43
1:L:106:PRO:HA	1:L:132:LEU:O	2.18	0.43
2:M:208:ALA:HB3	2:M:209:ARG:HH21	1.83	0.43
2:M:243:ARG:HB3	9:M:9892:HOH:O	2.18	0.43
2:M:444:PRO:CD	2:M:452:ILE:HG13	2.48	0.43
2:M:554:ASP:OD2	2:M:556:ASN:HB3	2.18	0.43
2:M:1013:TYR:HE1	2:M:1020:PRO:HG3	1.83	0.43
2:M:1015:LEU:HD12	5:P:333:ILE:CG2	2.48	0.43
2:M:1031:ARG:HA	3:N:621:LYS:O	2.17	0.43
3:N:471:GLU:HG2	9:N:9786:HOH:O	2.17	0.43
3:N:647:ARG:HH12	3:N:680:GLN:HG3	1.82	0.43
3:N:759:ALA:O	3:N:763:MET:HB3	2.18	0.43
3:N:822:ALA:HB2	9:N:9525:HOH:O	2.18	0.43
3:N:962:GLN:HA	9:N:9569:HOH:O	2.17	0.43
3:N:995:LEU:HA	3:N:998:GLU:OE1	2.18	0.43
3:N:1046:GLN:CA	3:N:1052:THR:HA	2.37	0.43
3:N:1273:VAL:O	3:N:1325:LEU:HB2	2.18	0.43
3:N:1303:TYR:HA	9:N:9699:HOH:O	2.18	0.43
5:P:192:LEU:HB3	9:P:4506:HOH:O	2.18	0.43
1:A:97:VAL:HG11	1:A:120:VAL:HG21	1.99	0.43
1:B:83:LYS:HE2	1:B:167:VAL:HG12	2.00	0.43
2:C:12:VAL:CG1	2:C:534:VAL:HG13	2.48	0.43
2:C:115:LEU:HD12	2:C:378:LEU:CD2	2.48	0.43
2:C:244:PRO:HD2	2:C:245:GLY:N	2.23	0.43
2:C:840:ALA:HB2	2:C:846:LYS:HG3	1.99	0.43
2:C:971:LYS:HG2	2:C:988:VAL:N	2.33	0.43
3:D:719:VAL:HG11	9:D:9572:HOH:O	2.17	0.43
3:D:1363:LEU:HD12	3:D:1363:LEU:O	2.19	0.43
3:D:1406:ARG:NE	3:D:1412:LYS:HB3	2.33	0.43
3:D:1425:THR:HB	9:D:9596:HOH:O	2.17	0.43
3:D:1481:VAL:HG12	4:E:21:VAL:HG21	1.99	0.43
4:E:48:MET:HB2	4:E:54:LEU:HD12	2.01	0.43
1:K:1:MET:O	1:K:6:LEU:HD22	2.18	0.43
1:K:24:VAL:HG22	1:K:196:THR:OG1	2.18	0.43
1:K:30:ARG:HD2	9:K:1388:HOH:O	2.17	0.43
1:K:112:ARG:NH1	9:K:3292:HOH:O	2.50	0.43
2:M:204:GLN:HE22	2:M:225:SER:HA	1.84	0.43
2:M:569:VAL:O	2:M:571:LEU:HD12	2.17	0.43
2:M:597:ALA:O	2:M:652:GLY:N	2.50	0.43
2:M:981:GLU:HA	9:M:9308:HOH:O	2.19	0.43
3:N:380:GLU:HA	9:N:9923:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:660:LYS:HD2	3:N:694:VAL:HG22	1.99	0.43
3:N:759:ALA:HA	3:N:763:MET:HE1	2.00	0.43
3:N:873:LEU:HD23	9:N:2208:HOH:O	2.18	0.43
4:O:53:GLY:HA3	9:O:4631:HOH:O	2.17	0.43
5:P:94:LEU:H	5:P:98:GLU:HB2	1.83	0.43
5:P:289:GLU:HG2	9:P:4194:HOH:O	2.18	0.43
1:B:17:GLY:C	1:B:19:GLU:H	2.21	0.43
2:C:336:VAL:HA	2:C:339:LEU:HD12	2.00	0.43
2:C:802:ARG:HB2	9:C:9590:HOH:O	2.17	0.43
2:C:869:VAL:HG22	2:C:871:LEU:CD1	2.48	0.43
2:C:881:ASN:HD22	2:C:881:ASN:N	2.12	0.43
3:D:107:ASP:O	3:D:108:VAL:C	2.56	0.43
3:D:123:LEU:O	3:D:126:VAL:HB	2.19	0.43
3:D:193:PRO:HG3	9:D:3106:HOH:O	2.17	0.43
3:D:1310:ARG:HE	3:D:1310:ARG:HB2	1.69	0.43
1:K:60:ASP:HA	9:K:3216:HOH:O	2.19	0.43
2:M:93:PRO:HB2	9:M:9852:HOH:O	2.19	0.43
2:M:103:LYS:HG3	9:M:2256:HOH:O	2.19	0.43
2:M:163:ILE:HG23	2:M:163:ILE:O	2.17	0.43
2:M:250:ARG:HB2	2:M:253:ALA:CB	2.49	0.43
2:M:305:PRO:O	2:M:308:ARG:HB3	2.18	0.43
2:M:498:GLN:CG	2:M:516:ARG:HE	2.31	0.43
2:M:999:HIS:HB3	2:M:1003:ASP:OD2	2.18	0.43
2:M:1105:LYS:HE3	9:M:9940:HOH:O	2.17	0.43
3:N:1147:ARG:H	3:N:1166:LEU:HG	1.83	0.43
5:P:276:ARG:HD2	9:P:2013:HOH:O	2.16	0.43
2:C:27:ARG:HG3	9:C:9641:HOH:O	2.19	0.43
2:C:73:LEU:HB2	9:C:2521:HOH:O	2.19	0.43
2:C:139:GLN:HG2	2:C:140:ILE:H	1.83	0.43
2:C:144:PRO:HA	2:C:163:ILE:O	2.19	0.43
2:C:256:TYR:HA	9:C:2199:HOH:O	2.17	0.43
2:C:1014:SER:HA	5:F:333:ILE:O	2.18	0.43
2:C:1034:GLU:HG3	2:C:1035:MET:H	1.83	0.43
3:D:460:ALA:O	3:D:464:LEU:HG	2.18	0.43
3:D:474:GLU:HG3	3:D:500:ARG:NE	2.32	0.43
3:D:523:ASP:HA	9:D:9853:HOH:O	2.18	0.43
3:D:850:LEU:O	3:D:853:VAL:HB	2.18	0.43
3:D:925:GLU:O	3:D:928:ALA:HB3	2.18	0.43
3:D:994:GLN:HE21	3:D:998:GLU:CD	2.21	0.43
3:D:1197:ARG:HG2	9:D:2561:HOH:O	2.18	0.43
3:D:1302:GLU:HG2	9:D:2309:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1397:LYS:HE2	9:D:3297:HOH:O	2.17	0.43
4:E:45:ARG:HB3	9:E:9659:HOH:O	2.18	0.43
5:F:260:ILE:HG12	5:F:264:MET:HB2	2.01	0.43
5:F:273:ARG:HB3	9:F:9601:HOH:O	2.18	0.43
1:K:139:ASN:HB2	9:K:2209:HOH:O	2.18	0.43
1:K:176:ARG:NH1	9:K:2274:HOH:O	2.50	0.43
2:M:14:PRO:HG3	9:M:2533:HOH:O	2.18	0.43
2:M:54:ILE:HD11	2:M:56:GLU:OE2	2.18	0.43
2:M:575:GLN:HA	2:M:662:GLU:HG3	2.00	0.43
2:M:811:PRO:HG3	9:M:9687:HOH:O	2.17	0.43
2:M:1001:VAL:HG13	9:M:9394:HOH:O	2.17	0.43
3:N:30:GLU:HB3	3:N:40:GLU:CB	2.48	0.43
3:N:441:ARG:O	3:N:443:VAL:N	2.47	0.43
3:N:459:GLU:OE2	5:P:144:ILE:HD12	2.19	0.43
3:N:719:VAL:O	3:N:721:VAL:HG13	2.18	0.43
3:N:1225:ALA:O	3:N:1229:ILE:HG13	2.18	0.43
3:N:1283:ILE:HG22	3:N:1284:GLU:N	2.34	0.43
5:P:253:ASP:HA	5:P:259:ARG:HE	1.83	0.43
5:P:356:LYS:O	5:P:360:LYS:HG2	2.18	0.43
1:B:50:GLY:HA2	9:B:9569:HOH:O	2.18	0.43
1:B:86:VAL:HA	9:B:9736:HOH:O	2.18	0.43
2:C:218:VAL:HB	9:C:2262:HOH:O	2.18	0.43
2:C:671:ASN:ND2	2:C:993:PHE:HD2	2.16	0.43
2:C:897:LEU:HB2	9:C:9860:HOH:O	2.17	0.43
3:D:101:HIS:CD2	3:D:103:TRP:HB2	2.53	0.43
3:D:101:HIS:CD2	3:D:582:LEU:HD13	2.53	0.43
3:D:209:ARG:HB3	3:D:210:ARG:H	1.62	0.43
3:D:380:GLU:O	3:D:382:GLU:N	2.51	0.43
3:D:442:ASN:HA	9:D:2613:HOH:O	2.19	0.43
3:D:787:LEU:HD21	3:D:947:ILE:CD1	2.36	0.43
3:D:1333:HIS:O	3:D:1336:LEU:HB3	2.19	0.43
4:E:50:THR:HA	9:E:9570:HOH:O	2.19	0.43
5:F:329:TYR:O	5:F:332:PHE:HB2	2.19	0.43
5:F:387:GLY:HA2	9:F:9617:HOH:O	2.18	0.43
5:F:406:ARG:HA	5:F:409:LYS:HD3	2.01	0.43
1:K:83:LYS:HZ1	1:K:168:ASP:HB2	1.84	0.43
2:M:247:PRO:HA	2:M:248:PRO:HD3	1.89	0.43
2:M:627:ARG:HD3	9:M:2410:HOH:O	2.18	0.43
2:M:755:LEU:HD21	2:M:792:VAL:HG22	2.01	0.43
2:M:1086:ARG:NH1	9:M:9565:HOH:O	2.52	0.43
3:N:14:SER:OG	3:N:17:LYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:422:ALA:HB2	9:N:9378:HOH:O	2.18	0.43
3:N:796:ARG:NE	3:N:862:ASP:OD2	2.51	0.43
3:N:812:ALA:O	3:N:816:HIS:HB2	2.19	0.43
3:N:863:VAL:HA	9:N:9938:HOH:O	2.18	0.43
3:N:1080:GLY:O	3:N:1084:THR:HG23	2.19	0.43
3:N:1161:GLU:HB3	9:N:9583:HOH:O	2.17	0.43
3:N:1320:GLU:N	3:N:1323:GLN:NE2	2.67	0.43
3:N:1357:ARG:HB3	9:N:2893:HOH:O	2.18	0.43
5:P:288:TYR:HE2	5:P:305:GLU:HA	1.84	0.43
1:A:201:THR:HG22	1:A:203:GLY:H	1.82	0.43
2:C:95:TYR:HE2	9:C:9699:HOH:O	2.01	0.43
2:C:165:LEU:HB2	9:C:2287:HOH:O	2.18	0.43
2:C:188:LYS:HE2	9:C:2731:HOH:O	2.18	0.43
2:C:358:ARG:HH12	2:C:374:ASN:CG	2.21	0.43
2:C:474:VAL:HB	2:C:479:VAL:HG12	1.99	0.43
2:C:534:VAL:N	2:C:538:GLN:NE2	2.67	0.43
3:D:137:PRO:HD2	3:D:453:ASP:CB	2.49	0.43
3:D:231:VAL:HA	3:D:378:ILE:CB	2.49	0.43
3:D:484:PRO:HG3	9:D:3258:HOH:O	2.18	0.43
3:D:806:PHE:N	9:D:2133:HOH:O	2.50	0.43
3:D:960:LYS:HG2	3:D:964:LEU:CD1	2.49	0.43
3:D:968:ASP:O	3:D:971:LEU:HB3	2.19	0.43
3:D:1096:ARG:NH1	3:D:1096:ARG:HB2	2.33	0.43
9:D:2183:HOH:O	5:F:349:LEU:HD13	2.19	0.43
9:D:2199:HOH:O	4:E:58:PRO:HA	2.19	0.43
4:E:45:ARG:HH22	4:E:72:ARG:HH21	1.66	0.43
5:F:142:ARG:HG3	9:F:2143:HOH:O	2.19	0.43
5:F:153:PRO:O	5:F:157:GLU:HG3	2.18	0.43
5:F:402:ASN:HB3	9:F:9689:HOH:O	2.17	0.43
5:F:419:ARG:HA	9:F:9727:HOH:O	2.18	0.43
1:L:47:SER:CB	1:L:217:ILE:HD13	2.48	0.43
1:L:55:SER:HB2	1:L:158:ILE:HB	2.01	0.43
1:L:176:ARG:HG3	1:L:200:TRP:CE3	2.53	0.43
1:L:227:ASN:HB2	9:L:1651:HOH:O	2.19	0.43
2:M:1085:PHE:HE1	2:M:1111:ILE:HG21	1.83	0.43
3:N:19:ARG:HH21	3:N:94:GLU:CD	2.21	0.43
3:N:137:PRO:HG2	9:N:2197:HOH:O	2.18	0.43
3:N:447:VAL:HG23	3:N:448:GLU:N	2.34	0.43
3:N:684:LYS:HE3	9:N:2460:HOH:O	2.18	0.43
3:N:792:ILE:HG23	3:N:793:THR:N	2.32	0.43
3:N:1103:HIS:HA	3:N:1223:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:6:ILE:HG23	4:O:7:ASP:N	2.33	0.43
5:P:333:ILE:HA	5:P:334:PRO:HD3	1.86	0.43
1:A:224:TYR:HB3	1:B:9:PRO:HB2	1.99	0.43
2:C:1:MET:N	9:C:9648:HOH:O	2.52	0.43
2:C:64:LEU:HB2	2:C:359:MET:SD	2.59	0.43
2:C:274:ARG:N	2:C:288:ARG:HH22	2.17	0.43
2:C:279:GLU:HG3	2:C:493:ARG:NH2	2.33	0.43
2:C:396:ASP:OD1	2:C:402:SER:HB3	2.18	0.43
2:C:520:GLU:HB2	9:C:9578:HOH:O	2.19	0.43
2:C:607:ASP:C	2:C:609:ASN:N	2.71	0.43
2:C:679:PHE:C	3:D:943:THR:HG22	2.38	0.43
2:C:773:LEU:HD21	5:F:354:LEU:HD11	2.00	0.43
2:C:861:LEU:HD21	2:C:925:TYR:CE1	2.54	0.43
3:D:155:ASP:HB3	9:D:2347:HOH:O	2.18	0.43
3:D:1431:THR:HB	3:D:1432:LYS:HE3	1.99	0.43
4:E:23:VAL:HG13	4:E:24:ALA:N	2.34	0.43
4:E:68:LEU:HA	4:E:73:LEU:HD12	2.00	0.43
5:F:291:ILE:CG2	5:F:304:VAL:HG21	2.48	0.43
1:K:88:ARG:NH2	9:K:1273:HOH:O	2.51	0.43
1:K:224:TYR:CD1	1:L:9:PRO:HD2	2.54	0.43
1:L:152:PRO:HB2	1:L:155:LYS:HG3	2.01	0.43
2:M:21:ILE:H	2:M:21:ILE:CD1	2.30	0.43
2:M:42:VAL:HG13	2:M:268:ASP:OD2	2.18	0.43
2:M:750:LYS:HG2	9:M:2076:HOH:O	2.18	0.43
2:M:790:LEU:HD12	2:M:790:LEU:HA	1.91	0.43
2:M:854:PRO:HB2	2:M:856:GLU:HB2	2.00	0.43
2:M:958:THR:HB	9:M:2134:HOH:O	2.18	0.43
2:M:1049:LEU:HD23	3:N:1472:ILE:HD11	2.00	0.43
2:M:1086:ARG:NH1	3:N:88:TYR:CZ	2.87	0.43
3:N:227:LEU:HA	9:P:1787:HOH:O	2.18	0.43
3:N:380:GLU:O	3:N:382:GLU:N	2.49	0.43
3:N:549:ASN:HD22	3:N:549:ASN:HA	1.65	0.43
3:N:601:ARG:CZ	3:N:613:ARG:HH21	2.31	0.43
3:N:1166:LEU:HD23	3:N:1166:LEU:N	2.27	0.43
4:O:47:LYS:C	4:O:54:LEU:HD13	2.39	0.43
5:P:83:GLN:O	5:P:86:HIS:HB2	2.19	0.43
5:P:138:SER:N	9:P:2295:HOH:O	2.52	0.43
5:P:309:LYS:HG3	9:P:5453:HOH:O	2.19	0.43
5:P:324:GLU:O	5:P:325:LYS:HD3	2.18	0.43
5:P:342:VAL:HG23	5:P:343:ASP:N	2.34	0.43
5:P:411:HIS:HB3	9:P:2127:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:O	1:A:12:THR:HG23	2.18	0.43
1:A:100:LEU:HD11	9:A:9576:HOH:O	2.18	0.43
1:B:1:MET:SD	1:B:5:LYS:HG2	2.59	0.43
2:C:549:PHE:HE2	2:C:887:GLU:HA	1.83	0.43
2:C:1083:GLU:OE1	2:C:1083:GLU:HA	2.17	0.43
3:D:396:VAL:CG2	3:D:447:VAL:HB	2.48	0.43
3:D:402:PRO:HG2	3:D:444:VAL:HG11	2.01	0.43
3:D:414:ARG:HH11	3:D:414:ARG:HG3	1.82	0.43
3:D:434:ARG:HB2	3:D:447:VAL:CG1	2.47	0.43
3:D:965:GLU:O	3:D:968:ASP:HB3	2.18	0.43
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.54	0.43
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.54	0.43
5:F:100:VAL:HG21	9:F:9872:HOH:O	2.17	0.43
5:F:151:LEU:O	5:F:155:THR:HB	2.19	0.43
5:F:155:THR:HG22	5:F:156:VAL:N	2.33	0.43
2:M:93:PRO:HG3	9:M:9555:HOH:O	2.19	0.43
2:M:160:ALA:CB	2:M:174:LEU:HD12	2.49	0.43
2:M:172:ILE:HG12	2:M:186:VAL:CG1	2.49	0.43
2:M:397:GLU:C	2:M:399:ASN:N	2.73	0.43
3:N:804:LEU:HD12	3:N:806:PHE:H	1.84	0.43
3:N:991:GLN:O	3:N:994:GLN:HB3	2.18	0.43
3:N:1442:ASN:HD22	3:N:1442:ASN:C	2.22	0.43
5:P:93:LEU:HD21	5:P:102:LEU:HD11	2.00	0.43
5:P:410:TYR:O	5:P:413:SER:HB2	2.19	0.43
1:A:41:ARG:HA	1:A:177:VAL:HG11	2.00	0.43
1:B:179:PHE:HB3	1:B:197:LEU:HB3	2.01	0.43
2:C:588:VAL:HG21	2:C:664:GLY:O	2.19	0.43
2:C:884:GLN:HG3	2:C:885:ILE:HD13	2.01	0.43
2:C:1002:GLU:HG3	3:D:744:GLN:NE2	2.33	0.43
2:C:1013:TYR:HE1	2:C:1020:PRO:HG3	1.84	0.43
3:D:30:GLU:HB3	3:D:40:GLU:CB	2.49	0.43
3:D:62:LYS:HA	9:D:2796:HOH:O	2.19	0.43
3:D:138:LYS:NZ	9:D:2617:HOH:O	2.52	0.43
3:D:213:VAL:HG22	9:D:2107:HOH:O	2.17	0.43
3:D:401:TYR:N	3:D:402:PRO:HD3	2.34	0.43
3:D:601:ARG:NH2	3:D:613:ARG:HE	2.17	0.43
3:D:658:LEU:O	3:D:661:MET:HB2	2.19	0.43
3:D:796:ARG:HD3	3:D:862:ASP:HA	2.00	0.43
3:D:1378:TYR:HB2	9:D:9729:HOH:O	2.19	0.43
4:E:59:ASN:N	9:E:9558:HOH:O	2.52	0.43
5:F:185:GLN:HB3	9:F:9576:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:25:LEU:HD12	9:L:2122:HOH:O	2.19	0.43
1:K:43:ILE:HD11	1:L:35:THR:HG21	2.01	0.43
1:L:70:GLY:HA3	9:L:1193:HOH:O	2.19	0.43
1:L:128:HIS:NE2	1:L:131:THR:HG23	2.34	0.43
2:M:166:PRO:HD2	9:M:9325:HOH:O	2.18	0.43
2:M:204:GLN:HG3	9:M:2070:HOH:O	2.19	0.43
2:M:288:ARG:HG3	9:M:9500:HOH:O	2.18	0.43
2:M:308:ARG:HD3	9:M:9332:HOH:O	2.19	0.43
2:M:625:LEU:O	2:M:627:ARG:N	2.52	0.43
2:M:813:VAL:HG23	9:M:9381:HOH:O	2.19	0.43
2:M:855:VAL:CG2	2:M:866:PRO:HG2	2.49	0.43
2:M:1020:PRO:HG3	3:N:624:ASP:OD1	2.19	0.43
3:N:107:ASP:O	3:N:108:VAL:C	2.57	0.43
3:N:122:GLU:HB2	9:N:9548:HOH:O	2.17	0.43
3:N:402:PRO:HG2	3:N:444:VAL:HG11	2.01	0.43
3:N:601:ARG:NH1	3:N:605:ASP:HB3	2.33	0.43
3:N:710:ARG:NH1	9:N:9333:HOH:O	2.46	0.43
3:N:821:VAL:HB	9:N:9577:HOH:O	2.17	0.43
3:N:1098:LEU:HD12	3:N:1098:LEU:N	2.34	0.43
3:N:1287:GLU:N	9:N:9657:HOH:O	2.52	0.43
3:N:1412:LYS:HD3	9:N:2853:HOH:O	2.19	0.43
9:N:2509:HOH:O	5:P:94:LEU:HD11	2.18	0.43
4:O:54:LEU:HD11	9:O:4249:HOH:O	2.18	0.43
1:A:22:GLU:HG3	9:A:9810:HOH:O	2.19	0.42
1:A:85:LEU:HD12	1:A:124:ASN:CB	2.49	0.42
1:A:88:ARG:HH11	1:A:90:LEU:HD23	1.83	0.42
1:A:91:ASN:ND2	1:A:92:PRO:HD2	2.34	0.42
1:B:92:PRO:HB3	9:B:9565:HOH:O	2.19	0.42
2:C:118:ILE:HA	2:C:119:PRO:HD3	1.92	0.42
2:C:146:VAL:HB	2:C:281:LEU:HD21	2.01	0.42
2:C:404:LEU:HA	2:C:407:LYS:CE	2.49	0.42
2:C:703:ILE:N	9:C:9875:HOH:O	2.51	0.42
2:C:728:HIS:HA	9:C:2290:HOH:O	2.19	0.42
2:C:783:ARG:O	2:C:785:VAL:N	2.50	0.42
2:C:945:ARG:HH11	2:C:945:ARG:CB	2.20	0.42
3:D:13:ALA:HB1	3:D:18:ILE:HD11	2.01	0.42
3:D:166:GLN:HG3	9:D:2963:HOH:O	2.19	0.42
3:D:423:ASP:HA	9:D:2049:HOH:O	2.18	0.42
3:D:424:GLY:N	3:D:437:VAL:HG23	2.34	0.42
3:D:827:ILE:HB	3:D:828:LYS:HD3	2.01	0.42
3:D:829:VAL:O	3:D:835:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:885:ILE:HG23	3:D:937:TYR:CE1	2.54	0.42
3:D:965:GLU:OE1	3:D:968:ASP:HB3	2.18	0.42
3:D:1211:MET:HB3	3:D:1213:ARG:NE	2.33	0.42
3:D:1333:HIS:N	9:D:9823:HOH:O	2.52	0.42
3:D:1436:SER:HB3	9:D:9873:HOH:O	2.19	0.42
4:E:91:ARG:HD2	9:E:9580:HOH:O	2.17	0.42
5:F:326:ASP:O	5:F:328:PHE:HD1	2.01	0.42
1:K:14:ARG:HG3	9:K:6203:HOH:O	2.18	0.42
1:K:34:VAL:HG22	1:K:181:VAL:HG21	2.00	0.42
1:K:182:GLU:N	9:K:1076:HOH:O	2.52	0.42
1:L:176:ARG:NH1	3:N:884:ARG:CZ	2.82	0.42
2:M:148:PHE:HA	9:M:9475:HOH:O	2.19	0.42
2:M:262:ALA:HB3	9:M:9600:HOH:O	2.18	0.42
2:M:427:VAL:HG23	9:M:2524:HOH:O	2.19	0.42
2:M:546:LEU:HA	2:M:581:THR:HG1	1.84	0.42
2:M:918:LEU:HD23	2:M:968:LEU:C	2.39	0.42
2:M:918:LEU:HD23	2:M:968:LEU:CA	2.49	0.42
3:N:39:PRO:HB2	9:N:9225:HOH:O	2.19	0.42
3:N:69:GLU:HA	9:N:9383:HOH:O	2.17	0.42
3:N:400:VAL:C	3:N:402:PRO:HD3	2.38	0.42
3:N:567:ILE:C	3:N:571:LYS:HE2	2.39	0.42
3:N:834:THR:HA	3:N:838:ARG:NH2	2.35	0.42
3:N:1459:LEU:HG	9:N:9608:HOH:O	2.19	0.42
5:P:113:ILE:HG23	5:P:127:ILE:CB	2.49	0.42
5:P:316:SER:HB3	5:P:319:THR:OG1	2.19	0.42
5:P:332:PHE:HD1	9:P:1466:HOH:O	2.00	0.42
5:P:373:LYS:HA	5:P:378:GLY:C	2.39	0.42
1:A:128:HIS:O	1:A:129:ILE:HD13	2.19	0.42
1:A:142:VAL:HG23	1:A:142:VAL:O	2.18	0.42
1:B:5:LYS:O	1:B:8:ALA:HB2	2.20	0.42
1:B:80:LEU:HG	3:D:844:ALA:CB	2.43	0.42
1:B:85:LEU:HD12	1:B:124:ASN:CB	2.49	0.42
2:C:288:ARG:HA	2:C:288:ARG:NH1	2.34	0.42
2:C:308:ARG:HB2	9:C:9614:HOH:O	2.18	0.42
2:C:614:ARG:HD3	9:C:9979:HOH:O	2.19	0.42
2:C:679:PHE:O	3:D:943:THR:HG22	2.19	0.42
2:C:776:SER:HA	2:C:780:GLU:CB	2.44	0.42
2:C:798:GLY:HA3	2:C:828:ALA:O	2.18	0.42
2:C:1009:SER:HB3	9:C:9882:HOH:O	2.19	0.42
3:D:2:LYS:HB3	9:D:2307:HOH:O	2.17	0.42
3:D:101:HIS:HD2	3:D:582:LEU:HD13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:127:LEU:HG	3:D:128:TYR:HD1	1.83	0.42
3:D:195:VAL:HG13	9:D:2043:HOH:O	2.18	0.42
3:D:413:ASP:OD1	3:D:421:LEU:HD22	2.19	0.42
3:D:520:LEU:CD1	3:D:521:PRO:HD2	2.40	0.42
3:D:669:ASN:O	3:D:672:ALA:HB3	2.19	0.42
3:D:866:VAL:O	3:D:873:LEU:HD12	2.19	0.42
3:D:1486:VAL:HG22	9:D:9984:HOH:O	2.19	0.42
5:F:94:LEU:H	5:F:98:GLU:HB2	1.83	0.42
5:F:111:GLU:HB3	9:F:9921:HOH:O	2.19	0.42
5:F:208:SER:HB2	5:F:211:ASP:OD1	2.19	0.42
5:F:369:LEU:HD21	5:F:401:GLU:OE1	2.19	0.42
1:K:39:PRO:HG3	1:L:39:PRO:HG3	2.01	0.42
1:K:53:VAL:HG21	1:K:82:LEU:HB3	2.00	0.42
1:L:48:ILE:HD13	1:L:210:ALA:HB1	2.00	0.42
1:L:61:VAL:HG13	9:L:6647:HOH:O	2.20	0.42
1:L:128:HIS:HB2	9:L:7862:HOH:O	2.18	0.42
2:M:208:ALA:HA	2:M:218:VAL:CG2	2.49	0.42
2:M:234:ALA:HB2	9:M:9679:HOH:O	2.19	0.42
2:M:651:LYS:HG2	9:M:9533:HOH:O	2.19	0.42
3:N:10:ILE:O	3:N:1454:GLY:HA2	2.19	0.42
3:N:79:GLU:HG2	9:N:2381:HOH:O	2.18	0.42
3:N:176:ASP:HA	9:N:9302:HOH:O	2.19	0.42
3:N:206:ARG:HB2	9:N:2716:HOH:O	2.19	0.42
3:N:489:ARG:NH1	9:N:9727:HOH:O	2.51	0.42
3:N:537:THR:HA	5:P:317:LEU:HD12	2.01	0.42
3:N:566:ILE:HG23	5:P:214:GLN:OE1	2.19	0.42
3:N:738:ALA:HB2	9:N:9228:HOH:O	2.19	0.42
3:N:1094:LEU:HD23	3:N:1230:GLY:HA2	2.01	0.42
3:N:1389:LEU:O	3:N:1391:GLU:N	2.52	0.42
5:P:93:LEU:HB2	9:P:2248:HOH:O	2.19	0.42
5:P:113:ILE:HA	5:P:116:LEU:HD12	2.01	0.42
1:A:133:GLU:HB3	9:A:9624:HOH:O	2.18	0.42
1:B:133:GLU:HG2	9:B:9650:HOH:O	2.19	0.42
2:C:72:ARG:HD3	9:C:2792:HOH:O	2.18	0.42
2:C:77:PRO:HD2	2:C:91:GLN:O	2.19	0.42
2:C:384:GLU:HA	2:C:388:ARG:NH2	2.34	0.42
2:C:734:LEU:HD12	9:C:9587:HOH:O	2.17	0.42
2:C:737:LEU:HD22	2:C:741:GLY:O	2.19	0.42
2:C:890:LEU:HG	2:C:901:TYR:CD1	2.53	0.42
2:C:971:LYS:HG2	2:C:988:VAL:HG12	2.02	0.42
3:D:190:GLU:HG3	3:D:210:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:613:ARG:HG3	3:D:613:ARG:HH11	1.83	0.42
3:D:890:VAL:HG11	3:D:922:LEU:HD13	2.01	0.42
3:D:898:GLU:HA	9:D:2154:HOH:O	2.19	0.42
3:D:1232:PRO:HB3	3:D:1361:VAL:CG2	2.50	0.42
3:D:1428:ALA:O	3:D:1430:SER:N	2.52	0.42
4:E:32:ARG:C	4:E:34:GLY:H	2.23	0.42
5:F:397:ILE:HD13	9:F:9936:HOH:O	2.19	0.42
5:F:416:ARG:HB3	9:F:9972:HOH:O	2.19	0.42
1:K:209:GLU:O	1:K:213:GLN:HG3	2.19	0.42
1:K:221:HIS:ND1	1:K:224:TYR:HE2	2.15	0.42
2:M:139:GLN:HA	2:M:411:SER:O	2.19	0.42
2:M:325:ILE:H	2:M:325:ILE:HG13	1.60	0.42
2:M:672:VAL:HG23	2:M:868:ASP:OD2	2.19	0.42
2:M:915:LYS:HB3	9:M:9311:HOH:O	2.19	0.42
3:N:58:CYS:SG	3:N:59:ALA:N	2.92	0.42
3:N:119:SER:N	3:N:123:LEU:HB2	2.34	0.42
3:N:424:GLY:CA	3:N:436:GLU:HA	2.37	0.42
3:N:669:ASN:O	3:N:672:ALA:HB3	2.18	0.42
3:N:813:LEU:HD11	9:N:9724:HOH:O	2.19	0.42
3:N:988:ARG:HD2	3:N:992:ILE:HD12	2.00	0.42
5:P:207:LEU:HD11	5:P:251:ILE:HA	2.01	0.42
5:P:335:ASP:CG	5:P:338:LEU:HD12	2.39	0.42
5:P:403:LYS:HA	5:P:403:LYS:HD3	1.84	0.42
1:A:72:LYS:HA	9:C:9832:HOH:O	2.18	0.42
1:B:44:LEU:HD23	1:B:48:ILE:CD1	2.45	0.42
2:C:793:PRO:HB2	9:C:9660:HOH:O	2.18	0.42
2:C:877:PRO:HD3	3:D:949:ILE:HD11	1.99	0.42
2:C:911:GLU:HB3	2:C:912:PRO:HD3	2.01	0.42
3:D:50:PHE:CB	3:D:522:PRO:HG2	2.50	0.42
3:D:105:VAL:HG12	3:D:106:LYS:HE3	2.01	0.42
3:D:212:ARG:HD2	3:D:445:ARG:NH1	2.34	0.42
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.85	0.42
3:D:583:ASP:HA	3:D:602:SER:CB	2.49	0.42
3:D:799:LYS:HD3	9:D:2211:HOH:O	2.18	0.42
3:D:1140:ILE:HD13	3:D:1175:ILE:HG12	2.02	0.42
3:D:1223:ILE:CD1	3:D:1462:LEU:HD12	2.50	0.42
3:D:1490:LYS:HB3	9:D:2818:HOH:O	2.19	0.42
5:F:159:ILE:O	5:F:163:LEU:HG	2.20	0.42
1:L:34:VAL:HG22	1:L:181:VAL:HG21	2.01	0.42
2:M:47:ALA:O	2:M:50:GLU:HB2	2.18	0.42
2:M:209:ARG:O	2:M:213:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:299:LYS:HE2	9:M:9257:HOH:O	2.20	0.42
2:M:321:GLU:HA	9:M:9664:HOH:O	2.20	0.42
2:M:617:ASP:HB2	9:M:9795:HOH:O	2.18	0.42
2:M:948:GLU:HB2	2:M:955:PRO:HG3	2.01	0.42
2:M:1082:PRO:HG2	3:N:1469:GLY:HA3	2.01	0.42
3:N:47:GLU:HA	3:N:51:GLY:O	2.19	0.42
3:N:139:GLY:HA3	3:N:452:ILE:HD12	2.01	0.42
3:N:167:GLU:HG2	9:N:2697:HOH:O	2.20	0.42
3:N:476:GLU:HA	9:N:9645:HOH:O	2.19	0.42
3:N:703:ASN:HD22	3:N:703:ASN:HA	1.73	0.42
3:N:850:LEU:O	3:N:853:VAL:HB	2.19	0.42
3:N:1442:ASN:ND2	3:N:1442:ASN:H	2.17	0.42
1:A:34:VAL:HG21	2:C:939:ARG:HD2	2.01	0.42
1:A:227:ASN:N	1:A:227:ASN:ND2	2.61	0.42
2:C:473:ARG:NE	2:C:531:PHE:HE1	2.11	0.42
2:C:478:VAL:CG1	2:C:506:ASN:HB3	2.49	0.42
2:C:557:ARG:CZ	2:C:560:MET:SD	3.07	0.42
2:C:578:VAL:CG2	2:C:579:VAL:HG12	2.49	0.42
2:C:606:VAL:HG22	2:C:645:VAL:HG13	2.01	0.42
2:C:678:PRO:O	3:D:943:THR:HA	2.19	0.42
3:D:15:PRO:HG3	9:D:9724:HOH:O	2.20	0.42
3:D:162:ARG:HB2	3:D:162:ARG:NH1	2.34	0.42
3:D:517:VAL:HG12	3:D:518:PRO:O	2.20	0.42
3:D:656:PHE:HB3	3:D:694:VAL:HG11	2.01	0.42
3:D:679:ARG:HH12	3:D:681:ARG:CD	2.24	0.42
3:D:1087:ARG:HH21	3:D:1238:MET:HB2	1.84	0.42
3:D:1138:ALA:O	3:D:1141:GLU:HB2	2.20	0.42
4:E:54:LEU:HG	4:E:58:PRO:CD	2.48	0.42
5:F:187:LEU:HD23	5:F:191:ASN:ND2	2.35	0.42
5:F:276:ARG:HG2	9:F:9570:HOH:O	2.18	0.42
2:M:15:LEU:HB2	2:M:586:ARG:NH2	2.33	0.42
2:M:30:LEU:HD11	9:M:9879:HOH:O	2.19	0.42
2:M:395:LYS:CG	2:M:397:GLU:HG2	2.47	0.42
2:M:418:LEU:HB3	9:M:9342:HOH:O	2.19	0.42
2:M:713:ARG:HG2	2:M:713:ARG:NH1	2.34	0.42
2:M:889:HIS:CD2	2:M:970:GLY:HA3	2.55	0.42
2:M:928:LYS:HA	9:M:9477:HOH:O	2.20	0.42
9:M:9885:HOH:O	3:N:628:ARG:HD3	2.19	0.42
3:N:36:THR:C	3:N:38:LYS:N	2.72	0.42
3:N:179:VAL:HG23	9:N:2700:HOH:O	2.18	0.42
3:N:858:VAL:HG12	3:N:859:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1197:ARG:HD2	3:N:1396:GLU:HB2	2.02	0.42
3:N:1331:ASP:OD1	3:N:1333:HIS:HB2	2.20	0.42
1:B:48:ILE:HD13	1:B:210:ALA:HB1	2.02	0.42
1:B:122:ILE:HD12	9:B:9579:HOH:O	2.18	0.42
2:C:115:LEU:H	2:C:115:LEU:HG	1.70	0.42
2:C:151:ASP:HB2	2:C:157:ARG:O	2.19	0.42
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.87	0.42
2:C:441:VAL:HG23	9:C:2264:HOH:O	2.20	0.42
2:C:525:SER:HA	9:C:9711:HOH:O	2.19	0.42
2:C:530:GLU:O	2:C:531:PHE:HD1	2.03	0.42
2:C:601:GLY:O	2:C:648:ARG:HA	2.19	0.42
3:D:48:ARG:HA	9:D:2217:HOH:O	2.19	0.42
3:D:65:ARG:HG3	3:D:66:GLN:H	1.84	0.42
3:D:112:ILE:HD11	3:D:116:LEU:HD12	2.00	0.42
3:D:205:TYR:CE2	3:D:393:ILE:HG12	2.55	0.42
3:D:421:LEU:HD21	9:D:9882:HOH:O	2.19	0.42
3:D:819:GLY:HA3	9:D:3219:HOH:O	2.18	0.42
3:D:1193:THR:N	9:D:9658:HOH:O	2.52	0.42
3:D:1462:LEU:HD22	3:D:1472:ILE:HG23	2.01	0.42
4:E:10:PHE:O	4:E:13:VAL:HG22	2.20	0.42
5:F:164:LYS:HA	5:F:171:LYS:HZ2	1.81	0.42
5:F:216:GLY:O	5:F:243:ILE:HG12	2.19	0.42
2:M:71:TYR:H	2:M:71:TYR:HD2	1.67	0.42
2:M:299:LYS:HG3	9:M:9257:HOH:O	2.18	0.42
2:M:435:TYR:CE1	2:M:539:VAL:HG22	2.54	0.42
2:M:651:LYS:HA	9:M:2442:HOH:O	2.19	0.42
2:M:685:GLU:HG3	3:N:783:ARG:HD2	2.01	0.42
2:M:1043:TYR:CE2	3:N:763:MET:HG3	2.54	0.42
2:M:1105:LYS:HB2	2:M:1107:ASN:ND2	2.35	0.42
3:N:231:VAL:HA	3:N:378:ILE:CB	2.50	0.42
3:N:426:LYS:HB3	3:N:426:LYS:HE2	1.90	0.42
3:N:546:ARG:O	3:N:550:ARG:HG2	2.20	0.42
3:N:699:VAL:HB	3:N:716:PHE:O	2.20	0.42
5:P:201:LYS:HD2	9:P:8888:HOH:O	2.19	0.42
5:P:358:LEU:O	5:P:358:LEU:HD23	2.19	0.42
1:A:34:VAL:HG23	9:A:9562:HOH:O	2.18	0.42
1:A:74:ASP:HB2	9:A:9794:HOH:O	2.19	0.42
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.53	0.42
1:B:75:VAL:O	1:B:79:ILE:HG23	2.19	0.42
1:B:90:LEU:CD2	1:B:91:ASN:HD22	2.33	0.42
2:C:514:VAL:HG13	9:C:9943:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:572:ILE:HG13	2:C:573:ARG:N	2.34	0.42
2:C:744:ARG:NE	9:C:9710:HOH:O	2.50	0.42
2:C:841:ASN:C	2:C:841:ASN:ND2	2.71	0.42
2:C:948:GLU:HB2	2:C:955:PRO:HG3	2.02	0.42
3:D:104:PHE:CE2	3:D:1448:THR:HG23	2.54	0.42
3:D:183:GLU:HA	3:D:186:VAL:CG1	2.49	0.42
3:D:205:TYR:HA	3:D:393:ILE:HD13	2.01	0.42
3:D:434:ARG:HB2	3:D:447:VAL:CG2	2.49	0.42
3:D:644:LEU:O	3:D:721:VAL:HG22	2.20	0.42
3:D:729:HIS:HE1	3:D:731:LEU:HG	1.83	0.42
3:D:894:LYS:HB3	9:D:2360:HOH:O	2.19	0.42
3:D:1194:CYS:HB2	9:D:2009:HOH:O	2.19	0.42
3:D:1250:ALA:HB3	9:D:3244:HOH:O	2.19	0.42
3:D:1275:SER:HA	3:D:1303:TYR:CE1	2.54	0.42
3:D:1336:LEU:HA	3:D:1344:VAL:HG22	2.01	0.42
4:E:40:LEU:HB2	4:E:45:ARG:CZ	2.49	0.42
5:F:299:TRP:CE3	5:F:303:ARG:HD3	2.54	0.42
1:K:33:GLY:HA2	1:K:195:LEU:HD22	2.01	0.42
1:K:178:ALA:HB2	2:M:864:GLY:CA	2.50	0.42
1:L:103:ALA:HB1	9:L:4720:HOH:O	2.20	0.42
2:M:165:LEU:HD12	2:M:166:PRO:HA	2.01	0.42
2:M:292:ARG:NH2	2:M:299:LYS:HD3	2.35	0.42
2:M:480:THR:HG22	2:M:481:ASP:N	2.35	0.42
2:M:517:ARG:O	2:M:519:GLY:N	2.52	0.42
2:M:724:ARG:HB2	2:M:740:GLU:CA	2.43	0.42
3:N:26:VAL:HG23	9:N:9259:HOH:O	2.19	0.42
3:N:480:GLU:O	3:N:484:PRO:HD2	2.19	0.42
3:N:559:ALA:O	5:P:132:ARG:NH1	2.52	0.42
3:N:645:PRO:HG2	3:N:724:GLN:O	2.19	0.42
3:N:796:ARG:HE	3:N:828:LYS:HZ3	1.68	0.42
4:O:84:ARG:HD2	9:O:3299:HOH:O	2.19	0.42
5:P:149:GLU:HB2	9:P:3104:HOH:O	2.18	0.42
1:A:72:LYS:N	9:A:9656:HOH:O	2.53	0.42
1:A:74:ASP:CB	9:A:9794:HOH:O	2.67	0.42
2:C:492:ASP:CA	2:C:518:LYS:HB3	2.47	0.42
2:C:599:GLU:HB2	9:C:2285:HOH:O	2.20	0.42
2:C:625:LEU:O	2:C:627:ARG:N	2.53	0.42
2:C:853:LEU:HB2	2:C:858:MET:HE3	2.01	0.42
3:D:1156:LEU:HD11	3:D:1177:ALA:HA	2.02	0.42
3:D:1300:SER:HB3	9:D:9737:HOH:O	2.20	0.42
3:D:1389:LEU:O	3:D:1391:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1503:VAL:HG21	9:D:9933:HOH:O	2.20	0.42
4:E:66:LYS:HB2	4:E:66:LYS:NZ	2.35	0.42
1:K:198:ARG:NE	9:K:1703:HOH:O	2.53	0.42
2:M:16:PRO:HB3	2:M:460:ARG:NH1	2.35	0.42
2:M:46:ALA:O	2:M:50:GLU:HG3	2.20	0.42
2:M:182:VAL:HG12	9:M:9802:HOH:O	2.19	0.42
2:M:575:GLN:HE21	2:M:671:ASN:HB2	1.85	0.42
2:M:753:ASP:OD2	3:N:681:ARG:HD2	2.20	0.42
2:M:939:ARG:CZ	9:M:9419:HOH:O	2.66	0.42
2:M:949:LYS:HZ2	3:N:796:ARG:HH22	1.67	0.42
3:N:10:ILE:HD11	3:N:1434:TRP:NE1	2.35	0.42
3:N:44:LEU:HG	9:N:9241:HOH:O	2.20	0.42
3:N:93:ILE:HG13	3:N:519:VAL:CG2	2.50	0.42
3:N:422:ALA:H	3:N:427:VAL:CG1	2.33	0.42
3:N:434:ARG:HB2	3:N:447:VAL:HG13	2.02	0.42
3:N:527:MET:CE	3:N:535:PHE:HB3	2.50	0.42
3:N:528:VAL:O	3:N:535:PHE:HA	2.20	0.42
3:N:728:LEU:HD12	3:N:729:HIS:N	2.34	0.42
3:N:1020:LEU:HG	3:N:1035:ILE:HD12	2.00	0.42
5:P:207:LEU:HD12	5:P:251:ILE:HG12	2.01	0.42
1:A:177:VAL:O	2:C:864:GLY:CA	2.68	0.42
1:A:177:VAL:HG12	1:A:178:ALA:N	2.35	0.42
2:C:418:LEU:HD12	9:C:2110:HOH:O	2.20	0.42
2:C:471:TYR:HB3	2:C:531:PHE:CD2	2.55	0.42
2:C:627:ARG:CG	2:C:628:PHE:H	2.33	0.42
2:C:714:ASP:HB2	2:C:818:GLY:O	2.20	0.42
2:C:906:PHE:N	9:C:9623:HOH:O	2.53	0.42
2:C:1014:SER:N	9:C:2050:HOH:O	2.52	0.42
2:C:1082:PRO:HA	9:C:9720:HOH:O	2.20	0.42
3:D:43:GLY:N	9:D:9655:HOH:O	2.53	0.42
3:D:111:LYS:HD3	3:D:111:LYS:HA	1.87	0.42
3:D:126:VAL:CG1	3:D:132:TYR:HB2	2.50	0.42
3:D:160:GLU:HA	9:D:2658:HOH:O	2.18	0.42
3:D:172:PRO:HA	3:D:173:PRO:HD3	1.75	0.42
3:D:525:ARG:N	3:D:526:PRO:HD3	2.35	0.42
3:D:601:ARG:HH22	3:D:613:ARG:HB2	1.84	0.42
3:D:1031:ASN:HB3	3:D:1034:GLN:CD	2.40	0.42
3:D:1166:LEU:HD23	3:D:1166:LEU:N	2.30	0.42
4:E:41:GLU:HA	4:E:45:ARG:HG3	2.02	0.42
4:E:54:LEU:HA	4:E:58:PRO:HG2	2.02	0.42
5:F:248:ASN:HB2	9:F:9828:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:421:PHE:C	5:F:423:ASP:N	2.72	0.42
1:K:106:PRO:HA	1:K:132:LEU:O	2.20	0.42
1:K:224:TYR:CD2	1:L:9:PRO:HG2	2.55	0.42
2:M:172:ILE:HG13	9:M:9595:HOH:O	2.20	0.42
2:M:207:LEU:HD13	2:M:221:LEU:CD1	2.50	0.42
2:M:649:VAL:HG12	2:M:650:ARG:HH21	1.85	0.42
2:M:913:GLU:O	2:M:916:GLU:HB3	2.20	0.42
2:M:929:ARG:HD3	9:M:9262:HOH:O	2.18	0.42
9:M:9896:HOH:O	5:P:373:LYS:HD2	2.19	0.42
3:N:438:ASP:OD2	3:N:440:VAL:HB	2.19	0.42
3:N:660:LYS:O	3:N:663:GLU:HB2	2.20	0.42
3:N:751:LEU:HD13	9:N:9380:HOH:O	2.19	0.42
3:N:838:ARG:HH11	3:N:863:VAL:HB	1.85	0.42
3:N:860:LEU:O	3:N:876:SER:OG	2.37	0.42
3:N:1033:GLN:O	3:N:1037:GLN:HG3	2.20	0.42
5:P:371:LEU:HD12	9:P:1495:HOH:O	2.19	0.42
1:A:30:ARG:HD2	9:D:9595:HOH:O	2.20	0.42
2:C:10:ARG:HA	2:C:10:ARG:HD2	1.80	0.42
2:C:359:MET:HB2	9:C:2205:HOH:O	2.18	0.42
2:C:780:GLU:HG3	2:C:781:LYS:N	2.31	0.42
2:C:1036:GLU:CD	2:C:1036:GLU:N	2.73	0.42
2:C:1085:PHE:CE2	3:D:1468:LEU:HA	2.54	0.42
3:D:55:ASP:HA	9:D:9689:HOH:O	2.20	0.42
3:D:445:ARG:HD3	9:D:2510:HOH:O	2.20	0.42
3:D:631:ILE:HG21	3:D:745:MET:CG	2.47	0.42
3:D:739:ASP:CG	3:D:741:ASP:OD1	2.58	0.42
3:D:914:LEU:HD23	3:D:914:LEU:O	2.19	0.42
3:D:983:LEU:N	9:D:2242:HOH:O	2.48	0.42
3:D:1103:HIS:HD2	3:D:1462:LEU:H	1.67	0.42
3:D:1284:GLU:OE1	3:D:1284:GLU:HA	2.20	0.42
3:D:1348:LEU:HD23	3:D:1375:MET:HE3	2.02	0.42
3:D:1466:VAL:HG22	3:D:1472:ILE:CD1	2.50	0.42
4:E:43:GLU:H	4:E:43:GLU:HG2	1.66	0.42
4:E:51:LEU:HD12	4:E:52:GLU:H	1.83	0.42
5:F:151:LEU:HB2	5:F:155:THR:CB	2.50	0.42
5:F:196:VAL:O	5:F:200:LYS:HB2	2.19	0.42
5:F:419:ARG:HG2	5:F:419:ARG:NH1	2.35	0.42
1:L:85:LEU:HD12	1:L:124:ASN:CB	2.50	0.42
1:L:175:ARG:O	3:N:851:LEU:HD21	2.20	0.42
1:L:176:ARG:NH1	3:N:884:ARG:NE	2.63	0.42
2:M:192:PRO:CB	2:M:195:LEU:HD13	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:248:PRO:HD3	9:M:9536:HOH:O	2.18	0.42
2:M:300:ASP:C	2:M:302:VAL:H	2.22	0.42
2:M:585:GLU:CG	2:M:586:ARG:H	2.33	0.42
2:M:601:GLY:O	2:M:648:ARG:HA	2.20	0.42
2:M:850:ALA:HB1	3:N:632:VAL:HG13	2.02	0.42
2:M:1067:TYR:O	2:M:1071:ILE:HG12	2.20	0.42
3:N:16:GLU:O	3:N:19:ARG:HB2	2.20	0.42
3:N:125:GLN:HG3	9:N:9692:HOH:O	2.20	0.42
3:N:128:TYR:HD2	3:N:128:TYR:HA	1.64	0.42
3:N:417:PRO:HB3	9:P:4142:HOH:O	2.20	0.42
3:N:565:ILE:H	3:N:565:ILE:CD1	2.20	0.42
3:N:715:ALA:HB3	3:N:764:LEU:CA	2.35	0.42
3:N:1234:THR:HA	9:N:2227:HOH:O	2.19	0.42
3:N:1314:LYS:HG3	9:N:2352:HOH:O	2.20	0.42
3:N:1428:ALA:O	3:N:1430:SER:N	2.53	0.42
5:P:256:ARG:HD3	5:P:260:ILE:HG22	2.02	0.42
5:P:367:MET:O	5:P:370:LYS:HG2	2.20	0.42
5:P:393:THR:CG2	5:P:394:ARG:N	2.83	0.42
1:A:106:PRO:HA	1:A:132:LEU:O	2.20	0.41
1:A:217:ILE:HG13	1:A:217:ILE:H	1.70	0.41
2:C:84:ARG:HH12	2:C:128:ILE:CD1	2.33	0.41
2:C:110:GLU:HB3	2:C:368:THR:HG22	2.02	0.41
2:C:130:ASN:CG	2:C:383:ARG:HH22	2.24	0.41
2:C:244:PRO:CD	2:C:245:GLY:N	2.82	0.41
2:C:264:PRO:HB2	9:C:9902:HOH:O	2.20	0.41
2:C:405:ARG:HD2	9:C:9844:HOH:O	2.19	0.41
2:C:431:HIS:O	2:C:434:HIS:HB2	2.19	0.41
2:C:872:ASN:HA	2:C:873:PRO:HD3	1.89	0.41
3:D:33:ASN:HA	9:F:9722:HOH:O	2.19	0.41
3:D:434:ARG:CB	3:D:447:VAL:HG13	2.49	0.41
3:D:486:ARG:HH21	3:D:489:ARG:CD	2.32	0.41
3:D:792:ILE:O	3:D:878:GLY:HA3	2.20	0.41
3:D:871:LYS:CG	3:D:873:LEU:HG	2.49	0.41
3:D:1274:ILE:H	3:D:1274:ILE:HG13	1.58	0.41
4:E:48:MET:HG2	4:E:49:GLN:N	2.34	0.41
5:F:104:ARG:NH2	9:F:9811:HOH:O	2.52	0.41
5:F:289:GLU:O	5:F:293:GLU:HG3	2.19	0.41
5:F:363:GLU:HA	9:F:9838:HOH:O	2.20	0.41
1:K:86:VAL:HG13	1:K:86:VAL:O	2.20	0.41
1:L:5:LYS:O	1:L:8:ALA:HB2	2.20	0.41
1:L:90:LEU:HB3	9:L:1485:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:18:LEU:HD21	2:M:542:VAL:HG11	2.01	0.41
2:M:246:ASP:HB2	9:M:9223:HOH:O	2.19	0.41
2:M:514:VAL:HG12	2:M:515:ALA:N	2.35	0.41
2:M:897:LEU:HB3	2:M:899:GLN:CG	2.50	0.41
2:M:1037:VAL:O	2:M:1041:GLU:HG3	2.20	0.41
3:N:30:GLU:HB3	3:N:40:GLU:CG	2.50	0.41
3:N:112:ILE:HD11	3:N:124:GLU:CG	2.50	0.41
3:N:168:THR:HB	3:N:170:PRO:HD3	2.03	0.41
3:N:186:VAL:HG23	3:N:211:VAL:CG1	2.49	0.41
3:N:399:ARG:HB3	3:N:402:PRO:CG	2.46	0.41
3:N:656:PHE:HB3	3:N:694:VAL:HG11	2.01	0.41
3:N:907:GLU:CD	3:N:909:ASN:HB2	2.40	0.41
3:N:1041:LEU:HD12	3:N:1058:ARG:HA	2.02	0.41
3:N:1278:ASP:HA	3:N:1319:VAL:O	2.20	0.41
4:O:87:LYS:HE2	4:O:91:ARG:NH2	2.28	0.41
5:P:80:PRO:O	5:P:83:GLN:HB2	2.20	0.41
5:P:253:ASP:HB3	5:P:259:ARG:HH21	1.85	0.41
5:P:287:THR:C	5:P:289:GLU:H	2.23	0.41
5:P:291:ILE:CG2	5:P:304:VAL:HG21	2.49	0.41
5:P:394:ARG:HA	5:P:397:ILE:CD1	2.45	0.41
1:A:3:ASP:HB3	1:A:4:SER:H	1.54	0.41
1:B:8:ALA:HB2	9:B:9765:HOH:O	2.20	0.41
1:B:41:ARG:HH11	1:B:41:ARG:HG3	1.85	0.41
1:B:55:SER:HB2	1:B:158:ILE:HB	2.02	0.41
1:B:132:LEU:HD21	1:B:138:LEU:HB2	2.02	0.41
2:C:384:GLU:HG3	2:C:388:ARG:HB2	2.02	0.41
2:C:887:GLU:HG3	9:C:9563:HOH:O	2.20	0.41
2:C:1016:ILE:HD11	5:F:330:GLY:CA	2.50	0.41
2:C:1067:TYR:CB	5:F:341:PRO:HB3	2.50	0.41
2:C:1087:VAL:O	2:C:1091:GLU:HG3	2.20	0.41
3:D:47:GLU:HA	3:D:51:GLY:O	2.20	0.41
3:D:168:THR:C	3:D:170:PRO:HD3	2.41	0.41
3:D:185:VAL:CG1	3:D:191:LEU:HD21	2.50	0.41
3:D:414:ARG:HB3	9:D:2090:HOH:O	2.20	0.41
3:D:794:GLN:NE2	3:D:795:VAL:N	2.68	0.41
3:D:996:TRP:CE3	3:D:996:TRP:HA	2.54	0.41
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.20	0.41
3:D:1335:LEU:HD21	9:D:9849:HOH:O	2.20	0.41
9:D:2988:HOH:O	4:E:58:PRO:HG3	2.19	0.41
5:F:366:ALA:HB3	9:F:9838:HOH:O	2.19	0.41
5:F:402:ASN:HB3	5:F:406:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:143:SER:CB	2:M:276:LYS:HE2	2.49	0.41
2:M:464:LEU:HD13	9:M:9893:HOH:O	2.20	0.41
2:M:524:VAL:HG22	2:M:528:GLU:HB2	2.01	0.41
2:M:757:GLY:HA2	2:M:789:SER:HB3	2.02	0.41
3:N:9:ARG:NH1	3:N:9:ARG:HG2	2.35	0.41
3:N:161:LEU:C	3:N:449:SER:HB2	2.41	0.41
3:N:209:ARG:NH1	3:N:397:LYS:HG3	2.35	0.41
3:N:213:VAL:HG13	9:N:2214:HOH:O	2.19	0.41
3:N:659:LYS:O	3:N:663:GLU:HG2	2.20	0.41
3:N:793:THR:HB	3:N:879:ARG:HD2	2.02	0.41
3:N:1007:VAL:HG23	3:N:1008:PHE:N	2.35	0.41
3:N:1146:GLY:N	9:N:2585:HOH:O	2.53	0.41
3:N:1301:LYS:HD3	9:N:2604:HOH:O	2.18	0.41
3:N:1307:LYS:HB2	3:N:1307:LYS:NZ	2.35	0.41
5:P:75:ILE:HG22	9:P:6479:HOH:O	2.18	0.41
5:P:367:MET:HA	5:P:370:LYS:CD	2.49	0.41
5:P:387:GLY:HA2	9:P:8096:HOH:O	2.19	0.41
2:C:73:LEU:HD23	2:C:118:ILE:HD11	2.01	0.41
2:C:249:LYS:HA	9:C:2727:HOH:O	2.19	0.41
2:C:516:ARG:HB3	9:C:9652:HOH:O	2.19	0.41
2:C:690:ILE:HG12	2:C:849:VAL:HG13	2.01	0.41
2:C:707:ARG:HD2	2:C:824:ARG:HD3	2.01	0.41
2:C:1008:ARG:NH1	3:D:624:ASP:OD1	2.53	0.41
2:C:1016:ILE:CD1	5:F:317:LEU:HD21	2.43	0.41
3:D:381:ALA:HA	9:D:2848:HOH:O	2.19	0.41
3:D:644:LEU:CG	3:D:718:PRO:HB3	2.50	0.41
3:D:1428:ALA:O	3:D:1431:THR:HG23	2.19	0.41
5:F:301:ALA:HB2	9:F:2002:HOH:O	2.19	0.41
5:F:317:LEU:O	5:F:329:TYR:HB3	2.21	0.41
2:M:137:VAL:HG13	2:M:409:ARG:O	2.20	0.41
2:M:230:ARG:CZ	2:M:237:ARG:HH22	2.32	0.41
2:M:241:LEU:HG	9:M:9694:HOH:O	2.21	0.41
2:M:366:SER:HB3	9:M:2384:HOH:O	2.20	0.41
2:M:460:ARG:HH11	2:M:460:ARG:HG3	1.85	0.41
2:M:497:ALA:HB3	2:M:532:MET:HG3	2.02	0.41
2:M:514:VAL:HG11	2:M:516:ARG:CZ	2.50	0.41
2:M:601:GLY:HA3	2:M:615:TYR:HA	2.02	0.41
2:M:854:PRO:C	2:M:856:GLU:N	2.73	0.41
2:M:928:LYS:HE2	9:M:9477:HOH:O	2.20	0.41
2:M:1035:MET:HA	2:M:1038:TRP:CE3	2.55	0.41
2:M:1115:LEU:CD2	3:N:85:VAL:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:116:LEU:CB	3:N:118:LEU:HD13	2.44	0.41
3:N:131:LYS:HB3	3:N:131:LYS:HZ3	1.85	0.41
3:N:427:VAL:HG21	3:N:435:VAL:HB	2.03	0.41
3:N:567:ILE:O	3:N:571:LYS:HG3	2.20	0.41
3:N:598:ARG:HA	3:N:599:PRO:HD3	1.92	0.41
3:N:829:VAL:HA	9:N:9736:HOH:O	2.19	0.41
3:N:907:GLU:OE2	3:N:909:ASN:HB2	2.21	0.41
3:N:1278:ASP:OD1	3:N:1321:ALA:HB2	2.20	0.41
3:N:1312:LEU:HD23	9:N:2549:HOH:O	2.20	0.41
3:N:1467:ILE:HD13	9:N:9712:HOH:O	2.20	0.41
5:P:313:GLU:OE1	5:P:313:GLU:HA	2.20	0.41
5:P:350:LEU:CD1	5:P:422:LEU:HD13	2.50	0.41
1:B:53:VAL:HG21	1:B:82:LEU:HB3	2.03	0.41
1:B:89:PHE:HD2	1:B:146:ARG:HH21	1.69	0.41
1:B:108:GLU:HB3	1:B:128:HIS:HE1	1.86	0.41
1:B:110:LYS:HG3	9:B:9637:HOH:O	2.20	0.41
2:C:19:THR:HG22	2:C:19:THR:O	2.20	0.41
2:C:47:ALA:O	2:C:50:GLU:HB3	2.20	0.41
2:C:121:MET:HA	2:C:127:PHE:CE2	2.56	0.41
2:C:193:LEU:HA	2:C:196:LEU:HD12	2.02	0.41
2:C:274:ARG:O	2:C:278:GLU:HG3	2.20	0.41
2:C:328:LEU:HD22	2:C:433:THR:C	2.41	0.41
2:C:455:LEU:HD22	2:C:459:ALA:HB1	2.02	0.41
2:C:988:VAL:HG13	9:C:9757:HOH:O	2.21	0.41
2:C:1091:GLU:O	2:C:1094:ALA:HB3	2.20	0.41
3:D:1110:ALA:O	3:D:1112:CYS:N	2.52	0.41
3:D:1209:LEU:HD23	3:D:1216:SER:H	1.85	0.41
4:E:48:MET:N	4:E:54:LEU:HB2	2.34	0.41
1:K:2:LEU:HA	1:K:6:LEU:CD2	2.50	0.41
9:K:5576:HOH:O	1:L:11:PHE:HB3	2.20	0.41
1:L:220:GLU:HA	1:L:223:THR:HG23	2.02	0.41
2:M:118:ILE:HA	2:M:119:PRO:HD3	1.88	0.41
2:M:130:ASN:N	9:M:9614:HOH:O	2.52	0.41
2:M:145:GLY:H	2:M:163:ILE:HG23	1.85	0.41
2:M:205:GLU:HG3	2:M:206:THR:N	2.36	0.41
2:M:205:GLU:HG3	9:M:9651:HOH:O	2.20	0.41
2:M:207:LEU:HD13	2:M:221:LEU:HD11	2.01	0.41
2:M:697:ARG:O	2:M:699:PHE:N	2.48	0.41
2:M:859:PRO:HB2	2:M:867:VAL:CG2	2.51	0.41
2:M:1047:HIS:O	2:M:1051:GLU:HG3	2.20	0.41
3:N:637:LEU:HD11	3:N:642:CYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1111:ASP:HB2	3:N:1203:LYS:HD2	2.03	0.41
5:P:94:LEU:HD12	5:P:97:GLU:H	1.83	0.41
1:A:48:ILE:HD13	1:A:210:ALA:HB1	2.03	0.41
1:A:88:ARG:HD2	1:A:123:MET:CE	2.50	0.41
1:B:151:VAL:HG12	1:B:156:HIS:ND1	2.36	0.41
2:C:666:LEU:HD11	2:C:668:LEU:HG	2.01	0.41
2:C:684:PHE:CG	2:C:685:GLU:N	2.86	0.41
2:C:807:ARG:HD2	9:C:2016:HOH:O	2.20	0.41
2:C:897:LEU:HD23	2:C:899:GLN:CD	2.41	0.41
2:C:1012:PRO:HB3	5:F:334:PRO:HB3	2.03	0.41
2:C:1095:LEU:HD12	3:D:603:LEU:HD13	2.03	0.41
3:D:99:ALA:CA	3:D:575:GLN:HE22	2.29	0.41
3:D:1164:ARG:HG2	9:D:2063:HOH:O	2.20	0.41
3:D:1381:VAL:HG23	3:D:1391:GLU:HB2	2.01	0.41
3:D:1394:VAL:CB	3:D:1397:LYS:HD2	2.51	0.41
5:F:80:PRO:O	5:F:83:GLN:HB3	2.20	0.41
1:K:71:VAL:HG13	9:K:1208:HOH:O	2.19	0.41
1:K:104:GLU:HA	1:K:136:GLY:O	2.21	0.41
1:K:184:THR:HG23	1:K:192:LEU:HB2	2.02	0.41
2:M:76:PRO:HB2	9:M:9838:HOH:O	2.19	0.41
2:M:176:VAL:HG12	2:M:178:PRO:HD3	2.03	0.41
2:M:246:ASP:HA	2:M:247:PRO:HD3	1.97	0.41
2:M:764:GLU:HG2	9:M:9355:HOH:O	2.21	0.41
2:M:926:PHE:O	2:M:930:LYS:HG3	2.21	0.41
2:M:927:GLY:HA2	2:M:930:LYS:HZ3	1.83	0.41
2:M:1092:LEU:CD1	2:M:1099:VAL:HG21	2.45	0.41
3:N:82:LYS:O	3:N:84:ILE:N	2.54	0.41
3:N:520:LEU:O	3:N:525:ARG:NH1	2.54	0.41
3:N:521:PRO:HB3	9:N:9625:HOH:O	2.20	0.41
3:N:704:ARG:CD	9:N:9228:HOH:O	2.69	0.41
3:N:1110:ALA:O	3:N:1112:CYS:N	2.53	0.41
3:N:1353:GLN:NE2	3:N:1365:ASP:OD2	2.53	0.41
9:N:2944:HOH:O	5:P:92:PRO:HG2	2.20	0.41
4:O:48:MET:HG2	4:O:49:GLN:N	2.33	0.41
4:O:59:ASN:HB2	9:O:4249:HOH:O	2.19	0.41
5:P:136:LEU:HD12	5:P:137:GLY:N	2.36	0.41
5:P:309:LYS:HA	5:P:312:GLN:OE1	2.20	0.41
1:A:69:PRO:O	1:A:71:VAL:HG23	2.21	0.41
1:A:79:ILE:HA	1:A:82:LEU:HD12	2.02	0.41
1:B:178:ALA:HB1	1:B:198:ARG:NH2	2.35	0.41
2:C:118:ILE:O	2:C:118:ILE:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:172:ILE:HG23	2:C:184:MET:CE	2.51	0.41
2:C:172:ILE:HA	2:C:185:LYS:O	2.20	0.41
2:C:279:GLU:OE2	2:C:489:THR:HG21	2.20	0.41
2:C:332:ARG:CZ	9:C:9819:HOH:O	2.69	0.41
2:C:701:THR:HG22	2:C:832:LYS:HG2	2.02	0.41
2:C:756:VAL:HG11	2:C:823:VAL:HG21	2.02	0.41
2:C:854:PRO:C	2:C:856:GLU:N	2.74	0.41
2:C:897:LEU:HD11	2:C:920:GLN:CG	2.49	0.41
2:C:942:GLU:HA	9:C:9752:HOH:O	2.19	0.41
3:D:205:TYR:OH	3:D:391:ALA:HB1	2.19	0.41
3:D:567:ILE:O	3:D:571:LYS:HG3	2.20	0.41
3:D:899:LEU:HD13	3:D:900:ILE:HG23	2.02	0.41
3:D:1223:ILE:HD12	3:D:1223:ILE:N	2.35	0.41
3:D:1487:VAL:HG12	3:D:1488:ASP:N	2.35	0.41
3:D:1497:GLU:OE1	3:D:1500:LYS:HD2	2.20	0.41
4:E:35:PHE:N	9:E:9641:HOH:O	2.52	0.41
5:F:125:ASP:N	9:F:9847:HOH:O	2.54	0.41
5:F:130:VAL:HG21	5:F:159:ILE:HD13	2.01	0.41
5:F:288:TYR:HE2	5:F:305:GLU:HA	1.86	0.41
5:F:406:ARG:O	5:F:409:LYS:HG2	2.20	0.41
5:F:419:ARG:O	5:F:421:PHE:N	2.53	0.41
1:K:180:GLN:NE2	9:K:1619:HOH:O	2.52	0.41
1:L:102:LYS:HB2	1:L:139:ASN:OD1	2.21	0.41
2:M:199:VAL:HG21	2:M:238:LEU:HD12	2.02	0.41
2:M:287:GLY:O	2:M:288:ARG:C	2.58	0.41
2:M:696:LYS:HA	9:M:9428:HOH:O	2.19	0.41
2:M:842:ARG:HD2	9:M:9367:HOH:O	2.21	0.41
2:M:858:MET:HB2	2:M:859:PRO:HD2	2.01	0.41
2:M:896:PHE:CD2	2:M:925:TYR:HB2	2.55	0.41
9:M:9803:HOH:O	3:N:1470:ARG:HA	2.21	0.41
3:N:191:LEU:HD22	3:N:195:VAL:HG21	2.02	0.41
3:N:550:ARG:NH1	3:N:573:MET:HB3	2.35	0.41
3:N:860:LEU:O	3:N:877:PRO:HD2	2.20	0.41
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.55	0.41
3:N:1483:PHE:CD1	3:N:1483:PHE:N	2.89	0.41
1:B:106:PRO:HA	1:B:132:LEU:O	2.20	0.41
1:B:108:GLU:O	1:B:110:LYS:HG3	2.20	0.41
2:C:200:LEU:HD13	2:C:300:ASP:OD1	2.20	0.41
2:C:205:GLU:HA	9:C:9874:HOH:O	2.20	0.41
2:C:546:LEU:HG	2:C:546:LEU:O	2.21	0.41
2:C:648:ARG:HB3	9:C:9827:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1016:ILE:HD11	5:F:330:GLY:HA2	2.03	0.41
3:D:3:LYS:HD3	3:D:3:LYS:N	2.34	0.41
3:D:27:GLU:O	3:D:28:LYS:HG2	2.21	0.41
3:D:35:ARG:HA	9:D:2169:HOH:O	2.21	0.41
3:D:191:LEU:HD22	3:D:195:VAL:HG21	2.03	0.41
3:D:421:LEU:N	3:D:421:LEU:HD23	2.36	0.41
3:D:684:LYS:HA	9:D:2441:HOH:O	2.19	0.41
3:D:711:LEU:C	3:D:713:ILE:N	2.74	0.41
3:D:890:VAL:HG22	3:D:926:LYS:HG2	2.02	0.41
3:D:991:GLN:O	3:D:994:GLN:HB3	2.20	0.41
3:D:1263:PHE:HD2	3:D:1424:VAL:HG21	1.85	0.41
3:D:1359:GLN:NE2	9:D:2889:HOH:O	2.52	0.41
5:F:131:VAL:HG22	5:F:178:ARG:HD3	2.03	0.41
1:K:48:ILE:CG2	1:K:173:PRO:HD2	2.49	0.41
1:L:117:VAL:HG12	9:L:3068:HOH:O	2.21	0.41
1:L:136:GLY:HA3	9:L:2881:HOH:O	2.19	0.41
1:L:198:ARG:HD3	9:L:1055:HOH:O	2.21	0.41
2:M:9:ILE:O	2:M:9:ILE:HG13	2.20	0.41
2:M:297:GLU:HB3	9:M:2030:HOH:O	2.19	0.41
2:M:420:ARG:H	2:M:420:ARG:CD	2.30	0.41
2:M:557:ARG:HD2	2:M:557:ARG:HA	1.95	0.41
2:M:950:LEU:HB3	2:M:952:LEU:CD2	2.50	0.41
2:M:1063:ARG:HG3	5:P:341:PRO:HG3	2.02	0.41
3:N:81:THR:HB	3:N:85:VAL:HG23	2.02	0.41
3:N:170:PRO:O	3:N:391:ALA:HB3	2.21	0.41
3:N:183:GLU:OE2	3:N:216:VAL:HG13	2.19	0.41
3:N:795:VAL:HA	3:N:861:GLN:O	2.20	0.41
9:N:9507:HOH:O	5:P:134:LYS:HA	2.20	0.41
1:A:35:THR:HG22	9:B:9638:HOH:O	2.20	0.41
1:A:189:ARG:HG2	9:A:9613:HOH:O	2.21	0.41
1:B:7:LYS:HB3	1:B:7:LYS:HZ2	1.86	0.41
2:C:290:LEU:H	2:C:290:LEU:CD1	2.25	0.41
2:C:384:GLU:CA	2:C:388:ARG:HH21	2.34	0.41
2:C:438:ILE:HG23	2:C:453:THR:OG1	2.20	0.41
2:C:1052:MET:CE	2:C:1056:LYS:HD3	2.47	0.41
3:D:16:GLU:O	3:D:19:ARG:HB2	2.20	0.41
3:D:119:SER:O	3:D:121:THR:N	2.54	0.41
3:D:884:ARG:O	3:D:888:GLU:N	2.53	0.41
3:D:1148:VAL:HG21	3:D:1203:LYS:HA	2.03	0.41
3:D:1258:ARG:HH11	3:D:1258:ARG:HG3	1.85	0.41
2:M:206:THR:HB	9:M:9651:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:462:ASP:OD1	2:M:463:GLU:N	2.54	0.41
2:M:502:PRO:HD3	9:M:2363:HOH:O	2.20	0.41
2:M:690:ILE:HG21	2:M:833:LEU:HD23	2.02	0.41
2:M:878:SER:HB3	8:N:9101:G4P:O2D	2.21	0.41
2:M:915:LYS:HD2	9:M:9311:HOH:O	2.20	0.41
2:M:958:THR:HG23	2:M:961:GLU:CG	2.51	0.41
3:N:13:ALA:O	3:N:511:TRP:HB3	2.21	0.41
3:N:141:ILE:HD11	3:N:431:VAL:O	2.20	0.41
3:N:190:GLU:HG3	3:N:210:ARG:CZ	2.50	0.41
3:N:644:LEU:HA	3:N:645:PRO:HD3	1.98	0.41
3:N:796:ARG:HD2	9:N:9384:HOH:O	2.20	0.41
3:N:799:LYS:HD2	9:N:2444:HOH:O	2.21	0.41
3:N:1314:LYS:HD3	3:N:1314:LYS:N	2.36	0.41
3:N:1372:VAL:HA	3:N:1375:MET:HE2	2.01	0.41
9:N:9844:HOH:O	5:P:92:PRO:HD3	2.21	0.41
5:P:155:THR:HG22	5:P:159:ILE:HD11	2.03	0.41
1:A:42:ARG:NE	1:B:35:THR:OG1	2.48	0.41
1:A:156:HIS:CD2	1:A:157:GLY:H	2.39	0.41
1:A:178:ALA:HB2	2:C:864:GLY:N	2.34	0.41
1:B:100:LEU:HB2	1:B:115:LEU:HD21	2.03	0.41
1:B:106:PRO:HD2	9:B:9677:HOH:O	2.20	0.41
1:B:189:ARG:HG3	9:B:9584:HOH:O	2.21	0.41
2:C:27:ARG:HG3	2:C:27:ARG:NH1	2.36	0.41
2:C:181:VAL:HG12	2:C:182:VAL:N	2.36	0.41
2:C:405:ARG:HH11	2:C:405:ARG:HG2	1.85	0.41
2:C:493:ARG:HB2	2:C:494:TYR:CE1	2.55	0.41
2:C:625:LEU:C	2:C:627:ARG:HH21	2.23	0.41
2:C:784:ASP:HB2	9:C:2121:HOH:O	2.19	0.41
2:C:889:HIS:CE1	3:D:951:ILE:H	2.28	0.41
2:C:964:LYS:O	2:C:968:LEU:HG	2.20	0.41
3:D:100:ALA:N	9:D:2106:HOH:O	2.53	0.41
3:D:119:SER:HB2	3:D:123:LEU:CB	2.42	0.41
3:D:162:ARG:NH1	9:D:9697:HOH:O	2.50	0.41
3:D:196:VAL:HG13	3:D:202:VAL:CG1	2.51	0.41
3:D:486:ARG:HA	3:D:489:ARG:HD3	2.03	0.41
3:D:520:LEU:O	3:D:525:ARG:NH1	2.54	0.41
3:D:527:MET:HE1	3:D:535:PHE:HB3	2.02	0.41
3:D:761:ILE:HD11	9:E:9593:HOH:O	2.20	0.41
3:D:780:LYS:NZ	3:D:912:LYS:HE3	2.36	0.41
3:D:785:ILE:N	9:D:2202:HOH:O	2.53	0.41
3:D:789:LEU:HD11	3:D:934:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.56	0.41
3:D:1103:HIS:CG	3:D:1104:GLU:N	2.89	0.41
3:D:1105:ILE:HD13	9:D:9754:HOH:O	2.20	0.41
3:D:1123:PHE:CD1	3:D:1134:LEU:HA	2.56	0.41
3:D:1197:ARG:C	3:D:1199:GLY:H	2.24	0.41
3:D:1500:LYS:HA	9:D:9806:HOH:O	2.20	0.41
4:E:25:LYS:HA	4:E:28:GLN:OE1	2.21	0.41
5:F:84:TYR:CD2	5:F:192:LEU:HD13	2.56	0.41
5:F:170:HIS:HA	5:F:173:TYR:HD1	1.85	0.41
5:F:276:ARG:HD2	9:F:9563:HOH:O	2.21	0.41
5:F:320:PRO:HA	9:F:9771:HOH:O	2.20	0.41
5:F:361:LEU:HB3	9:F:9838:HOH:O	2.21	0.41
1:K:128:HIS:O	1:K:129:ILE:HD13	2.20	0.41
1:K:165:ILE:HA	1:K:166:PRO:HD3	1.95	0.41
1:L:48:ILE:HA	1:L:49:PRO:HD3	1.86	0.41
1:L:50:GLY:O	1:L:146:ARG:HA	2.20	0.41
2:M:61:LYS:HB2	9:M:9741:HOH:O	2.20	0.41
2:M:166:PRO:HB2	9:M:9681:HOH:O	2.21	0.41
2:M:200:LEU:HD22	2:M:300:ASP:OD1	2.20	0.41
2:M:204:GLN:HB2	9:M:9986:HOH:O	2.20	0.41
2:M:397:GLU:N	2:M:633:GLN:OE1	2.54	0.41
2:M:504:GLU:HB2	9:M:9322:HOH:O	2.20	0.41
2:M:710:ILE:HB	2:M:790:LEU:HB2	2.02	0.41
2:M:850:ALA:CB	3:N:632:VAL:HG13	2.51	0.41
2:M:916:GLU:O	2:M:919:ALA:HB3	2.21	0.41
3:N:162:ARG:HG2	9:N:9455:HOH:O	2.20	0.41
3:N:416:ALA:HB3	3:N:417:PRO:HD3	2.02	0.41
3:N:737:ASN:N	9:N:9545:HOH:O	2.51	0.41
3:N:823:LEU:HD11	9:N:2306:HOH:O	2.20	0.41
3:N:851:LEU:N	3:N:851:LEU:HD23	2.35	0.41
3:N:1033:GLN:HB2	9:N:2467:HOH:O	2.21	0.41
3:N:1124:GLN:NE2	9:N:2426:HOH:O	2.53	0.41
3:N:1379:VAL:O	3:N:1392:GLY:HA2	2.21	0.41
4:O:33:HIS:HB2	4:O:37:ASN:ND2	2.35	0.41
4:O:87:LYS:HA	9:O:4487:HOH:O	2.20	0.41
5:P:115:LYS:HD2	5:P:118:GLU:OE2	2.21	0.41
5:P:157:GLU:O	5:P:161:GLN:HG3	2.21	0.41
5:P:276:ARG:HG3	5:P:276:ARG:HH11	1.86	0.41
1:A:35:THR:CG2	9:B:9638:HOH:O	2.68	0.41
1:A:65:PHE:CE2	2:C:830:LYS:HG3	2.56	0.41
2:C:300:ASP:C	2:C:302:VAL:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:547:ILE:HA	2:C:548:PRO:HD3	1.96	0.41
2:C:778:PHE:HE1	5:F:418:LEU:O	2.04	0.41
2:C:820:ARG:HG2	2:C:820:ARG:HH11	1.85	0.41
3:D:36:THR:C	3:D:38:LYS:N	2.73	0.41
3:D:54:LYS:CD	3:D:55:ASP:H	2.27	0.41
3:D:172:PRO:HB3	3:D:178:LEU:HB2	2.03	0.41
3:D:235:ALA:HA	9:D:2001:HOH:O	2.20	0.41
3:D:652:LEU:HB3	3:D:653:PHE:HD1	1.86	0.41
3:D:785:ILE:HD12	9:D:2202:HOH:O	2.19	0.41
3:D:890:VAL:HG21	3:D:922:LEU:CD1	2.51	0.41
3:D:995:LEU:HD23	9:D:2129:HOH:O	2.21	0.41
3:D:1384:PRO:HG3	3:D:1389:LEU:CA	2.51	0.41
5:F:110:MET:HG2	5:F:114:LYS:HE3	2.03	0.41
5:F:288:TYR:HA	5:F:291:ILE:HG22	2.03	0.41
1:K:18:ARG:CZ	1:K:88:ARG:HH21	2.34	0.41
1:L:10:VAL:O	1:L:12:THR:HG23	2.20	0.41
2:M:208:ALA:O	2:M:218:VAL:HG21	2.21	0.41
2:M:385:PHE:O	2:M:389:SER:HB3	2.21	0.41
2:M:721:ARG:HB2	2:M:759:THR:OG1	2.21	0.41
2:M:759:THR:HB	2:M:785:VAL:CG1	2.49	0.41
2:M:843:HIS:CD2	2:M:884:GLN:HA	2.56	0.41
3:N:457:GLY:HA3	3:N:568:ARG:HH12	1.86	0.41
3:N:589:ALA:N	9:N:2734:HOH:O	2.54	0.41
3:N:795:VAL:HG13	3:N:863:VAL:HG13	2.02	0.41
3:N:853:VAL:HG11	3:N:860:LEU:CD2	2.51	0.41
3:N:1036:ARG:HD3	9:N:2161:HOH:O	2.21	0.41
3:N:1311:LEU:HD22	9:N:9440:HOH:O	2.19	0.41
4:O:54:LEU:HA	4:O:58:PRO:HG2	2.03	0.41
5:P:88:ILE:O	5:P:92:PRO:HG3	2.21	0.41
5:P:153:PRO:HG2	5:P:154:LYS:H	1.86	0.41
5:P:292:ALA:HA	5:P:299:TRP:HB3	2.03	0.41
5:P:342:VAL:O	5:P:345:ALA:HB3	2.21	0.41
1:A:132:LEU:HD23	1:A:136:GLY:O	2.22	0.40
1:B:90:LEU:HD22	9:B:9609:HOH:O	2.21	0.40
2:C:162:ILE:O	2:C:164:PRO:HD3	2.21	0.40
2:C:193:LEU:HD12	2:C:307:LEU:HD22	2.03	0.40
2:C:266:ARG:HD3	2:C:288:ARG:NE	2.32	0.40
2:C:287:GLY:O	2:C:288:ARG:C	2.59	0.40
2:C:462:ASP:CG	2:C:468:ARG:HE	2.23	0.40
2:C:471:TYR:HE1	2:C:491:GLU:HG3	1.86	0.40
2:C:482:GLU:HG2	2:C:483:VAL:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:532:MET:HG3	2:C:533:ASP:N	2.36	0.40
2:C:628:PHE:HA	9:C:2384:HOH:O	2.21	0.40
2:C:927:GLY:HA3	9:C:2426:HOH:O	2.20	0.40
9:C:9574:HOH:O	3:D:582:LEU:HD21	2.21	0.40
3:D:470:LEU:HD22	3:D:499:VAL:HG13	2.02	0.40
3:D:764:LEU:HG	3:D:765:SER:N	2.36	0.40
3:D:998:GLU:HG2	9:D:3028:HOH:O	2.21	0.40
3:D:1093:TYR:O	3:D:1097:LYS:HG2	2.21	0.40
3:D:1097:LYS:HE2	9:D:9630:HOH:O	2.21	0.40
3:D:1112:CYS:HB2	9:D:9694:HOH:O	2.21	0.40
3:D:1343:ALA:N	9:D:9670:HOH:O	2.54	0.40
5:F:333:ILE:HA	5:F:334:PRO:HD3	1.81	0.40
1:K:5:LYS:NZ	9:K:1872:HOH:O	2.54	0.40
1:K:5:LYS:O	1:K:8:ALA:HB2	2.21	0.40
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.55	0.40
2:M:44:ILE:N	2:M:44:ILE:HD12	2.36	0.40
2:M:157:ARG:HB3	9:M:2325:HOH:O	2.21	0.40
2:M:197:LEU:CD1	2:M:207:LEU:HD11	2.52	0.40
2:M:321:GLU:HB3	9:M:9404:HOH:O	2.20	0.40
2:M:360:LEU:HD11	9:M:2160:HOH:O	2.19	0.40
2:M:577:PRO:HG3	2:M:993:PHE:CD1	2.56	0.40
2:M:1086:ARG:NH1	2:M:1086:ARG:HG3	2.36	0.40
3:N:128:TYR:O	3:N:568:ARG:NH2	2.54	0.40
3:N:221:ALA:HB3	3:N:367:ILE:CB	2.52	0.40
3:N:824:ASN:ND2	9:N:9277:HOH:O	2.53	0.40
3:N:1308:GLU:HG2	9:N:2487:HOH:O	2.21	0.40
5:P:94:LEU:HD12	5:P:97:GLU:CB	2.50	0.40
1:A:18:ARG:NH2	1:A:88:ARG:NH2	2.69	0.40
1:B:10:VAL:HG12	1:B:12:THR:HG23	2.02	0.40
2:C:140:ILE:HD11	2:C:412:ALA:HB2	2.03	0.40
2:C:300:ASP:HB2	2:C:303:PHE:CD1	2.56	0.40
2:C:358:ARG:NH2	2:C:373:VAL:N	2.66	0.40
2:C:686:ASP:N	9:C:2345:HOH:O	2.53	0.40
2:C:743:VAL:HG11	2:C:755:LEU:HD13	2.03	0.40
2:C:855:VAL:CG2	2:C:866:PRO:HG2	2.52	0.40
2:C:917:LEU:HG	9:C:9726:HOH:O	2.21	0.40
3:D:70:GLY:HA3	9:D:2046:HOH:O	2.20	0.40
3:D:211:VAL:HG12	3:D:212:ARG:N	2.36	0.40
3:D:493:ARG:HE	3:D:1389:LEU:HD21	1.86	0.40
3:D:795:VAL:HA	3:D:861:GLN:O	2.22	0.40
3:D:1198:TYR:OH	3:D:1394:VAL:HG21	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1278:ASP:N	3:D:1278:ASP:OD1	2.54	0.40
5:F:78:SER:O	5:F:82:ARG:HG3	2.21	0.40
5:F:256:ARG:HB3	9:F:9562:HOH:O	2.22	0.40
5:F:373:LYS:HA	5:F:378:GLY:C	2.42	0.40
5:F:396:ARG:HB2	9:F:9739:HOH:O	2.21	0.40
1:K:18:ARG:CZ	9:K:2975:HOH:O	2.70	0.40
1:L:13:VAL:HG12	1:L:14:ARG:N	2.36	0.40
2:M:44:ILE:HG23	9:M:9747:HOH:O	2.20	0.40
2:M:609:ASN:HB3	9:M:9455:HOH:O	2.20	0.40
2:M:637:LEU:CD2	2:M:659:PRO:HG2	2.51	0.40
2:M:786:LYS:NZ	9:M:2081:HOH:O	2.54	0.40
2:M:1107:ASN:HB3	9:M:9373:HOH:O	2.20	0.40
3:N:55:ASP:O	3:N:82:LYS:HA	2.22	0.40
3:N:671:LYS:HE3	5:P:421:PHE:O	2.22	0.40
3:N:736:PHE:HA	9:N:9545:HOH:O	2.21	0.40
3:N:935:LYS:HG2	3:N:939:PHE:CE1	2.57	0.40
3:N:1424:VAL:HG13	3:N:1425:THR:N	2.36	0.40
5:P:110:MET:HE2	9:P:2076:HOH:O	2.20	0.40
5:P:208:SER:HB2	5:P:211:ASP:OD1	2.20	0.40
1:A:5:LYS:O	1:A:8:ALA:HB2	2.21	0.40
1:A:68:ILE:O	1:A:71:VAL:HB	2.21	0.40
1:A:146:ARG:HG3	9:A:9628:HOH:O	2.21	0.40
1:B:81:ASN:ND2	9:B:9670:HOH:O	2.54	0.40
2:C:117:HIS:HB2	9:C:2237:HOH:O	2.21	0.40
2:C:280:LYS:HB3	9:C:2065:HOH:O	2.21	0.40
2:C:442:GLU:HG3	9:C:9844:HOH:O	2.21	0.40
2:C:473:ARG:HG2	2:C:473:ARG:HH11	1.86	0.40
2:C:636:ALA:C	2:C:637:LEU:HD23	2.41	0.40
2:C:1014:SER:HB2	5:F:331:ASP:OD1	2.21	0.40
3:D:806:PHE:HE1	3:D:813:LEU:HB3	1.84	0.40
3:D:1159:ARG:HG3	3:D:1159:ARG:NH1	2.35	0.40
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	2.22	0.40
4:E:35:PHE:HE2	4:E:63:TRP:CD2	2.40	0.40
5:F:234:LYS:CD	5:F:236:SER:HB2	2.49	0.40
1:K:100:LEU:HD11	9:K:7148:HOH:O	2.22	0.40
1:L:17:GLY:C	1:L:19:GLU:H	2.25	0.40
1:L:104:GLU:HA	1:L:136:GLY:O	2.21	0.40
2:M:44:ILE:HD12	2:M:44:ILE:H	1.86	0.40
2:M:49:ARG:HG2	9:M:2240:HOH:O	2.21	0.40
2:M:575:GLN:HE21	2:M:671:ASN:HD22	1.69	0.40
2:M:719:PRO:HG3	9:M:9740:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:724:ARG:HD2	2:M:738:ASP:O	2.21	0.40
2:M:737:LEU:O	2:M:738:ASP:C	2.59	0.40
3:N:64:LYS:HD3	5:P:376:ILE:O	2.21	0.40
3:N:85:VAL:HG12	3:N:89:ARG:NE	2.36	0.40
3:N:96:ALA:CB	3:N:554:LEU:HG	2.51	0.40
3:N:115:LEU:HD12	9:N:9458:HOH:O	2.21	0.40
3:N:396:VAL:CG2	3:N:447:VAL:HB	2.51	0.40
3:N:416:ALA:HA	3:N:442:ASN:ND2	2.36	0.40
3:N:456:MET:CG	3:N:568:ARG:HD3	2.51	0.40
3:N:930:LEU:HD12	3:N:930:LEU:O	2.21	0.40
3:N:983:LEU:HG	9:N:2329:HOH:O	2.21	0.40
3:N:1345:GLU:HG2	3:N:1376:MET:SD	2.62	0.40
4:O:40:LEU:HG	4:O:67:GLU:HG2	2.04	0.40
5:P:364:ARG:O	5:P:368:VAL:HG23	2.22	0.40
5:P:392:VAL:CG1	5:P:396:ARG:HB2	2.51	0.40
1:A:76:VAL:HA	1:A:79:ILE:HG12	2.03	0.40
1:B:170:VAL:N	9:B:9602:HOH:O	2.54	0.40
2:C:122:THR:HG22	2:C:123:GLU:N	2.37	0.40
2:C:427:VAL:HG22	9:C:2153:HOH:O	2.20	0.40
2:C:432:ARG:H	2:C:432:ARG:HG2	1.50	0.40
2:C:551:GLU:HB2	9:C:9690:HOH:O	2.21	0.40
2:C:1013:TYR:CE1	2:C:1020:PRO:HG3	2.57	0.40
3:D:80:VAL:HA	9:D:9665:HOH:O	2.21	0.40
3:D:116:LEU:C	3:D:118:LEU:HD13	2.41	0.40
3:D:586:ARG:NE	9:D:2208:HOH:O	2.48	0.40
3:D:683:ILE:HB	9:D:9721:HOH:O	2.22	0.40
3:D:789:LEU:CD1	3:D:934:LEU:HD22	2.51	0.40
3:D:836:VAL:HA	3:D:839:LEU:HD12	2.03	0.40
3:D:995:LEU:HB3	9:D:2129:HOH:O	2.20	0.40
5:F:93:LEU:HD11	5:F:187:LEU:HA	2.03	0.40
5:F:215:GLU:HA	5:F:215:GLU:OE1	2.21	0.40
1:K:57:TYR:CG	1:K:161:ARG:HD3	2.56	0.40
1:K:196:THR:HG23	1:K:196:THR:O	2.20	0.40
1:L:198:ARG:HG2	9:L:1453:HOH:O	2.21	0.40
1:L:206:THR:HG22	1:L:209:GLU:H	1.86	0.40
2:M:413:LEU:HD22	9:M:2205:HOH:O	2.22	0.40
2:M:473:ARG:HH21	2:M:484:VAL:HG21	1.86	0.40
2:M:516:ARG:HD2	3:N:1068:LEU:HD22	2.02	0.40
9:M:2038:HOH:O	3:N:680:GLN:HB2	2.22	0.40
3:N:116:LEU:HB3	3:N:118:LEU:CD1	2.41	0.40
3:N:126:VAL:HG13	3:N:132:TYR:CB	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:239:GLY:HA2	9:N:9367:HOH:O	2.21	0.40
3:N:601:ARG:NH2	3:N:613:ARG:NH2	2.69	0.40
3:N:704:ARG:CG	3:N:705:ALA:N	2.84	0.40
3:N:1087:ARG:HE	3:N:1238:MET:CB	2.34	0.40
4:O:10:PHE:O	4:O:13:VAL:HG22	2.22	0.40
4:O:25:LYS:HA	4:O:28:GLN:CD	2.41	0.40
5:P:253:ASP:HB3	5:P:259:ARG:NH2	2.36	0.40
5:P:294:ALA:HA	9:P:4602:HOH:O	2.21	0.40
2:C:165:LEU:HD12	2:C:166:PRO:CA	2.51	0.40
2:C:216:GLU:O	2:C:219:GLN:HG3	2.21	0.40
2:C:420:ARG:HA	9:C:2134:HOH:O	2.20	0.40
2:C:435:TYR:HD1	3:D:1071:PHE:CE2	2.40	0.40
2:C:724:ARG:O	2:C:734:LEU:HD11	2.21	0.40
2:C:739:GLU:N	9:C:9982:HOH:O	2.55	0.40
2:C:829:GLN:HB2	9:C:9705:HOH:O	2.20	0.40
3:D:130:SER:HB3	3:D:132:TYR:CE1	2.56	0.40
3:D:175:VAL:HG21	9:D:3255:HOH:O	2.21	0.40
3:D:554:LEU:O	3:D:557:LEU:HB2	2.20	0.40
3:D:702:LEU:HD12	3:D:702:LEU:N	2.36	0.40
3:D:729:HIS:CE1	3:D:730:PRO:HG2	2.57	0.40
3:D:1192:LEU:N	9:D:9658:HOH:O	2.54	0.40
3:D:1440:PHE:O	3:D:1443:THR:HG23	2.21	0.40
3:D:1489:GLN:HA	3:D:1489:GLN:NE2	2.35	0.40
5:F:281:GLU:HB2	9:F:9741:HOH:O	2.21	0.40
5:F:316:SER:HB3	5:F:319:THR:OG1	2.22	0.40
1:K:9:PRO:HD2	1:L:224:TYR:CG	2.56	0.40
1:K:85:LEU:HD12	1:K:124:ASN:CB	2.51	0.40
1:K:185:ARG:O	1:K:185:ARG:HD2	2.22	0.40
2:M:510:ALA:HB3	2:M:513:VAL:CG2	2.52	0.40
2:M:631:SER:OG	2:M:635:THR:N	2.55	0.40
2:M:722:ILE:HD12	2:M:823:VAL:HG21	2.03	0.40
2:M:837:ASP:O	2:M:849:VAL:HG23	2.21	0.40
2:M:881:ASN:HD22	2:M:881:ASN:N	2.11	0.40
2:M:906:PHE:CD1	3:N:1067:VAL:HG22	2.57	0.40
2:M:958:THR:O	2:M:962:GLN:HG3	2.22	0.40
2:M:1005:MET:HG3	3:N:629:SER:CB	2.44	0.40
3:N:49:ILE:HD13	9:N:9259:HOH:O	2.22	0.40
3:N:190:GLU:HG3	3:N:210:ARG:NH1	2.35	0.40
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.56	0.40
3:N:1121:PRO:HG3	9:N:9490:HOH:O	2.21	0.40
3:N:1378:TYR:CE2	3:N:1394:VAL:HG22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1417:TRP:HA	9:N:9243:HOH:O	2.21	0.40
3:N:1478:SER:O	3:N:1480:PHE:N	2.54	0.40
5:P:329:TYR:CE2	5:P:333:ILE:HD11	2.57	0.40
5:P:350:LEU:HG	5:P:354:LEU:CD1	2.50	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%)	187 (82%)	33 (14%)	7 (3%)	4	9
1	B	227/315 (72%)	183 (81%)	38 (17%)	6 (3%)	5	13
1	K	227/315 (72%)	186 (82%)	32 (14%)	9 (4%)	3	6
1	L	227/315 (72%)	185 (82%)	37 (16%)	5 (2%)	6	17
2	C	1117/1119 (100%)	856 (77%)	194 (17%)	67 (6%)	1	2
2	M	1117/1119 (100%)	863 (77%)	187 (17%)	67 (6%)	1	2
3	D	1388/1524 (91%)	1047 (75%)	248 (18%)	93 (7%)	1	1
3	N	1388/1524 (91%)	1042 (75%)	251 (18%)	95 (7%)	1	1
4	E	93/99 (94%)	72 (77%)	11 (12%)	10 (11%)	0	0
4	O	93/99 (94%)	70 (75%)	13 (14%)	10 (11%)	0	0
5	F	341/423 (81%)	264 (77%)	53 (16%)	24 (7%)	1	1
5	P	341/423 (81%)	267 (78%)	53 (16%)	21 (6%)	1	2
All	All	6786/7590 (89%)	5222 (77%)	1150 (17%)	414 (6%)	1	2

All (414) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA
1	A	188	GLN
1	B	118	ALA
2	C	10	ARG
2	C	59	LYS
2	C	111	ASP
2	C	152	PRO
2	C	178	PRO
2	C	231	PRO
2	C	244	PRO
2	C	251	ASP
2	C	253	ALA
2	C	261	ILE
2	C	265	ARG
2	C	267	TYR
2	C	290	LEU
2	C	316	GLY
2	C	363	SER
2	C	369	PRO
2	C	419	THR
2	C	462	ASP
2	C	518	LYS
2	C	627	ARG
2	C	684	PHE
2	C	735	ARG
2	C	738	ASP
2	C	740	GLU
2	C	762	LYS
2	C	864	GLY
2	C	905	ILE
3	D	55	ASP
3	D	83	SER
3	D	98	PRO
3	D	120	ALA
3	D	136	ASP
3	D	140	ALA
3	D	177	ALA
3	D	208	PRO
3	D	209	ARG
3	D	233	LYS
3	D	234	GLU
3	D	238	PRO
3	D	246	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	370	ALA
3	D	373	PRO
3	D	385	VAL
3	D	417	PRO
3	D	487	ALA
3	D	807	ALA
3	D	832	ARG
3	D	1028	ALA
3	D	1125	PRO
3	D	1197	ARG
3	D	1208	ASP
3	D	1243	THR
3	D	1388	ARG
3	D	1389	LEU
3	D	1390	LEU
4	E	42	PRO
4	E	58	PRO
5	F	75	ILE
5	F	76	SER
5	F	77	THR
5	F	145	PRO
5	F	148	LYS
5	F	153	PRO
5	F	297	PRO
5	F	324	GLU
5	F	341	PRO
5	F	364	ARG
5	F	390	PHE
1	K	118	ALA
1	K	187	GLY
1	L	118	ALA
2	M	10	ARG
2	M	59	LYS
2	M	111	ASP
2	M	152	PRO
2	M	178	PRO
2	M	231	PRO
2	M	244	PRO
2	M	251	ASP
2	M	253	ALA
2	M	261	ILE
2	M	265	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	M	267	TYR
2	M	290	LEU
2	M	316	GLY
2	M	363	SER
2	M	369	PRO
2	M	419	THR
2	M	462	ASP
2	M	518	LYS
2	M	627	ARG
2	M	684	PHE
2	M	735	ARG
2	M	738	ASP
2	M	740	GLU
2	M	762	LYS
2	M	864	GLY
2	M	905	ILE
3	N	40	GLU
3	N	55	ASP
3	N	120	ALA
3	N	136	ASP
3	N	140	ALA
3	N	177	ALA
3	N	208	PRO
3	N	209	ARG
3	N	233	LYS
3	N	234	GLU
3	N	238	PRO
3	N	246	PRO
3	N	370	ALA
3	N	373	PRO
3	N	385	VAL
3	N	417	PRO
3	N	487	ALA
3	N	807	ALA
3	N	832	ARG
3	N	1028	ALA
3	N	1066	THR
3	N	1125	PRO
3	N	1197	ARG
3	N	1208	ASP
3	N	1243	THR
3	N	1287	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	N	1389	LEU
3	N	1390	LEU
4	O	42	PRO
4	O	58	PRO
5	P	75	ILE
5	P	76	SER
5	P	77	THR
5	P	145	PRO
5	P	148	LYS
5	P	153	PRO
5	P	232	ARG
5	P	297	PRO
5	P	324	GLU
5	P	341	PRO
5	P	364	ARG
5	P	390	PHE
1	A	11	PHE
1	A	187	GLY
1	A	191	ASP
2	C	7	GLY
2	C	11	GLU
2	C	129	ILE
2	C	144	PRO
2	C	262	ALA
2	C	288	ARG
2	C	292	ARG
2	C	465	GLY
2	C	548	PRO
2	C	575	GLN
2	C	598	GLU
2	C	626	ARG
2	C	727	PRO
2	C	1005	MET
2	C	1016	ILE
2	C	1106	ASP
3	D	37	LEU
3	D	40	GLU
3	D	43	GLY
3	D	88	TYR
3	D	119	SER
3	D	135	LEU
3	D	202	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	424	GLY
3	D	440	VAL
3	D	601	ARG
3	D	782	SER
3	D	1066	THR
3	D	1067	VAL
3	D	1111	ASP
3	D	1127	GLU
3	D	1129	THR
3	D	1265	ALA
3	D	1287	GLU
3	D	1475	GLY
4	E	43	GLU
5	F	147	LEU
5	F	232	ARG
5	F	255	ALA
1	K	188	GLN
2	M	7	GLY
2	M	11	GLU
2	M	23	VAL
2	M	129	ILE
2	M	130	ASN
2	M	262	ALA
2	M	292	ARG
2	M	465	GLY
2	M	548	PRO
2	M	598	GLU
2	M	626	ARG
2	M	727	PRO
2	M	1005	MET
2	M	1016	ILE
2	M	1106	ASP
3	N	37	LEU
3	N	43	GLY
3	N	82	LYS
3	N	83	SER
3	N	88	TYR
3	N	98	PRO
3	N	119	SER
3	N	135	LEU
3	N	202	VAL
3	N	217	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	N	424	GLY
3	N	440	VAL
3	N	601	ARG
3	N	782	SER
3	N	1067	VAL
3	N	1089	ALA
3	N	1111	ASP
3	N	1127	GLU
3	N	1137	ARG
3	N	1265	ALA
3	N	1385	GLY
3	N	1388	ARG
3	N	1475	GLY
4	O	43	GLU
5	P	95	THR
5	P	420	ASP
2	C	130	ASN
2	C	164	PRO
2	C	170	PRO
2	C	457	ALA
2	C	739	GLU
2	C	767	PRO
2	C	1079	PRO
3	D	110	SER
3	D	115	LEU
3	D	117	ASP
3	D	137	PRO
3	D	190	GLU
3	D	410	SER
3	D	416	ALA
3	D	504	ASP
3	D	521	PRO
3	D	594	PRO
3	D	705	ALA
3	D	922	LEU
3	D	1089	ALA
3	D	1385	GLY
3	D	1429	LEU
4	E	5	GLY
4	E	33	HIS
4	E	41	GLU
4	E	46	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	F	95	THR
5	F	286	PRO
5	F	420	ASP
5	F	421	PHE
1	K	11	PHE
1	L	191	ASP
2	M	144	PRO
2	M	164	PRO
2	M	170	PRO
2	M	223	ASP
2	M	288	ARG
2	M	381	ALA
2	M	457	ALA
2	M	699	PHE
2	M	739	GLU
2	M	767	PRO
3	N	115	LEU
3	N	137	PRO
3	N	189	GLN
3	N	206	ARG
3	N	410	SER
3	N	416	ALA
3	N	594	PRO
3	N	705	ALA
3	N	869	MET
3	N	922	LEU
3	N	1429	LEU
4	O	5	GLY
4	O	33	HIS
4	O	41	GLU
4	O	46	PRO
5	P	147	LEU
5	P	255	ALA
5	P	285	GLU
5	P	286	PRO
5	P	329	TYR
1	A	59	GLU
1	B	11	PHE
1	B	59	GLU
1	B	191	ASP
2	C	23	VAL
2	C	277	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	381	ALA
2	C	415	PRO
2	C	699	PHE
3	D	31	THR
3	D	82	LYS
3	D	189	GLN
3	D	206	ARG
3	D	381	ALA
3	D	560	GLN
3	D	808	THR
3	D	869	MET
3	D	919	PHE
3	D	1051	GLU
3	D	1155	VAL
3	D	1248	GLY
3	D	1288	GLU
4	E	82	GLU
5	F	155	THR
5	F	285	GLU
5	F	329	TYR
1	K	59	GLU
1	K	191	ASP
1	L	11	PHE
1	L	59	GLU
2	M	277	ALA
2	M	415	PRO
2	M	1079	PRO
3	N	110	SER
3	N	133	ILE
3	N	149	LYS
3	N	190	GLU
3	N	504	ASP
3	N	521	PRO
3	N	560	GLN
3	N	801	GLY
3	N	806	PHE
3	N	808	THR
3	N	936	TYR
3	N	1051	GLU
3	N	1155	VAL
3	N	1248	GLY
5	P	416	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	106	PRO
1	B	106	PRO
2	C	113	VAL
2	C	180	GLY
2	C	377	PRO
3	D	149	LYS
3	D	522	PRO
3	D	801	GLY
3	D	822	ALA
4	E	32	ARG
4	E	57	ASP
5	F	97	GLU
5	F	416	ARG
1	K	93	SER
1	K	106	PRO
2	M	180	GLY
2	M	434	HIS
2	M	1004	LYS
3	N	31	THR
3	N	522	PRO
3	N	822	ALA
3	N	919	PHE
3	N	945	SER
3	N	1019	PRO
4	O	32	ARG
4	O	57	ASP
4	O	82	GLU
2	C	202	TYR
2	C	1020	PRO
3	D	133	ILE
3	D	138	LYS
3	D	936	TYR
3	D	1213	ARG
1	K	172	SER
1	L	106	PRO
2	M	113	VAL
2	M	377	PRO
2	M	575	GLN
3	N	117	ASP
3	N	381	ALA
3	N	406	ASP
3	N	1205	TYR

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Mol	Chain	Res	Type
3	N	1213	ARG
5	P	167	PRO
2	C	779	GLY
3	D	245	LEU
3	D	509	PRO
3	D	1019	PRO
5	F	167	PRO
2	M	777	ILE
2	M	779	GLY
1	B	48	ILE
2	C	42	VAL
3	D	141	ILE
2	M	1020	PRO
3	N	245	LEU
2	C	811	PRO
2	C	876	VAL
3	D	175	VAL
2	M	42	VAL
2	M	876	VAL
3	N	78	VAL
3	N	108	VAL
3	N	141	ILE
3	N	173	PRO
2	C	777	ILE
3	D	78	VAL
3	D	425	GLY
3	D	670	VAL
3	N	425	GLY
3	N	526	PRO
2	C	1060	ILE
3	D	52	PRO
3	D	530	VAL
3	N	175	VAL
2	M	166	PRO
2	C	166	PRO

### 5.3.2 Protein sidechains [i](#)

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%)	181 (90%)	21 (10%)	7	16
1	B	202/273 (74%)	186 (92%)	16 (8%)	12	28
1	K	202/273 (74%)	187 (93%)	15 (7%)	13	32
1	L	202/273 (74%)	190 (94%)	12 (6%)	19	43
2	C	941/941 (100%)	827 (88%)	114 (12%)	5	11
2	M	941/941 (100%)	838 (89%)	103 (11%)	6	14
3	D	1123/1279 (88%)	992 (88%)	131 (12%)	5	12
3	N	1123/1279 (88%)	987 (88%)	136 (12%)	5	11
4	E	83/87 (95%)	73 (88%)	10 (12%)	5	11
4	O	83/87 (95%)	73 (88%)	10 (12%)	5	11
5	F	295/370 (80%)	263 (89%)	32 (11%)	6	15
5	P	295/370 (80%)	273 (92%)	22 (8%)	13	31
All	All	5692/6446 (88%)	5070 (89%)	622 (11%)	6	14

All (622) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	5	LYS
1	A	9	PRO
1	A	15	THR
1	A	26	GLU
1	A	62	LEU
1	A	92	PRO
1	A	95	GLN
1	A	96	THR
1	A	124	ASN
1	A	145	ASP
1	A	146	ARG
1	A	156	HIS
1	A	160	ASP
1	A	170	VAL
1	A	185	ARG
1	A	196	THR
1	A	197	LEU
1	A	206	THR
1	A	208	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	227	ASN
1	B	7	LYS
1	B	9	PRO
1	B	26	GLU
1	B	62	LEU
1	B	95	GLN
1	B	96	THR
1	B	119	ASP
1	B	124	ASN
1	B	134	GLU
1	B	138	LEU
1	B	140	MET
1	B	145	ASP
1	B	159	LYS
1	B	160	ASP
1	B	189	ARG
1	B	206	THR
2	C	6	PHE
2	C	8	ARG
2	C	26	TYR
2	C	30	LEU
2	C	41	ASN
2	C	48	PHE
2	C	52	PHE
2	C	81	ASP
2	C	87	ASP
2	C	95	TYR
2	C	107	LEU
2	C	113	VAL
2	C	114	PHE
2	C	115	LEU
2	C	118	ILE
2	C	134	ARG
2	C	152	PRO
2	C	157	ARG
2	C	158	TYR
2	C	163	ILE
2	C	168	ARG
2	C	178	PRO
2	C	184	MET
2	C	186	VAL
2	C	190	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	198	ARG
2	C	203	ASP
2	C	207	LEU
2	C	216	GLU
2	C	217	LEU
2	C	218	VAL
2	C	224	GLU
2	C	243	ARG
2	C	246	ASP
2	C	247	PRO
2	C	256	TYR
2	C	261	ILE
2	C	266	ARG
2	C	268	ASP
2	C	281	LEU
2	C	288	ARG
2	C	289	THR
2	C	290	LEU
2	C	309	TYR
2	C	321	GLU
2	C	333	ILE
2	C	344	PHE
2	C	359	MET
2	C	367	LEU
2	C	388	ARG
2	C	389	SER
2	C	393	GLN
2	C	402	SER
2	C	418	LEU
2	C	420	ARG
2	C	425	PHE
2	C	432	ARG
2	C	455	LEU
2	C	460	ARG
2	C	469	THR
2	C	471	TYR
2	C	500	ASN
2	C	507	ARG
2	C	527	GLU
2	C	533	ASP
2	C	559	LEU
2	C	564	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	579	VAL
2	C	584	GLU
2	C	620	LEU
2	C	627	ARG
2	C	637	LEU
2	C	640	ARG
2	C	645	VAL
2	C	650	ARG
2	C	657	ASP
2	C	689	VAL
2	C	693	GLU
2	C	699	PHE
2	C	701	THR
2	C	719	PRO
2	C	727	PRO
2	C	739	GLU
2	C	744	ARG
2	C	755	LEU
2	C	773	LEU
2	C	785	VAL
2	C	807	ARG
2	C	815	LEU
2	C	824	ARG
2	C	841	ASN
2	C	862	PRO
2	C	865	THR
2	C	881	ASN
2	C	886	LEU
2	C	887	GLU
2	C	900	ARG
2	C	917	LEU
2	C	934	PHE
2	C	945	ARG
2	C	950	LEU
2	C	952	LEU
2	C	959	PRO
2	C	962	GLN
2	C	982	PRO
2	C	988	VAL
2	C	999	HIS
2	C	1003	ASP
2	C	1016	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	1017	THR
2	C	1019	GLN
2	C	1020	PRO
2	C	1052	MET
2	C	1115	LEU
3	D	3	LYS
3	D	6	ARG
3	D	12	LEU
3	D	25	GLU
3	D	27	GLU
3	D	42	ASP
3	D	56	TYR
3	D	66	GLN
3	D	76	CYS
3	D	87	ARG
3	D	98	PRO
3	D	103	TRP
3	D	121	THR
3	D	127	LEU
3	D	135	LEU
3	D	136	ASP
3	D	145	VAL
3	D	149	LYS
3	D	152	LEU
3	D	163	TYR
3	D	168	THR
3	D	169	TYR
3	D	171	LEU
3	D	185	VAL
3	D	199	LEU
3	D	208	PRO
3	D	389	GLU
3	D	393	ILE
3	D	403	PHE
3	D	423	ASP
3	D	426	LYS
3	D	445	ARG
3	D	447	VAL
3	D	456	MET
3	D	465	LEU
3	D	476	GLU
3	D	486	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	488	ARG
3	D	521	PRO
3	D	523	ASP
3	D	528	VAL
3	D	554	LEU
3	D	569	ASN
3	D	594	PRO
3	D	602	SER
3	D	605	ASP
3	D	624	ASP
3	D	626	SER
3	D	629	SER
3	D	635	PRO
3	D	651	GLU
3	D	662	GLU
3	D	676	MET
3	D	679	ARG
3	D	685	ASP
3	D	710	ARG
3	D	725	SER
3	D	727	GLN
3	D	754	PHE
3	D	770	LEU
3	D	781	PRO
3	D	782	SER
3	D	792	ILE
3	D	794	GLN
3	D	796	ARG
3	D	828	LYS
3	D	829	VAL
3	D	834	THR
3	D	863	VAL
3	D	865	THR
3	D	873	LEU
3	D	899	LEU
3	D	904	VAL
3	D	935	LYS
3	D	961	LYS
3	D	986	ARG
3	D	988	ARG
3	D	1029	ARG
3	D	1044	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	1046	GLN
3	D	1058	ARG
3	D	1062	ARG
3	D	1096	ARG
3	D	1097	LYS
3	D	1109	GLU
3	D	1112	CYS
3	D	1127	GLU
3	D	1134	LEU
3	D	1135	ARG
3	D	1152	GLU
3	D	1159	ARG
3	D	1166	LEU
3	D	1182	GLU
3	D	1183	ILE
3	D	1194	CYS
3	D	1196	THR
3	D	1207	TYR
3	D	1209	LEU
3	D	1211	MET
3	D	1213	ARG
3	D	1231	GLU
3	D	1238	MET
3	D	1243	THR
3	D	1252	ILE
3	D	1253	THR
3	D	1257	PRO
3	D	1267	ARG
3	D	1278	ASP
3	D	1285	GLU
3	D	1299	PHE
3	D	1304	LYS
3	D	1306	PRO
3	D	1314	LYS
3	D	1315	ASP
3	D	1317	ASP
3	D	1326	THR
3	D	1337	GLU
3	D	1344	VAL
3	D	1346	ARG
3	D	1375	MET
3	D	1388	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	1389	LEU
3	D	1390	LEU
3	D	1396	GLU
3	D	1406	ARG
3	D	1412	LYS
3	D	1427	SER
3	D	1432	LYS
3	D	1434	TRP
3	D	1442	ASN
3	D	1487	VAL
4	E	42	PRO
4	E	46	PRO
4	E	47	LYS
4	E	51	LEU
4	E	57	ASP
4	E	58	PRO
4	E	59	ASN
4	E	61	GLU
4	E	66	LYS
4	E	79	LEU
5	F	84	TYR
5	F	87	GLU
5	F	94	LEU
5	F	120	THR
5	F	124	PRO
5	F	125	ASP
5	F	142	ARG
5	F	149	GLU
5	F	156	VAL
5	F	174	LEU
5	F	203	THR
5	F	234	LYS
5	F	280	GLN
5	F	282	LEU
5	F	285	GLU
5	F	295	MET
5	F	297	PRO
5	F	307	THR
5	F	312	GLN
5	F	341	PRO
5	F	347	GLN
5	F	352	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	F	361	LEU
5	F	362	SER
5	F	364	ARG
5	F	370	LYS
5	F	375	LEU
5	F	392	VAL
5	F	396	ARG
5	F	398	ARG
5	F	405	LEU
5	F	409	LYS
1	K	12	THR
1	K	15	THR
1	K	26	GLU
1	K	62	LEU
1	K	95	GLN
1	K	96	THR
1	K	124	ASN
1	K	143	ARG
1	K	146	ARG
1	K	167	VAL
1	K	186	LEU
1	K	201	THR
1	K	216	GLU
1	K	223	THR
1	K	227	ASN
1	L	1	MET
1	L	2	LEU
1	L	3	ASP
1	L	5	LYS
1	L	26	GLU
1	L	62	LEU
1	L	95	GLN
1	L	96	THR
1	L	124	ASN
1	L	145	ASP
1	L	189	ARG
1	L	196	THR
2	M	26	TYR
2	M	28	ARG
2	M	30	LEU
2	M	31	GLN
2	M	34	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	M	39	ARG
2	M	41	ASN
2	M	52	PHE
2	M	68	PHE
2	M	107	LEU
2	M	115	LEU
2	M	129	ILE
2	M	144	PRO
2	M	147	TYR
2	M	152	PRO
2	M	158	TYR
2	M	167	LYS
2	M	168	ARG
2	M	170	PRO
2	M	178	PRO
2	M	185	LYS
2	M	186	VAL
2	M	189	ARG
2	M	194	VAL
2	M	198	ARG
2	M	203	ASP
2	M	207	LEU
2	M	209	ARG
2	M	216	GLU
2	M	221	LEU
2	M	230	ARG
2	M	243	ARG
2	M	254	VAL
2	M	256	TYR
2	M	257	VAL
2	M	288	ARG
2	M	290	LEU
2	M	309	TYR
2	M	328	LEU
2	M	333	ILE
2	M	343	GLN
2	M	359	MET
2	M	384	GLU
2	M	393	GLN
2	M	397	GLU
2	M	407	LYS
2	M	418	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	M	420	ARG
2	M	426	ASP
2	M	432	ARG
2	M	455	LEU
2	M	481	ASP
2	M	503	LEU
2	M	523	ILE
2	M	533	ASP
2	M	542	VAL
2	M	548	PRO
2	M	564	MET
2	M	607	ASP
2	M	609	ASN
2	M	620	LEU
2	M	629	TYR
2	M	633	GLN
2	M	650	ARG
2	M	663	ASN
2	M	678	PRO
2	M	679	PHE
2	M	680	ASP
2	M	686	ASP
2	M	701	THR
2	M	716	LYS
2	M	727	PRO
2	M	728	HIS
2	M	729	LEU
2	M	737	LEU
2	M	750	LYS
2	M	765	SER
2	M	774	LEU
2	M	785	VAL
2	M	799	ILE
2	M	839	LEU
2	M	841	ASN
2	M	848	VAL
2	M	865	THR
2	M	871	LEU
2	M	876	VAL
2	M	881	ASN
2	M	886	LEU
2	M	928	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	M	937	ASP
2	M	948	GLU
2	M	950	LEU
2	M	958	THR
2	M	981	GLU
2	M	984	GLU
2	M	988	VAL
2	M	1015	LEU
2	M	1026	GLN
2	M	1057	SER
2	M	1079	PRO
2	M	1098	ASP
2	M	1110	ASP
2	M	1119	ARG
3	N	12	LEU
3	N	19	ARG
3	N	23	TYR
3	N	25	GLU
3	N	34	TYR
3	N	47	GLU
3	N	65	ARG
3	N	71	LYS
3	N	76	CYS
3	N	98	PRO
3	N	109	PRO
3	N	115	LEU
3	N	122	GLU
3	N	126	VAL
3	N	128	TYR
3	N	131	LYS
3	N	135	LEU
3	N	138	LYS
3	N	142	LEU
3	N	143	ASN
3	N	145	VAL
3	N	149	LYS
3	N	154	THR
3	N	155	ASP
3	N	168	THR
3	N	185	VAL
3	N	190	GLU
3	N	197	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	N	199	LEU
3	N	205	TYR
3	N	208	PRO
3	N	394	LEU
3	N	403	PHE
3	N	406	ASP
3	N	432	TYR
3	N	442	ASN
3	N	445	ARG
3	N	452	ILE
3	N	456	MET
3	N	474	GLU
3	N	502	PHE
3	N	503	LEU
3	N	510	GLU
3	N	513	ILE
3	N	521	PRO
3	N	549	ASN
3	N	554	LEU
3	N	581	LEU
3	N	594	PRO
3	N	601	ARG
3	N	602	SER
3	N	604	THR
3	N	605	ASP
3	N	611	GLN
3	N	624	ASP
3	N	644	LEU
3	N	660	LYS
3	N	676	MET
3	N	679	ARG
3	N	681	ARG
3	N	682	ASP
3	N	703	ASN
3	N	707	THR
3	N	709	HIS
3	N	711	LEU
3	N	722	GLU
3	N	724	GLN
3	N	737	ASN
3	N	739	ASP
3	N	754	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	N	794	GLN
3	N	800	LYS
3	N	828	LYS
3	N	845	ASN
3	N	847	ASP
3	N	859	ASP
3	N	863	VAL
3	N	864	VAL
3	N	865	THR
3	N	879	ARG
3	N	880	ILE
3	N	897	TRP
3	N	899	LEU
3	N	902	LEU
3	N	907	GLU
3	N	919	PHE
3	N	942	SER
3	N	951	ILE
3	N	970	LYS
3	N	1005	GLN
3	N	1029	ARG
3	N	1045	MET
3	N	1058	ARG
3	N	1062	ARG
3	N	1066	THR
3	N	1068	LEU
3	N	1083	ASP
3	N	1087	ARG
3	N	1096	ARG
3	N	1109	GLU
3	N	1112	CYS
3	N	1124	GLN
3	N	1127	GLU
3	N	1134	LEU
3	N	1137	ARG
3	N	1164	ARG
3	N	1166	LEU
3	N	1169	ASP
3	N	1183	ILE
3	N	1197	ARG
3	N	1207	TYR
3	N	1211	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	N	1231	GLU
3	N	1243	THR
3	N	1252	ILE
3	N	1253	THR
3	N	1267	ARG
3	N	1274	ILE
3	N	1278	ASP
3	N	1285	GLU
3	N	1287	GLU
3	N	1297	GLU
3	N	1304	LYS
3	N	1308	GLU
3	N	1311	LEU
3	N	1314	LYS
3	N	1318	TYR
3	N	1342	GLU
3	N	1350	GLU
3	N	1376	MET
3	N	1389	LEU
3	N	1396	GLU
3	N	1415	VAL
3	N	1442	ASN
3	N	1468	LEU
3	N	1497	GLU
4	O	3	GLU
4	O	32	ARG
4	O	40	LEU
4	O	42	PRO
4	O	46	PRO
4	O	51	LEU
4	O	58	PRO
4	O	59	ASN
4	O	61	GLU
4	O	85	LEU
5	P	84	TYR
5	P	86	HIS
5	P	91	VAL
5	P	120	THR
5	P	122	LEU
5	P	142	ARG
5	P	148	LYS
5	P	149	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	P	174	LEU
5	P	194	LEU
5	P	208	SER
5	P	280	GLN
5	P	281	GLU
5	P	295	MET
5	P	302	LYS
5	P	318	GLU
5	P	341	PRO
5	P	353	GLU
5	P	401	GLU
5	P	406	ARG
5	P	409	LYS
5	P	411	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	95	GLN
1	A	124	ASN
1	A	156	HIS
1	A	163	ASN
1	A	180	GLN
1	A	212	ASN
1	A	213	GLN
1	A	227	ASN
1	A	229	GLN
1	B	63	HIS
1	B	95	GLN
1	B	124	ASN
1	B	163	ASN
1	B	212	ASN
1	B	221	HIS
1	B	227	ASN
2	C	31	GLN
2	C	41	ASN
2	C	45	GLN
2	C	91	GLN
2	C	204	GLN
2	C	343	GLN
2	C	431	HIS
2	C	434	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	498	GLN
2	C	538	GLN
2	C	552	HIS
2	C	609	ASN
2	C	632	ASN
2	C	671	ASN
2	C	704	HIS
2	C	829	GLN
2	C	834	GLN
2	C	841	ASN
2	C	843	HIS
2	C	881	ASN
2	C	889	HIS
2	C	969	GLN
2	C	991	GLN
2	C	1018	GLN
2	C	1019	GLN
2	C	1100	GLN
3	D	166	GLN
3	D	507	ASN
3	D	549	ASN
3	D	575	GLN
3	D	616	GLN
3	D	669	ASN
3	D	696	HIS
3	D	717	GLN
3	D	744	GLN
3	D	756	GLN
3	D	768	ASN
3	D	816	HIS
3	D	824	ASN
3	D	845	ASN
3	D	962	GLN
3	D	976	GLN
3	D	991	GLN
3	D	994	GLN
3	D	1005	GLN
3	D	1124	GLN
3	D	1202	GLN
3	D	1465	ASN
3	D	1489	GLN
4	E	33	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	E	86	GLN
5	F	90	GLN
5	F	191	ASN
5	F	217	ASN
5	F	218	GLN
5	F	245	GLN
5	F	269	ASN
5	F	337	HIS
5	F	402	ASN
1	K	81	ASN
1	K	95	GLN
1	K	124	ASN
1	K	163	ASN
1	K	180	GLN
1	K	212	ASN
1	K	227	ASN
1	L	81	ASN
1	L	95	GLN
1	L	124	ASN
1	L	163	ASN
1	L	180	GLN
1	L	221	HIS
1	L	229	GLN
2	M	31	GLN
2	M	41	ASN
2	M	80	GLN
2	M	99	GLN
2	M	187	ASN
2	M	204	GLN
2	M	330	ASN
2	M	343	GLN
2	M	390	GLN
2	M	431	HIS
2	M	434	HIS
2	M	538	GLN
2	M	545	ASN
2	M	552	HIS
2	M	565	GLN
2	M	567	GLN
2	M	575	GLN
2	M	663	ASN
2	M	829	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	M	841	ASN
2	M	881	ASN
2	M	969	GLN
2	M	1018	GLN
2	M	1026	GLN
2	M	1050	GLN
2	M	1093	GLN
2	M	1107	ASN
3	N	101	HIS
3	N	151	GLN
3	N	166	GLN
3	N	442	ASN
3	N	462	GLN
3	N	529	GLN
3	N	552	ASN
3	N	569	ASN
3	N	575	GLN
3	N	636	GLN
3	N	703	ASN
3	N	709	HIS
3	N	724	GLN
3	N	727	GLN
3	N	737	ASN
3	N	744	GLN
3	N	756	GLN
3	N	767	HIS
3	N	768	ASN
3	N	794	GLN
3	N	901	GLN
3	N	962	GLN
3	N	991	GLN
3	N	994	GLN
3	N	1005	GLN
3	N	1010	ASN
3	N	1014	ASN
3	N	1184	GLN
3	N	1323	GLN
3	N	1442	ASN
3	N	1465	ASN
4	O	28	GLN
4	O	29	GLN
4	O	33	HIS

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Mol	Chain	Res	Type
4	O	37	ASN
5	P	83	GLN
5	P	90	GLN
5	P	161	GLN
5	P	191	ASN
5	P	254	GLN
5	P	277	GLN
5	P	280	GLN
5	P	312	GLN
5	P	337	HIS
5	P	399	GLN
5	P	411	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 368 ligands modelled in this entry, 366 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
8	G4P	N	9101	6	30,38,38	1.55	5 (16%)	42,61,61	1.52	6 (14%)
8	G4P	N	9100	6	30,38,38	1.37	4 (13%)	42,61,61	1.61	9 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	G4P	N	9101	6	-	8/23/43/43	0/3/3/3
8	G4P	N	9100	6	-	8/23/43/43	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	9101	G4P	O4'-C1'	3.85	1.46	1.41
8	N	9101	G4P	C5-C6	-3.57	1.40	1.47
8	N	9101	G4P	C6-N1	3.50	1.43	1.37
8	N	9100	G4P	O4'-C1'	3.17	1.45	1.41
8	N	9101	G4P	C8-N7	-3.09	1.29	1.35
8	N	9100	G4P	C8-N7	-3.06	1.29	1.35
8	N	9100	G4P	PD-O3D	2.70	1.65	1.54
8	N	9101	G4P	PD-O3D	2.38	1.64	1.54
8	N	9100	G4P	C5-C4	-2.05	1.37	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	9101	G4P	PC-O3C-PD	-5.30	114.65	132.83
8	N	9100	G4P	PA-O3A-PB	-4.40	117.73	132.83
8	N	9101	G4P	O3'-C3'-C4'	4.26	125.47	110.08
8	N	9100	G4P	O3B-PB-O3A	-3.07	94.35	104.64
8	N	9100	G4P	C2'-C3'-C4'	3.06	108.65	103.22
8	N	9100	G4P	O5'-PA-O1A	2.81	120.03	109.07
8	N	9101	G4P	PA-O3A-PB	-2.48	124.33	132.83
8	N	9100	G4P	O3'-C3'-C2'	2.45	120.57	111.68
8	N	9100	G4P	O3'-PC-O1C	-2.36	100.61	109.47
8	N	9100	G4P	O3'-C3'-C4'	2.33	118.52	110.08
8	N	9101	G4P	C2'-C3'-C4'	2.27	107.24	103.22
8	N	9100	G4P	O3B-PB-O1B	2.18	119.20	110.68
8	N	9101	G4P	O2D-PD-O3C	2.14	111.81	104.64
8	N	9101	G4P	O2'-C2'-C3'	2.09	117.11	111.17
8	N	9100	G4P	O4'-C4'-C3'	-2.00	100.58	104.87

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	N	9100	G4P	PA-O3A-PB-O2B
8	N	9100	G4P	C5'-O5'-PA-O1A
8	N	9100	G4P	C4'-C5'-O5'-PA
8	N	9100	G4P	PC-O3C-PD-O3D
8	N	9101	G4P	PA-O3A-PB-O3B
8	N	9101	G4P	C5'-O5'-PA-O1A
8	N	9101	G4P	C5'-O5'-PA-O2A
8	N	9101	G4P	C2'-C3'-O3'-PC
8	N	9101	G4P	C3'-O3'-PC-O3C
8	N	9101	G4P	C4'-C5'-O5'-PA
8	N	9100	G4P	C5'-O5'-PA-O3A
8	N	9100	G4P	C5'-O5'-PA-O2A
8	N	9100	G4P	PC-O3C-PD-O1D
8	N	9100	G4P	PA-O3A-PB-O3B
8	N	9101	G4P	C5'-O5'-PA-O3A
8	N	9101	G4P	PA-O3A-PB-O1B

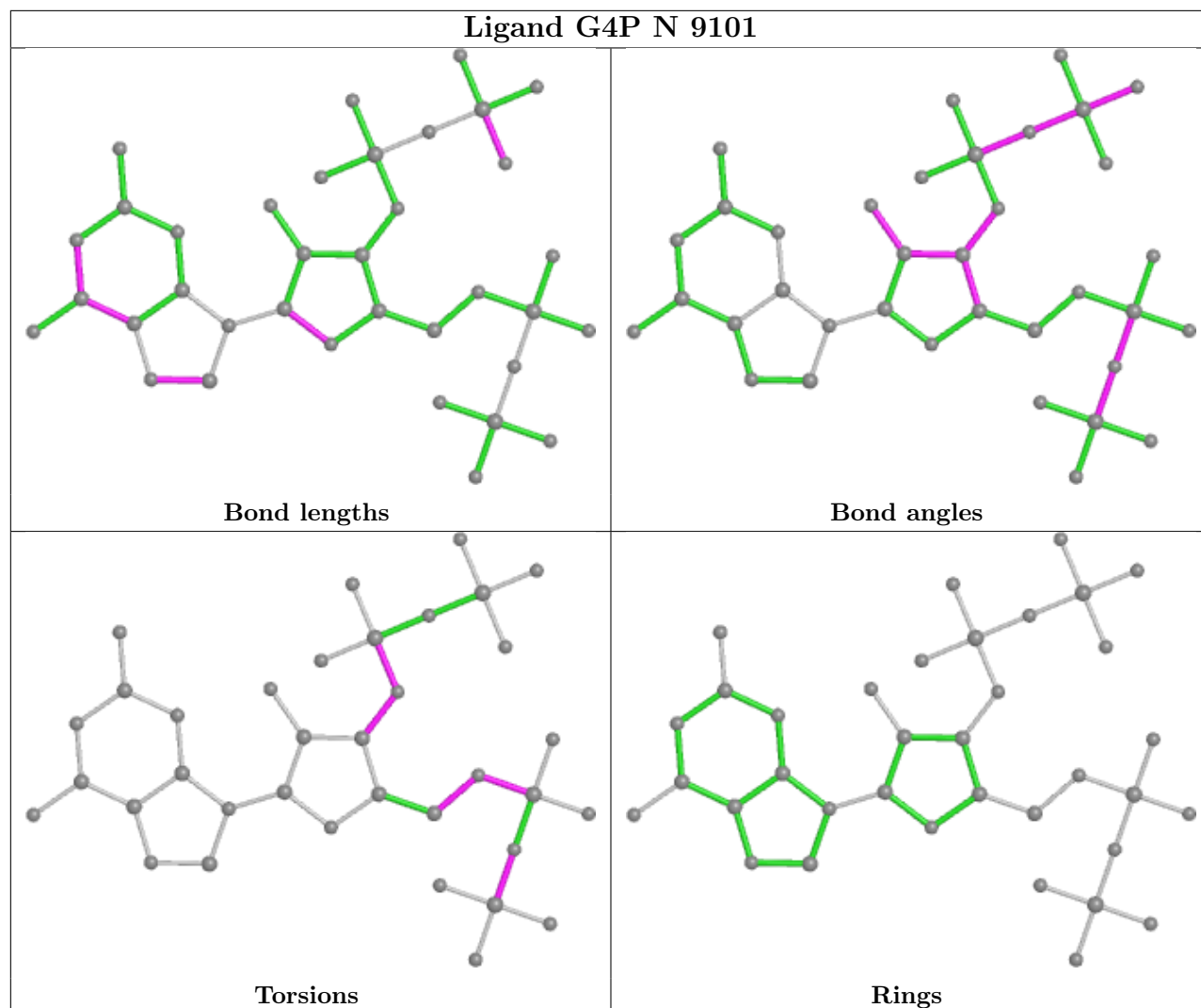
There are no ring outliers.

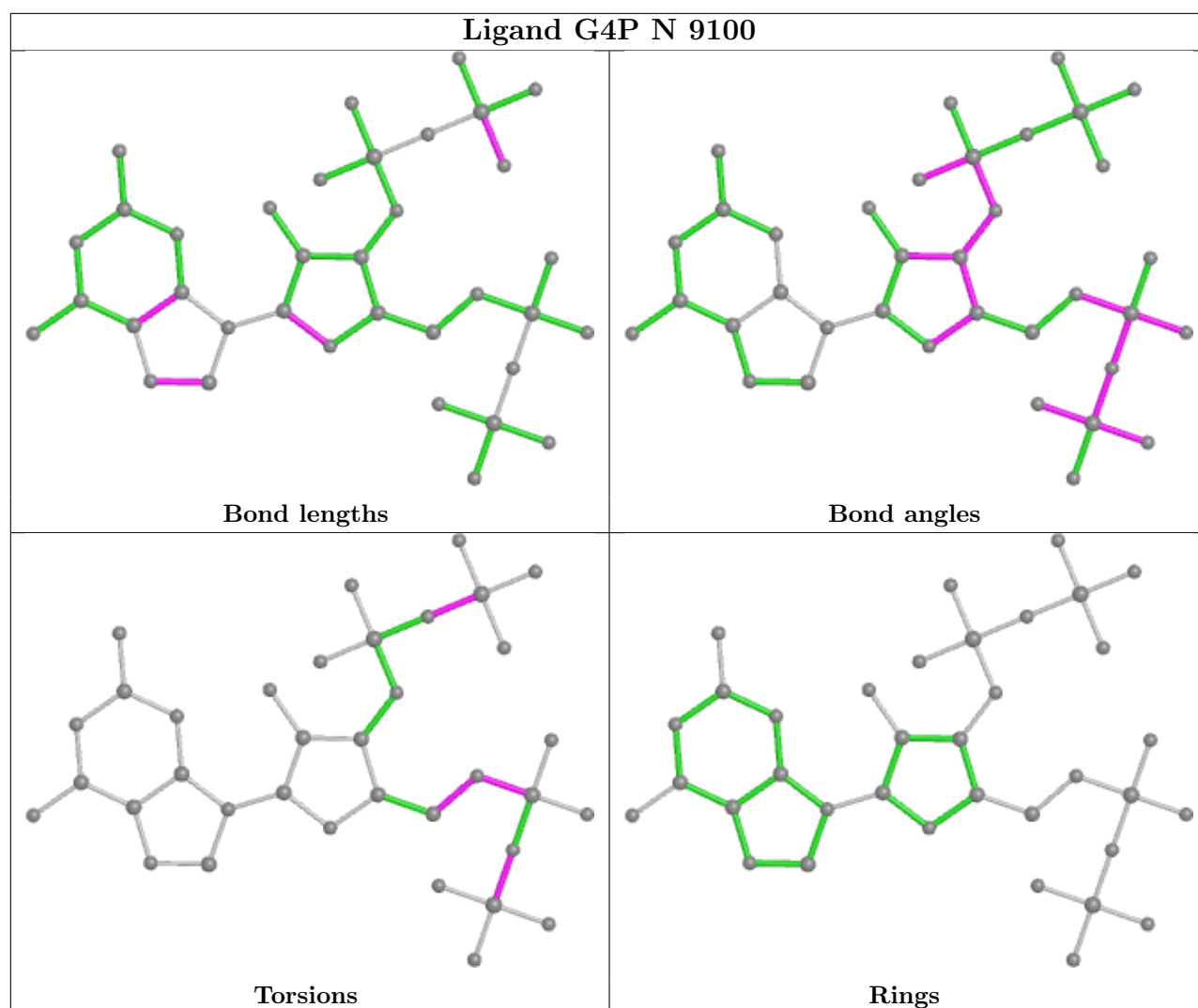
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	9101	G4P	5	0
8	N	9100	G4P	4	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 i

### 6.1 Protein, DNA and RNA chains i

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%)	-0.74	2 (0%) 84 85	39, 65, 90, 121	0
1	B	229/315 (72%)	-0.70	3 (1%) 77 78	58, 82, 103, 129	0
1	K	229/315 (72%)	-0.72	1 (0%) 92 93	42, 65, 87, 117	0
1	L	229/315 (72%)	-0.71	2 (0%) 84 85	54, 88, 104, 122	0
2	C	1119/1119 (100%)	-0.80	1 (0%) 95 96	31, 73, 106, 124	0
2	M	1119/1119 (100%)	-0.76	7 (0%) 89 91	30, 75, 110, 122	0
3	D	1392/1524 (91%)	-0.70	16 (1%) 80 82	33, 71, 108, 152	0
3	N	1392/1524 (91%)	-0.72	17 (1%) 79 80	35, 71, 108, 145	0
4	E	95/99 (95%)	-0.90	0 100 100	49, 79, 103, 109	0
4	O	95/99 (95%)	-0.77	0 100 100	42, 81, 111, 119	0
5	F	345/423 (81%)	-0.61	7 (2%) 65 67	53, 84, 111, 126	0
5	P	345/423 (81%)	-0.66	2 (0%) 89 91	41, 83, 110, 117	0
All	All	6818/7590 (89%)	-0.73	58 (0%) 84 85	30, 74, 108, 152	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	1246	VAL	7.3
3	D	1245	GLY	7.2
3	D	1246	VAL	6.5
3	N	1247	ALA	6.2
3	D	1243	THR	5.3
1	K	1	MET	5.3
3	N	1245	GLY	5.1
3	N	407	VAL	4.8
3	D	1247	ALA	4.6
3	N	1244	GLY	4.4
3	D	1242	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.2
2	M	39	ARG	4.2
3	N	1242	HIS	4.1
3	N	1243	THR	4.1
1	B	2	LEU	4.0
5	F	389	PHE	3.9
1	L	97	VAL	3.7
2	M	269	LEU	3.5
3	D	1398	TRP	3.4
2	M	268	ASP	3.4
2	M	40	GLU	3.3
2	C	39	ARG	3.3
1	B	1	MET	3.2
3	D	1244	GLY	3.1
3	N	1408	ILE	3.1
1	A	2	LEU	2.9
3	D	1407	LEU	2.9
3	D	594	PRO	2.8
5	F	391	GLY	2.8
3	D	816	HIS	2.8
3	D	410	SER	2.7
5	P	365	GLU	2.6
3	D	1408	ILE	2.6
5	F	394	ARG	2.6
3	N	1241	PHE	2.6
3	D	1241	PHE	2.5
3	N	403	PHE	2.5
3	N	900	ILE	2.4
3	N	401	TYR	2.4
2	M	270	GLY	2.4
5	P	408	LEU	2.4
5	F	397	ILE	2.4
5	F	388	ALA	2.3
3	D	1240	THR	2.3
3	N	405	ASP	2.3
3	D	403	PHE	2.2
2	M	186	VAL	2.2
3	N	594	PRO	2.2
5	F	151	LEU	2.2
3	D	72	VAL	2.2
1	L	94	LEU	2.2
5	F	384	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	N	61	GLY	2.1
1	B	119	ASP	2.1
3	N	71	LYS	2.1
3	N	899	LEU	2.0
2	M	267	TYR	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 monosaccharides 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	C	9202	1/1	0.96	0.07	43,43,43,43	0
6	MG	D	9204	1/1	0.96	0.05	38,38,38,38	0
6	MG	D	9240	1/1	0.96	0.08	20,20,20,20	0
6	MG	D	9384	1/1	0.96	0.07	20,20,20,20	0
6	MG	D	9416	1/1	0.96	0.08	20,20,20,20	0
7	ZN	D	9102	1/1	0.96	0.06	115,115,115,115	0
6	MG	A	9394	1/1	0.97	0.09	20,20,20,20	0
6	MG	C	9257	1/1	0.97	0.06	20,20,20,20	0
6	MG	C	9272	1/1	0.97	0.07	20,20,20,20	0
6	MG	C	9525	1/1	0.97	0.05	20,20,20,20	0
6	MG	D	9528	1/1	0.97	0.06	20,20,20,20	0
6	MG	F	9250	1/1	0.97	0.06	20,20,20,20	0
6	MG	M	9206	1/1	0.97	0.10	38,38,38,38	0
6	MG	D	9201	1/1	0.97	0.11	30,30,30,30	0
6	MG	C	9441	1/1	0.98	0.05	20,20,20,20	0
6	MG	C	9519	1/1	0.98	0.05	20,20,20,20	0
6	MG	B	9235	1/1	0.98	0.06	20,20,20,20	0
6	MG	C	9554	1/1	0.98	0.06	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	C	9210	1/1	0.98	0.05	20,20,20,20	0
6	MG	C	9238	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9214	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9216	1/1	0.98	0.08	20,20,20,20	0
6	MG	D	9220	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9226	1/1	0.98	0.04	20,20,20,20	0
6	MG	D	9237	1/1	0.98	0.05	20,20,20,20	0
6	MG	B	9413	1/1	0.98	0.05	20,20,20,20	0
6	MG	D	9241	1/1	0.98	0.06	20,20,20,20	0
6	MG	D	9271	1/1	0.98	0.06	20,20,20,20	0
6	MG	D	9294	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9301	1/1	0.98	0.05	20,20,20,20	0
6	MG	D	9355	1/1	0.98	0.13	20,20,20,20	0
6	MG	B	9485	1/1	0.98	0.05	20,20,20,20	0
6	MG	D	9386	1/1	0.98	0.04	20,20,20,20	0
6	MG	D	9390	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9406	1/1	0.98	0.05	20,20,20,20	0
6	MG	C	9299	1/1	0.98	0.06	20,20,20,20	0
6	MG	D	9460	1/1	0.98	0.04	20,20,20,20	0
6	MG	D	9480	1/1	0.98	0.07	20,20,20,20	0
6	MG	D	9518	1/1	0.98	0.06	20,20,20,20	0
6	MG	C	9320	1/1	0.98	0.06	20,20,20,20	0
6	MG	D	9532	1/1	0.98	0.04	20,20,20,20	0
6	MG	E	9249	1/1	0.98	0.09	20,20,20,20	0
6	MG	E	9341	1/1	0.98	0.06	20,20,20,20	0
6	MG	E	9431	1/1	0.98	0.07	20,20,20,20	0
6	MG	C	9354	1/1	0.98	0.07	20,20,20,20	0
6	MG	F	9290	1/1	0.98	0.06	20,20,20,20	0
6	MG	F	9305	1/1	0.98	0.07	20,20,20,20	0
6	MG	F	9398	1/1	0.98	0.07	20,20,20,20	0
6	MG	F	9496	1/1	0.98	0.05	20,20,20,20	0
6	MG	F	9500	1/1	0.98	0.08	20,20,20,20	0
6	MG	F	9545	1/1	0.98	0.08	20,20,20,20	0
6	MG	C	9356	1/1	0.98	0.07	20,20,20,20	0
6	MG	C	9364	1/1	0.98	0.06	20,20,20,20	0
7	ZN	D	9103	1/1	0.98	0.09	87,87,87,87	0
7	ZN	N	9104	1/1	0.98	0.05	116,116,116,116	0
7	ZN	N	9105	1/1	0.98	0.10	80,80,80,80	0
8	G4P	N	9100	36/36	0.98	0.11	35,45,54,55	0
6	MG	C	9316	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9423	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9321	1/1	0.99	0.06	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	C	9328	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9330	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9339	1/1	0.99	0.11	20,20,20,20	0
6	MG	C	9345	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9348	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9442	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9464	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9358	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9359	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9473	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9367	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9371	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9378	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9381	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9383	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9385	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9387	1/1	0.99	0.10	20,20,20,20	0
6	MG	C	9395	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9396	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9405	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9408	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9422	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9430	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9438	1/1	0.99	0.11	20,20,20,20	0
6	MG	A	9486	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9444	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9451	1/1	0.99	0.11	20,20,20,20	0
6	MG	C	9454	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9465	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9466	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9474	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9476	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9489	1/1	0.99	0.11	20,20,20,20	0
6	MG	C	9497	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9501	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9507	1/1	0.99	0.03	20,20,20,20	0
6	MG	C	9511	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9514	1/1	0.99	0.04	20,20,20,20	0
6	MG	A	9487	1/1	0.99	0.09	20,20,20,20	0
6	MG	C	9524	1/1	0.99	0.06	20,20,20,20	0
6	MG	A	9517	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9542	1/1	0.99	0.07	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	9550	1/1	0.99	0.08	20,20,20,20	0
6	MG	A	9520	1/1	0.99	0.08	20,20,20,20	0
6	MG	C	9561	1/1	0.99	0.04	20,20,20,20	0
6	MG	A	9543	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9203	1/1	0.99	0.08	25,25,25,25	0
6	MG	B	9230	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9211	1/1	0.99	0.06	20,20,20,20	0
6	MG	A	9227	1/1	0.99	0.05	20,20,20,20	0
6	MG	B	9256	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9218	1/1	0.99	0.07	20,20,20,20	0
6	MG	B	9260	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9225	1/1	0.99	0.06	20,20,20,20	0
6	MG	B	9280	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9233	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9236	1/1	0.99	0.08	20,20,20,20	0
6	MG	B	9306	1/1	0.99	0.10	20,20,20,20	0
6	MG	B	9311	1/1	0.99	0.11	20,20,20,20	0
6	MG	A	9273	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9246	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9247	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9252	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9253	1/1	0.99	0.08	20,20,20,20	0
6	MG	D	9258	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9261	1/1	0.99	0.10	20,20,20,20	0
6	MG	D	9262	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9265	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9269	1/1	0.99	0.05	20,20,20,20	0
6	MG	B	9427	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9274	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9277	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9283	1/1	0.99	0.10	20,20,20,20	0
6	MG	D	9285	1/1	0.99	0.11	20,20,20,20	0
6	MG	D	9286	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9291	1/1	0.99	0.07	20,20,20,20	0
6	MG	B	9446	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9296	1/1	0.99	0.06	20,20,20,20	0
6	MG	B	9458	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9304	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9307	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9308	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9315	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9317	1/1	0.99	0.12	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9325	1/1	0.99	0.10	20,20,20,20	0
6	MG	D	9331	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9332	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9333	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9336	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9337	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9342	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9344	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9353	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9295	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9357	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9361	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9362	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9363	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9369	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9370	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9372	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9377	1/1	0.99	0.07	20,20,20,20	0
6	MG	B	9488	1/1	0.99	0.05	20,20,20,20	0
6	MG	B	9491	1/1	0.99	0.08	20,20,20,20	0
6	MG	B	9552	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9391	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9393	1/1	0.99	0.08	20,20,20,20	0
6	MG	D	9399	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9400	1/1	0.99	0.08	20,20,20,20	0
6	MG	D	9401	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9403	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9404	1/1	0.99	0.09	20,20,20,20	0
6	MG	A	9318	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9409	1/1	0.99	0.11	20,20,20,20	0
6	MG	D	9410	1/1	0.99	0.04	20,20,20,20	0
6	MG	A	9327	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9417	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9419	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9421	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9433	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9434	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9439	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9440	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9443	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9448	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9452	1/1	0.99	0.07	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9456	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9217	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9467	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9469	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9470	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9472	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9475	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9477	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9478	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9479	1/1	0.99	0.10	20,20,20,20	0
6	MG	C	9219	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9481	1/1	0.99	0.08	20,20,20,20	0
6	MG	D	9482	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9490	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9498	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9499	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9502	1/1	0.99	0.10	20,20,20,20	0
6	MG	D	9503	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9505	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9506	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9512	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9515	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9221	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9523	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9526	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9527	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9222	1/1	0.99	0.04	20,20,20,20	0
6	MG	D	9529	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9223	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9533	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9536	1/1	0.99	0.06	20,20,20,20	0
6	MG	D	9539	1/1	0.99	0.03	20,20,20,20	0
6	MG	D	9546	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9548	1/1	0.99	0.09	20,20,20,20	0
6	MG	D	9556	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9557	1/1	0.99	0.05	20,20,20,20	0
6	MG	D	9559	1/1	0.99	0.07	20,20,20,20	0
6	MG	D	9562	1/1	0.99	0.06	20,20,20,20	0
6	MG	A	9334	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9239	1/1	0.99	0.04	20,20,20,20	0
6	MG	E	9352	1/1	0.99	0.08	20,20,20,20	0
6	MG	E	9373	1/1	0.99	0.06	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	E	9389	1/1	0.99	0.05	20,20,20,20	0
6	MG	E	9415	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9243	1/1	0.99	0.06	20,20,20,20	0
6	MG	E	9432	1/1	0.99	0.06	20,20,20,20	0
6	MG	E	9449	1/1	0.99	0.07	20,20,20,20	0
6	MG	E	9484	1/1	0.99	0.07	20,20,20,20	0
6	MG	E	9494	1/1	0.99	0.05	20,20,20,20	0
6	MG	E	9538	1/1	0.99	0.09	20,20,20,20	0
6	MG	E	9551	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9229	1/1	0.99	0.11	20,20,20,20	0
6	MG	F	9244	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9245	1/1	0.99	0.09	20,20,20,20	0
6	MG	C	9255	1/1	0.99	0.10	20,20,20,20	0
6	MG	F	9251	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9365	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9297	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9298	1/1	0.99	0.08	20,20,20,20	0
6	MG	F	9302	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9303	1/1	0.99	0.06	20,20,20,20	0
6	MG	C	9263	1/1	0.99	0.08	20,20,20,20	0
6	MG	F	9309	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9310	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9323	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9326	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9340	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9374	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9375	1/1	0.99	0.10	20,20,20,20	0
6	MG	F	9382	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9264	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9407	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9414	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9424	1/1	0.99	0.09	20,20,20,20	0
6	MG	F	9425	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9445	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9450	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9453	1/1	0.99	0.09	20,20,20,20	0
6	MG	F	9463	1/1	0.99	0.08	20,20,20,20	0
6	MG	F	9468	1/1	0.99	0.06	20,20,20,20	0
6	MG	F	9483	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9495	1/1	0.99	0.04	20,20,20,20	0
6	MG	C	9267	1/1	0.99	0.09	20,20,20,20	0
6	MG	A	9368	1/1	0.99	0.04	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	F	9504	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9508	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9513	1/1	0.99	0.07	20,20,20,20	0
6	MG	F	9516	1/1	0.99	0.09	20,20,20,20	0
6	MG	F	9530	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9531	1/1	0.99	0.04	20,20,20,20	0
6	MG	F	9540	1/1	0.99	0.05	20,20,20,20	0
6	MG	C	9282	1/1	0.99	0.05	20,20,20,20	0
6	MG	F	9558	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9287	1/1	0.99	0.04	20,20,20,20	0
6	MG	N	9205	1/1	0.99	0.08	16,16,16,16	0
6	MG	C	9289	1/1	0.99	0.09	20,20,20,20	0
6	MG	C	9293	1/1	0.99	0.05	20,20,20,20	0
6	MG	A	9212	1/1	0.99	0.07	20,20,20,20	0
6	MG	C	9300	1/1	0.99	0.03	20,20,20,20	0
6	MG	C	9313	1/1	0.99	0.10	20,20,20,20	0
8	G4P	N	9101	36/36	0.99	0.11	35,45,50,50	0
6	MG	D	9547	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9380	1/1	1.00	0.10	20,20,20,20	0
6	MG	D	9242	1/1	1.00	0.11	20,20,20,20	0
6	MG	B	9228	1/1	1.00	0.08	20,20,20,20	0
6	MG	C	9346	1/1	1.00	0.10	20,20,20,20	0
6	MG	D	9248	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9392	1/1	1.00	0.07	20,20,20,20	0
6	MG	E	9275	1/1	1.00	0.10	20,20,20,20	0
6	MG	E	9288	1/1	1.00	0.08	20,20,20,20	0
6	MG	C	9347	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9209	1/1	1.00	0.20	20,20,20,20	0
6	MG	E	9366	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9259	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9493	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9402	1/1	1.00	0.05	20,20,20,20	0
6	MG	A	9254	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9268	1/1	1.00	0.10	20,20,20,20	0
6	MG	C	9266	1/1	1.00	0.07	20,20,20,20	0
6	MG	E	9457	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9509	1/1	1.00	0.06	20,20,20,20	0
6	MG	B	9541	1/1	1.00	0.07	20,20,20,20	0
6	MG	D	9276	1/1	1.00	0.05	20,20,20,20	0
6	MG	A	9329	1/1	1.00	0.08	20,20,20,20	0
6	MG	D	9279	1/1	1.00	0.06	20,20,20,20	0
6	MG	B	9560	1/1	1.00	0.03	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9428	1/1	1.00	0.03	20,20,20,20	0
6	MG	C	9522	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9284	1/1	1.00	0.07	20,20,20,20	0
6	MG	F	9270	1/1	1.00	0.03	20,20,20,20	0
6	MG	F	9278	1/1	1.00	0.07	20,20,20,20	0
6	MG	D	9435	1/1	1.00	0.04	20,20,20,20	0
6	MG	A	9437	1/1	1.00	0.07	20,20,20,20	0
6	MG	C	9534	1/1	1.00	0.05	20,20,20,20	0
6	MG	B	9281	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9447	1/1	1.00	0.06	20,20,20,20	0
6	MG	C	9549	1/1	1.00	0.05	20,20,20,20	0
6	MG	C	9292	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9455	1/1	1.00	0.10	20,20,20,20	0
6	MG	C	9553	1/1	1.00	0.05	20,20,20,20	0
6	MG	F	9324	1/1	1.00	0.07	20,20,20,20	0
6	MG	C	9213	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9461	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9312	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9314	1/1	1.00	0.05	20,20,20,20	0
6	MG	A	9224	1/1	1.00	0.07	20,20,20,20	0
6	MG	F	9388	1/1	1.00	0.09	20,20,20,20	0
6	MG	A	9521	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9319	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9322	1/1	1.00	0.09	20,20,20,20	0
6	MG	C	9397	1/1	1.00	0.05	20,20,20,20	0
6	MG	B	9412	1/1	1.00	0.06	20,20,20,20	0
6	MG	F	9436	1/1	1.00	0.11	20,20,20,20	0
6	MG	D	9208	1/1	1.00	0.10	20,20,20,20	0
6	MG	A	9462	1/1	1.00	0.07	20,20,20,20	0
6	MG	C	9411	1/1	1.00	0.11	20,20,20,20	0
6	MG	D	9215	1/1	1.00	0.08	20,20,20,20	0
6	MG	D	9492	1/1	1.00	0.08	20,20,20,20	0
6	MG	F	9471	1/1	1.00	0.08	20,20,20,20	0
6	MG	C	9418	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9343	1/1	1.00	0.05	20,20,20,20	0
6	MG	B	9420	1/1	1.00	0.07	20,20,20,20	0
6	MG	D	9349	1/1	1.00	0.03	20,20,20,20	0
6	MG	D	9350	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9351	1/1	1.00	0.09	20,20,20,20	0
6	MG	D	9510	1/1	1.00	0.08	20,20,20,20	0
6	MG	C	9429	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9231	1/1	1.00	0.10	20,20,20,20	0

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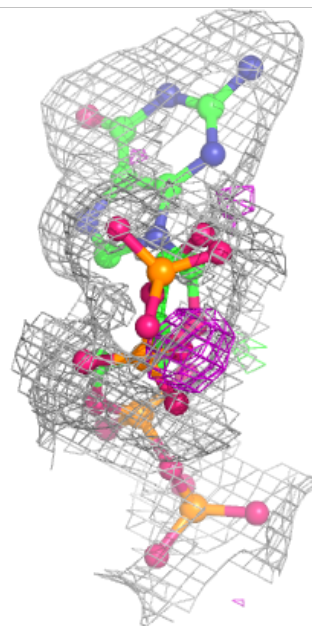
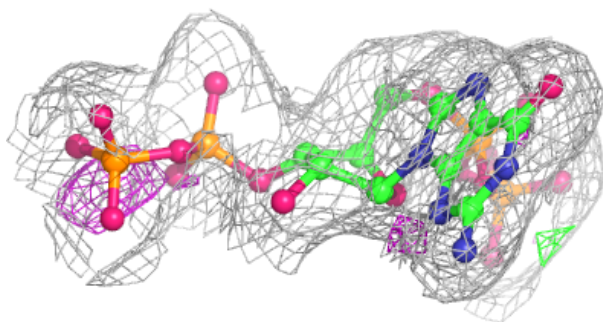
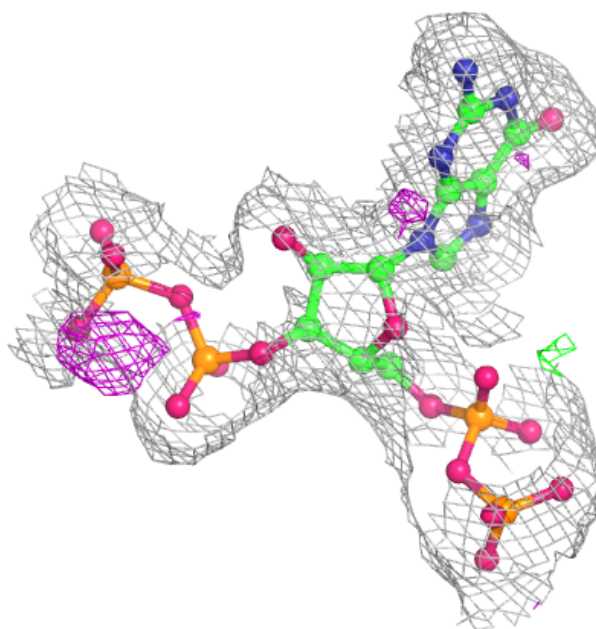
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	B	9426	1/1	1.00	0.06	20,20,20,20	0
6	MG	F	9537	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9360	1/1	1.00	0.05	20,20,20,20	0
6	MG	D	9232	1/1	1.00	0.10	20,20,20,20	0
6	MG	A	9544	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9234	1/1	1.00	0.09	20,20,20,20	0
6	MG	C	9335	1/1	1.00	0.08	20,20,20,20	0
6	MG	N	9207	1/1	1.00	0.07	37,37,37,37	0
6	MG	C	9338	1/1	1.00	0.06	20,20,20,20	0
6	MG	A	9555	1/1	1.00	0.04	20,20,20,20	0
6	MG	D	9535	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9376	1/1	1.00	0.04	20,20,20,20	0
6	MG	C	9459	1/1	1.00	0.06	20,20,20,20	0
6	MG	D	9379	1/1	1.00	0.07	20,20,20,20	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.

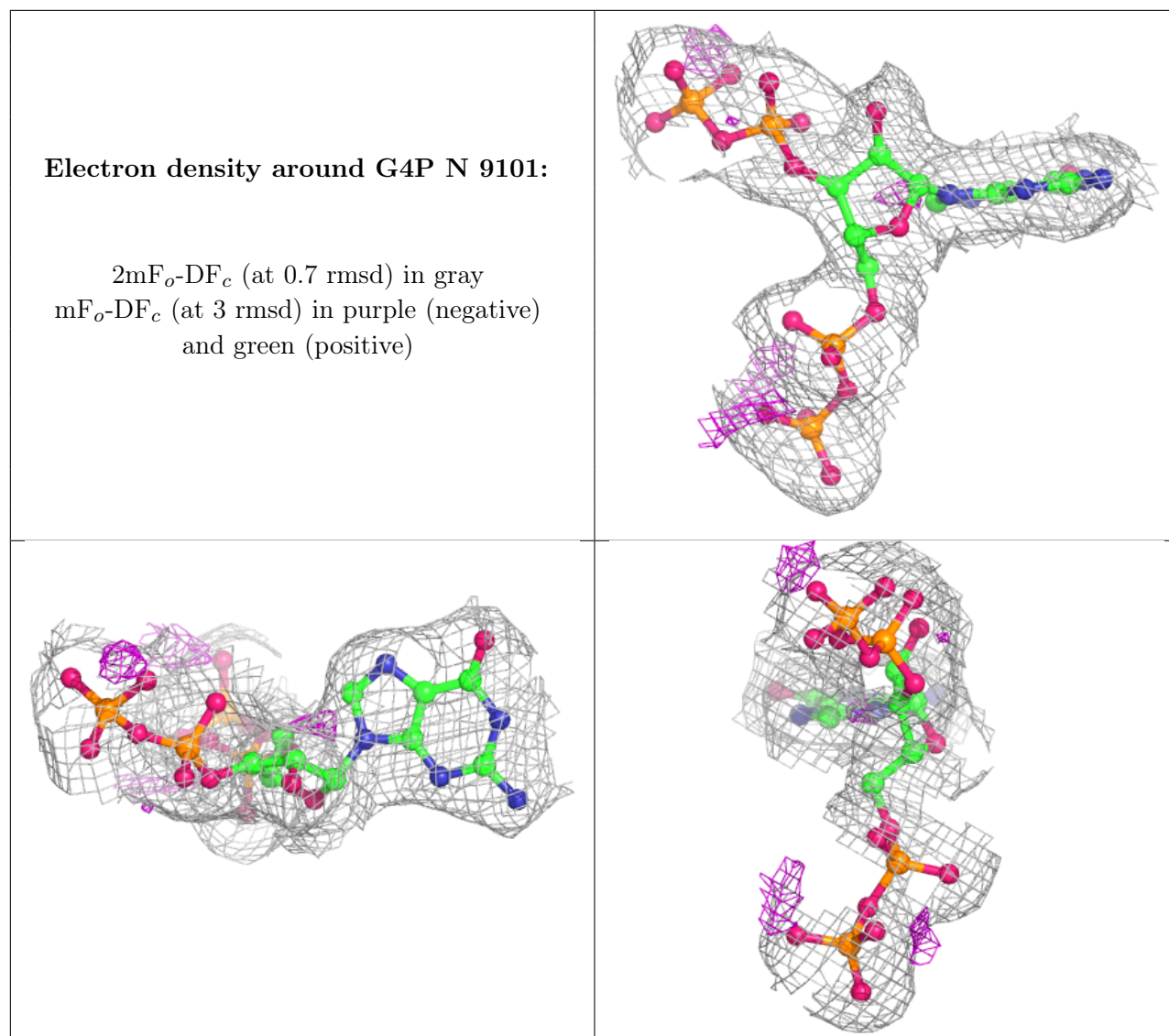


**Electron density around G4P N 9100:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







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

There are no such residues in this entry.