



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2020 – 11:19 pm BST

PDB ID : 2A6H
Title : Crystal structure of the T. thermophilus RNA polymerase holoenzyme in complex with antibiotic sterptolydigin
Authors : Temiakov, D.; Zenkin, N.; Vassilyeva, M.N.; Perederina, A.; Tahirov, T.H.; Savkina, M.; Zorov, S.; Nikiforov, V.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Severinov, K.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-02
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

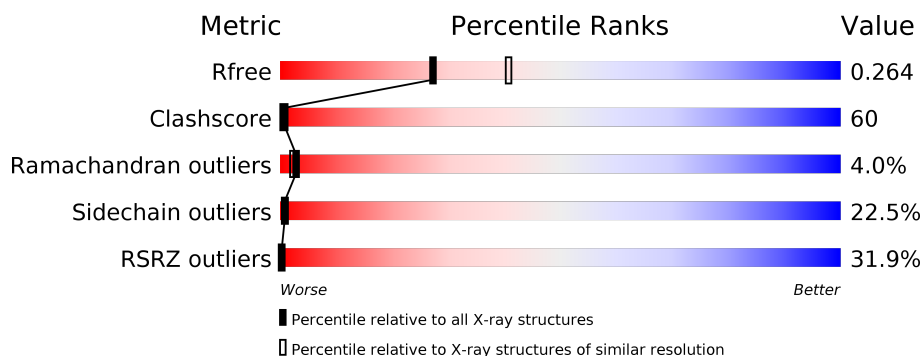
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	315	<div> <div>21%</div> <div>16% 43% 13% 27%</div> </div>
1	B	315	<div> <div>23%</div> <div>16% 43% 13% 27%</div> </div>
1	K	315	<div> <div>19%</div> <div>23% 41% 8% 27%</div> </div>
1	L	315	<div> <div>26%</div> <div>20% 39% 12% 27%</div> </div>
2	C	1119	<div> <div>38%</div> <div>24% 57% 19%</div> </div>
2	M	1119	<div> <div>35%</div> <div>25% 55% 19%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1524	<div><div></div><div>23%</div><div></div><div>22%</div><div>52%</div><div>15%</div><div>•</div><div>9%</div></div>
3	N	1524	<div><div></div><div>24%</div><div></div><div>25%</div><div>49%</div><div>15%</div><div>•</div><div>9%</div></div>
4	E	99	<div><div></div><div>28%</div><div></div><div>27%</div><div>53%</div><div>15%</div><div>•</div><div>•</div></div>
4	O	99	<div><div></div><div>32%</div><div></div><div>24%</div><div>53%</div><div>18%</div><div>•</div><div>•</div></div>
5	F	423	<div><div></div><div>35%</div><div></div><div>20%</div><div>49%</div><div>11%</div><div>•</div><div>18%</div></div>
5	P	423	<div><div></div><div>30%</div><div></div><div>21%</div><div>49%</div><div>11%</div><div></div><div>18%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60908 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase alpha chain.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1381	Total	C	N	O	S	0	0	0
			10728	6776	1912	2007	33			
3	N	1381	Total	C	N	O	S	0	0	0
			10728	6776	1912	2007	33			

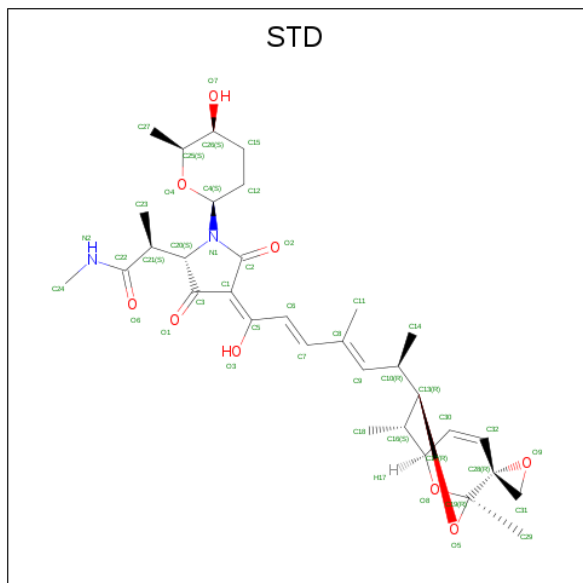
- Molecule 4 is a protein called RNA polymerase omega chain.

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

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

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

- Molecule 6 is STREPTOLYDIGIN (three-letter code: STD) (formula: C₃₂H₄₄N₂O₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			43	32	2	9		
6	N	1	Total	C	N	O	0	0
			43	32	2	9		

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

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Mg 1 1	0	0
8	N	1	Total Mg 1 1	0	0

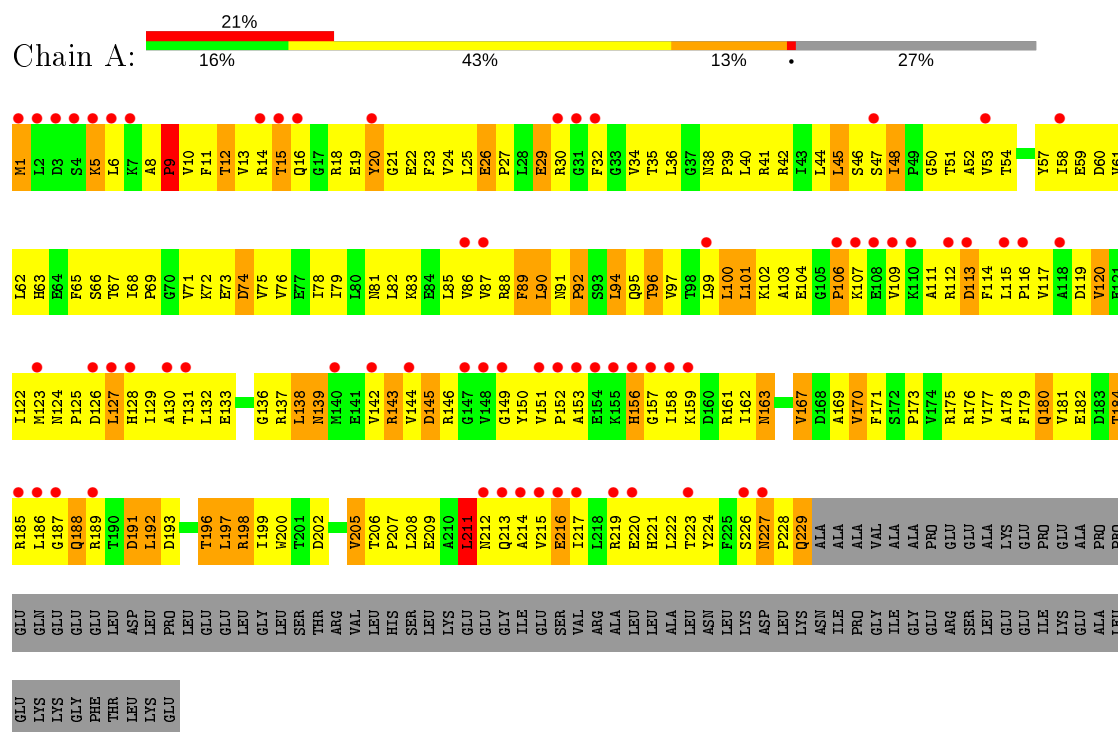
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	232	Total O 232 232	0	0
9	B	304	Total O 304 304	0	0
9	C	1144	Total O 1144 1144	0	0
9	D	1546	Total O 1546 1546	0	0
9	E	130	Total O 130 130	0	0
9	F	491	Total O 491 491	0	0
9	K	229	Total O 229 229	0	0
9	L	274	Total O 274 274	0	0
9	M	1072	Total O 1072 1072	0	0
9	N	1392	Total O 1392 1392	0	0
9	O	137	Total O 137 137	0	0
9	P	447	Total O 447 447	0	0

3 Residue-property plots

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

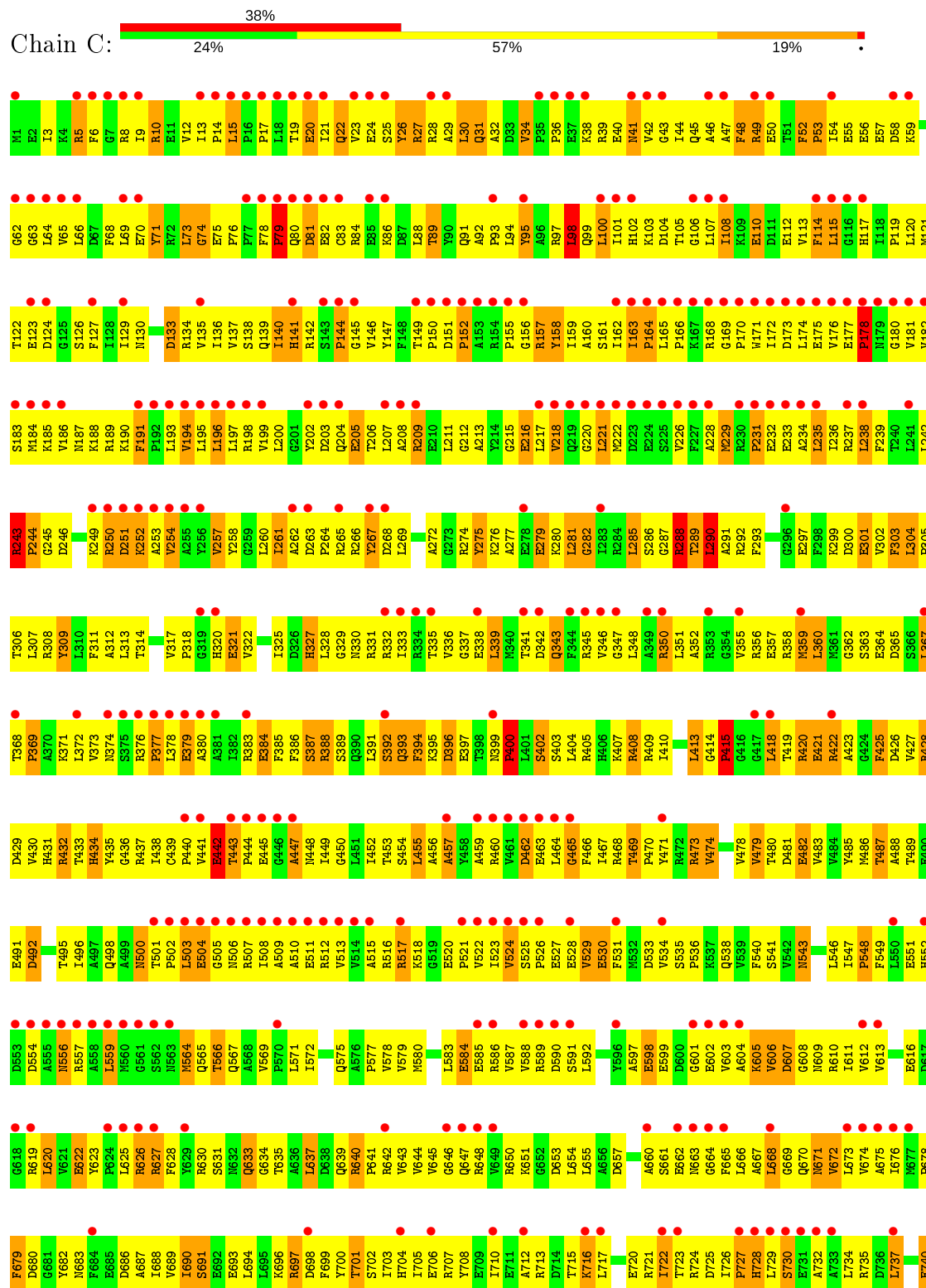
• Molecule 1: DNA-directed RNA polymerase alpha chain

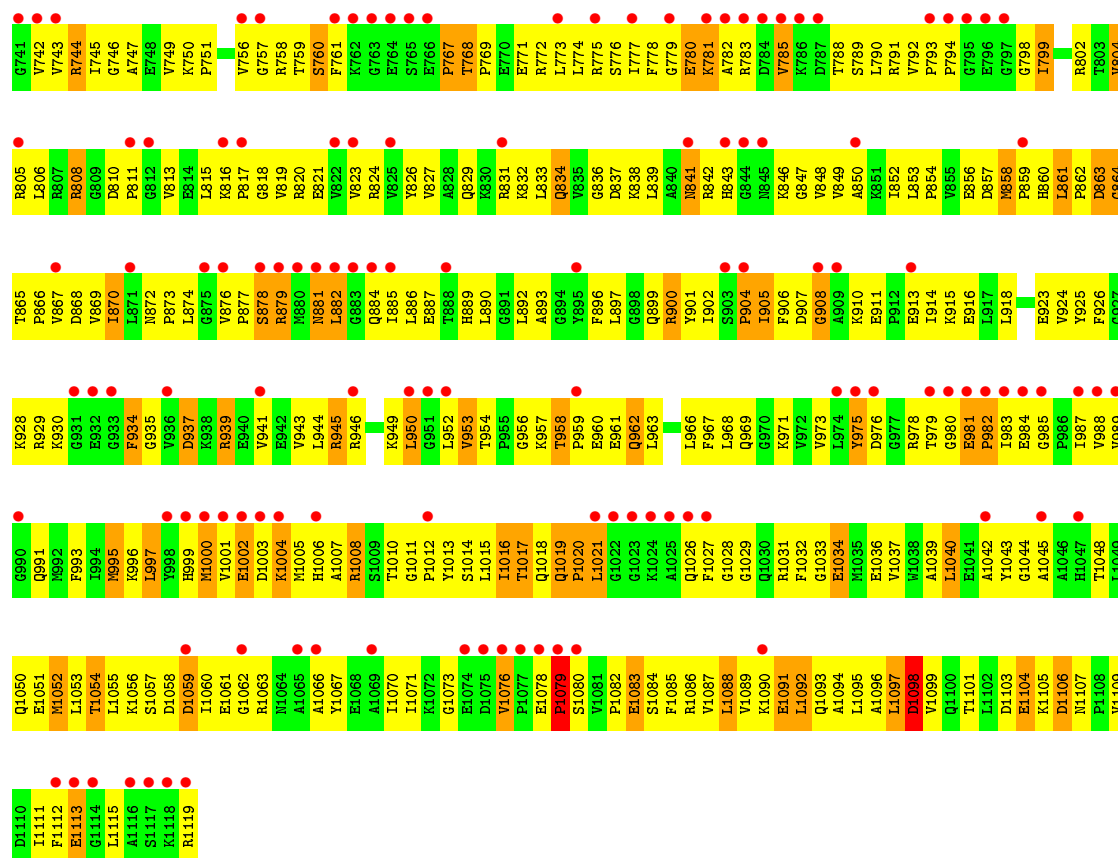




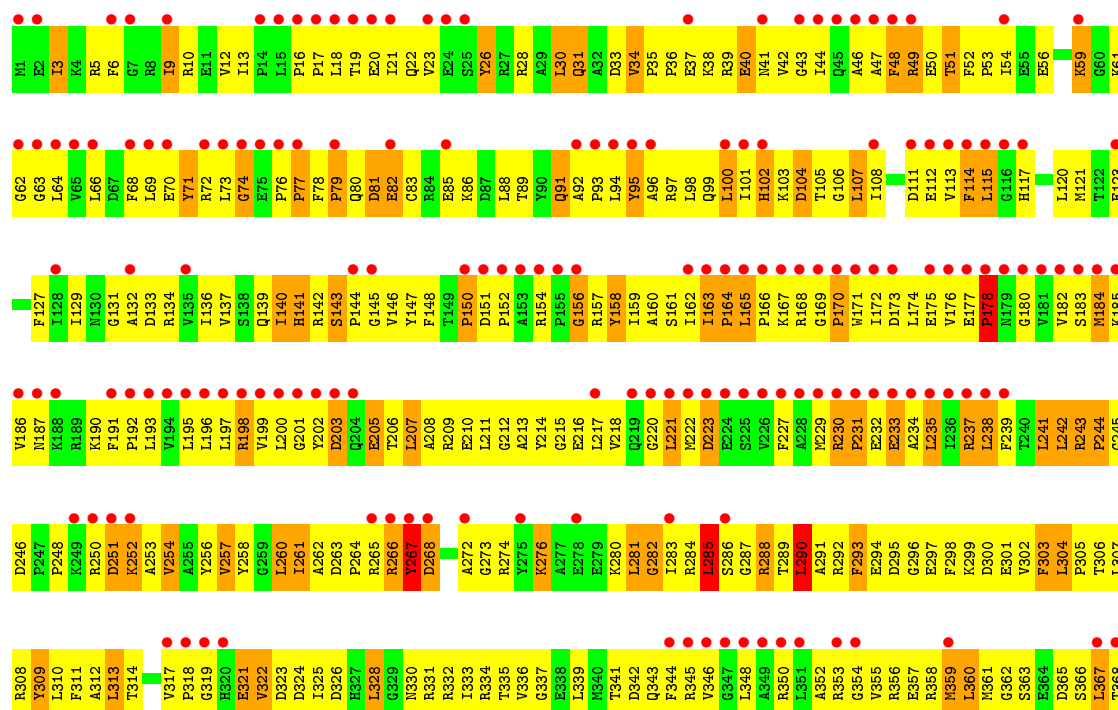
LYS
LYS
GLY
PHE
THR
LEU
LYS
GLU

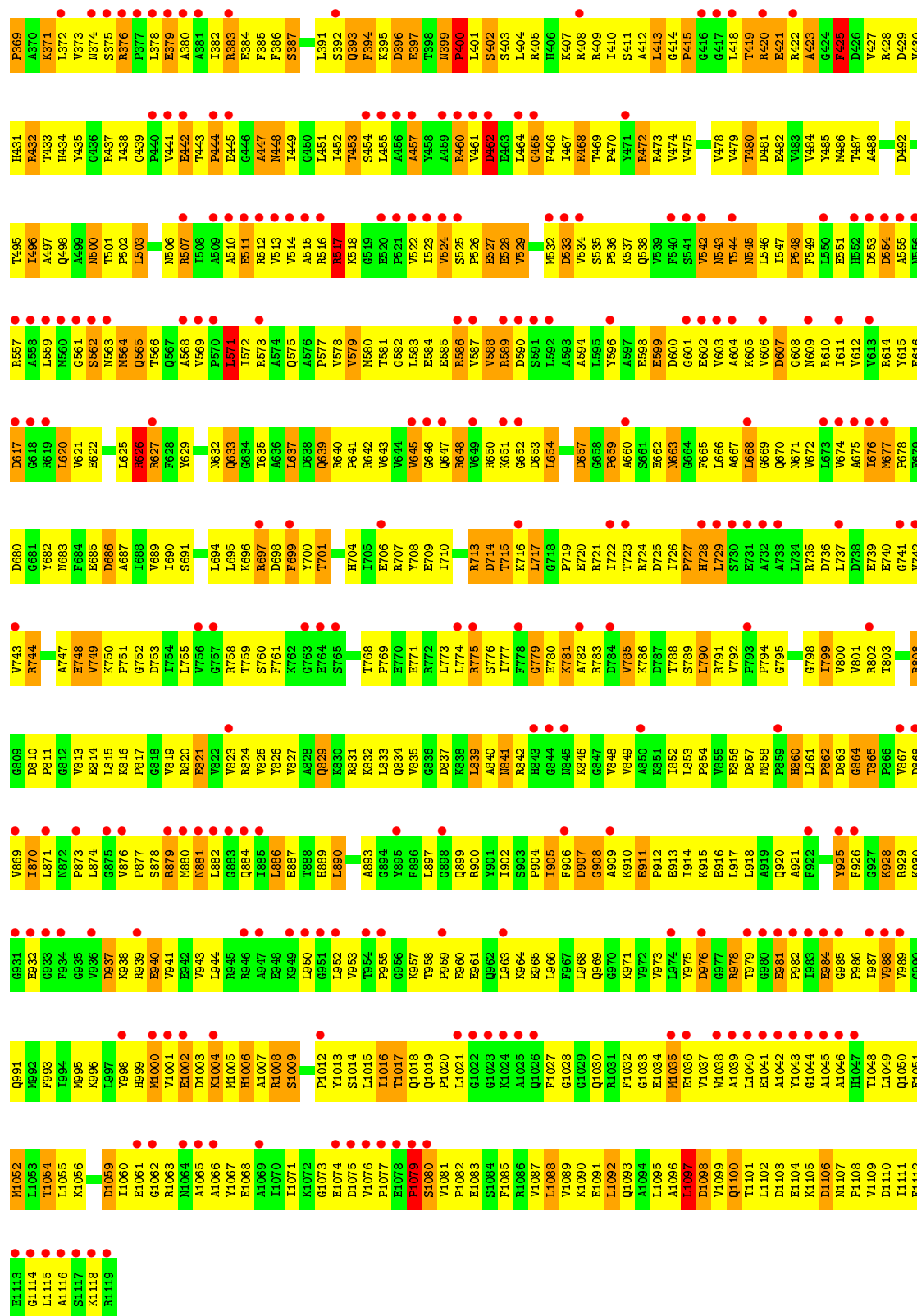
● Molecule 2: DNA-directed RNA polymerase beta chain





• Molecule 2: DNA-directed RNA polymerase beta chain

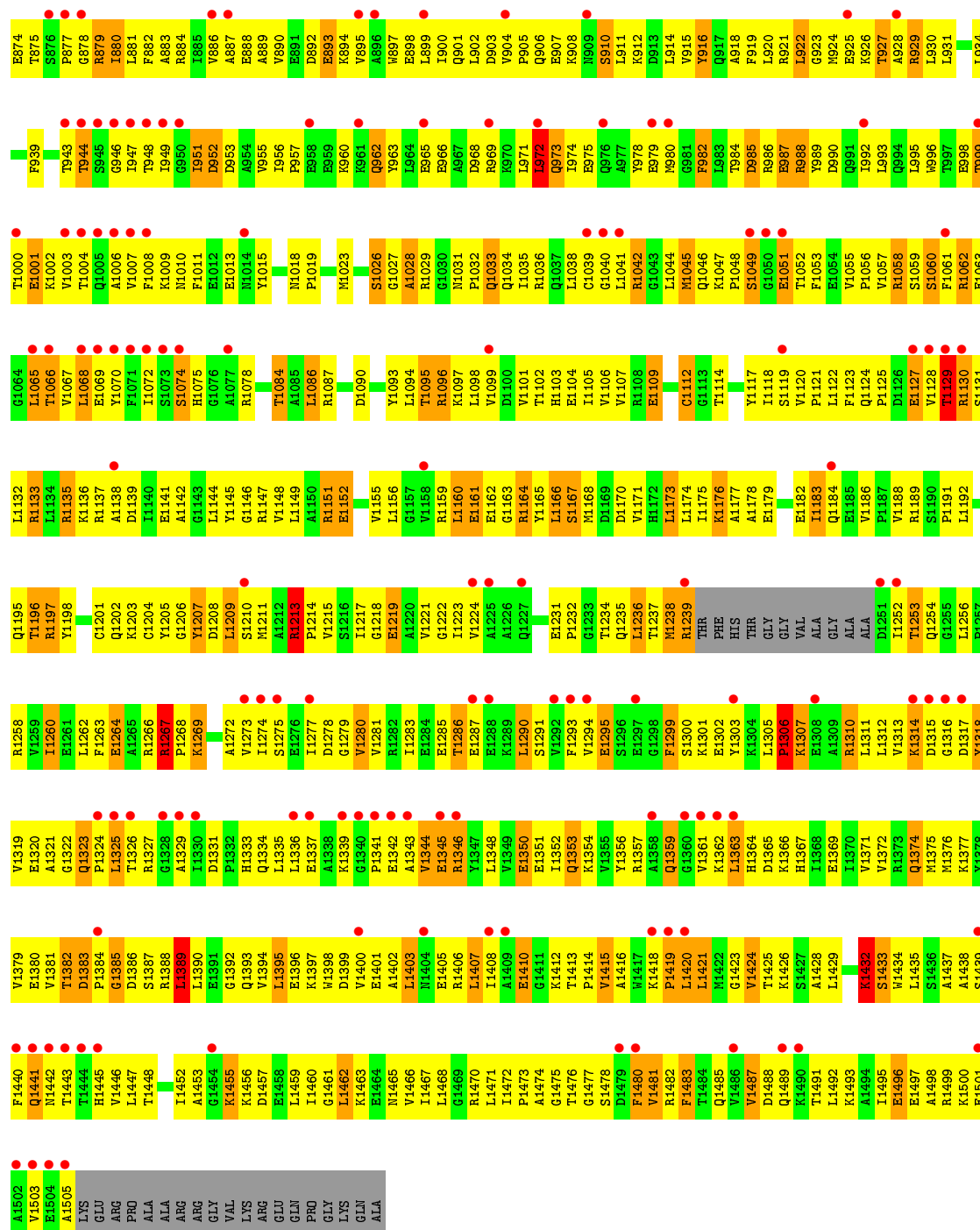




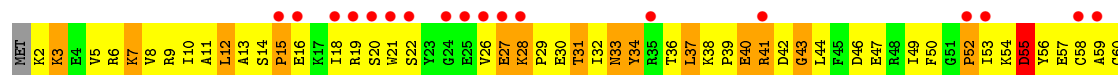
• Molecule 3: DNA-directed RNA polymerase beta' chain

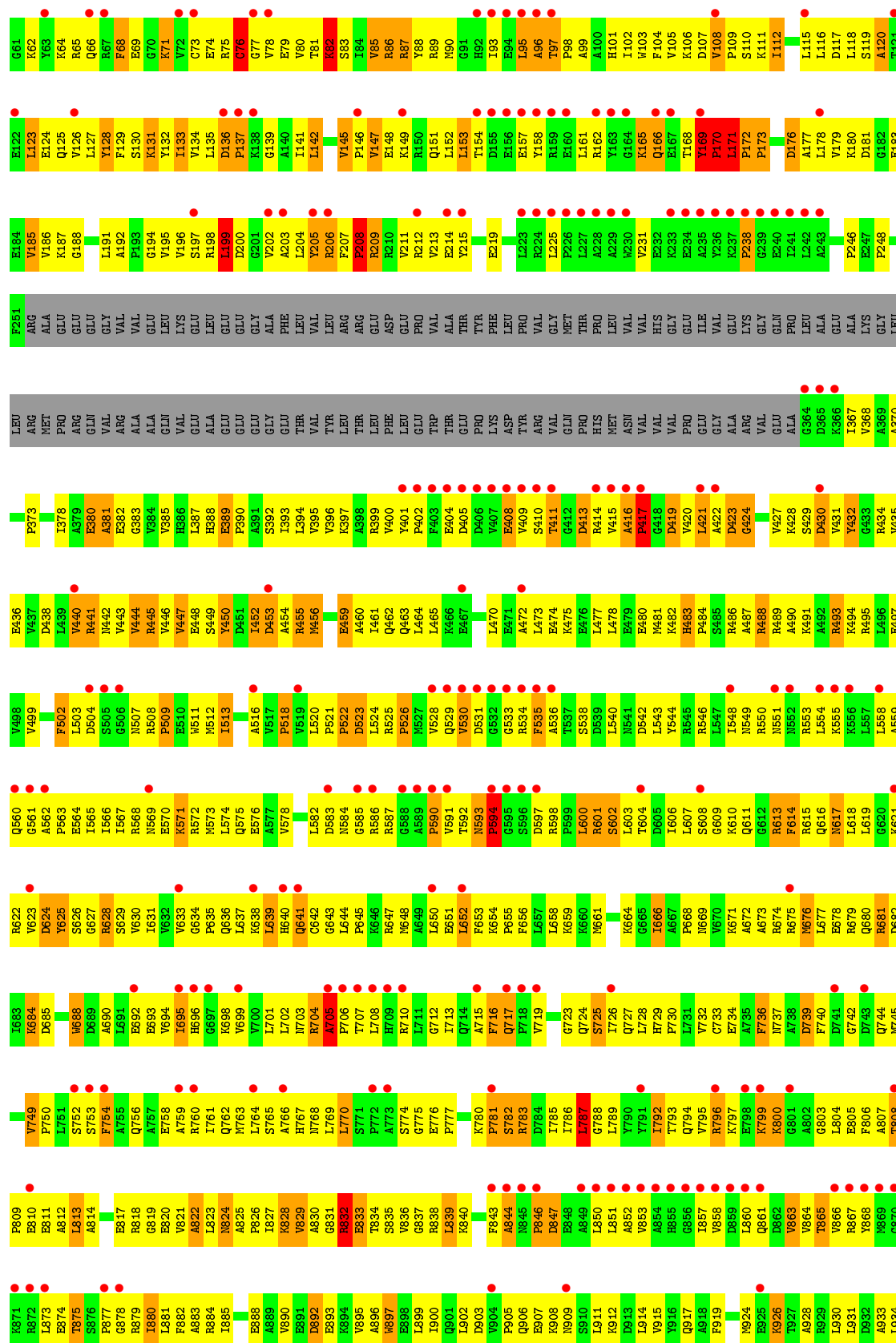


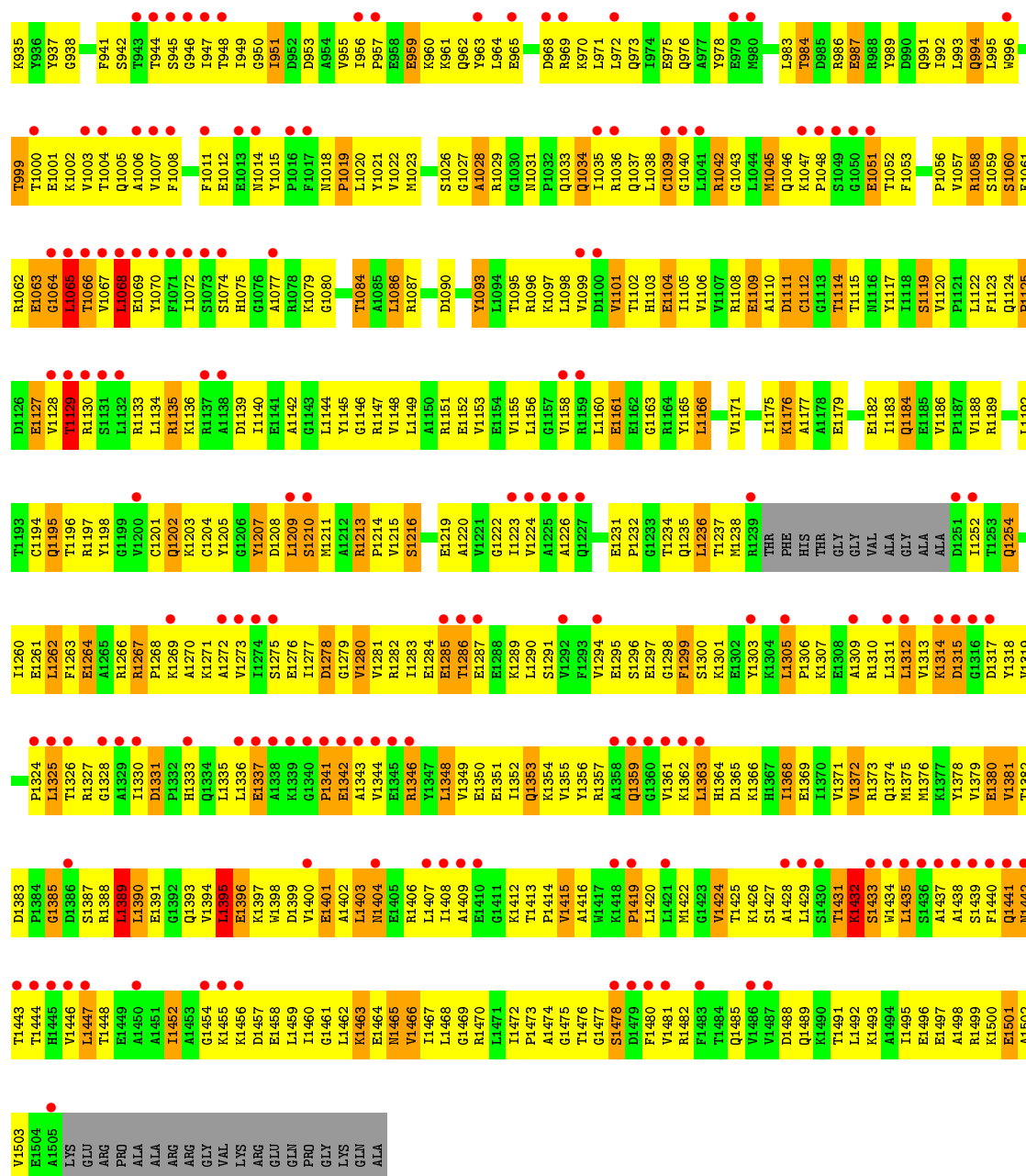
A812	A813	A814	A815	B816	B817	B818	B819	B820	B821	A822	A823	A824	A825	B826	B827	B828	B829	A830	G831	R832	E833	T834	S835	S836	G837	R838	L839	F843	A844	F845	D847	E848	A849	L850	L851	A852	V853	A854	H855	G856	B857	V858	D859	L860	Q861	D862	V863	T864	V865	R866	R867	V868	B869	G870	R871	R872	L873	K621	R622	D623	D624	S625	S626	G627	R628	S629	S630	V631	V632	V633	G634	P635	G636	L637	R638	L639	R640	Q641	G642	G643	K646	R647	M648	A649	L650	B651	L652	F653	A654	P655	F656	L657	L658	K659	R660	M661	B662	B663	K664	G665	L666	L667	V669	G670	D671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	Q724	S725	L726	L727	L728	L729	P730	L731	E734	A735	F736	T737	L738	E739	S740	L741	L742	L743	L744	L745	L751	S752	T753	F754	A755	T756	A757	D758	A759	L760	L761	Q762	M763	H764	S765	G766	A767	H768	L769	L770	S771	T772	A773	S774	G775	E776	P777	F781	S782	R783	D784	L785	L786	L787	G788	L789	L790	Y791	L792	L793	Q794	L795	R796	K797	E798	Q800	G801	A802	T803	R804	E805	L806	Q806	L807	S808	G809	G812	R813	F814	R815	R816	M817	L818	L819	G820	Q860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	L873	Q81	R82	G83	K84	R85	Q86	R87	F88	E89	G90	K91	L92	L93	L94	L95	A96	R97	R98	A99	H100	H101	I102	W103	F104	V105	K106	D107	V108	P109	S110	K111	I112	G113	L114	L115	L116	L117	L118	S119	A120	G121	E122	L123	E124	L125	L126	L127	L128	F129	S130	K131	L132	L133	L134	L135	D136	P137	K138	G139	A140	I141	L204	Y205	R206	F207	P208	R209	R210	V211	R212	V213	E214	L215	T216	E217	E155	E156	E157	Y158	R159	E160	L161	R162	Y163	G164	K165	Q166	E167	T168	Y169	L171	P172	P173	P174	V175	D176	A177	L178	V179	K180	D181	G182	E183	Q81	R82	G83	K84	R85	Q86	R87	F88	E89	G90	K91	L92	L93	L94	L95	A96	R97	R98	A99	H100	H101	I102	W103	F104	V105	K106	D107	V108	P109	S110	K111	I112	G113	L114	L115	L116	L117	L118	S119	A120	G121	E122	L123	E124	L125	L126	L127	L128	F129	S130	K131	L132	L133	L134	L135	D136	P137	K138	G139	A140	I141	L204	Y205	R206	F207	P208	R209	R210	V211	R212	V213	E214	L215	T216	E217	E155	E156	E157	Y158	R159	E160	L161	R162	Y163	G164	K165	Q166	E167	T168	Y169	L171	P172	P173	P174	V175	D176	A177	L178	V179	K180	D181	G182	E183	Q81	R82	G83	K84	R85	Q86	R87	F88	E89	G90	K91	L92	L93	L94	L95	A96	R97	R98	A99	H100	H101	I102	W103	F104	V105	K106	D107	V108	P109	S110	K111	I112	G113	L114	L115	L116	L117	L118	S119	A120	G121	E122	L123	E124	L125	L126	L127	L128	F129	S130	K131	L132	L133	L134	L135	D136	P137	K138	G139	A140	I141	L204	Y205	R206	F207	P208	R209	R210	V211	R212	V213	E214	L215	T216	E217	E155	E156	E157	Y158	R159	E160	L161	R162	Y163	G164	K165	Q166	E167	T168	Y169	L171	P172	P173	P174	V175	D176	A177	L178	V179	K180	D181	G182	E183	Q81	R82	G83	K84	R85	Q86	R87	F88	E89	G90	K91	L92	L93	L94	L95	A96	R97	R98	A99	H100	H101	I102	W103	F104	V105	K106	D107	V108	P109	S110	K111	I112	G113	L114	L115	L116	L117	L118	S119	A120	G121	E122	L123	E124	L125	L126	L127	L128	F129	S130	K131	L132	L133	L134	L135	D136	P137	K138	G139	A140	I141	L204	Y205	R206	F207	P208	R209	R210	V211	R212	V213	E214	L215	T216	E217	E155	E156	E157	Y158	R159	E160	L161	R162	Y163	G164	K165	Q166	E167	T168	Y169	L171	P172	P173	P174	V175	D176	A177	L178	V179	K180	D181	G182	E183	Q81	R82	G83	K84	R85	Q86	R87	F88	E89	G90	K91	L92	L93	L94	L95	A96	R97	R98	A99	H100	H101	I102	W103	F104	V105	K106	D107	V108	P109	S110	K111	I112	G113	L114	L115	L116	L117	L118	S119	A120	G121	E122	L123	E124	L125	L126	L127	L128	F129	S130	K131	L132	L133	L134	L135	D136	P137	K138	G139	A140	I141	L204	Y205	R206	F207	P208	R209	R210	V211	R212	V213	E214	L215	T216	E217	E155	E156	E157	Y158	R159	E160	L161	R162	Y163	G164	K165	Q166	E167	T168	Y169	L171	P172	P173	P174	V175	D176	A177	L178	V179	K180	D181	G182	E183	Q81	R82	G83	K84	R85	Q86	R87	F88	E89	G90	K91	L92	L93	L94	L95	A96	R97	R98	A99	H100	H101	I102	W103	F104	V105	K106	D107	V108	P109	S110	K111	I112	G113	L114	L115	L116	L117	L118	S119	A120	G121	E122	L123	E124	L125	L126	L127	L128	F129	S130	K131	L132	L133	L134	L135	D136	P137	K138	G139	A140	I141	L204	Y205	R206	F207	P208	R209	R210	V211	R212	V213	E214	L215	T216	E217	E155	E156	E157	Y158	R159	E160	L161	R162	Y163	G164	K165	Q166	E167	T168	Y169	L171	P172	P173	P174	V175	D176	A177	L178	V179	K180	D181	G182	E183	Q81	R82	G83	K84	R85	Q86	R87	F88	E89	G90	K91	L92	L93	L94	L95	A96	R97	R98	A99	H100	H101	I102	W103	F104	V105	K106	D107	V108	P109	S110	K111	I112	G113	L114	L115	L116	L117	L118	S119	A120	G121	E122	L123	E124	L125	L126	L127	L128	F129	S130	K131	L132	L133	L134	L135	D136	P137	K138	G139	A140	I141	L204	Y205	R206	F207	P208	R209	R210	V211	R212	V213	E214	L215	T216	E217	E155	E156	E157	Y158	R159	E160	L161	R162	Y163	G164	K165	Q166	E167	T168	Y169	L171	P172	P173	P174	V175	D176	A177	L178	V179	K180	D181	G182	E183	Q81	R82	G83	K84	R85	Q86	R87	F88	E89	G90	K91	L92	L93	L94	L95	A96	R97	R98	A99	H100	H101	I102	W103	F104	V105	K106	D107	V108	P109	S110	K111	I112	G113	L114	L115	L116	L117	L118	S119	A120	G121	E122	L123	E124	L125	L126	L127	L128	F129	S130	K131	L132	L133	L134	L1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- Molecule 3: DNA-directed RNA polymerase beta' chain



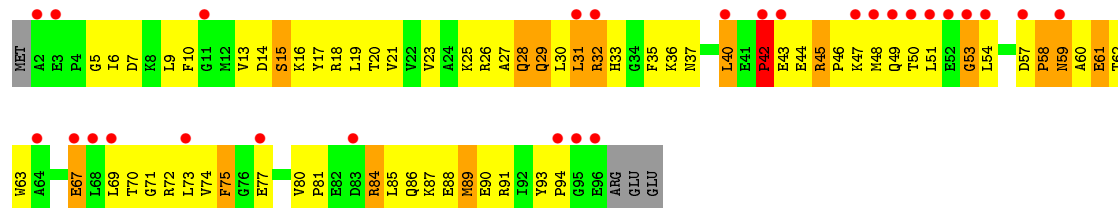




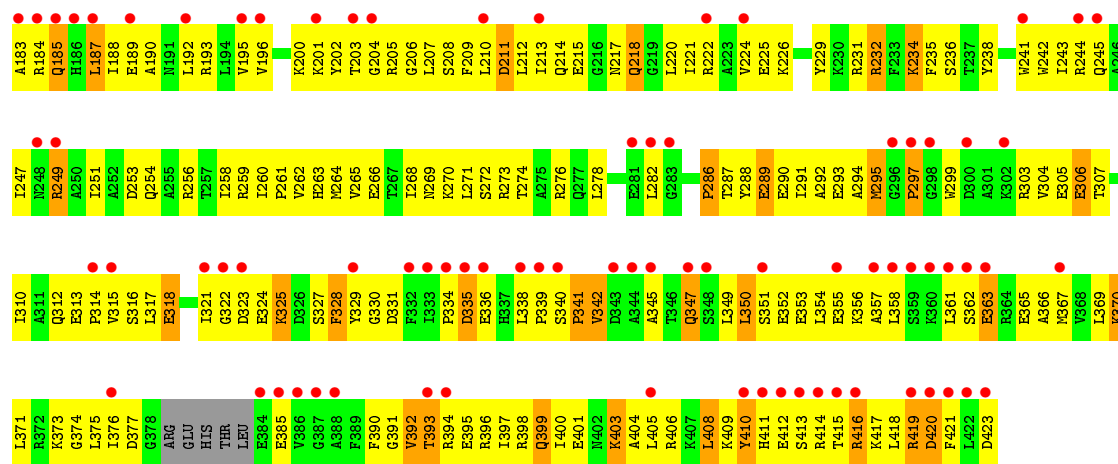
- Molecule 4: RNA polymerase omega chain



Chain E:



- Molecule 4: RNA polymerase omega chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.40 34.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.40) 91.0 (34.69-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.268 0.230 , 0.264	Depositor DCC
R_{free} test set	33251 reflections (5.76%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.079 for h,-h-k,-l 0.079 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	60908	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: STD, ZN, 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	0.80	1/1838 (0.1%)	0.87	3/2498 (0.1%)
1	B	0.75	0/1838	0.84	6/2498 (0.2%)
1	K	0.75	0/1838	0.83	1/2498 (0.0%)
1	L	0.73	1/1838 (0.1%)	0.77	3/2498 (0.1%)
2	C	0.83	1/8997 (0.0%)	0.89	7/12164 (0.1%)
2	M	0.82	0/8997	0.90	10/12164 (0.1%)
3	D	0.82	0/10903	0.93	18/14736 (0.1%)
3	N	0.81	0/10903	0.93	19/14736 (0.1%)
4	E	0.82	0/783	0.96	0/1054
4	O	0.84	1/783 (0.1%)	0.95	1/1054 (0.1%)
5	F	0.72	0/2812	0.83	4/3781 (0.1%)
5	P	0.73	0/2812	0.82	3/3781 (0.1%)
All	All	0.80	4/54342 (0.0%)	0.90	75/73462 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	17	TYR	CD1-CE1	6.19	1.48	1.39
1	A	48	ILE	C-N	5.79	1.45	1.34
1	L	172	SER	N-CA	-5.30	1.35	1.46
2	C	191	PHE	C-N	5.26	1.44	1.34

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1389	LEU	CA-CB-CG	8.52	134.89	115.30
3	D	76	CYS	CA-CB-SG	8.24	128.84	114.00
3	D	199	LEU	CA-CB-CG	-8.01	96.89	115.30
2	M	165	LEU	C-N-CD	-7.94	103.13	120.60
3	N	199	LEU	CA-CB-CG	-7.89	97.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	813	LEU	CA-CB-CG	7.73	133.08	115.30
3	D	637	LEU	CA-CB-CG	7.49	132.53	115.30
5	P	136	LEU	CA-CB-CG	7.46	132.45	115.30
1	A	192	LEU	CA-CB-CG	7.40	132.33	115.30
1	B	138	LEU	CA-CB-CG	7.37	132.24	115.30
3	D	1389	LEU	CA-CB-CG	7.19	131.84	115.30
1	B	25	LEU	CA-CB-CG	6.78	130.89	115.30
3	D	73	CYS	CA-CB-SG	6.39	125.51	114.00
2	M	571	LEU	CA-CB-CG	6.28	129.75	115.30
3	N	705	ALA	C-N-CD	6.13	141.27	128.40
1	K	211	LEU	CA-CB-CG	6.11	129.36	115.30
5	F	354	LEU	CA-CB-CG	6.04	129.19	115.30
5	P	354	LEU	CA-CB-CG	6.04	129.19	115.30
5	P	85	LEU	CA-CB-CG	5.93	128.95	115.30
1	B	2	LEU	CA-CB-CG	5.91	128.89	115.30
3	D	238	PRO	N-CA-CB	5.88	110.35	103.30
3	D	1395	LEU	CA-CB-CG	5.86	128.77	115.30
3	N	238	PRO	N-CA-CB	5.84	110.31	103.30
3	D	208	PRO	CA-N-CD	-5.78	103.41	111.50
2	M	207	LEU	CA-CB-CG	5.77	128.57	115.30
3	N	171	LEU	CA-CB-CG	5.75	128.54	115.30
3	N	1209	LEU	N-CA-C	-5.75	95.48	111.00
5	F	136	LEU	CA-CB-CG	5.68	128.37	115.30
3	N	1065	LEU	CA-CB-CG	5.67	128.35	115.30
3	D	209	ARG	N-CA-C	5.67	126.30	111.00
2	M	243	ARG	C-N-CD	-5.66	108.14	120.60
3	N	76	CYS	CA-CB-SG	5.66	124.19	114.00
3	D	581	LEU	CA-CB-CG	5.65	128.30	115.30
3	N	209	ARG	N-CA-C	5.64	126.24	111.00
3	D	1209	LEU	N-CA-C	-5.62	95.81	111.00
1	B	171	PHE	CA-C-N	5.58	129.48	117.20
2	M	423	ALA	N-CA-C	5.58	126.06	111.00
3	N	1068	LEU	CA-CB-CG	-5.49	102.69	115.30
3	D	972	LEU	CA-CB-CG	5.46	127.87	115.30
3	N	380	GLU	N-CA-C	-5.46	96.25	111.00
3	N	82	LYS	C-N-CA	-5.44	108.10	121.70
5	F	174	LEU	CA-CB-CG	5.43	127.78	115.30
2	C	861	LEU	CA-CB-CG	5.41	127.73	115.30
1	L	2	LEU	CA-CB-CG	5.38	127.67	115.30
1	B	36	LEU	CA-CB-CG	5.37	127.65	115.30
3	N	423	ASP	N-CA-C	5.37	125.50	111.00
1	L	197	LEU	CA-CB-CG	5.32	127.53	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	208	PRO	CA-N-CD	-5.32	104.06	111.50
2	C	243	ARG	C-N-CD	-5.29	108.97	120.60
3	D	380	GLU	N-CA-C	-5.29	96.72	111.00
3	D	423	ASP	N-CA-C	5.25	125.19	111.00
3	N	1395	LEU	CA-CB-CG	5.21	127.29	115.30
5	F	361	LEU	CA-CB-CG	5.21	127.28	115.30
2	C	58	ASP	C-N-CA	5.20	134.70	121.70
3	D	248	PRO	N-CA-CB	5.20	109.53	103.30
3	N	248	PRO	N-CA-CB	5.18	109.52	103.30
2	M	728	HIS	N-CA-C	5.18	124.98	111.00
1	L	132	LEU	CA-CB-CG	5.17	127.19	115.30
2	C	728	HIS	N-CA-C	5.15	124.90	111.00
3	N	1363	LEU	CA-CB-CG	5.15	127.14	115.30
2	C	394	PHE	CB-CG-CD1	-5.14	117.20	120.80
1	A	90	LEU	CA-CB-CG	-5.13	103.50	115.30
2	C	1098	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	211	LEU	CB-CG-CD2	-5.11	102.32	111.00
2	M	360	LEU	CA-CB-CG	5.10	127.02	115.30
2	M	285	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	132	LEU	CA-CB-CG	5.09	127.00	115.30
3	D	1305	LEU	CA-CB-CG	5.08	126.98	115.30
3	N	813	LEU	CA-CB-CG	5.05	126.92	115.30
3	D	839	LEU	CA-CB-CG	5.05	126.91	115.30
4	O	49	GLN	N-CA-C	5.05	124.63	111.00
2	M	267	TYR	CA-CB-CG	5.03	122.95	113.40
2	M	423	ALA	CA-C-N	5.02	126.23	116.20
3	N	787	LEU	CA-CB-CG	5.02	126.84	115.30
2	C	98	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	239	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1806	0	1861	210	0
1	K	1806	0	1861	178	0
1	L	1806	0	1861	205	0
2	C	8829	0	8933	1211	0
2	M	8829	0	8933	1154	0
3	D	10728	0	10809	1434	0
3	N	10728	0	10809	1309	0
4	E	769	0	775	89	0
4	O	769	0	775	118	0
5	F	2771	0	2844	364	0
5	P	2771	0	2844	336	0
6	D	43	0	31	4	0
6	N	43	0	31	6	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	D	1	0	0	0	0
8	N	1	0	0	0	0
9	A	232	0	0	42	0
9	B	304	0	0	53	0
9	C	1144	0	0	274	0
9	D	1546	0	0	310	0
9	E	130	0	0	20	0
9	F	491	0	0	108	0
9	K	229	0	0	33	0
9	L	274	0	0	51	0
9	M	1072	0	0	223	0
9	N	1392	0	0	261	0
9	O	137	0	0	26	0
9	P	447	0	0	72	0
All	All	60908	0	54228	6435	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 60.

All (6435) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:131:LYS:HG2	3:N:568:ARG:HG2	1.30	1.08
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.09	1.06
2:M:169:GLY:HA2	2:M:263:ASP:HB3	1.36	1.05
1:K:42:ARG:HH12	2:M:857:ASP:HB3	1.22	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.38	1.03
3:D:197:SER:HB3	3:D:203:ALA:HB3	1.41	1.03
1:K:100:LEU:HB2	1:K:115:LEU:HD11	1.39	1.02
2:C:630:ARG:HE	2:C:705:ILE:HB	1.24	1.02
2:C:150:PRO:HA	2:C:158:TYR:HB3	1.39	1.02
3:N:197:SER:HB3	3:N:203:ALA:HB3	1.37	1.02
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.38	1.01
2:M:1114:GLY:H	2:M:1115:LEU:HD12	1.22	1.00
3:N:55:ASP:HA	3:N:82:LYS:HG3	1.42	0.99
3:N:1101:VAL:HG21	3:N:1424:VAL:HG22	1.45	0.99
2:M:150:PRO:HA	2:M:158:TYR:HB3	1.46	0.98
2:M:685:GLU:HG2	3:N:739:ASP:HB2	1.43	0.98
2:M:350:ARG:HD3	2:M:353:ARG:HH22	1.26	0.97
5:F:268:ILE:HA	5:F:271:LEU:HD12	1.46	0.97
1:A:68:ILE:HD13	1:A:138:LEU:HD11	1.46	0.97
3:D:1412:LYS:HA	9:D:9761:HOH:O	1.65	0.97
5:P:88:ILE:HD13	5:P:193:ARG:HB2	1.46	0.97
2:C:232:GLU:HA	2:C:235:LEU:HD12	1.45	0.97
3:N:1481:VAL:HG13	4:O:18:ARG:HE	1.29	0.97
3:N:637:LEU:HD21	3:N:642:CYS:HA	1.46	0.96
2:C:126:SER:HB3	2:C:407:LYS:HE2	1.47	0.96
2:C:775:ARG:HH21	2:C:782:ALA:HB1	1.31	0.95
2:C:1016:ILE:HD11	5:F:330:GLY:HA3	1.49	0.95
2:M:176:VAL:HG12	2:M:182:VAL:HG13	1.49	0.95
2:M:49:ARG:HH11	2:M:49:ARG:HB2	1.32	0.95
3:D:422:ALA:HB3	3:D:427:VAL:HG22	1.46	0.95
2:M:154:ARG:HH21	2:M:156:GLY:HA3	1.31	0.94
2:M:626:ARG:HB2	2:M:639:GLN:HE22	1.31	0.94
1:A:14:ARG:HH21	1:A:22:GLU:HB3	1.31	0.94
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.50	0.94
3:D:127:LEU:HD11	3:D:461:ILE:HD11	1.49	0.94
2:C:135:VAL:HG11	2:C:407:LYS:HA	1.47	0.93
3:N:422:ALA:HB3	3:N:427:VAL:HG22	1.49	0.93
2:M:1102:LEU:HB2	3:N:7:LYS:HG3	1.50	0.93
2:M:1054:THR:HG22	2:M:1059:ASP:HB2	1.49	0.93
2:C:890:LEU:HA	2:C:914:ILE:HD11	1.50	0.93
3:D:101:HIS:HD1	3:D:103:TRP:HB2	1.34	0.93
3:D:1124:GLN:HE21	3:D:1135:ARG:HG2	1.32	0.93
2:M:412:ALA:CB	2:M:451:LEU:HB3	1.99	0.92
5:P:394:ARG:HA	5:P:397:ILE:HD12	1.49	0.92
2:C:146:VAL:HG22	2:C:162:ILE:HA	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:800:LYS:HE3	3:D:830:ALA:HB3	1.52	0.92
3:N:141:ILE:HG12	3:N:449:SER:HA	1.51	0.92
3:N:65:ARG:HG3	3:N:66:GLN:H	1.31	0.92
5:P:347:GLN:HA	5:P:350:LEU:HD22	1.52	0.92
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.52	0.92
3:N:1033:GLN:HE21	3:N:1036:ARG:HH11	1.08	0.91
3:N:1262:LEU:HD21	3:N:1351:GLU:HG3	1.52	0.91
1:K:219:ARG:HH22	1:L:223:THR:HG22	1.35	0.91
1:B:152:PRO:HD2	1:B:155:LYS:HD3	1.50	0.91
3:D:795:VAL:HG23	3:D:879:ARG:HH12	1.34	0.91
2:C:979:THR:HG23	2:C:981:GLU:H	1.36	0.91
2:M:578:VAL:HG23	2:M:579:VAL:HG12	1.52	0.91
3:D:119:SER:HB2	3:D:123:LEU:H	1.34	0.90
3:N:41:ARG:HD3	3:N:43:GLY:H	1.36	0.90
2:C:328:LEU:HB2	2:C:488:ALA:HB2	1.52	0.90
3:D:661:MET:HE1	3:D:677:LEU:HD11	1.53	0.90
5:F:205:ARG:HD2	5:F:251:ILE:HD13	1.53	0.90
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.36	0.90
2:M:115:LEU:HD22	2:M:373:VAL:HG11	1.53	0.90
3:N:978:TYR:HA	9:N:2283:HOH:O	1.70	0.90
2:M:196:LEU:HD23	2:M:200:LEU:HD11	1.54	0.89
3:N:214:GLU:HB2	3:N:390:PRO:HD2	1.52	0.89
2:C:773:LEU:HB2	5:F:373:LYS:HB3	1.52	0.89
1:L:152:PRO:HD2	1:L:155:LYS:HD3	1.52	0.89
2:C:479:VAL:HG21	2:C:503:LEU:HD11	1.54	0.89
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.55	0.89
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.54	0.89
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.36	0.89
3:N:1111:ASP:HB2	3:N:1203:LYS:HG3	1.55	0.88
2:C:49:ARG:HH11	2:C:49:ARG:HB2	1.36	0.88
2:M:979:THR:HG23	2:M:981:GLU:H	1.38	0.88
2:C:439:CYS:HB3	2:C:442:GLU:HB2	1.54	0.88
2:M:905:ILE:HD12	2:M:905:ILE:H	1.37	0.88
3:D:1481:VAL:HG11	4:E:18:ARG:HA	1.56	0.87
1:B:41:ARG:HG3	1:B:177:VAL:HG21	1.57	0.87
2:C:578:VAL:HG11	2:C:991:GLN:HB3	1.53	0.87
1:B:87:VAL:HG21	1:B:144:VAL:HG11	1.57	0.87
3:N:875:THR:HG21	3:N:902:LEU:HD13	1.57	0.87
1:A:95:GLN:HA	1:A:146:ARG:HH12	1.39	0.86
1:L:87:VAL:HG21	1:L:144:VAL:HG11	1.57	0.86
3:N:52:PRO:HG3	3:N:78:VAL:HG13	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:422:ALA:HB1	5:P:178:ARG:HH12	1.38	0.86
2:C:305:PRO:HB3	2:C:308:ARG:HH21	1.38	0.86
2:M:572:ILE:HD11	2:M:698:ASP:HB3	1.58	0.86
1:K:67:THR:H	2:M:627:ARG:NH2	1.73	0.86
3:D:1311:LEU:HA	9:D:9040:HOH:O	1.76	0.86
3:D:598:ARG:NH1	5:F:319:THR:HA	1.91	0.86
3:N:1018:ASN:HB3	3:N:1021:TYR:HB3	1.58	0.86
3:N:119:SER:HB2	3:N:123:LEU:H	1.41	0.86
1:B:86:VAL:HG12	1:B:124:ASN:HD22	1.41	0.86
2:C:631:SER:HB3	2:C:637:LEU:HD21	1.55	0.85
3:D:1466:VAL:HG23	3:D:1472:ILE:HD11	1.55	0.85
5:F:125:ASP:HA	5:F:128:ARG:NH1	1.91	0.85
3:D:973:GLN:HA	9:D:2386:HOH:O	1.76	0.85
5:F:394:ARG:HA	5:F:397:ILE:HD12	1.58	0.85
3:N:1481:VAL:HG11	4:O:18:ARG:HA	1.58	0.85
5:P:361:LEU:HD22	5:P:366:ALA:HB2	1.58	0.85
2:C:66:LEU:HD22	2:C:372:LEU:HD23	1.57	0.85
2:C:818:GLY:HA3	9:C:1150:HOH:O	1.77	0.85
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.56	0.85
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.57	0.85
1:B:27:PRO:HG2	1:B:186:LEU:HD12	1.57	0.85
5:F:85:LEU:HA	5:F:88:ILE:HD12	1.57	0.85
2:M:412:ALA:HB2	2:M:451:LEU:HB3	1.57	0.85
2:M:199:VAL:HG13	2:M:235:LEU:HG	1.58	0.85
2:M:409:ARG:HA	2:M:454:SER:HA	1.59	0.84
2:M:573:ARG:HH21	2:M:697:ARG:HB2	1.42	0.84
2:M:573:ARG:NH2	2:M:697:ARG:HB2	1.92	0.84
3:N:973:GLN:HA	3:N:976:GLN:HE21	1.42	0.84
2:C:41:ASN:HD22	2:C:41:ASN:H	1.22	0.84
3:D:86:ARG:O	3:D:522:PRO:HD2	1.77	0.84
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.59	0.84
3:D:1160:LEU:HD11	3:D:1174:LEU:HD21	1.57	0.84
2:C:1090:LYS:HZ2	3:D:90:MET:HG3	1.42	0.84
2:M:860:HIS:HB2	9:M:1390:HOH:O	1.75	0.84
2:M:964:LYS:O	2:M:968:LEU:HG	1.77	0.84
5:F:361:LEU:HD23	5:F:362:SER:H	1.43	0.84
1:A:42:ARG:NH1	2:C:857:ASP:HB3	1.92	0.84
3:D:1173:LEU:HD23	3:D:1174:LEU:HD23	1.59	0.84
5:P:163:LEU:HD13	5:P:174:LEU:HD21	1.60	0.84
2:M:904:PRO:HD2	2:M:908:GLY:HA2	1.60	0.84
2:C:721:ARG:HH21	2:C:783:ARG:HH21	1.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:118:LEU:HB3	3:D:123:LEU:HD22	1.60	0.84
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.57	0.84
2:C:436:GLY:HA2	2:C:538:GLN:O	1.77	0.84
3:N:1290:LEU:HD23	3:N:1291:SER:H	1.40	0.83
2:C:651:LYS:HA	9:C:1155:HOH:O	1.79	0.83
1:L:57:TYR:HB3	1:L:141:GLU:HG3	1.58	0.83
2:M:689:VAL:HB	2:M:870:ILE:HG13	1.60	0.83
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.61	0.83
3:D:1495:ILE:HD11	9:E:161:HOH:O	1.77	0.83
9:C:1150:HOH:O	3:D:532:GLY:HA2	1.77	0.83
3:D:397:LYS:HG2	9:D:9673:HOH:O	1.79	0.83
5:P:133:ALA:HA	9:P:4452:HOH:O	1.79	0.83
2:C:54:ILE:HD11	2:C:356:ARG:HG2	1.61	0.83
2:C:804:VAL:HG23	2:C:824:ARG:HB2	1.58	0.83
2:C:630:ARG:HH21	2:C:705:ILE:HG22	1.43	0.83
2:M:22:GLN:NE2	2:M:336:VAL:HG21	1.93	0.83
2:M:853:LEU:HD23	2:M:858:MET:HB3	1.58	0.83
2:C:350:ARG:HB3	2:C:350:ARG:HH11	1.42	0.83
2:C:943:VAL:HG23	2:C:985:GLY:H	1.42	0.83
3:N:187:LYS:HE2	3:N:213:VAL:HG12	1.61	0.83
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.60	0.83
2:M:1096:ALA:O	3:N:13:ALA:HB2	1.78	0.83
1:K:89:PHE:HB3	1:K:94:LEU:HD22	1.59	0.82
3:N:1210:SER:HA	9:N:9085:HOH:O	1.78	0.82
2:C:244:PRO:HD2	2:C:245:GLY:H	1.44	0.82
2:C:671:ASN:HD22	2:C:671:ASN:N	1.78	0.82
3:N:1205:TYR:HD2	3:N:1215:VAL:HG21	1.43	0.82
2:M:1018:GLN:HE21	2:M:1060:ILE:HD11	1.44	0.82
2:M:715:THR:HB	2:M:717:LEU:HG	1.61	0.82
3:N:1277:ILE:HD12	3:N:1301:LYS:HB2	1.59	0.82
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.59	0.82
2:M:428:ARG:NH1	6:N:8002:STD:H292	1.94	0.82
5:P:160:ASP:HA	5:P:163:LEU:HD12	1.59	0.82
1:B:57:TYR:HB3	1:B:141:GLU:HG3	1.62	0.82
3:D:561:GLY:HA3	5:F:184:ARG:HH22	1.43	0.82
5:P:120:THR:HG22	5:P:122:LEU:HD13	1.60	0.82
1:B:185:ARG:HA	9:B:592:HOH:O	1.78	0.82
1:B:74:ASP:HB3	9:B:475:HOH:O	1.77	0.82
3:N:704:ARG:HD2	3:N:705:ALA:H	1.44	0.82
3:D:720:LEU:H	3:D:720:LEU:HD12	1.45	0.82
2:C:847:GLY:HA2	9:C:1260:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:227:PHE:HA	2:M:230:ARG:HE	1.43	0.81
1:B:206:THR:HG22	1:B:209:GLU:HB2	1.61	0.81
4:E:67:GLU:HB2	4:E:73:LEU:HD11	1.60	0.81
3:D:133:ILE:HG21	3:D:454:ALA:HB1	1.62	0.81
3:N:699:VAL:H	3:N:756:GLN:NE2	1.77	0.81
5:P:260:ILE:HD11	5:P:310:ILE:HG22	1.63	0.81
2:C:1054:THR:HG23	2:C:1082:PRO:HG3	1.60	0.81
3:N:434:ARG:HB2	3:N:447:VAL:HG22	1.62	0.81
5:P:166:LEU:HB3	5:P:170:HIS:HB2	1.63	0.81
1:L:45:LEU:HD21	1:L:177:VAL:HG22	1.63	0.81
1:A:95:GLN:HA	1:A:146:ARG:NH1	1.94	0.81
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.63	0.81
3:D:135:LEU:HD13	3:D:147:VAL:HG23	1.62	0.81
5:P:358:LEU:HD13	5:P:370:LYS:HG3	1.63	0.81
2:M:232:GLU:HA	2:M:235:LEU:HD12	1.62	0.81
2:C:328:LEU:HD13	2:C:433:THR:HB	1.60	0.81
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.61	0.81
5:F:196:VAL:HG13	5:F:213:ILE:HD11	1.61	0.81
3:D:1277:ILE:HD12	3:D:1301:LYS:HB2	1.62	0.80
3:D:149:LYS:HA	9:D:9019:HOH:O	1.81	0.80
2:C:1099:VAL:HG23	9:C:1503:HOH:O	1.81	0.80
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.62	0.80
1:L:89:PHE:HB2	1:L:94:LEU:HD13	1.63	0.80
1:B:179:PHE:HB3	1:B:197:LEU:HG	1.63	0.80
3:N:18:ILE:HG23	3:N:518:PRO:HG3	1.61	0.80
2:C:710:ILE:HB	2:C:790:LEU:HD13	1.62	0.80
5:F:166:LEU:HB3	5:F:170:HIS:HB2	1.64	0.80
2:M:146:VAL:HG22	2:M:162:ILE:HA	1.64	0.80
3:N:565:ILE:H	3:N:565:ILE:HD12	1.46	0.80
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.63	0.80
1:K:87:VAL:HG21	1:K:144:VAL:HG11	1.63	0.80
2:M:250:ARG:HG2	2:M:253:ALA:HB3	1.63	0.80
3:N:493:ARG:HH21	3:N:1388:ARG:HB3	1.45	0.80
2:M:873:PRO:HB3	3:N:949:ILE:HG12	1.63	0.80
3:D:1046:GLN:HG2	3:D:1052:THR:HG22	1.63	0.80
5:P:142:ARG:HH11	5:P:142:ARG:HB3	1.46	0.80
3:N:396:VAL:HG21	3:N:447:VAL:HB	1.64	0.80
2:C:64:LEU:HD22	2:C:359:MET:HG3	1.64	0.80
5:F:337:HIS:CD2	5:F:337:HIS:H	2.00	0.80
1:L:133:GLU:HB3	9:L:5271:HOH:O	1.81	0.80
2:M:1097:LEU:HD22	2:M:1097:LEU:H	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:THR:HA	9:B:592:HOH:O	1.82	0.79
3:D:87:ARG:HB3	3:D:523:ASP:HB2	1.64	0.79
1:A:186:LEU:HB2	1:A:192:LEU:HD11	1.62	0.79
3:D:1320:GLU:HG2	3:D:1339:LYS:HE2	1.63	0.79
3:D:208:PRO:HB2	3:D:395:VAL:HG22	1.64	0.79
3:D:464:LEU:HA	9:D:2108:HOH:O	1.81	0.79
1:L:26:GLU:HB3	1:L:194:LYS:HG3	1.64	0.79
3:N:1205:TYR:CD2	3:N:1215:VAL:HG21	2.16	0.79
3:N:169:TYR:HD1	3:N:169:TYR:H	1.30	0.79
1:K:88:ARG:HE	1:K:121:GLU:HG2	1.46	0.79
2:C:597:ALA:HB2	2:C:655:LEU:HD21	1.63	0.79
3:D:1234:THR:HA	9:D:9918:HOH:O	1.81	0.79
3:N:1147:ARG:HB3	3:N:1188:VAL:HG21	1.64	0.79
3:D:1136:LYS:HB2	9:D:2265:HOH:O	1.82	0.79
2:M:312:ALA:HB1	2:M:318:PRO:HG2	1.64	0.79
2:M:412:ALA:HA	9:M:1151:HOH:O	1.82	0.79
3:N:1476:THR:HG23	4:O:21:VAL:HG22	1.65	0.79
3:N:1033:GLN:HE21	3:N:1036:ARG:NH1	1.80	0.79
2:C:413:LEU:HD12	2:C:413:LEU:H	1.46	0.79
2:C:603:VAL:HG21	2:C:643:VAL:HG11	1.65	0.79
3:N:86:ARG:O	3:N:522:PRO:HD2	1.81	0.79
4:E:85:LEU:HA	9:E:161:HOH:O	1.81	0.79
2:M:650:ARG:HG2	2:M:653:ASP:HB2	1.64	0.79
3:N:1261:GLU:HG2	9:N:9222:HOH:O	1.83	0.79
2:C:1054:THR:HG22	2:C:1059:ASP:HB2	1.63	0.79
2:C:124:ASP:HB3	2:C:592:LEU:HD12	1.63	0.79
4:O:54:LEU:HG	4:O:58:PRO:HG2	1.65	0.79
2:C:750:LYS:HB2	3:D:681:ARG:HH21	1.48	0.78
3:N:558:LEU:HD13	5:P:145:PRO:HB3	1.64	0.78
3:N:535:PHE:HB3	5:P:314:PRO:HB3	1.65	0.78
5:F:156:VAL:HA	5:F:159:ILE:HD12	1.65	0.78
1:K:117:VAL:HB	1:K:120:VAL:HG12	1.65	0.78
2:M:512:ARG:HB3	2:M:523:ILE:HD11	1.65	0.78
2:M:943:VAL:HG23	2:M:985:GLY:H	1.48	0.78
3:N:1412:LYS:O	3:N:1414:PRO:HD3	1.82	0.78
3:N:644:LEU:HD12	3:N:645:PRO:HD2	1.64	0.78
3:N:806:PHE:CE1	3:N:813:LEU:HB3	2.18	0.78
3:D:1147:ARG:HB2	3:D:1166:LEU:HD21	1.66	0.78
3:D:554:LEU:HA	9:D:9564:HOH:O	1.82	0.78
1:L:206:THR:HG22	1:L:209:GLU:H	1.47	0.78
2:M:422:ARG:HA	9:M:1373:HOH:O	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:33:HIS:HB3	9:O:5639:HOH:O	1.81	0.78
2:M:274:ARG:HD2	2:M:285:LEU:HD22	1.63	0.78
2:M:768:THR:HB	2:M:771:GLU:HB3	1.64	0.78
3:N:133:ILE:HG21	3:N:454:ALA:HB1	1.66	0.78
3:N:186:VAL:HG21	3:N:213:VAL:HB	1.63	0.78
1:A:54:THR:HG22	1:A:158:ILE:HG13	1.66	0.78
3:D:101:HIS:ND1	3:D:103:TRP:HB2	1.99	0.78
5:F:93:LEU:HD22	5:F:98:GLU:HB3	1.64	0.78
2:M:752:GLY:H	2:M:792:VAL:HB	1.47	0.78
3:N:152:LEU:HD23	3:N:152:LEU:H	1.44	0.78
1:B:94:LEU:HD21	1:B:119:ASP:HB2	1.64	0.78
3:N:1109:GLU:HG2	3:N:1201:CYS:HA	1.66	0.78
1:K:54:THR:HG22	1:K:158:ILE:HG13	1.66	0.78
3:N:1372:VAL:HA	3:N:1375:MET:HE3	1.66	0.78
2:C:137:VAL:HG23	2:C:391:LEU:HG	1.66	0.77
2:C:703:ILE:HG22	9:C:1760:HOH:O	1.84	0.77
4:O:93:TYR:HB2	9:O:5639:HOH:O	1.84	0.77
2:C:69:LEU:HG	9:C:1321:HOH:O	1.84	0.77
3:D:1374:GLN:HE22	3:D:1377:LYS:HD2	1.48	0.77
3:D:65:ARG:HG3	3:D:66:GLN:H	1.49	0.77
1:A:222:LEU:HD12	1:B:215:VAL:HB	1.65	0.77
5:P:131:VAL:HG12	5:P:181:GLU:HG3	1.67	0.77
3:N:1296:SER:HB3	9:N:9049:HOH:O	1.84	0.77
2:C:500:ASN:HD21	3:D:1067:VAL:HG23	1.50	0.77
3:D:616:GLN:HG3	3:D:619:LEU:HB3	1.67	0.77
2:M:197:LEU:HB3	2:M:202:TYR:HB2	1.66	0.77
2:M:281:LEU:HD11	2:M:306:THR:HA	1.65	0.77
3:D:1061:PHE:HA	9:D:9012:HOH:O	1.85	0.77
5:F:88:ILE:HD13	5:F:193:ARG:HB2	1.65	0.77
5:F:260:ILE:HG23	5:F:264:MET:HB2	1.67	0.77
5:F:76:SER:O	5:F:80:PRO:HD2	1.83	0.77
1:L:156:HIS:ND1	1:L:158:ILE:HG12	1.99	0.77
2:M:589:ARG:HB2	2:M:589:ARG:HH11	1.49	0.77
3:N:1112:CYS:HB2	3:N:1195:GLN:OE1	1.84	0.77
3:N:1438:ALA:O	3:N:1443:THR:HG22	1.84	0.77
3:N:53:ILE:HG23	3:N:54:LYS:H	1.47	0.77
3:N:566:ILE:HD11	5:P:192:LEU:HD21	1.65	0.77
1:A:27:PRO:HG2	1:A:186:LEU:HD22	1.66	0.76
2:C:332:ARG:HE	2:C:464:LEU:HD11	1.49	0.76
1:L:65:PHE:HD1	3:N:813:LEU:HD22	1.50	0.76
2:M:197:LEU:HA	2:M:200:LEU:HD12	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:244:PRO:HD2	2:M:245:GLY:H	1.49	0.76
3:N:535:PHE:O	5:P:315:VAL:N	2.17	0.76
3:D:1311:LEU:HD23	3:D:1311:LEU:H	1.51	0.76
3:D:756:GLN:O	3:D:760:ARG:HG2	1.85	0.76
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.67	0.76
1:A:20:TYR:HD2	1:A:21:GLY:N	1.83	0.76
3:D:598:ARG:HH12	5:F:319:THR:HA	1.49	0.76
1:K:102:LYS:HG3	1:K:139:ASN:HB2	1.65	0.76
1:K:42:ARG:NH1	2:M:857:ASP:HB3	1.99	0.76
3:N:208:PRO:HB2	3:N:395:VAL:HG13	1.66	0.76
1:A:177:VAL:O	2:C:864:GLY:HA3	1.85	0.76
3:D:704:ARG:HB3	9:D:9490:HOH:O	1.84	0.76
1:B:13:VAL:HG23	9:B:396:HOH:O	1.85	0.76
1:L:194:LYS:HG2	9:L:6021:HOH:O	1.84	0.76
2:M:94:LEU:HD11	9:M:1826:HOH:O	1.84	0.76
2:C:626:ARG:H	2:C:639:GLN:NE2	1.83	0.76
3:D:445:ARG:HB2	3:D:445:ARG:HH11	1.50	0.76
2:M:939:ARG:HD3	2:M:982:PRO:HD3	1.66	0.76
4:O:12:MET:HG3	9:O:7062:HOH:O	1.86	0.76
2:C:21:ILE:HD12	2:C:21:ILE:H	1.49	0.76
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.68	0.76
3:D:111:LYS:HE2	3:D:1452:ILE:HG12	1.68	0.76
2:M:675:ALA:HA	2:M:989:VAL:HG12	1.66	0.76
3:N:145:VAL:HG22	3:N:146:PRO:HD2	1.65	0.76
3:N:37:LEU:HA	9:N:9522:HOH:O	1.86	0.76
1:A:14:ARG:NH2	1:A:22:GLU:HB3	1.99	0.76
3:D:564:GLU:HA	3:D:567:ILE:HD12	1.68	0.76
2:M:1016:ILE:HD11	5:P:330:GLY:O	1.85	0.76
2:C:144:PRO:HA	2:C:163:ILE:HG12	1.68	0.76
2:C:768:THR:HB	2:C:771:GLU:HB3	1.68	0.76
3:D:1372:VAL:HA	3:D:1375:MET:SD	2.25	0.76
3:D:795:VAL:HG23	3:D:879:ARG:NH1	2.01	0.76
5:P:406:ARG:HA	5:P:409:LYS:HG2	1.66	0.76
3:D:186:VAL:HG21	3:D:213:VAL:HB	1.68	0.75
3:D:906:GLN:HB3	3:D:911:LEU:HD11	1.68	0.75
2:M:897:LEU:HD21	2:M:920:GLN:HE21	1.50	0.75
3:N:1109:GLU:OE1	3:N:1201:CYS:HB2	1.86	0.75
3:N:830:ALA:HA	9:N:2273:HOH:O	1.84	0.75
3:D:1136:LYS:HA	9:D:9116:HOH:O	1.86	0.75
3:D:493:ARG:HH12	3:D:1389:LEU:HD12	1.51	0.75
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:139:GLY:O	3:N:147:VAL:HB	1.86	0.75
3:N:191:LEU:HD13	3:N:195:VAL:HG11	1.65	0.75
3:N:192:ALA:O	3:N:195:VAL:HG23	1.86	0.75
1:B:102:LYS:HE3	9:B:503:HOH:O	1.86	0.75
1:K:123:MET:HG2	9:K:4125:HOH:O	1.85	0.75
1:B:89:PHE:HB3	1:B:94:LEU:HD13	1.68	0.75
3:D:1236:LEU:HD12	3:D:1256:LEU:HD13	1.69	0.75
3:D:1273:VAL:HG22	3:D:1326:THR:OG1	1.87	0.75
2:C:1109:VAL:HG23	3:D:3:LYS:HG2	1.67	0.75
3:D:572:ARG:HH12	5:F:79:ASP:CG	1.90	0.75
2:M:774:LEU:HA	2:M:777:ILE:HD12	1.68	0.75
2:C:211:LEU:HD11	2:C:308:ARG:HA	1.68	0.75
3:D:187:LYS:HE2	3:D:213:VAL:HG12	1.69	0.75
3:D:436:GLU:HB2	3:D:445:ARG:HB3	1.68	0.75
5:F:163:LEU:HB3	5:F:174:LEU:HG	1.69	0.75
2:M:350:ARG:HD3	2:M:353:ARG:NH2	2.01	0.75
3:N:817:GLU:HG3	3:N:839:LEU:HD13	1.67	0.75
3:D:1412:LYS:O	3:D:1414:PRO:HD3	1.87	0.75
1:K:67:THR:H	2:M:627:ARG:HH21	1.32	0.75
3:N:1057:VAL:HG13	3:N:1069:GLU:HB3	1.67	0.75
2:M:1115:LEU:HB3	3:N:85:VAL:HG12	1.68	0.75
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.69	0.75
1:L:103:ALA:HB1	1:L:107:LYS:HE3	1.69	0.75
2:M:837:ASP:HB2	9:M:1208:HOH:O	1.86	0.75
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	1.68	0.74
2:C:846:LYS:HD3	3:D:741:ASP:HB2	1.68	0.74
2:M:397:GLU:H	2:M:633:GLN:NE2	1.84	0.74
3:N:1040:GLY:O	3:N:1060:SER:HB3	1.86	0.74
1:B:176:ARG:HH22	3:D:884:ARG:HD3	1.50	0.74
3:D:1236:LEU:HD23	3:D:1359:GLN:HE21	1.49	0.74
2:C:1096:ALA:O	3:D:13:ALA:HB2	1.87	0.74
2:M:810:ASP:HB3	2:M:813:VAL:HG22	1.69	0.74
2:M:96:ALA:HB2	9:M:1826:HOH:O	1.86	0.74
3:N:41:ARG:CZ	3:N:42:ASP:HB2	2.18	0.74
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.51	0.74
2:C:430:VAL:HG13	3:D:1075:HIS:HA	1.69	0.74
2:C:504:GLU:OE2	2:C:509:ALA:HB2	1.88	0.74
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.69	0.74
2:M:404:LEU:HA	2:M:407:LYS:HD2	1.69	0.74
2:M:721:ARG:HH21	2:M:783:ARG:HH21	1.34	0.74
4:E:88:GLU:HB2	9:E:161:HOH:O	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:410:ILE:O	2:M:452:ILE:HA	1.88	0.74
3:N:119:SER:HB2	3:N:123:LEU:HB2	1.69	0.74
2:C:579:VAL:HB	2:C:890:LEU:HD22	1.70	0.74
3:D:808:THR:HB	3:D:809:PRO:HD3	1.69	0.74
5:P:270:LYS:HA	5:P:273:ARG:HD2	1.69	0.74
1:A:14:ARG:NH2	1:A:24:VAL:HG23	2.03	0.74
3:D:806:PHE:CE1	3:D:813:LEU:HB3	2.23	0.74
2:C:546:LEU:HD21	2:C:587:VAL:HG21	1.70	0.74
2:C:751:PRO:HB2	3:D:680:GLN:HG3	1.69	0.74
5:F:191:ASN:HB2	9:F:598:HOH:O	1.86	0.74
2:M:423:ALA:HB1	9:M:1180:HOH:O	1.86	0.74
2:C:1005:MET:HE1	3:D:648:MET:HB2	1.69	0.74
2:C:329:GLY:HA3	2:C:489:THR:HG23	1.70	0.74
2:C:705:ILE:HG13	9:C:1760:HOH:O	1.87	0.74
3:D:1127:GLU:HG3	9:D:9015:HOH:O	1.87	0.74
3:D:210:ARG:HH11	3:D:210:ARG:HB3	1.53	0.74
3:N:13:ALA:HA	9:N:9038:HOH:O	1.87	0.74
3:N:903:ASP:HA	9:N:9909:HOH:O	1.87	0.74
2:C:678:PRO:HG3	3:D:947:ILE:HD11	1.69	0.74
3:D:530:VAL:HA	9:D:2446:HOH:O	1.87	0.74
2:M:926:PHE:HE2	2:M:960:GLU:HG3	1.53	0.74
3:N:704:ARG:HG3	3:N:736:PHE:HB3	1.70	0.74
1:A:150:TYR:HE2	1:A:152:PRO:HG3	1.51	0.73
2:C:322:VAL:HA	9:C:1224:HOH:O	1.88	0.73
2:C:724:ARG:HD2	2:C:740:GLU:HA	1.70	0.73
2:C:41:ASN:N	2:C:41:ASN:HD22	1.86	0.73
3:N:141:ILE:HD13	3:N:450:TYR:HB2	1.70	0.73
2:M:1056:LYS:O	3:N:624:ASP:HB2	1.88	0.73
3:D:465:LEU:HD22	9:D:9443:HOH:O	1.89	0.73
5:P:269:ASN:HB3	5:P:273:ARG:HE	1.50	0.73
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.70	0.73
3:D:795:VAL:HG11	3:D:863:VAL:HG13	1.69	0.73
9:D:9529:HOH:O	4:E:61:GLU:HG2	1.87	0.73
3:N:131:LYS:HG3	3:N:572:ARG:HH21	1.54	0.73
1:B:199:ILE:HD11	1:B:211:LEU:HD13	1.70	0.73
2:C:83:CYS:HA	2:C:88:LEU:HB3	1.71	0.73
2:C:945:ARG:HG3	2:C:946:ARG:N	2.04	0.73
3:D:1438:ALA:O	3:D:1443:THR:HG22	1.88	0.73
3:D:775:GLY:HA2	9:D:9258:HOH:O	1.87	0.73
4:O:31:LEU:HD21	4:O:60:ALA:HB2	1.70	0.73
5:P:358:LEU:HD11	5:P:370:LYS:HZ2	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1374:GLN:HE21	3:D:1374:GLN:HA	1.54	0.73
3:D:461:ILE:HG22	9:D:9464:HOH:O	1.89	0.73
3:D:679:ARG:HB2	3:D:682:ASP:OD1	1.89	0.73
4:E:87:LYS:HZ3	4:E:91:ARG:HE	1.37	0.73
3:N:108:VAL:HG23	3:N:109:PRO:HD3	1.70	0.73
2:M:1090:LYS:HE3	3:N:90:MET:HG2	1.68	0.73
2:C:616:GLU:HG3	9:C:1986:HOH:O	1.88	0.73
2:M:1016:ILE:HD13	2:M:1016:ILE:H	1.54	0.73
2:M:164:PRO:HA	9:M:1138:HOH:O	1.88	0.73
2:M:614:ARG:HG3	2:M:620:LEU:HD12	1.69	0.73
3:N:650:LEU:HD13	3:N:688:TRP:HZ3	1.52	0.73
3:N:875:THR:HG22	3:N:879:ARG:HE	1.51	0.73
1:A:95:GLN:HG2	1:A:146:ARG:HH22	1.54	0.73
2:C:478:VAL:HG13	2:C:506:ASN:HB3	1.71	0.73
2:C:630:ARG:NE	2:C:705:ILE:HB	2.03	0.73
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.71	0.73
5:P:185:GLN:HA	5:P:188:ILE:HD12	1.70	0.73
5:P:361:LEU:HG	5:P:408:LEU:HD21	1.70	0.73
2:C:1111:ILE:HG13	2:C:1112:PHE:H	1.54	0.72
3:D:58:CYS:SG	3:D:59:ALA:N	2.62	0.72
5:F:337:HIS:HD2	5:F:337:HIS:H	1.36	0.72
3:N:1209:LEU:HD23	3:N:1210:SER:H	1.54	0.72
3:N:1209:LEU:HG	3:N:1219:GLU:OE1	1.89	0.72
3:D:1096:ARG:HH11	3:D:1096:ARG:HB2	1.52	0.72
4:E:30:LEU:O	4:E:35:PHE:HA	1.89	0.72
2:M:1005:MET:HB2	3:N:648:MET:HE1	1.71	0.72
3:N:838:ARG:HB2	9:N:2269:HOH:O	1.88	0.72
2:C:479:VAL:CG2	2:C:503:LEU:HD11	2.19	0.72
2:C:771:GLU:O	2:C:775:ARG:HG2	1.88	0.72
3:D:209:ARG:NH2	3:D:397:LYS:HG3	2.04	0.72
2:M:438:ILE:HD11	2:M:467:ILE:HD12	1.72	0.72
3:D:1109:GLU:HG2	3:D:1201:CYS:HA	1.72	0.72
2:C:1098:ASP:HB2	3:D:21:TRP:HZ2	1.55	0.72
3:D:210:ARG:CZ	3:D:398:ALA:HB3	2.19	0.72
2:M:704:HIS:HA	9:M:1178:HOH:O	1.88	0.72
3:N:135:LEU:HD13	3:N:147:VAL:HG23	1.72	0.72
3:N:549:ASN:HB2	9:N:9149:HOH:O	1.89	0.72
3:N:639:LEU:HD12	3:N:639:LEU:H	1.53	0.72
1:A:24:VAL:HG22	1:A:196:THR:HB	1.70	0.72
3:D:396:VAL:HG21	3:D:447:VAL:HB	1.70	0.72
3:D:673:ALA:HB2	9:D:9062:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:73:CYS:HB3	3:D:76:CYS:O	1.89	0.72
2:M:603:VAL:HG21	2:M:643:VAL:HG11	1.70	0.72
2:C:1008:ARG:NH2	2:C:1028:GLY:HA2	2.04	0.72
3:D:513:ILE:HG23	9:D:9117:HOH:O	1.89	0.72
1:L:86:VAL:HG12	1:L:124:ASN:HD22	1.53	0.72
3:N:1394:VAL:HG11	9:N:2250:HOH:O	1.88	0.72
1:B:78:ILE:HA	9:B:385:HOH:O	1.90	0.72
2:C:175:GLU:HA	9:C:2004:HOH:O	1.90	0.72
2:C:551:GLU:HB3	2:C:906:PHE:HD2	1.53	0.72
2:C:873:PRO:HG2	3:D:947:ILE:HD12	1.71	0.72
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.71	0.72
3:D:141:ILE:HD13	3:D:450:TYR:HB2	1.72	0.72
5:F:247:ILE:HG22	5:F:251:ILE:HD11	1.72	0.72
1:L:97:VAL:HG11	1:L:120:VAL:HG21	1.71	0.72
2:M:132:ALA:HB1	2:M:632:ASN:HD21	1.54	0.72
3:N:1223:ILE:H	3:N:1223:ILE:HD12	1.55	0.72
2:M:1015:LEU:HB2	5:P:334:PRO:O	1.89	0.72
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.71	0.72
2:M:511:GLU:O	2:M:526:PRO:HD3	1.89	0.72
5:P:361:LEU:HD21	5:P:404:ALA:HB1	1.71	0.72
5:F:108:GLU:HG3	5:F:176:ILE:HG21	1.72	0.72
2:M:478:VAL:HA	2:M:506:ASN:O	1.90	0.72
3:N:207:PHE:HB3	3:N:208:PRO:HD2	1.71	0.72
2:C:158:TYR:HB2	9:C:1570:HOH:O	1.89	0.72
5:F:388:ALA:HB3	9:F:553:HOH:O	1.89	0.72
1:L:41:ARG:HG3	1:L:177:VAL:HG21	1.71	0.72
3:N:723:GLY:HA3	9:N:9632:HOH:O	1.90	0.72
2:C:1000:MET:HB3	2:C:1002:GLU:HG3	1.71	0.71
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.72	0.71
9:C:1389:HOH:O	3:D:630:VAL:HG23	1.89	0.71
2:M:72:ARG:HH21	2:M:112:GLU:HG3	1.54	0.71
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.70	0.71
3:N:808:THR:HB	3:N:809:PRO:HD3	1.73	0.71
2:C:274:ARG:HB2	2:C:285:LEU:HD13	1.72	0.71
2:C:557:ARG:NH2	2:C:879:ARG:HD3	2.05	0.71
3:D:1350:GLU:O	3:D:1354:LYS:HG2	1.90	0.71
2:M:1030:GLN:HB2	3:N:626:SER:HB2	1.70	0.71
2:M:1056:LYS:HD3	3:N:623:VAL:HG13	1.72	0.71
2:M:139:GLN:NE2	2:M:334:ARG:HH11	1.87	0.71
3:N:1189:ARG:CZ	3:N:1203:LYS:HB2	2.20	0.71
3:N:142:LEU:HD11	9:N:9710:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:95:GLN:H	1:L:95:GLN:HE21	1.38	0.71
3:N:148:GLU:HB3	3:N:151:GLN:HB3	1.73	0.71
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.71	0.71
2:C:720:GLU:HG2	2:C:760:SER:HB3	1.70	0.71
3:D:562:ALA:HB1	3:D:567:ILE:HD11	1.73	0.71
1:K:27:PRO:HB2	9:K:4607:HOH:O	1.90	0.71
2:M:207:LEU:HD13	2:M:221:LEU:HD13	1.72	0.71
2:M:289:THR:HG22	2:M:290:LEU:HD23	1.71	0.71
3:N:1272:ALA:HA	3:N:1326:THR:HB	1.71	0.71
3:N:158:TYR:HA	9:N:9313:HOH:O	1.89	0.71
5:F:100:VAL:HG21	9:F:478:HOH:O	1.89	0.71
2:M:605:LYS:HD3	2:M:610:ARG:CZ	2.20	0.71
3:N:117:ASP:HB2	3:N:495:ARG:NH2	2.04	0.71
3:N:1485:GLN:HE21	4:O:80:VAL:H	1.36	0.71
5:P:164:LYS:HA	5:P:171:LYS:HE2	1.71	0.71
5:P:102:LEU:HD13	5:P:187:LEU:HG	1.72	0.71
3:D:1236:LEU:HD23	3:D:1359:GLN:NE2	2.04	0.71
3:D:1399:ASP:O	3:D:1403:LEU:HB2	1.90	0.71
3:N:165:LYS:HE2	3:N:165:LYS:HA	1.73	0.71
2:M:755:LEU:HB2	2:M:790:LEU:HD23	1.73	0.71
3:N:400:VAL:HG11	3:N:441:ARG:NH1	2.06	0.71
5:P:312:GLN:HB2	9:P:4816:HOH:O	1.90	0.71
1:A:219:ARG:HH22	1:B:223:THR:HG22	1.53	0.71
1:B:103:ALA:HB1	1:B:107:LYS:HE3	1.73	0.71
3:D:1321:ALA:O	3:D:1339:LYS:HD3	1.91	0.71
1:K:198:ARG:HB2	1:K:200:TRP:CZ3	2.25	0.71
2:M:399:ASN:O	2:M:402:SER:HB3	1.90	0.71
3:N:119:SER:HB2	3:N:123:LEU:N	2.05	0.71
1:B:24:VAL:HG13	1:B:196:THR:HG22	1.71	0.71
2:C:186:VAL:HG23	2:C:187:ASN:H	1.54	0.71
2:C:346:VAL:O	2:C:350:ARG:HG3	1.91	0.71
3:D:1137:ARG:O	3:D:1141:GLU:HG3	1.90	0.71
2:M:144:PRO:HB3	9:M:1138:HOH:O	1.91	0.71
5:P:291:ILE:HG21	5:P:304:VAL:HG11	1.71	0.71
3:D:1047:LYS:HZ1	3:D:1053:PHE:HA	1.55	0.71
3:D:1166:LEU:HD12	3:D:1171:VAL:HG22	1.71	0.71
2:M:786:LYS:HA	9:M:1196:HOH:O	1.91	0.71
3:N:572:ARG:HH22	5:P:83:GLN:HG3	1.55	0.71
1:A:53:VAL:HG23	9:A:481:HOH:O	1.90	0.70
3:D:191:LEU:HD12	3:D:211:VAL:HG21	1.73	0.70
3:D:699:VAL:HG12	3:D:717:GLN:HA	1.70	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:146:VAL:HG11	2:M:306:THR:HG22	1.71	0.70
2:M:17:PRO:O	2:M:20:GLU:HB2	1.90	0.70
2:M:292:ARG:HD2	2:M:299:LYS:HD3	1.71	0.70
2:M:437:ARG:NH2	2:M:488:ALA:HA	2.06	0.70
3:D:1205:TYR:CD2	3:D:1215:VAL:HG21	2.26	0.70
3:D:449:SER:HB2	9:D:9007:HOH:O	1.90	0.70
1:K:103:ALA:HB1	1:K:107:LYS:HD3	1.73	0.70
2:M:136:ILE:HD13	2:M:392:SER:HB2	1.72	0.70
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.72	0.70
5:P:393:THR:HG22	5:P:394:ARG:H	1.56	0.70
2:C:329:GLY:H	2:C:488:ALA:HB3	1.53	0.70
3:D:150:ARG:HH11	3:D:150:ARG:HG3	1.55	0.70
3:D:55:ASP:HA	3:D:82:LYS:HG3	1.73	0.70
3:D:877:PRO:HA	9:D:9080:HOH:O	1.90	0.70
2:M:707:ARG:HH21	2:M:709:GLU:HB2	1.55	0.70
2:M:741:GLY:HA3	9:M:1428:HOH:O	1.90	0.70
2:M:820:ARG:HB2	9:M:1453:HOH:O	1.91	0.70
1:K:226:SER:O	1:K:228:PRO:HD3	1.91	0.70
3:N:1432:LYS:HD2	3:N:1433:SER:H	1.54	0.70
2:C:308:ARG:HH12	2:C:309:TYR:HD1	1.39	0.70
2:C:352:ALA:O	2:C:356:ARG:HG3	1.91	0.70
1:K:83:LYS:HE3	1:K:167:VAL:HG12	1.72	0.70
2:M:83:CYS:HA	2:M:88:LEU:HB3	1.73	0.70
2:C:313:LEU:HA	2:C:321:GLU:HG3	1.73	0.70
3:D:194:GLY:H	3:D:206:ARG:HA	1.56	0.70
2:M:362:GLY:HA3	2:M:367:LEU:HD23	1.73	0.70
2:M:457:ALA:HB3	2:M:538:GLN:HA	1.74	0.70
2:M:876:VAL:HA	9:M:1223:HOH:O	1.92	0.70
3:N:1095:THR:O	3:N:1099:VAL:HG23	1.90	0.70
3:N:185:VAL:HG12	3:N:191:LEU:HD21	1.73	0.70
2:C:478:VAL:HA	2:C:506:ASN:O	1.92	0.70
3:D:1099:VAL:HG13	3:D:1223:ILE:HD11	1.73	0.70
4:E:87:LYS:NZ	4:E:91:ARG:HE	1.88	0.70
3:N:1273:VAL:HG22	3:N:1326:THR:OG1	1.90	0.70
3:N:559:ALA:HA	9:P:4209:HOH:O	1.91	0.70
2:C:804:VAL:HG22	9:C:1991:HOH:O	1.92	0.70
2:M:710:ILE:HB	2:M:790:LEU:HD13	1.74	0.70
3:D:1166:LEU:HD23	3:D:1166:LEU:H	1.56	0.70
3:N:171:LEU:HD22	3:N:390:PRO:HG3	1.74	0.70
3:N:810:GLU:O	3:N:813:LEU:HG	1.92	0.70
3:N:906:GLN:HB3	3:N:911:LEU:HD11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:VAL:HG21	1:A:82:LEU:HD22	1.71	0.70
2:C:333:ILE:CD1	2:C:467:ILE:HG13	2.22	0.70
3:N:430:ASP:HB3	9:N:9129:HOH:O	1.92	0.70
9:N:9045:HOH:O	4:O:84:ARG:HG2	1.91	0.70
5:F:361:LEU:HD22	5:F:366:ALA:HB2	1.74	0.69
3:N:124:GLU:HB2	9:N:2068:HOH:O	1.90	0.69
3:N:483:HIS:HB2	3:N:484:PRO:HD3	1.73	0.69
3:N:46:ASP:HB3	3:N:49:ILE:HG13	1.74	0.69
2:C:1050:GLN:HA	9:D:9467:HOH:O	1.92	0.69
2:C:231:PRO:HB3	9:C:1979:HOH:O	1.91	0.69
2:M:357:GLU:HG3	9:M:1526:HOH:O	1.92	0.69
2:M:551:GLU:HB3	2:M:906:PHE:HD2	1.56	0.69
3:N:795:VAL:HG11	3:N:863:VAL:HG13	1.73	0.69
3:N:850:LEU:H	3:N:850:LEU:HD12	1.56	0.69
3:N:561:GLY:HA3	5:P:184:ARG:HH22	1.57	0.69
2:C:432:ARG:HH12	3:D:1047:LYS:HG2	1.56	0.69
3:D:1267:ARG:HB2	3:D:1267:ARG:HH11	1.56	0.69
5:F:112:ALA:HA	5:F:173:TYR:HD2	1.57	0.69
2:M:95:TYR:CD2	2:M:114:PHE:HB3	2.28	0.69
3:N:866:VAL:HG11	9:N:9036:HOH:O	1.93	0.69
2:M:1090:LYS:HE2	3:N:88:TYR:O	1.91	0.69
2:C:108:ILE:HB	2:C:368:THR:OG1	1.92	0.69
2:C:325:ILE:HG21	9:C:1414:HOH:O	1.91	0.69
2:C:939:ARG:HG3	9:C:1124:HOH:O	1.90	0.69
1:K:24:VAL:HG22	1:K:196:THR:HB	1.73	0.69
3:N:1068:LEU:O	3:N:1072:ILE:HG12	1.92	0.69
3:N:171:LEU:HB2	3:N:390:PRO:HA	1.74	0.69
3:N:470:LEU:HG	3:N:508:ARG:HH21	1.57	0.69
5:P:168:LYS:HG3	9:P:5800:HOH:O	1.92	0.69
5:P:76:SER:O	5:P:80:PRO:HD2	1.92	0.69
5:F:363:GLU:O	5:F:367:MET:HG2	1.92	0.69
2:M:724:ARG:HG3	2:M:741:GLY:H	1.58	0.69
3:N:1115:THR:HG22	9:N:9343:HOH:O	1.93	0.69
3:N:1156:LEU:HB3	9:N:9178:HOH:O	1.92	0.69
9:M:2105:HOH:O	5:P:409:LYS:HB2	1.93	0.69
1:B:27:PRO:HB3	1:B:192:LEU:HD22	1.75	0.69
2:C:115:LEU:HD22	2:C:373:VAL:HG11	1.74	0.69
3:D:1376:MET:HG2	9:D:9649:HOH:O	1.92	0.69
3:D:65:ARG:HB3	9:D:9625:HOH:O	1.91	0.69
2:M:186:VAL:HG23	2:M:187:ASN:H	1.57	0.69
2:M:736:ASP:O	2:M:744:ARG:HG2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1192:LEU:HD12	3:N:1346:ARG:HH22	1.56	0.69
3:N:400:VAL:HG12	3:N:401:TYR:HD1	1.58	0.69
3:N:488:ARG:HH11	3:N:488:ARG:HB3	1.58	0.69
2:C:1090:LYS:HE2	2:C:1112:PHE:HE1	1.58	0.69
3:D:1101:VAL:HG22	3:D:1428:ALA:HB2	1.75	0.69
3:D:15:PRO:HB2	9:D:9069:HOH:O	1.92	0.69
3:D:477:LEU:HD22	3:D:492:ALA:HB1	1.75	0.69
3:N:206:ARG:O	3:N:206:ARG:HD3	1.92	0.69
3:N:28:LYS:HB2	3:N:41:ARG:NH1	2.07	0.69
5:P:321:ILE:HG22	5:P:322:GLY:H	1.57	0.69
1:A:128:HIS:HE1	1:A:131:THR:HG23	1.57	0.69
1:B:58:ILE:HD13	1:B:140:MET:HB3	1.73	0.69
1:B:77:GLU:HB3	9:B:475:HOH:O	1.92	0.69
2:C:1062:GLY:HA2	9:C:1248:HOH:O	1.93	0.69
5:F:125:ASP:HA	5:F:128:ARG:HH12	1.55	0.69
5:F:398:ARG:HG2	5:F:402:ASN:HD22	1.57	0.69
2:M:474:VAL:HG11	2:M:529:VAL:HG12	1.74	0.69
2:M:802:ARG:HB3	9:M:1993:HOH:O	1.91	0.69
3:N:1112:CYS:HB3	3:N:1201:CYS:SG	2.31	0.69
1:A:214:ALA:HA	1:A:217:ILE:HD12	1.74	0.69
1:B:36:LEU:O	1:B:39:PRO:HD2	1.93	0.69
2:C:101:ILE:HG23	2:C:107:LEU:HD22	1.73	0.69
2:C:110:GLU:HG2	2:C:369:PRO:HB3	1.74	0.69
3:D:1132:LEU:HA	9:D:2445:HOH:O	1.92	0.69
3:D:153:LEU:CD1	3:D:157:GLU:HB2	2.22	0.69
3:D:434:ARG:HB2	3:D:447:VAL:HG22	1.73	0.69
1:L:184:THR:HG23	1:L:192:LEU:HB3	1.74	0.69
3:N:1098:LEU:HD23	3:N:1226:ALA:HA	1.73	0.69
2:C:841:ASN:HD22	2:C:843:HIS:H	1.39	0.69
3:D:1314:LYS:HB2	9:D:9368:HOH:O	1.93	0.69
3:D:9:ARG:HA	3:D:1434:TRP:HH2	1.58	0.69
5:F:82:ARG:HG2	5:F:86:HIS:NE2	2.07	0.69
2:M:1015:LEU:HA	5:P:335:ASP:HB3	1.75	0.69
2:M:35:PRO:HD2	2:M:38:LYS:HG3	1.73	0.69
3:N:1402:ALA:HB3	9:N:9219:HOH:O	1.93	0.69
5:P:303:ARG:HD2	9:P:4749:HOH:O	1.93	0.69
3:D:423:ASP:HB2	5:F:178:ARG:HD2	1.75	0.69
1:K:206:THR:HG23	1:K:209:GLU:HB2	1.74	0.69
2:M:346:VAL:O	2:M:350:ARG:HG2	1.92	0.69
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.28	0.69
3:N:1087:ARG:HD2	3:N:1234:THR:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:194:GLY:H	3:N:206:ARG:HA	1.57	0.69
2:C:676:ILE:HG23	3:D:948:THR:HB	1.75	0.68
2:C:758:ARG:HB3	2:C:788:THR:O	1.93	0.68
2:M:18:LEU:HD23	2:M:404:LEU:HD21	1.74	0.68
3:N:1020:LEU:HB3	9:N:9262:HOH:O	1.93	0.68
3:N:1232:PRO:HB3	3:N:1361:VAL:HG21	1.74	0.68
3:N:1434:TRP:CZ3	3:N:1457:ASP:HB2	2.28	0.68
2:C:1080:SER:HA	9:C:1199:HOH:O	1.93	0.68
2:C:516:ARG:HH11	2:C:521:PRO:HB3	1.56	0.68
3:D:1410:GLU:HA	9:D:2415:HOH:O	1.93	0.68
2:M:157:ARG:HG3	9:M:1827:HOH:O	1.93	0.68
3:N:1102:THR:HG22	3:N:1222:GLY:HA2	1.75	0.68
3:N:561:GLY:HA3	5:P:184:ARG:NH2	2.08	0.68
3:N:619:LEU:HB2	9:N:9336:HOH:O	1.91	0.68
5:P:260:ILE:HG23	5:P:264:MET:HB2	1.74	0.68
1:A:91:ASN:OD1	1:A:92:PRO:HD2	1.92	0.68
2:C:329:GLY:N	2:C:488:ALA:HB3	2.08	0.68
3:D:119:SER:HB2	3:D:123:LEU:N	2.05	0.68
3:D:1354:LYS:HD2	9:D:9073:HOH:O	1.92	0.68
3:D:704:ARG:HE	3:D:705:ALA:H	1.42	0.68
2:M:412:ALA:HB1	2:M:419:THR:HG23	1.74	0.68
2:M:944:LEU:HD21	2:M:963:LEU:HD22	1.75	0.68
3:N:1194:CYS:HB3	3:N:1373:ARG:NH2	2.08	0.68
2:C:421:GLU:HA	9:C:1472:HOH:O	1.92	0.68
3:D:207:PHE:HB3	3:D:208:PRO:HD2	1.76	0.68
5:F:392:VAL:HG11	5:F:396:ARG:HE	1.58	0.68
3:N:1287:GLU:HA	9:N:9009:HOH:O	1.93	0.68
3:N:478:LEU:HD22	3:N:1388:ARG:HH21	1.59	0.68
1:A:9:PRO:HD2	1:B:224:TYR:CZ	2.28	0.68
2:C:601:GLY:HA2	2:C:616:GLU:HG2	1.74	0.68
3:D:1197:ARG:HG3	9:D:9004:HOH:O	1.92	0.68
3:D:1487:VAL:HG11	3:D:1492:LEU:HG	1.74	0.68
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.75	0.68
5:F:113:ILE:HA	5:F:116:LEU:HD12	1.75	0.68
3:N:1492:LEU:HA	9:N:9942:HOH:O	1.92	0.68
3:N:1493:LYS:O	3:N:1497:GLU:HG2	1.93	0.68
3:N:804:LEU:HB2	3:N:830:ALA:O	1.94	0.68
3:N:838:ARG:HD3	3:N:865:THR:HG23	1.75	0.68
3:N:846:PRO:HA	9:N:9036:HOH:O	1.93	0.68
1:B:214:ALA:HA	1:B:217:ILE:HD12	1.76	0.68
2:C:1104:GLU:HA	3:D:6:ARG:HD2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.76	0.68
3:D:469:ASP:HA	9:D:9515:HOH:O	1.93	0.68
3:D:810:GLU:HA	3:D:813:LEU:HD23	1.74	0.68
2:M:780:GLU:HG3	2:M:781:LYS:H	1.58	0.68
3:N:761:ILE:HG21	9:O:5032:HOH:O	1.94	0.68
3:D:1299:PHE:HB2	9:D:9155:HOH:O	1.93	0.68
3:D:598:ARG:NH1	3:D:598:ARG:HG2	2.09	0.68
3:D:63:TYR:HB3	3:D:68:PHE:CE1	2.28	0.68
3:D:650:LEU:HD13	3:D:688:TRP:HZ3	1.59	0.68
3:D:67:ARG:HD3	9:D:2035:HOH:O	1.94	0.68
4:E:48:MET:HB2	4:E:54:LEU:HD12	1.76	0.68
3:N:800:LYS:HE3	3:N:830:ALA:HB3	1.74	0.68
1:A:184:THR:HG23	1:A:192:LEU:HB2	1.76	0.68
3:D:1478:SER:O	3:D:1482:ARG:HG3	1.94	0.68
3:D:478:LEU:HA	9:D:9267:HOH:O	1.94	0.68
3:D:78:VAL:HG23	9:D:2450:HOH:O	1.93	0.68
3:D:889:ALA:O	3:D:929:ARG:HD2	1.93	0.68
5:F:358:LEU:HD13	5:F:370:LYS:HG3	1.75	0.68
5:F:78:SER:HA	9:F:735:HOH:O	1.93	0.68
1:L:110:LYS:HG3	9:L:6714:HOH:O	1.93	0.68
2:M:36:PRO:HG2	2:M:70:GLU:HB3	1.75	0.68
2:M:1085:PHE:CD2	3:N:1468:LEU:HA	2.29	0.68
5:P:401:GLU:O	5:P:405:LEU:HB2	1.92	0.68
1:B:156:HIS:ND1	1:B:158:ILE:HG12	2.09	0.68
2:C:1042:ALA:HB3	3:D:710:ARG:HB3	1.74	0.68
2:C:1087:VAL:HG22	2:C:1091:GLU:OE2	1.94	0.68
2:C:428:ARG:HD3	2:C:450:GLY:H	1.58	0.68
3:D:543:LEU:HA	3:D:546:ARG:HG3	1.76	0.68
5:F:144:ILE:HB	5:F:145:PRO:HD3	1.75	0.68
2:M:412:ALA:HB3	2:M:451:LEU:HB3	1.75	0.68
2:M:913:GLU:O	2:M:916:GLU:HB3	1.94	0.68
3:N:633:VAL:HG22	3:N:635:PRO:HD3	1.75	0.68
3:N:661:MET:HG2	3:N:666:ILE:HD12	1.74	0.68
1:B:99:LEU:HD12	1:B:114:PHE:HB3	1.76	0.68
2:C:1015:LEU:HA	9:C:1234:HOH:O	1.93	0.68
2:C:41:ASN:H	2:C:41:ASN:ND2	1.92	0.68
3:D:139:GLY:O	3:D:147:VAL:HB	1.94	0.68
3:D:172:PRO:HD2	3:D:389:GLU:O	1.93	0.68
9:C:1170:HOH:O	3:D:648:MET:HE3	1.94	0.68
2:M:525:SER:H	2:M:528:GLU:HG3	1.59	0.68
3:N:30:GLU:HB3	3:N:40:GLU:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:HG3	1:A:139:ASN:HB2	1.75	0.67
3:D:1316:GLY:HA3	9:D:9350:HOH:O	1.92	0.67
3:D:728:LEU:HD22	3:D:745:MET:SD	2.34	0.67
3:D:854:ALA:HB3	9:D:9283:HOH:O	1.94	0.67
4:E:10:PHE:HE2	4:E:16:LYS:HG3	1.59	0.67
5:F:314:PRO:HD2	9:F:481:HOH:O	1.93	0.67
5:F:94:LEU:HD23	5:F:96:LEU:H	1.59	0.67
1:L:94:LEU:HD21	1:L:119:ASP:HB2	1.76	0.67
2:M:1082:PRO:HG2	3:N:1469:GLY:HA3	1.74	0.67
3:N:191:LEU:HB3	3:N:195:VAL:HG21	1.75	0.67
3:N:658:LEU:HA	3:N:661:MET:HE3	1.76	0.67
5:P:155:THR:HA	9:P:3694:HOH:O	1.92	0.67
3:N:1383:ASP:HB2	3:N:1416:ALA:HB3	1.76	0.67
3:N:622:ARG:HD2	9:P:5569:HOH:O	1.93	0.67
3:N:715:ALA:HB3	3:N:764:LEU:HA	1.76	0.67
3:D:1306:PRO:HB3	3:D:1307:LYS:HE3	1.76	0.67
3:D:145:VAL:HB	9:D:2447:HOH:O	1.93	0.67
3:D:1462:LEU:HD22	3:D:1472:ILE:HG23	1.75	0.67
3:D:386:HIS:HA	9:D:2147:HOH:O	1.94	0.67
3:D:161:LEU:HD22	3:D:452:ILE:HG21	1.76	0.67
2:M:432:ARG:HH11	3:N:1048:PRO:HG2	1.58	0.67
3:N:95:LEU:HD21	3:N:574:LEU:HD11	1.75	0.67
1:A:100:LEU:HD11	9:A:408:HOH:O	1.94	0.67
2:C:1000:MET:SD	2:C:1001:VAL:HG22	2.34	0.67
2:C:379:GLU:HG3	2:C:383:ARG:HH12	1.60	0.67
2:C:511:GLU:O	2:C:526:PRO:HD3	1.94	0.67
3:D:1324:PRO:HA	9:D:9450:HOH:O	1.94	0.67
3:D:195:VAL:HG13	9:D:9209:HOH:O	1.94	0.67
3:D:554:LEU:HD22	9:D:9564:HOH:O	1.94	0.67
3:D:978:TYR:HE1	3:D:985:ASP:HA	1.60	0.67
5:F:215:GLU:HB2	9:F:482:HOH:O	1.95	0.67
1:A:30:ARG:NH1	1:A:191:ASP:HB2	2.10	0.67
2:C:71:TYR:HB2	9:C:1203:HOH:O	1.93	0.67
3:D:1412:LYS:HG2	3:D:1414:PRO:HG3	1.76	0.67
1:K:117:VAL:HB	1:K:120:VAL:CG1	2.25	0.67
1:A:130:ALA:HB1	9:A:328:HOH:O	1.92	0.67
2:C:420:ARG:HD2	2:C:420:ARG:H	1.59	0.67
2:C:712:ALA:O	2:C:820:ARG:HB3	1.94	0.67
5:F:220:LEU:HB2	5:F:243:ILE:HD11	1.76	0.67
3:N:1409:ALA:HB1	9:N:9241:HOH:O	1.94	0.67
3:N:906:GLN:HB3	3:N:911:LEU:CD1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:88:ILE:CD1	5:P:193:ARG:HB2	2.22	0.67
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.76	0.67
2:C:358:ARG:HH22	2:C:374:ASN:HB3	1.58	0.67
2:C:36:PRO:HG2	2:C:70:GLU:HB3	1.75	0.67
3:D:214:GLU:HB2	3:D:390:PRO:HD2	1.75	0.67
3:D:676:MET:HG3	9:D:9271:HOH:O	1.92	0.67
3:D:899:LEU:HD12	3:D:900:ILE:HG23	1.76	0.67
4:E:36:LYS:HB3	9:E:130:HOH:O	1.95	0.67
2:M:169:GLY:HA2	2:M:263:ASP:CB	2.20	0.67
3:N:690:ALA:O	3:N:694:VAL:HG23	1.95	0.67
4:O:70:THR:HG21	4:O:72:ARG:CZ	2.25	0.67
5:P:130:VAL:HG21	5:P:159:ILE:HG21	1.76	0.67
1:B:30:ARG:HE	2:C:854:PRO:HG3	1.59	0.67
3:D:667:ALA:HB2	9:D:9271:HOH:O	1.93	0.67
1:K:9:PRO:HB2	1:L:224:TYR:HB3	1.76	0.67
1:L:168:ASP:HA	9:L:6431:HOH:O	1.94	0.67
2:M:1054:THR:HG21	2:M:1079:PRO:CB	2.18	0.67
2:M:251:ASP:HB3	2:M:252:LYS:HD2	1.77	0.67
2:M:263:ASP:HB2	2:M:264:PRO:HD3	1.76	0.67
3:N:381:ALA:HA	9:N:2123:HOH:O	1.93	0.67
5:P:138:SER:H	5:P:140:ARG:CZ	2.08	0.67
2:C:145:GLY:O	2:C:163:ILE:HG23	1.94	0.67
2:C:676:ILE:CG2	2:C:988:VAL:HG22	2.24	0.67
3:D:1498:ALA:HB1	9:E:165:HOH:O	1.94	0.67
3:D:486:ARG:HH21	3:D:489:ARG:NH2	1.92	0.67
1:L:46:SER:HB2	9:L:4292:HOH:O	1.95	0.67
2:M:177:GLU:HB2	9:M:1718:HOH:O	1.95	0.67
2:M:265:ARG:HG2	2:M:266:ARG:N	2.10	0.67
5:P:208:SER:HB2	5:P:211:ASP:CG	2.14	0.67
3:D:12:LEU:HD21	3:D:104:PHE:HE1	1.59	0.67
3:N:1393:GLN:HB2	3:N:1398:TRP:NE1	2.10	0.67
2:C:1008:ARG:HH21	2:C:1028:GLY:HA2	1.60	0.66
2:C:1084:SER:O	2:C:1087:VAL:HG12	1.94	0.66
3:D:165:LYS:HB3	3:D:395:VAL:HG11	1.75	0.66
3:D:500:ARG:HG3	9:D:2428:HOH:O	1.94	0.66
2:M:144:PRO:HA	2:M:163:ILE:HG13	1.77	0.66
2:M:207:LEU:HD22	2:M:221:LEU:HD22	1.77	0.66
2:M:42:VAL:HG12	2:M:43:GLY:H	1.60	0.66
5:P:138:SER:H	5:P:140:ARG:NH2	1.93	0.66
1:A:128:HIS:CE1	1:A:131:THR:HG23	2.30	0.66
1:B:85:LEU:HD12	1:B:124:ASN:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:586:ARG:HD3	9:C:1768:HOH:O	1.94	0.66
3:D:171:LEU:HD11	3:D:388:HIS:CB	2.24	0.66
2:M:162:ILE:HB	2:M:172:ILE:HB	1.76	0.66
2:M:140:ILE:HA	2:M:332:ARG:O	1.95	0.66
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.77	0.66
3:N:416:ALA:HB2	9:N:2085:HOH:O	1.94	0.66
2:C:470:PRO:HG2	2:C:538:GLN:OE1	1.96	0.66
3:D:955:VAL:HB	3:D:1011:PHE:HE1	1.60	0.66
3:D:544:TYR:O	3:D:548:ILE:HG12	1.94	0.66
3:D:824:ASN:HB3	9:D:9067:HOH:O	1.96	0.66
5:F:363:GLU:HA	5:F:367:MET:HE2	1.75	0.66
3:N:828:LYS:HD2	9:N:9243:HOH:O	1.95	0.66
5:P:151:LEU:HD13	5:P:154:LYS:HB3	1.75	0.66
2:C:500:ASN:HB2	9:C:1931:HOH:O	1.95	0.66
2:C:773:LEU:HB2	5:F:373:LYS:CB	2.26	0.66
3:D:191:LEU:HD13	3:D:195:VAL:HG11	1.77	0.66
3:D:233:LYS:HA	9:D:9066:HOH:O	1.96	0.66
3:D:787:LEU:HD21	3:D:947:ILE:HD13	1.78	0.66
4:E:87:LYS:HZ2	4:E:91:ARG:HH21	1.42	0.66
5:F:273:ARG:HA	5:F:276:ARG:HD2	1.77	0.66
5:F:291:ILE:HG21	5:F:304:VAL:HG11	1.77	0.66
5:F:363:GLU:HA	5:F:367:MET:CE	2.26	0.66
1:L:102:LYS:HG3	1:L:139:ASN:HB2	1.78	0.66
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	1.77	0.66
2:M:326:ASP:HB2	2:M:431:HIS:ND1	2.10	0.66
2:M:492:ASP:HB3	2:M:518:LYS:HD3	1.76	0.66
2:M:724:ARG:HG3	2:M:740:GLU:HA	1.75	0.66
3:N:983:LEU:HA	9:N:9324:HOH:O	1.95	0.66
1:K:58:ILE:HD12	1:K:138:LEU:HD11	1.78	0.66
2:M:262:ALA:HB3	9:M:1344:HOH:O	1.96	0.66
3:N:928:ALA:HA	3:N:931:LEU:HD12	1.78	0.66
1:A:8:ALA:HB1	1:B:224:TYR:HE1	1.59	0.66
1:B:57:TYR:HB3	1:B:141:GLU:CG	2.26	0.66
2:M:200:LEU:HD13	2:M:300:ASP:CG	2.16	0.66
2:M:453:THR:HA	9:M:1130:HOH:O	1.94	0.66
2:M:507:ARG:HB2	2:M:507:ARG:HH11	1.60	0.66
2:M:773:LEU:O	2:M:777:ILE:HG13	1.96	0.66
1:A:30:ARG:HH11	1:A:191:ASP:HB2	1.58	0.66
1:A:219:ARG:HH22	1:B:223:THR:CG2	2.08	0.66
3:D:1144:LEU:HB3	3:D:1166:LEU:HD11	1.76	0.66
3:D:1495:ILE:HG12	4:E:80:VAL:HG11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:80:PRO:HA	5:F:83:GLN:HB2	1.78	0.66
1:K:89:PHE:HD1	1:K:120:VAL:HG23	1.60	0.66
1:L:20:TYR:OH	1:L:198:ARG:HD2	1.96	0.66
1:K:218:LEU:HD23	1:L:222:LEU:HD21	1.77	0.66
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.76	0.66
5:P:350:LEU:HD23	5:P:351:SER:N	2.11	0.66
1:A:63:HIS:HB3	2:C:746:GLY:HA2	1.78	0.66
2:C:1090:LYS:HZ2	3:D:90:MET:CG	2.09	0.66
3:D:996:TRP:CE3	3:D:999:THR:HG21	2.31	0.66
3:D:996:TRP:HE3	3:D:999:THR:HG21	1.59	0.66
3:D:572:ARG:HH21	5:F:83:GLN:NE2	1.94	0.66
1:L:178:ALA:HA	9:L:6698:HOH:O	1.96	0.66
2:M:34:VAL:HB	2:M:38:LYS:HG3	1.78	0.66
2:M:437:ARG:HB3	2:M:467:ILE:HB	1.77	0.66
5:P:358:LEU:HD21	5:P:370:LYS:HE3	1.78	0.66
2:C:12:VAL:HG12	2:C:13:ILE:HG23	1.77	0.66
2:C:276:LYS:HB3	9:C:1659:HOH:O	1.96	0.66
2:C:264:PRO:HB3	2:C:289:THR:HG21	1.76	0.66
2:C:676:ILE:HG21	2:C:988:VAL:HG22	1.78	0.66
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.31	0.66
3:D:1124:GLN:NE2	3:D:1135:ARG:HG2	2.07	0.66
3:N:1147:ARG:HB3	3:N:1188:VAL:CG2	2.25	0.66
5:P:207:LEU:HB3	5:P:212:LEU:HG	1.78	0.66
3:D:175:VAL:HG12	3:D:176:ASP:OD1	1.96	0.66
3:D:177:ALA:HB1	3:D:199:LEU:HD22	1.78	0.66
3:D:421:LEU:HD12	3:D:435:VAL:HG11	1.78	0.66
2:M:150:PRO:HG3	2:M:158:TYR:HD2	1.60	0.66
3:N:422:ALA:H	3:N:427:VAL:HG11	1.59	0.66
4:O:30:LEU:O	4:O:35:PHE:HA	1.94	0.66
1:A:143:ARG:HG3	1:A:144:VAL:N	2.10	0.65
1:A:46:SER:HB3	2:C:856:GLU:HG3	1.78	0.65
3:D:100:ALA:HA	9:D:2414:HOH:O	1.96	0.65
5:F:213:ILE:HG22	5:F:217:ASN:HD21	1.60	0.65
1:L:99:LEU:HA	9:L:4894:HOH:O	1.95	0.65
2:M:139:GLN:HE21	2:M:334:ARG:HH11	1.43	0.65
3:N:119:SER:H	3:N:123:LEU:HB2	1.61	0.65
3:N:1468:LEU:HD22	3:N:1470:ARG:HB2	1.77	0.65
4:O:34:GLY:HA3	9:O:5632:HOH:O	1.96	0.65
2:C:291:ALA:O	2:C:299:LYS:HE2	1.96	0.65
2:C:588:VAL:HB	9:C:1450:HOH:O	1.96	0.65
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1072:ILE:HA	3:D:1075:HIS:HD2	1.61	0.65
3:D:1209:LEU:HD22	3:D:1211:MET:HB3	1.77	0.65
3:D:980:MET:HE1	9:D:9118:HOH:O	1.96	0.65
1:K:161:ARG:NH1	1:K:161:ARG:HB2	2.10	0.65
1:K:58:ILE:HB	1:K:61:VAL:HB	1.78	0.65
1:L:84:GLU:HB2	9:N:9385:HOH:O	1.94	0.65
5:P:144:ILE:HB	5:P:145:PRO:HD3	1.78	0.65
1:A:156:HIS:HD2	1:A:157:GLY:H	1.43	0.65
1:B:27:PRO:O	1:B:28:LEU:HD23	1.97	0.65
2:C:384:GLU:HG3	2:C:388:ARG:HE	1.62	0.65
2:C:571:LEU:HD21	2:C:700:TYR:HD2	1.61	0.65
2:C:605:LYS:HD3	2:C:612:VAL:HB	1.78	0.65
2:C:769:PRO:HA	9:F:832:HOH:O	1.94	0.65
2:C:836:GLY:HA2	3:D:725:SER:OG	1.96	0.65
3:D:1214:PRO:HB2	9:D:9171:HOH:O	1.96	0.65
3:D:33:ASN:HB2	3:D:40:GLU:OE1	1.96	0.65
2:M:1007:ALA:HB2	3:N:648:MET:HG3	1.77	0.65
3:N:1403:LEU:HD23	3:N:1407:LEU:HD22	1.78	0.65
1:A:226:SER:O	1:A:228:PRO:HD3	1.95	0.65
1:B:59:GLU:HG2	1:B:139:ASN:O	1.96	0.65
2:C:516:ARG:HD3	2:C:521:PRO:HA	1.79	0.65
2:C:945:ARG:HB2	2:C:945:ARG:CZ	2.26	0.65
3:D:1314:LYS:NZ	3:D:1317:ASP:H	1.94	0.65
5:F:196:VAL:HG22	5:F:213:ILE:HD13	1.79	0.65
1:K:161:ARG:HH11	1:K:161:ARG:HB2	1.60	0.65
2:M:1098:ASP:HB3	9:N:9038:HOH:O	1.95	0.65
2:M:218:VAL:HA	2:M:221:LEU:HD23	1.77	0.65
2:M:714:ASP:HB2	9:M:1453:HOH:O	1.97	0.65
2:M:694:LEU:HD11	2:M:868:ASP:HB3	1.78	0.65
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.79	0.65
3:N:474:GLU:O	3:N:478:LEU:HG	1.97	0.65
3:N:699:VAL:H	3:N:756:GLN:HE22	1.42	0.65
3:N:73:CYS:HB2	9:N:9191:HOH:O	1.96	0.65
5:P:371:LEU:HD22	5:P:375:LEU:HD22	1.79	0.65
2:C:717:LEU:HB3	9:C:2169:HOH:O	1.97	0.65
2:C:99:GLN:HG2	9:C:1321:HOH:O	1.95	0.65
3:D:1055:VAL:HG13	9:D:9713:HOH:O	1.96	0.65
2:M:431:HIS:CD2	2:M:433:THR:H	2.13	0.65
1:A:11:PHE:CD1	1:B:225:PHE:HA	2.32	0.65
1:A:8:ALA:HB1	1:B:224:TYR:CE1	2.31	0.65
1:B:123:MET:C	1:B:125:PRO:HD3	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:961:GLU:HG3	9:C:1815:HOH:O	1.97	0.65
3:D:36:THR:HB	3:D:38:LYS:HG3	1.78	0.65
3:D:537:THR:C	5:F:317:LEU:HB2	2.17	0.65
3:D:699:VAL:HG22	3:D:756:GLN:NE2	2.12	0.65
2:M:444:PRO:HA	9:M:2038:HOH:O	1.95	0.65
2:M:464:LEU:HG	9:M:1433:HOH:O	1.96	0.65
2:M:728:HIS:HB3	2:M:729:LEU:HD12	1.77	0.65
3:N:1117:TYR:HD2	9:N:9343:HOH:O	1.79	0.65
3:N:475:LYS:HA	3:N:478:LEU:HD12	1.78	0.65
3:N:52:PRO:CG	3:N:78:VAL:HG13	2.26	0.65
1:A:57:TYR:CE2	1:A:161:ARG:HD2	2.31	0.65
2:C:197:LEU:HB3	2:C:202:TYR:HB2	1.79	0.65
3:D:171:LEU:HB2	3:D:390:PRO:HA	1.77	0.65
3:D:546:ARG:O	3:D:550:ARG:HG2	1.96	0.65
3:D:579:ASP:HB2	9:D:9169:HOH:O	1.96	0.65
3:D:598:ARG:HH22	5:F:318:GLU:C	2.00	0.65
1:L:7:LYS:HD2	9:L:3648:HOH:O	1.95	0.65
2:M:290:LEU:HB3	2:M:302:VAL:CG1	2.27	0.65
2:M:428:ARG:NH1	6:N:8002:STD:C29	2.60	0.65
2:M:626:ARG:NH1	2:M:637:LEU:HD12	2.11	0.65
2:M:739:GLU:HB3	9:M:1183:HOH:O	1.96	0.65
3:N:125:GLN:HE22	3:N:587:ARG:HE	1.44	0.65
3:N:1465:ASN:HD21	3:N:1470:ARG:HD3	1.62	0.65
4:O:78:ASN:HB3	9:O:3505:HOH:O	1.96	0.65
2:C:405:ARG:CZ	2:C:566:THR:HG21	2.26	0.65
3:D:704:ARG:NE	3:D:705:ALA:H	1.94	0.65
1:L:192:LEU:HD12	9:L:5714:HOH:O	1.97	0.65
3:N:963:TYR:CD2	3:N:1002:LYS:HB3	2.32	0.65
3:N:1063:GLU:HG3	3:N:1064:GLY:H	1.62	0.65
3:N:455:ARG:HH12	3:N:463:GLN:HG3	1.62	0.65
1:A:71:VAL:HG13	9:A:328:HOH:O	1.96	0.65
1:B:129:ILE:HG12	9:B:474:HOH:O	1.95	0.65
2:C:274:ARG:HD2	2:C:285:LEU:HD22	1.79	0.65
2:C:93:PRO:HG3	2:C:117:HIS:HE1	1.62	0.65
3:D:1384:PRO:HG2	9:D:9535:HOH:O	1.97	0.65
3:D:211:VAL:HG13	3:D:393:ILE:HA	1.78	0.65
3:D:422:ALA:HB3	3:D:427:VAL:CG2	2.24	0.65
9:C:1690:HOH:O	3:D:5:VAL:HA	1.94	0.65
4:E:6:ILE:HA	4:E:9:LEU:HD12	1.79	0.65
5:F:321:ILE:HB	5:F:327:SER:OG	1.95	0.65
5:F:317:LEU:O	5:F:329:TYR:HB3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:67:THR:N	2:M:627:ARG:HH21	1.94	0.65
2:M:289:THR:HB	9:M:1731:HOH:O	1.97	0.65
2:M:584:GLU:H	2:M:584:GLU:CD	1.99	0.65
3:N:153:LEU:HD11	3:N:158:TYR:N	2.12	0.65
3:N:800:LYS:HE2	3:N:804:LEU:HD22	1.79	0.65
5:P:403:LYS:NZ	5:P:403:LYS:HA	2.11	0.65
1:B:3:ASP:HA	9:B:538:HOH:O	1.97	0.65
2:C:1085:PHE:CD2	3:D:1468:LEU:HA	2.31	0.65
2:C:1090:LYS:HE2	2:C:1112:PHE:CE1	2.31	0.65
2:C:701:THR:HG23	2:C:832:LYS:HG3	1.79	0.65
2:C:945:ARG:HB2	2:C:945:ARG:NH1	2.12	0.65
3:D:531:ASP:H	3:D:534:ARG:HB2	1.62	0.65
2:C:423:ALA:HB2	6:D:8001:STD:H10	1.77	0.65
3:N:1267:ARG:HH21	3:N:1271:LYS:HD2	1.62	0.65
3:N:136:ASP:CB	3:N:137:PRO:HD3	2.27	0.65
3:N:1105:ILE:HD11	3:N:1374:GLN:NE2	2.12	0.65
3:N:592:THR:HA	9:N:9335:HOH:O	1.95	0.65
2:C:1097:LEU:HD22	2:C:1097:LEU:H	1.62	0.64
2:C:198:ARG:NH2	2:C:204:GLN:H	1.96	0.64
2:C:671:ASN:ND2	2:C:671:ASN:N	2.45	0.64
2:C:926:PHE:O	2:C:930:LYS:HG3	1.95	0.64
3:D:153:LEU:HD12	3:D:154:THR:N	2.12	0.64
3:D:97:THR:HG21	3:D:571:LYS:HD3	1.78	0.64
2:M:192:PRO:HB3	9:M:1875:HOH:O	1.96	0.64
2:M:227:PHE:HA	2:M:230:ARG:NE	2.11	0.64
3:N:950:GLY:H	3:N:953:ASP:HB2	1.62	0.64
1:A:76:VAL:HB	9:A:404:HOH:O	1.97	0.64
2:C:301:GLU:HG2	9:C:1862:HOH:O	1.96	0.64
2:C:627:ARG:HG2	9:C:1542:HOH:O	1.96	0.64
3:D:1106:VAL:HG13	9:D:9516:HOH:O	1.96	0.64
3:D:1393:GLN:HB2	3:D:1398:TRP:CZ2	2.32	0.64
3:D:1468:LEU:HD13	3:D:1470:ARG:HD3	1.79	0.64
3:D:394:LEU:HD13	9:D:9961:HOH:O	1.98	0.64
3:D:487:ALA:HB3	9:D:9146:HOH:O	1.97	0.64
4:E:25:LYS:HA	4:E:28:GLN:HE21	1.63	0.64
2:M:139:GLN:O	2:M:333:ILE:HA	1.98	0.64
2:M:328:LEU:HD21	2:M:434:HIS:HA	1.80	0.64
3:N:1146:GLY:HA3	3:N:1207:TYR:HB2	1.80	0.64
3:N:15:PRO:HA	3:N:18:ILE:HG12	1.78	0.64
3:N:860:LEU:HB2	3:N:861:GLN:NE2	2.12	0.64
3:N:984:THR:HG22	3:N:987:GLU:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:664:GLY:HA2	9:C:1145:HOH:O	1.97	0.64
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.78	0.64
1:K:78:ILE:HA	1:K:81:ASN:ND2	2.12	0.64
1:L:132:LEU:HB2	9:L:5877:HOH:O	1.97	0.64
2:M:549:PHE:CD2	2:M:886:LEU:HB3	2.33	0.64
3:N:33:ASN:HB2	3:N:40:GLU:OE1	1.98	0.64
2:C:605:LYS:HE2	2:C:610:ARG:NH1	2.12	0.64
3:D:1132:LEU:HD12	9:D:2445:HOH:O	1.98	0.64
3:D:1264:GLU:OE1	3:D:1425:THR:HB	1.97	0.64
3:D:1474:ALA:HB1	9:D:9516:HOH:O	1.97	0.64
2:C:778:PHE:CZ	5:F:409:LYS:HB2	2.32	0.64
2:M:779:GLY:HA3	9:M:1784:HOH:O	1.96	0.64
9:N:9881:HOH:O	4:O:5:GLY:HA2	1.96	0.64
5:P:416:ARG:HH11	5:P:419:ARG:HB2	1.63	0.64
5:P:85:LEU:HD23	9:P:5610:HOH:O	1.97	0.64
1:B:102:LYS:HG3	1:B:139:ASN:HB2	1.80	0.64
2:C:151:ASP:HB2	2:C:157:ARG:O	1.98	0.64
2:C:212:GLY:HA3	2:C:218:VAL:HG23	1.79	0.64
2:C:505:GLY:HA3	9:C:1255:HOH:O	1.98	0.64
3:D:379:ALA:HA	9:D:9392:HOH:O	1.98	0.64
5:F:395:GLU:O	5:F:399:GLN:HB2	1.97	0.64
1:K:20:TYR:HD2	1:K:21:GLY:H	1.45	0.64
1:L:107:LYS:HB2	9:L:4679:HOH:O	1.96	0.64
1:L:80:LEU:HB3	3:N:867:ARG:NH2	2.12	0.64
2:M:92:ALA:HB1	9:M:2075:HOH:O	1.96	0.64
3:N:367:ILE:HA	9:N:9641:HOH:O	1.98	0.64
3:N:705:ALA:HB3	3:N:706:PRO:HD3	1.80	0.64
2:C:810:ASP:HB3	2:C:813:VAL:HG22	1.80	0.64
3:D:1264:GLU:HG2	3:D:1266:ARG:NH2	2.13	0.64
3:D:721:VAL:HA	9:D:2048:HOH:O	1.96	0.64
3:D:838:ARG:HH11	3:D:874:GLU:HB3	1.61	0.64
5:F:87:GLU:O	5:F:91:VAL:HG23	1.98	0.64
1:L:185:ARG:HG3	1:L:190:THR:HG22	1.78	0.64
2:M:148:PHE:HZ	2:M:281:LEU:HD13	1.62	0.64
2:M:139:GLN:NE2	2:M:418:LEU:HD22	2.12	0.64
2:M:610:ARG:HB2	9:M:1533:HOH:O	1.97	0.64
2:M:650:ARG:HB2	9:M:1692:HOH:O	1.96	0.64
3:N:2:LYS:HB2	9:N:9354:HOH:O	1.98	0.64
5:P:128:ARG:HD2	9:P:4586:HOH:O	1.96	0.64
2:C:150:PRO:CA	2:C:158:TYR:HB3	2.22	0.64
2:C:517:ARG:NH1	2:C:522:VAL:HG11	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:810:GLU:O	3:D:813:LEU:HG	1.98	0.64
2:M:30:LEU:HB3	2:M:44:ILE:HD12	1.77	0.64
3:N:12:LEU:HD22	3:N:511:TRP:HB2	1.80	0.64
3:N:630:VAL:HA	3:N:744:GLN:HG2	1.79	0.64
2:C:267:TYR:HB2	9:C:1724:HOH:O	1.98	0.64
3:D:161:LEU:HD13	3:D:452:ILE:HD12	1.78	0.64
5:F:214:GLN:HA	5:F:217:ASN:HD22	1.62	0.64
2:M:1110:ASP:HA	9:M:1272:HOH:O	1.97	0.64
3:N:1031:ASN:HB3	3:N:1034:GLN:CD	2.17	0.64
3:N:1109:GLU:HA	9:N:9975:HOH:O	1.97	0.64
3:N:119:SER:CB	3:N:123:LEU:HB2	2.28	0.64
3:N:52:PRO:CB	3:N:80:VAL:HG13	2.27	0.64
1:A:54:THR:HG21	9:A:409:HOH:O	1.98	0.64
2:C:286:SER:HB3	2:C:299:LYS:HE3	1.79	0.64
2:C:30:LEU:HB3	2:C:44:ILE:HD12	1.80	0.64
2:C:348:LEU:HD21	9:C:1976:HOH:O	1.97	0.64
2:C:433:THR:HG21	2:C:488:ALA:HB1	1.80	0.64
2:C:958:THR:HG23	2:C:961:GLU:HB2	1.80	0.64
1:L:58:ILE:HB	1:L:61:VAL:HB	1.80	0.64
2:M:197:LEU:HD12	2:M:207:LEU:HD11	1.79	0.64
2:M:285:LEU:O	2:M:285:LEU:HD23	1.98	0.64
2:M:31:GLN:HB3	2:M:71:TYR:OH	1.97	0.64
1:A:18:ARG:O	1:A:207:PRO:HD3	1.97	0.64
2:C:1067:TYR:CG	5:F:341:PRO:HB3	2.33	0.64
3:D:478:LEU:HD22	3:D:1388:ARG:NH2	2.14	0.64
5:F:398:ARG:HB2	9:F:818:HOH:O	1.97	0.64
1:K:26:GLU:HB3	1:K:194:LYS:HG3	1.80	0.64
2:M:674:VAL:HG21	2:M:871:LEU:HD12	1.80	0.64
3:N:1267:ARG:HH11	3:N:1267:ARG:HB2	1.63	0.64
3:N:179:VAL:HG22	3:N:389:GLU:HG3	1.80	0.64
3:N:197:SER:HB2	3:N:205:TYR:CZ	2.33	0.64
2:C:437:ARG:HG2	2:C:467:ILE:HG22	1.80	0.63
3:D:1406:ARG:HA	9:D:9761:HOH:O	1.98	0.63
3:D:448:GLU:HB3	9:D:9158:HOH:O	1.98	0.63
3:D:60:CYS:HA	9:D:2260:HOH:O	1.97	0.63
5:F:278:LEU:O	5:F:282:LEU:HG	1.98	0.63
3:N:1415:VAL:HG23	9:N:9100:HOH:O	1.97	0.63
3:N:1493:LYS:HB3	9:N:9467:HOH:O	1.96	0.63
1:L:175:ARG:O	3:N:851:LEU:HD21	1.98	0.63
3:D:369:ALA:HB2	9:D:9232:HOH:O	1.99	0.63
3:N:1166:LEU:HD23	3:N:1166:LEU:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:584:ASN:HD21	3:N:590:PRO:HB2	1.63	0.63
3:N:726:ILE:HD11	9:N:9650:HOH:O	1.97	0.63
5:P:87:GLU:O	5:P:91:VAL:HG23	1.97	0.63
1:B:56:VAL:HG13	1:B:142:VAL:HG12	1.80	0.63
2:C:14:PRO:HD2	9:C:1805:HOH:O	1.98	0.63
3:D:956:ILE:HG12	3:D:1039:CYS:O	1.98	0.63
3:D:1258:ARG:CZ	3:D:1262:LEU:HD11	2.27	0.63
3:D:1272:ALA:CA	3:D:1326:THR:HB	2.28	0.63
3:D:1399:ASP:HA	9:D:2120:HOH:O	1.98	0.63
5:F:314:PRO:HB3	9:F:515:HOH:O	1.98	0.63
2:M:953:VAL:HG13	2:M:966:LEU:HD13	1.81	0.63
3:N:996:TRP:CE2	3:N:1056:PRO:HG2	2.33	0.63
5:P:366:ALA:HB3	5:P:367:MET:HE2	1.81	0.63
1:A:83:LYS:HE2	1:A:167:VAL:HG12	1.80	0.63
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.78	0.63
1:K:151:VAL:HG23	9:K:3798:HOH:O	1.97	0.63
1:K:78:ILE:O	1:K:82:LEU:HG	1.97	0.63
2:M:1068:GLU:OE1	5:P:345:ALA:HA	1.98	0.63
2:M:151:ASP:HB2	2:M:157:ARG:O	1.98	0.63
2:M:428:ARG:HD3	2:M:449:ILE:HG22	1.79	0.63
2:M:528:GLU:HB3	9:M:1417:HOH:O	1.97	0.63
2:M:89:THR:O	2:M:91:GLN:HG3	1.99	0.63
3:N:449:SER:HB2	9:N:9454:HOH:O	1.98	0.63
3:N:502:PHE:HZ	3:N:512:MET:HE2	1.63	0.63
3:N:462:GLN:HA	3:N:513:ILE:HD13	1.80	0.63
2:C:612:VAL:HG22	2:C:622:GLU:HA	1.81	0.63
3:D:116:LEU:HB3	3:D:118:LEU:HD21	1.79	0.63
3:D:1491:THR:O	3:D:1495:ILE:HD13	1.99	0.63
3:D:528:VAL:O	3:D:535:PHE:HA	1.99	0.63
3:D:529:GLN:OE1	3:D:533:GLY:HA2	1.99	0.63
5:F:227:PHE:HA	9:F:638:HOH:O	1.98	0.63
5:F:93:LEU:HG	5:F:190:ALA:CB	2.28	0.63
1:K:120:VAL:HG13	9:K:7313:HOH:O	1.98	0.63
3:N:119:SER:OG	3:N:123:LEU:HD12	1.98	0.63
3:N:1458:GLU:HG2	9:N:9361:HOH:O	1.98	0.63
3:N:198:ARG:HA	9:N:9071:HOH:O	1.97	0.63
4:O:95:GLY:HA3	9:O:5632:HOH:O	1.99	0.63
2:C:276:LYS:O	2:C:280:LYS:HB2	1.99	0.63
2:C:565:GLN:HG2	2:C:995:MET:HE1	1.81	0.63
2:C:862:PRO:HG3	2:C:975:TYR:HE1	1.62	0.63
3:D:1130:ARG:NH1	3:D:1130:ARG:HB2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1139:ASP:HB2	9:D:2265:HOH:O	1.98	0.63
3:D:15:PRO:HA	3:D:18:ILE:HG12	1.80	0.63
4:E:72:ARG:HD3	9:E:186:HOH:O	1.98	0.63
2:M:607:ASP:HB2	2:M:610:ARG:HG3	1.79	0.63
3:N:1267:ARG:HH12	3:N:1331:ASP:HB2	1.63	0.63
3:N:807:ALA:HB2	3:N:833:GLU:OE1	1.98	0.63
3:N:877:PRO:O	3:N:880:ILE:HG22	1.98	0.63
9:N:9114:HOH:O	5:P:140:ARG:HB3	1.96	0.63
5:P:358:LEU:HD11	5:P:370:LYS:NZ	2.14	0.63
1:A:11:PHE:HD1	1:A:25:LEU:HD13	1.63	0.63
2:C:162:ILE:O	2:C:164:PRO:HD3	1.99	0.63
3:D:633:VAL:HB	3:D:740:PHE:CE1	2.34	0.63
1:L:216:GLU:HB2	9:L:4700:HOH:O	1.99	0.63
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.80	0.63
2:M:378:LEU:HG	2:M:382:ILE:HD11	1.80	0.63
5:P:102:LEU:O	5:P:106:VAL:HG23	1.99	0.63
1:A:123:MET:O	1:A:125:PRO:HD3	1.99	0.63
2:C:110:GLU:OE2	2:C:369:PRO:HG3	1.98	0.63
2:C:627:ARG:HG3	2:C:628:PHE:H	1.64	0.63
3:D:478:LEU:HD22	3:D:1388:ARG:CZ	2.29	0.63
5:F:147:LEU:HG	9:F:845:HOH:O	1.99	0.63
2:M:1105:LYS:HG2	9:M:1472:HOH:O	1.97	0.63
2:M:532:MET:HG3	2:M:533:ASP:N	2.13	0.63
2:M:710:ILE:HD11	2:M:758:ARG:HE	1.63	0.63
3:N:1305:LEU:HD21	3:N:1326:THR:OG1	1.98	0.63
2:C:1066:ALA:O	2:C:1070:ILE:HG13	1.99	0.63
2:C:588:VAL:HG21	2:C:664:GLY:O	1.99	0.63
2:C:580:MET:O	2:C:902:ILE:HA	1.99	0.63
3:D:462:GLN:HA	3:D:513:ILE:HD13	1.81	0.63
2:M:1111:ILE:HG13	2:M:1112:PHE:H	1.63	0.63
3:N:536:ALA:HA	5:P:315:VAL:O	1.99	0.63
4:O:70:THR:HG21	4:O:72:ARG:NH2	2.13	0.63
5:P:131:VAL:O	5:P:135:ILE:HG22	1.99	0.63
5:P:163:LEU:HB3	5:P:174:LEU:CG	2.29	0.63
2:C:937:ASP:O	2:C:941:VAL:HG23	1.99	0.62
2:M:41:ASN:O	2:M:46:ALA:HB2	1.99	0.62
3:N:1122:LEU:O	3:N:1134:LEU:HD23	1.98	0.62
3:N:185:VAL:CG1	3:N:191:LEU:HD21	2.29	0.62
3:N:395:VAL:HG12	9:N:2032:HOH:O	1.99	0.62
4:O:48:MET:N	4:O:54:LEU:HB2	2.14	0.62
4:O:51:LEU:HG	4:O:53:GLY:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:694:LEU:HD11	2:C:868:ASP:HB3	1.81	0.62
2:M:64:LEU:HD22	2:M:359:MET:HG3	1.81	0.62
3:N:181:ASP:OD2	3:N:199:LEU:HB2	1.99	0.62
3:N:383:GLY:HA2	9:N:2057:HOH:O	1.98	0.62
3:N:127:LEU:HD21	3:N:461:ILE:HD11	1.81	0.62
2:C:3:ILE:HG23	9:C:1258:HOH:O	1.99	0.62
2:C:587:VAL:HA	9:C:1272:HOH:O	1.98	0.62
2:C:676:ILE:HG23	2:C:676:ILE:O	2.00	0.62
3:D:459:GLU:HB3	9:D:9210:HOH:O	1.98	0.62
3:D:637:LEU:HD12	3:D:641:GLN:OE1	1.99	0.62
1:K:36:LEU:O	1:K:39:PRO:HD2	2.00	0.62
2:M:332:ARG:HH21	2:M:464:LEU:HD11	1.64	0.62
2:M:889:HIS:HE1	3:N:951:ILE:HB	1.64	0.62
2:M:578:VAL:HG11	2:M:991:GLN:HB3	1.80	0.62
3:N:1314:LYS:HD3	3:N:1314:LYS:H	1.65	0.62
3:N:1390:LEU:HB3	9:N:2333:HOH:O	1.98	0.62
3:N:52:PRO:HB2	9:N:9016:HOH:O	1.98	0.62
4:O:54:LEU:HG	4:O:58:PRO:CG	2.29	0.62
3:D:1209:LEU:HD13	3:D:1211:MET:HE1	1.81	0.62
2:M:254:VAL:HG21	9:M:1618:HOH:O	1.99	0.62
2:M:447:ALA:HB1	9:M:1423:HOH:O	1.97	0.62
2:M:49:ARG:NH1	2:M:49:ARG:HB2	2.09	0.62
2:M:546:LEU:O	2:M:546:LEU:HD23	1.99	0.62
3:N:131:LYS:CG	3:N:572:ARG:HH21	2.12	0.62
3:N:1399:ASP:O	3:N:1403:LEU:HB2	1.99	0.62
2:C:120:LEU:HD11	9:C:2187:HOH:O	1.98	0.62
2:C:172:ILE:HG23	9:C:1676:HOH:O	1.99	0.62
2:C:141:HIS:HB3	2:C:418:LEU:HG	1.81	0.62
2:C:62:GLY:O	2:C:103:LYS:HG3	1.99	0.62
3:D:9:ARG:HA	3:D:1434:TRP:CH2	2.34	0.62
3:D:441:ARG:O	3:D:443:VAL:HG23	1.99	0.62
3:D:477:LEU:HD23	9:D:9334:HOH:O	1.99	0.62
3:D:565:ILE:HD11	5:F:189:GLU:OE1	2.00	0.62
2:M:603:VAL:HG21	2:M:643:VAL:CG1	2.30	0.62
3:N:422:ALA:HB3	3:N:427:VAL:CG2	2.26	0.62
3:N:587:ARG:HD2	9:N:9886:HOH:O	2.00	0.62
5:P:415:THR:O	5:P:417:LYS:HG3	1.99	0.62
1:B:100:LEU:HD12	1:B:115:LEU:HD21	1.80	0.62
1:B:153:ALA:HB3	9:B:402:HOH:O	1.99	0.62
2:C:557:ARG:CZ	2:C:879:ARG:HD3	2.30	0.62
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.80	0.62
3:D:1423:GLY:HA2	9:D:9071:HOH:O	1.97	0.62
3:D:553:ARG:HH12	5:F:211:ASP:HA	1.63	0.62
5:F:366:ALA:HB1	9:F:616:HOH:O	1.98	0.62
1:L:86:VAL:HG12	1:L:124:ASN:ND2	2.14	0.62
2:M:683:ASN:HA	2:M:687:ALA:HB3	1.81	0.62
2:M:571:LEU:HG	2:M:700:TYR:HA	1.82	0.62
3:N:1500:LYS:HA	9:N:9743:HOH:O	2.00	0.62
5:P:244:ARG:HH11	5:P:244:ARG:HG3	1.64	0.62
1:A:161:ARG:HB2	1:A:161:ARG:NH1	2.14	0.62
2:C:810:ASP:HB3	9:C:1294:HOH:O	2.00	0.62
3:D:699:VAL:HG22	3:D:756:GLN:HE22	1.65	0.62
5:F:408:LEU:O	5:F:412:GLU:HG2	2.00	0.62
2:M:64:LEU:HA	9:M:2181:HOH:O	2.00	0.62
2:M:910:LYS:HB3	2:M:912:PRO:HD2	1.82	0.62
3:N:192:ALA:HB3	9:N:9113:HOH:O	2.00	0.62
3:N:404:GLU:HB3	3:N:414:ARG:HD2	1.82	0.62
3:N:538:SER:HB2	9:N:9315:HOH:O	1.99	0.62
4:O:17:TYR:HD2	4:O:17:TYR:N	1.97	0.62
2:C:199:VAL:HG22	2:C:235:LEU:HG	1.81	0.62
2:C:265:ARG:HB3	2:C:267:TYR:CD2	2.34	0.62
2:C:427:VAL:HG23	9:C:1138:HOH:O	1.98	0.62
2:C:432:ARG:HH11	3:D:1048:PRO:HD3	1.63	0.62
1:B:38:ASN:OD1	2:C:979:THR:HA	1.99	0.62
3:D:1290:LEU:HD22	3:D:1291:SER:H	1.64	0.62
5:F:117:SER:OG	5:F:124:PRO:HG3	2.00	0.62
1:L:70:GLY:HA2	9:L:5271:HOH:O	2.00	0.62
2:M:196:LEU:O	2:M:200:LEU:HG	1.99	0.62
2:M:265:ARG:HG2	2:M:266:ARG:H	1.64	0.62
2:M:343:GLN:HG2	2:M:385:PHE:HB2	1.80	0.62
2:M:44:ILE:HG22	9:M:1699:HOH:O	1.99	0.62
2:C:510:ALA:HB3	9:C:2128:HOH:O	1.99	0.62
2:C:606:VAL:HG11	2:C:643:VAL:O	1.99	0.62
3:D:131:LYS:HA	3:D:456:MET:HG3	1.81	0.62
3:D:503:LEU:HB3	9:D:9451:HOH:O	2.00	0.62
3:D:517:VAL:HG23	9:D:9427:HOH:O	1.98	0.62
1:L:19:GLU:HG3	1:L:201:THR:O	2.00	0.62
1:L:208:LEU:HD23	9:L:4122:HOH:O	2.00	0.62
2:M:166:PRO:HD3	2:M:265:ARG:HB2	1.82	0.62
2:M:916:GLU:HA	9:M:1386:HOH:O	1.99	0.62
3:N:1231:GLU:HB3	3:N:1232:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:558:LEU:HB2	9:N:9146:HOH:O	2.00	0.62
2:M:1090:LYS:HE3	3:N:90:MET:CG	2.30	0.62
2:C:42:VAL:HG12	2:C:43:GLY:H	1.65	0.62
2:C:954:THR:OG1	2:C:957:LYS:HG3	2.00	0.62
3:D:963:TYR:CD2	3:D:1002:LYS:HB3	2.35	0.62
1:L:123:MET:C	1:L:125:PRO:HD3	2.19	0.62
2:M:182:VAL:HG12	2:M:193:LEU:HD13	1.82	0.62
2:M:286:SER:HB3	2:M:299:LYS:HE3	1.82	0.62
2:M:350:ARG:HD2	9:M:2100:HOH:O	2.00	0.62
2:M:62:GLY:O	2:M:103:LYS:HG3	1.99	0.62
2:M:723:THR:HG21	9:M:1504:HOH:O	2.00	0.62
2:M:874:LEU:CD1	3:N:783:ARG:HB2	2.30	0.62
2:M:976:ASP:CB	2:M:979:THR:HG22	2.30	0.62
3:N:1063:GLU:HG3	3:N:1064:GLY:N	2.15	0.62
3:N:1459:LEU:HD22	3:N:1465:ASN:HA	1.81	0.62
5:P:321:ILE:HD11	5:P:329:TYR:HB2	1.81	0.62
1:A:117:VAL:HB	1:A:120:VAL:HG12	1.82	0.61
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.80	0.61
2:C:707:ARG:HG3	2:C:826:TYR:CE1	2.35	0.61
3:D:1123:PHE:HE2	3:D:1184:GLN:HA	1.64	0.61
3:D:179:VAL:HG22	3:D:389:GLU:HG3	1.81	0.61
3:D:48:ARG:HB2	9:D:9499:HOH:O	2.00	0.61
3:D:550:ARG:HD3	3:D:553:ARG:NH2	2.15	0.61
3:D:675:ARG:O	3:D:678:GLU:HG2	2.00	0.61
3:D:955:VAL:HG11	3:D:1015:TYR:HE2	1.65	0.61
5:F:412:GLU:HG3	5:F:418:LEU:HD22	1.82	0.61
2:M:998:TYR:HE2	2:M:1000:MET:HG2	1.65	0.61
2:M:578:VAL:HG13	2:M:671:ASN:CG	2.21	0.61
2:M:966:LEU:HD11	2:M:986:PRO:HG2	1.82	0.61
3:N:52:PRO:HG2	3:N:80:VAL:HG22	1.81	0.61
4:O:60:ALA:O	4:O:63:TRP:HB2	2.00	0.61
1:A:20:TYR:CE2	1:A:22:GLU:HG3	2.35	0.61
1:A:25:LEU:HG	9:A:350:HOH:O	2.00	0.61
1:B:97:VAL:HG11	1:B:120:VAL:HG21	1.81	0.61
2:C:254:VAL:HG22	2:C:258:TYR:HE1	1.64	0.61
3:D:422:ALA:H	3:D:427:VAL:HG11	1.65	0.61
2:M:274:ARG:HB2	2:M:285:LEU:HD13	1.81	0.61
2:C:515:ALA:HB3	9:C:1200:HOH:O	2.00	0.61
3:D:1102:THR:HG22	3:D:1222:GLY:HA2	1.82	0.61
5:F:108:GLU:HG3	5:F:176:ILE:CG2	2.30	0.61
1:L:109:VAL:HG23	9:L:5877:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:358:ARG:HH22	2:M:374:ASN:CB	2.13	0.61
2:M:534:VAL:HB	2:M:538:GLN:NE2	2.14	0.61
2:C:431:HIS:H	2:C:434:HIS:CE1	2.18	0.61
2:C:578:VAL:HA	2:C:900:ARG:HD2	1.81	0.61
3:D:136:ASP:CB	3:D:137:PRO:HD3	2.30	0.61
3:D:928:ALA:HB2	9:D:9129:HOH:O	1.99	0.61
1:K:106:PRO:HD3	9:K:4436:HOH:O	1.99	0.61
2:M:245:GLY:HA3	9:M:1762:HOH:O	2.00	0.61
2:M:290:LEU:HB3	2:M:302:VAL:HG11	1.80	0.61
2:M:367:LEU:HD23	2:M:371:LYS:HZ2	1.65	0.61
2:M:777:ILE:HG22	9:M:2105:HOH:O	1.99	0.61
2:M:905:ILE:N	2:M:905:ILE:HD12	2.13	0.61
3:N:441:ARG:O	3:N:443:VAL:HG23	2.00	0.61
3:N:572:ARG:NH1	5:P:80:PRO:HD3	2.15	0.61
4:O:17:TYR:CD2	4:O:17:TYR:N	2.68	0.61
2:C:437:ARG:NE	2:C:469:THR:HB	2.16	0.61
2:C:678:PRO:O	3:D:943:THR:HA	2.01	0.61
2:C:71:TYR:H	2:C:71:TYR:HD2	1.47	0.61
2:C:953:VAL:HB	2:C:962:GLN:HG2	1.82	0.61
2:M:642:ARG:HG3	2:M:657:ASP:OD2	2.00	0.61
3:N:536:ALA:HA	5:P:315:VAL:H	1.65	0.61
3:N:832:ARG:HA	9:N:2061:HOH:O	2.01	0.61
3:D:211:VAL:HG13	3:D:393:ILE:HG13	1.81	0.61
3:D:404:GLU:HB3	3:D:414:ARG:CD	2.31	0.61
3:D:477:LEU:HD13	3:D:492:ALA:O	2.01	0.61
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.83	0.61
2:M:150:PRO:CA	2:M:158:TYR:HB3	2.27	0.61
2:M:354:GLY:HA2	9:M:1526:HOH:O	1.98	0.61
2:M:583:LEU:O	2:M:587:VAL:HG23	2.00	0.61
1:A:20:TYR:HD2	1:A:21:GLY:H	1.48	0.61
1:B:52:ALA:HB2	1:B:170:VAL:O	2.01	0.61
2:C:1014:SER:OG	5:F:331:ASP:HA	2.01	0.61
2:C:722:ILE:HG22	2:C:820:ARG:HH12	1.65	0.61
2:C:432:ARG:HH12	3:D:1047:LYS:CG	2.14	0.61
3:D:168:THR:OG1	3:D:393:ILE:HB	2.01	0.61
3:D:584:ASN:HB2	3:D:602:SER:HB3	1.81	0.61
3:D:785:ILE:HG22	3:D:789:LEU:HD12	1.81	0.61
3:D:800:LYS:HG2	9:D:9141:HOH:O	2.00	0.61
3:D:975:GLU:O	3:D:979:GLU:HG3	2.00	0.61
5:F:171:LYS:HE3	5:F:175:HIS:NE2	2.16	0.61
1:K:226:SER:HA	9:K:5223:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:291:ALA:HB2	9:M:1720:HOH:O	2.00	0.61
3:N:28:LYS:HB3	3:N:41:ARG:HD2	1.82	0.61
3:N:831:GLY:HA3	9:N:9026:HOH:O	2.00	0.61
1:A:158:ILE:HA	9:A:339:HOH:O	1.99	0.61
2:C:716:LYS:HD3	9:C:1399:HOH:O	1.99	0.61
2:C:750:LYS:HB2	3:D:681:ARG:NH2	2.16	0.61
4:E:26:ARG:HD2	4:E:29:GLN:OE1	2.01	0.61
1:L:67:THR:HG22	1:L:74:ASP:OD1	2.00	0.61
3:N:11:ALA:HB1	3:N:507:ASN:OD1	2.00	0.61
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.36	0.61
3:D:192:ALA:O	3:D:195:VAL:HG23	2.01	0.61
3:D:466:LYS:HG2	9:D:9178:HOH:O	2.00	0.61
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.81	0.61
3:D:470:LEU:HD11	3:D:509:PRO:HG3	1.82	0.61
5:F:398:ARG:HG2	5:F:402:ASN:ND2	2.14	0.61
3:N:1264:GLU:OE2	3:N:1424:VAL:HG12	2.00	0.61
3:N:1495:ILE:HG12	4:O:80:VAL:HG11	1.83	0.61
2:M:1009:SER:OG	3:N:655:PRO:HD3	2.00	0.61
3:D:1318:TYR:HD1	3:D:1319:VAL:N	1.97	0.61
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.01	0.61
3:D:802:ALA:HB1	9:D:2302:HOH:O	2.01	0.61
3:D:860:LEU:HA	3:D:877:PRO:HB2	1.81	0.61
1:L:136:GLY:HA2	9:L:5776:HOH:O	2.00	0.61
1:K:224:TYR:HB3	1:L:9:PRO:HB2	1.83	0.61
1:B:62:LEU:HD12	1:B:62:LEU:H	1.65	0.60
2:C:1008:ARG:HE	2:C:1029:GLY:N	1.98	0.60
2:C:579:VAL:HB	2:C:890:LEU:CD2	2.31	0.60
3:D:1341:PRO:HA	3:D:1344:VAL:HG23	1.83	0.60
1:K:7:LYS:HE2	9:K:4607:HOH:O	2.00	0.60
2:M:139:GLN:HE22	2:M:415:PRO:HG2	1.66	0.60
2:M:429:ASP:HB3	3:N:1079:LYS:NZ	2.16	0.60
3:N:835:SER:HA	9:N:9026:HOH:O	2.01	0.60
1:B:73:GLU:HB3	1:B:77:GLU:HG3	1.82	0.60
2:C:535:SER:OG	2:C:538:GLN:HG2	2.01	0.60
2:C:944:LEU:HD21	2:C:963:LEU:HD22	1.84	0.60
3:D:149:LYS:HB3	9:D:9547:HOH:O	2.00	0.60
3:D:178:LEU:HG	3:D:200:ASP:H	1.66	0.60
3:D:399:ARG:HG3	9:D:9673:HOH:O	2.00	0.60
2:M:1018:GLN:NE2	2:M:1060:ILE:HD11	2.14	0.60
2:M:260:LEU:HB2	2:M:291:ALA:HB1	1.81	0.60
3:N:834:THR:HG22	3:N:838:ARG:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:90:GLN:HA	5:P:90:GLN:HE21	1.65	0.60
3:D:1335:LEU:HD23	3:D:1344:VAL:HA	1.84	0.60
3:D:134:VAL:HG12	3:D:152:LEU:HB3	1.83	0.60
3:D:148:GLU:CB	3:D:151:GLN:HB2	2.30	0.60
3:D:560:GLN:HG3	5:F:221:ILE:HG21	1.83	0.60
3:D:906:GLN:HB3	3:D:911:LEU:CD1	2.30	0.60
5:F:220:LEU:O	5:F:224:VAL:HG23	2.01	0.60
3:D:545:ARG:NH2	5:F:257:THR:HA	2.16	0.60
2:M:281:LEU:HD12	2:M:309:TYR:HB2	1.82	0.60
3:N:1393:GLN:HB2	3:N:1398:TRP:HE1	1.66	0.60
4:O:45:ARG:HD2	4:O:47:LYS:HE3	1.84	0.60
1:A:86:VAL:HG12	1:A:124:ASN:HB2	1.83	0.60
2:C:317:VAL:HG22	9:C:1726:HOH:O	2.01	0.60
2:C:54:ILE:HB	9:C:1122:HOH:O	2.01	0.60
2:C:9:ILE:HD11	9:C:1162:HOH:O	2.01	0.60
3:D:1130:ARG:HB2	3:D:1130:ARG:HH11	1.65	0.60
3:D:1287:GLU:HB2	9:D:9218:HOH:O	2.01	0.60
3:D:1336:LEU:HA	3:D:1344:VAL:HG22	1.82	0.60
3:D:510:GLU:O	3:D:513:ILE:HD12	2.00	0.60
3:D:572:ARG:HH21	5:F:83:GLN:HE21	1.49	0.60
1:K:62:LEU:H	1:K:62:LEU:HD12	1.66	0.60
2:M:503:LEU:HB3	9:M:2107:HOH:O	2.01	0.60
2:M:573:ARG:HG3	2:M:698:ASP:O	2.00	0.60
3:N:546:ARG:HG3	9:N:9308:HOH:O	2.00	0.60
3:N:60:CYS:HB3	9:N:2111:HOH:O	2.02	0.60
2:M:1035:MET:HG2	3:N:707:THR:O	2.02	0.60
5:P:392:VAL:HA	9:P:5909:HOH:O	2.00	0.60
2:C:181:VAL:HB	9:C:1469:HOH:O	2.01	0.60
2:C:683:ASN:HA	2:C:687:ALA:HB3	1.82	0.60
3:D:1044:LEU:HD21	3:D:1056:PRO:HG3	1.82	0.60
3:D:1094:LEU:O	3:D:1098:LEU:HD13	2.01	0.60
3:D:1152:GLU:HB3	9:D:9312:HOH:O	2.01	0.60
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.37	0.60
5:F:356:LYS:O	5:F:360:LYS:HG2	2.01	0.60
1:K:123:MET:O	1:K:125:PRO:HD3	2.01	0.60
1:K:175:ARG:HG2	9:K:4053:HOH:O	2.01	0.60
2:M:815:LEU:HB3	9:M:1820:HOH:O	2.01	0.60
2:M:905:ILE:H	2:M:905:ILE:CD1	2.01	0.60
3:N:1277:ILE:CD1	3:N:1301:LYS:HB2	2.31	0.60
3:N:427:VAL:CG2	3:N:435:VAL:HB	2.32	0.60
3:N:434:ARG:HB2	3:N:447:VAL:CG2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:814:ALA:HB2	9:N:9899:HOH:O	2.01	0.60
4:O:86:GLN:O	4:O:90:GLU:HG3	2.02	0.60
3:N:420:VAL:HA	5:P:164:LYS:HD3	1.83	0.60
2:C:328:LEU:HD22	2:C:433:THR:HG22	1.83	0.60
3:D:493:ARG:NH2	3:D:1388:ARG:HB3	2.16	0.60
4:E:60:ALA:O	4:E:63:TRP:HB2	2.02	0.60
2:M:127:PHE:HB3	9:M:1515:HOH:O	2.00	0.60
2:M:13:ILE:HG22	9:M:1164:HOH:O	2.01	0.60
2:M:157:ARG:CZ	2:M:157:ARG:HA	2.31	0.60
2:M:265:ARG:HB3	2:M:267:TYR:CD2	2.36	0.60
2:M:959:PRO:O	2:M:963:LEU:HD23	2.02	0.60
3:N:1156:LEU:HD21	3:N:1177:ALA:HA	1.82	0.60
3:N:188:GLY:HA3	9:N:9221:HOH:O	2.00	0.60
3:N:524:LEU:C	3:N:526:PRO:HD3	2.22	0.60
3:N:608:SER:HA	9:N:9404:HOH:O	2.02	0.60
5:P:268:ILE:HA	5:P:271:LEU:HD12	1.83	0.60
5:P:94:LEU:HD22	5:P:97:GLU:HB2	1.81	0.60
1:A:208:LEU:HD13	9:B:442:HOH:O	2.01	0.60
2:C:254:VAL:O	2:C:257:VAL:HG23	2.01	0.60
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.84	0.60
3:D:127:LEU:CD1	3:D:461:ILE:HD11	2.28	0.60
3:D:694:VAL:HG13	9:D:9037:HOH:O	2.02	0.60
1:K:156:HIS:CD2	1:K:158:ILE:HG12	2.35	0.60
2:M:56:GLU:HB3	9:M:1232:HOH:O	2.00	0.60
2:M:721:ARG:NH2	2:M:785:VAL:HG21	2.16	0.60
3:N:783:ARG:HE	3:N:1029:ARG:HD2	1.67	0.60
3:N:1379:VAL:HG12	3:N:1419:PRO:HA	1.84	0.60
3:N:1435:LEU:HD23	3:N:1464:GLU:HB2	1.82	0.60
3:N:57:GLU:HG3	3:N:64:LYS:HG2	1.83	0.60
1:B:184:THR:HG23	1:B:192:LEU:HB3	1.83	0.60
1:B:2:LEU:HD12	1:B:3:ASP:N	2.17	0.60
2:C:913:GLU:O	2:C:916:GLU:HB3	2.02	0.60
3:D:1147:ARG:O	3:D:1165:TYR:HA	2.02	0.60
3:D:1279:GLY:O	3:D:1318:TYR:HA	2.02	0.60
3:D:156:GLU:CD	3:D:156:GLU:H	2.05	0.60
2:M:423:ALA:HB2	6:N:8002:STD:H10	1.82	0.60
2:M:555:ALA:HA	3:N:1070:TYR:OH	2.00	0.60
3:N:1124:GLN:N	3:N:1133:ARG:O	2.33	0.60
3:N:1441:GLN:NE2	3:N:1442:ASN:HB2	2.16	0.60
3:N:961:LYS:HG2	9:N:9759:HOH:O	2.02	0.60
4:O:25:LYS:HA	4:O:28:GLN:NE2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:151:LEU:HD22	5:P:153:PRO:HD2	1.83	0.60
5:P:163:LEU:HB3	5:P:174:LEU:HG	1.84	0.60
1:B:228:PRO:O	1:B:229:GLN:HG3	2.02	0.60
2:C:305:PRO:HA	2:C:308:ARG:HB3	1.84	0.60
2:C:599:GLU:HG3	9:C:1839:HOH:O	2.01	0.60
2:C:901:TYR:HA	9:C:1258:HOH:O	2.02	0.60
2:C:987:ILE:HD11	3:D:946:GLY:HA2	1.84	0.60
3:D:1109:GLU:OE1	3:D:1201:CYS:HB2	2.02	0.60
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	1.83	0.60
3:D:524:LEU:C	3:D:526:PRO:HD3	2.22	0.60
3:D:572:ARG:NH1	5:F:80:PRO:HD3	2.17	0.60
2:C:1033:GLY:HA2	3:D:619:LEU:O	2.01	0.60
3:D:633:VAL:HG22	3:D:635:PRO:HD3	1.82	0.60
5:F:166:LEU:O	5:F:171:LYS:HB2	2.01	0.60
5:F:132:ARG:HD3	5:F:181:GLU:CD	2.23	0.60
5:F:352:GLU:O	5:F:356:LYS:HG3	2.02	0.60
5:F:420:ASP:O	5:F:422:LEU:HD23	2.02	0.60
1:K:158:ILE:HD11	9:K:4923:HOH:O	2.02	0.60
1:L:136:GLY:HA3	9:L:4988:HOH:O	2.00	0.60
2:M:1054:THR:HG22	2:M:1059:ASP:CB	2.29	0.60
3:N:1101:VAL:HG21	3:N:1424:VAL:CG2	2.27	0.60
3:N:1147:ARG:O	3:N:1166:LEU:HD23	2.02	0.60
2:M:1005:MET:HE3	3:N:648:MET:HB2	1.82	0.60
5:P:321:ILE:HA	9:P:4225:HOH:O	2.01	0.60
2:C:263:ASP:HA	9:C:1161:HOH:O	2.00	0.60
2:C:483:VAL:HG23	9:C:1834:HOH:O	2.02	0.60
3:D:662:GLU:HB3	9:D:9278:HOH:O	2.01	0.60
5:F:305:GLU:O	5:F:309:LYS:HG3	2.01	0.60
2:M:212:GLY:HA3	2:M:218:VAL:HG23	1.82	0.60
2:M:411:SER:HA	2:M:452:ILE:HG23	1.83	0.60
2:M:546:LEU:HD22	2:M:565:GLN:HE22	1.66	0.60
2:M:579:VAL:HG11	2:M:887:GLU:HG3	1.84	0.60
3:N:1090:ASP:O	3:N:1093:TYR:HB3	2.01	0.60
3:N:422:ALA:HB1	5:P:178:ARG:NH1	2.15	0.60
3:N:491:LYS:HB2	9:N:2246:HOH:O	2.02	0.60
3:N:817:GLU:O	3:N:821:VAL:HG23	2.02	0.60
3:N:899:LEU:HD12	3:N:900:ILE:HG23	1.83	0.60
2:C:300:ASP:HB2	9:C:1479:HOH:O	2.01	0.59
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.83	0.59
3:D:1118:ILE:HG21	3:D:1346:ARG:NH2	2.16	0.59
3:D:1260:ILE:HG21	9:D:9360:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1379:VAL:HG11	3:D:1395:LEU:HD23	1.84	0.59
3:D:396:VAL:HB	9:D:9961:HOH:O	1.99	0.59
3:D:756:GLN:HE21	3:D:760:ARG:HD2	1.67	0.59
3:D:1209:LEU:HD21	4:E:16:LYS:NZ	2.17	0.59
5:F:213:ILE:HG22	5:F:217:ASN:ND2	2.17	0.59
2:M:113:VAL:HG12	9:M:1967:HOH:O	2.01	0.59
2:M:114:PHE:HB2	9:M:1431:HOH:O	2.01	0.59
2:M:114:PHE:H	2:M:114:PHE:HD1	1.47	0.59
2:M:16:PRO:HB3	2:M:460:ARG:HH22	1.67	0.59
2:M:516:ARG:NH2	3:N:1068:LEU:HB2	2.17	0.59
2:M:707:ARG:HD2	2:M:824:ARG:HD3	1.83	0.59
3:N:963:TYR:HD2	3:N:1002:LYS:HB3	1.67	0.59
3:N:628:ARG:HG2	3:N:744:GLN:NE2	2.17	0.59
5:P:151:LEU:HB2	5:P:155:THR:OG1	2.02	0.59
2:C:717:LEU:HD21	9:C:1599:HOH:O	2.02	0.59
3:D:813:LEU:HD12	9:D:9578:HOH:O	2.02	0.59
2:M:49:ARG:HB3	2:M:266:ARG:HH12	1.67	0.59
3:N:53:ILE:HG23	3:N:54:LYS:N	2.15	0.59
9:N:9942:HOH:O	4:O:80:VAL:HG21	2.02	0.59
1:A:191:ASP:O	1:A:192:LEU:HD23	2.02	0.59
1:A:41:ARG:HD3	9:C:1607:HOH:O	2.03	0.59
2:C:113:VAL:HG12	9:C:1672:HOH:O	2.01	0.59
2:C:342:ASP:O	2:C:346:VAL:HG23	2.02	0.59
2:C:605:LYS:HE2	2:C:610:ARG:HH12	1.67	0.59
2:C:742:VAL:HG11	9:C:1692:HOH:O	2.02	0.59
3:D:908:LYS:CB	3:D:1027:GLY:HA3	2.32	0.59
3:D:116:LEU:O	3:D:118:LEU:HG	2.01	0.59
5:F:151:LEU:HD11	9:F:834:HOH:O	2.02	0.59
3:D:572:ARG:NH2	5:F:83:GLN:HE21	1.99	0.59
1:K:9:PRO:HD2	1:L:224:TYR:CD1	2.37	0.59
2:M:1050:GLN:CG	2:M:1079:PRO:HG2	2.32	0.59
2:M:137:VAL:HG23	2:M:391:LEU:HG	1.84	0.59
2:M:498:GLN:O	2:M:501:THR:HG23	2.01	0.59
3:N:1149:LEU:HD12	3:N:1161:GLU:O	2.03	0.59
3:N:1289:LYS:HB2	9:N:9234:HOH:O	2.02	0.59
2:C:1016:ILE:HD11	5:F:330:GLY:CA	2.27	0.59
2:C:102:HIS:HB2	2:C:106:GLY:O	2.03	0.59
2:C:244:PRO:HG2	2:C:246:ASP:OD2	2.02	0.59
2:C:261:ILE:HD11	9:C:2158:HOH:O	2.02	0.59
2:C:672:VAL:HG23	2:C:868:ASP:HB2	1.85	0.59
3:D:1112:CYS:HB3	3:D:1201:CYS:SG	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1236:LEU:HA	3:D:1359:GLN:NE2	2.17	0.59
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.84	0.59
3:D:822:ALA:HA	9:D:9977:HOH:O	2.02	0.59
5:F:351:SER:O	5:F:355:GLU:HB2	2.02	0.59
1:K:150:TYR:CE2	1:K:152:PRO:HG3	2.37	0.59
2:M:196:LEU:CD2	2:M:200:LEU:HD11	2.29	0.59
3:N:1466:VAL:HG23	3:N:1472:ILE:HD11	1.83	0.59
4:O:48:MET:HB3	4:O:54:LEU:HB2	1.82	0.59
5:P:158:GLU:HB2	9:P:3694:HOH:O	2.03	0.59
5:P:222:ARG:HA	9:P:3558:HOH:O	2.01	0.59
1:B:58:ILE:HB	1:B:61:VAL:HB	1.85	0.59
3:D:1278:ASP:HB2	3:D:1318:TYR:HE1	1.68	0.59
2:M:882:LEU:HD11	3:N:1038:LEU:HD22	1.84	0.59
3:N:1425:THR:HG23	3:N:1426:LYS:N	2.18	0.59
3:N:1464:GLU:HG2	9:N:9277:HOH:O	2.03	0.59
3:N:211:VAL:HG22	3:N:393:ILE:HG23	1.84	0.59
3:N:637:LEU:HD11	3:N:642:CYS:N	2.17	0.59
5:P:365:GLU:OE1	5:P:400:ILE:HD12	2.03	0.59
2:C:1043:TYR:CE2	3:D:763:MET:HA	2.38	0.59
2:C:91:GLN:HG2	2:C:119:PRO:HG3	1.83	0.59
2:C:640:ARG:NH1	2:C:642:ARG:HH22	2.00	0.59
2:C:690:ILE:HG12	2:C:694:LEU:HD12	1.83	0.59
3:D:1381:VAL:HB	3:D:1389:LEU:O	2.02	0.59
3:D:1448:THR:O	3:D:1452:ILE:HD13	2.03	0.59
3:D:127:LEU:HD21	3:D:461:ILE:HD11	1.83	0.59
3:D:67:ARG:HA	9:D:9049:HOH:O	2.02	0.59
3:D:820:GLU:HB2	3:D:836:VAL:HG11	1.85	0.59
2:M:195:LEU:HD12	2:M:234:ALA:HB1	1.84	0.59
2:M:19:THR:HG22	2:M:22:GLN:HB2	1.85	0.59
2:M:257:VAL:HG11	9:M:1540:HOH:O	2.01	0.59
2:M:301:GLU:HG2	9:M:1719:HOH:O	2.03	0.59
3:N:1036:ARG:HH21	3:N:1043:GLY:H	1.49	0.59
3:N:1102:THR:HG22	3:N:1222:GLY:CA	2.33	0.59
3:N:1267:ARG:HH11	3:N:1267:ARG:CB	2.16	0.59
3:N:1495:ILE:HG23	9:N:9045:HOH:O	2.02	0.59
3:N:178:LEU:HD11	3:N:203:ALA:HB2	1.83	0.59
3:N:566:ILE:HG12	5:P:217:ASN:HD22	1.68	0.59
2:M:1115:LEU:HD23	3:N:85:VAL:HG13	1.84	0.59
1:A:145:ASP:HB3	9:A:453:HOH:O	2.01	0.59
1:A:206:THR:HG22	1:A:209:GLU:CG	2.32	0.59
1:A:36:LEU:O	1:A:39:PRO:HD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:ARG:NH1	2:C:49:ARG:HB2	2.12	0.59
2:C:959:PRO:O	2:C:963:LEU:HD23	2.03	0.59
3:D:1359:GLN:HB3	9:D:9147:HOH:O	2.02	0.59
3:D:530:VAL:N	3:D:534:ARG:O	2.31	0.59
3:D:663:GLU:HA	9:D:9822:HOH:O	2.02	0.59
5:F:321:ILE:HD11	5:F:329:TYR:HB2	1.85	0.59
3:N:1462:LEU:HD22	3:N:1472:ILE:CG2	2.32	0.59
1:A:178:ALA:HB2	2:C:864:GLY:H	1.68	0.59
1:A:9:PRO:HD2	1:B:224:TYR:CE1	2.38	0.59
2:C:1067:TYR:CE1	2:C:1071:ILE:HD11	2.37	0.59
2:C:222:MET:HB3	9:C:1348:HOH:O	2.01	0.59
2:C:643:VAL:HB	9:C:1217:HOH:O	2.03	0.59
3:D:1063:GLU:HB3	9:D:9027:HOH:O	2.03	0.59
3:D:534:ARG:HG3	9:D:9100:HOH:O	2.03	0.59
3:D:537:THR:O	5:F:317:LEU:HB2	2.03	0.59
5:F:138:SER:O	5:F:141:VAL:HG12	2.02	0.59
2:M:1115:LEU:HD12	2:M:1115:LEU:N	2.18	0.59
2:M:140:ILE:HG23	2:M:333:ILE:HG13	1.85	0.59
2:M:151:ASP:HB3	9:M:1442:HOH:O	2.03	0.59
3:N:127:LEU:HD12	3:N:128:TYR:N	2.18	0.59
3:N:440:VAL:HG13	9:N:9604:HOH:O	2.01	0.59
3:N:548:ILE:HG23	9:N:9055:HOH:O	2.01	0.59
3:N:574:LEU:O	3:N:578:VAL:HG23	2.02	0.59
3:N:62:LYS:NZ	3:N:75:ARG:HD2	2.18	0.59
2:C:244:PRO:CD	2:C:245:GLY:H	2.14	0.59
3:D:887:ALA:HB1	3:D:893:GLU:HG3	1.84	0.59
1:L:5:LYS:O	1:L:8:ALA:HB2	2.02	0.59
2:M:1104:GLU:HA	3:N:6:ARG:NH1	2.17	0.59
2:M:367:LEU:HB3	2:M:371:LYS:HG2	1.83	0.59
3:N:423:ASP:OD2	5:P:174:LEU:HD22	2.03	0.59
3:N:764:LEU:HD23	3:N:767:HIS:NE2	2.17	0.59
1:A:207:PRO:HB2	9:A:444:HOH:O	2.03	0.59
2:C:1059:ASP:O	2:C:1063:ARG:HG2	2.03	0.59
2:C:626:ARG:H	2:C:639:GLN:HE21	1.49	0.59
2:C:572:ILE:HG23	2:C:703:ILE:HD13	1.85	0.59
3:D:183:GLU:O	3:D:186:VAL:HG12	2.03	0.59
3:D:369:ALA:HB3	9:D:9915:HOH:O	2.01	0.59
3:D:536:ALA:HA	9:D:9452:HOH:O	2.03	0.59
1:K:88:ARG:NE	1:K:121:GLU:HG2	2.15	0.59
2:M:187:ASN:HB2	9:M:1971:HOH:O	2.03	0.59
2:M:208:ALA:O	2:M:218:VAL:HG21	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:305:PRO:HG3	2:M:308:ARG:HH21	1.67	0.59
2:M:5:ARG:HB3	2:M:902:ILE:HB	1.85	0.59
2:M:537:LYS:HG3	2:M:905:ILE:HD11	1.85	0.59
3:N:1381:VAL:HG23	3:N:1391:GLU:O	2.03	0.59
3:N:55:ASP:O	3:N:82:LYS:HA	2.03	0.59
5:P:220:LEU:O	5:P:224:VAL:HG23	2.02	0.59
2:C:640:ARG:HH11	2:C:642:ARG:HH22	1.51	0.58
3:D:1213:ARG:HB2	3:D:1214:PRO:CD	2.33	0.58
1:L:103:ALA:HB1	1:L:107:LYS:CE	2.32	0.58
2:M:439:CYS:HB3	2:M:442:GLU:HB2	1.85	0.58
3:N:481:MET:SD	3:N:1388:ARG:HG2	2.43	0.58
3:N:529:GLN:HA	9:N:9510:HOH:O	2.02	0.58
3:N:948:THR:O	3:N:1019:PRO:HG2	2.03	0.58
5:P:82:ARG:HG2	5:P:86:HIS:CD2	2.38	0.58
1:A:53:VAL:HG11	1:A:82:LEU:HD13	1.84	0.58
2:C:433:THR:HG21	2:C:488:ALA:CB	2.33	0.58
2:C:820:ARG:HB2	9:C:1318:HOH:O	2.02	0.58
2:C:838:LYS:HG3	2:C:997:LEU:HB2	1.85	0.58
3:D:996:TRP:CD2	3:D:1056:PRO:HG2	2.39	0.58
3:D:235:ALA:HB3	9:D:2396:HOH:O	2.03	0.58
3:D:133:ILE:HG23	3:D:456:MET:SD	2.43	0.58
3:D:624:ASP:HB3	3:D:625:TYR:CD1	2.38	0.58
9:B:433:HOH:O	3:D:813:LEU:HD21	2.03	0.58
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.85	0.58
1:K:101:LEU:HG	1:K:114:PHE:HA	1.84	0.58
1:K:20:TYR:HD2	1:K:21:GLY:N	2.01	0.58
1:L:156:HIS:CE1	1:L:166:PRO:HB3	2.38	0.58
3:N:1481:VAL:HG13	4:O:18:ARG:NE	2.10	0.58
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.85	0.58
3:N:546:ARG:HA	9:N:9149:HOH:O	2.02	0.58
3:N:681:ARG:HH11	3:N:681:ARG:HB3	1.68	0.58
2:M:1043:TYR:HE1	3:N:710:ARG:O	1.86	0.58
2:C:976:ASP:CB	2:C:979:THR:HG22	2.33	0.58
3:D:17:LYS:HD3	9:D:9746:HOH:O	2.03	0.58
4:E:48:MET:CB	4:E:54:LEU:HB2	2.33	0.58
9:D:2009:HOH:O	5:F:147:LEU:HD11	2.02	0.58
9:C:1615:HOH:O	5:F:354:LEU:HD21	2.03	0.58
1:K:100:LEU:HD12	9:K:4767:HOH:O	2.02	0.58
1:K:150:TYR:HE2	1:K:152:PRO:HG3	1.66	0.58
2:M:13:ILE:HB	9:M:1979:HOH:O	2.02	0.58
2:M:716:LYS:HB2	9:M:1462:HOH:O	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:862:PRO:HA	2:M:975:TYR:HE1	1.67	0.58
3:N:783:ARG:HE	3:N:1029:ARG:CD	2.16	0.58
3:N:809:PRO:HB2	3:N:812:ALA:HB2	1.85	0.58
3:N:875:THR:HG22	3:N:879:ARG:NE	2.17	0.58
1:B:212:ASN:O	1:B:215:VAL:HG22	2.03	0.58
2:C:209:ARG:O	2:C:213:ALA:HB2	2.03	0.58
2:C:235:LEU:HA	9:C:1222:HOH:O	2.03	0.58
3:D:598:ARG:HH11	3:D:598:ARG:HG2	1.67	0.58
1:K:100:LEU:HB3	9:K:3995:HOH:O	2.01	0.58
2:M:141:HIS:HB3	2:M:418:LEU:HG	1.84	0.58
2:M:191:PHE:HB3	2:M:241:LEU:HD13	1.84	0.58
3:N:119:SER:N	3:N:123:LEU:HB2	2.17	0.58
3:N:1441:GLN:CD	3:N:1442:ASN:HB2	2.23	0.58
3:N:860:LEU:HA	3:N:877:PRO:HB2	1.84	0.58
1:A:191:ASP:HA	9:A:327:HOH:O	2.03	0.58
2:C:137:VAL:HG22	2:C:391:LEU:O	2.02	0.58
2:C:332:ARG:HH22	2:C:338:GLU:CD	2.06	0.58
2:C:440:PRO:HB2	3:D:1074:SER:HB3	1.84	0.58
2:C:512:ARG:HB2	9:C:1379:HOH:O	2.04	0.58
3:D:658:LEU:HD11	3:D:674:ARG:NH1	2.19	0.58
3:D:699:VAL:N	3:D:756:GLN:HE22	2.00	0.58
3:D:804:LEU:HB2	3:D:830:ALA:O	2.04	0.58
3:D:813:LEU:O	3:D:817:GLU:HB2	2.03	0.58
3:D:965:GLU:HA	3:D:968:ASP:HB2	1.85	0.58
5:F:250:ALA:HA	9:F:629:HOH:O	2.04	0.58
5:F:403:LYS:HB3	9:F:714:HOH:O	2.03	0.58
1:L:110:LYS:HD2	1:L:112:ARG:NH1	2.18	0.58
2:M:1006:HIS:O	3:N:627:GLY:HA2	2.04	0.58
2:M:1101:THR:HB	3:N:5:VAL:CG1	2.32	0.58
2:M:1115:LEU:HD12	2:M:1115:LEU:H	1.69	0.58
2:M:294:GLU:HG3	9:M:1411:HOH:O	2.03	0.58
2:M:367:LEU:O	2:M:372:LEU:HD13	2.03	0.58
2:M:382:ILE:HD12	9:M:1347:HOH:O	2.03	0.58
3:N:1342:GLU:CD	3:N:1342:GLU:H	2.07	0.58
3:N:1106:VAL:HG21	3:N:1474:ALA:HB2	1.85	0.58
4:O:54:LEU:HA	4:O:58:PRO:HG2	1.86	0.58
5:P:181:GLU:O	5:P:184:ARG:HB3	2.03	0.58
5:P:342:VAL:HG21	9:P:6462:HOH:O	2.01	0.58
1:B:109:VAL:HG21	1:B:138:LEU:HD21	1.85	0.58
2:C:112:GLU:HG3	9:C:1263:HOH:O	2.03	0.58
2:C:129:ILE:HD13	2:C:134:ARG:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:260:LEU:HB2	2:C:291:ALA:HB1	1.86	0.58
3:D:542:ASP:O	3:D:546:ARG:HG2	2.04	0.58
3:D:963:TYR:CE2	3:D:1002:LYS:HB3	2.39	0.58
3:N:1220:ALA:HB1	3:N:1223:ILE:HD13	1.86	0.58
3:N:1101:VAL:HG13	3:N:1428:ALA:HB2	1.85	0.58
4:O:42:PRO:HG3	9:O:4652:HOH:O	2.03	0.58
5:P:271:LEU:HD23	5:P:291:ILE:HD11	1.86	0.58
2:C:441:VAL:HG13	2:C:559:LEU:HA	1.84	0.58
3:D:1003:VAL:O	3:D:1007:VAL:HG13	2.03	0.58
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.84	0.58
3:D:178:LEU:HD21	9:D:9048:HOH:O	2.03	0.58
3:D:204:LEU:HD12	9:D:2356:HOH:O	2.04	0.58
3:D:209:ARG:CZ	3:D:397:LYS:HG3	2.33	0.58
3:D:562:ALA:HB1	3:D:567:ILE:CD1	2.32	0.58
2:C:1043:TYR:HE1	3:D:710:ARG:O	1.86	0.58
3:D:965:GLU:O	3:D:968:ASP:HB2	2.04	0.58
9:C:1403:HOH:O	5:F:373:LYS:HB3	2.03	0.58
1:L:56:VAL:HG13	1:L:142:VAL:HG12	1.85	0.58
1:L:91:ASN:H	1:L:94:LEU:HD12	1.69	0.58
2:M:21:ILE:HD12	2:M:21:ILE:H	1.68	0.58
2:M:352:ALA:HA	2:M:355:VAL:HG12	1.86	0.58
2:M:478:VAL:HG13	2:M:506:ASN:HB3	1.85	0.58
2:M:510:ALA:HB3	2:M:513:VAL:HG23	1.85	0.58
3:N:971:LEU:HG	3:N:975:GLU:OE2	2.01	0.58
2:C:598:GLU:O	2:C:651:LYS:HG3	2.04	0.58
2:C:78:PHE:HB2	2:C:88:LEU:HD21	1.86	0.58
3:D:6:ARG:NH1	3:D:6:ARG:HB2	2.19	0.58
2:C:874:LEU:HD13	3:D:783:ARG:HB2	1.85	0.58
2:M:1054:THR:HG23	9:M:1191:HOH:O	2.03	0.58
2:M:134:ARG:NH1	2:M:387:SER:HA	2.19	0.58
2:M:379:GLU:HA	9:M:1347:HOH:O	2.03	0.58
3:N:119:SER:H	3:N:123:LEU:HD13	1.69	0.58
3:N:890:VAL:HG12	3:N:926:LYS:HG2	1.86	0.58
5:P:80:PRO:HA	5:P:83:GLN:HB2	1.86	0.58
1:A:101:LEU:HG	1:A:114:PHE:HA	1.86	0.58
1:B:132:LEU:HG	1:B:136:GLY:HA3	1.84	0.58
1:B:83:LYS:HE3	1:B:167:VAL:HG12	1.86	0.58
2:C:238:LEU:HB2	9:C:1222:HOH:O	2.02	0.58
2:C:479:VAL:HG22	2:C:508:ILE:HD13	1.84	0.58
3:D:850:LEU:HD12	3:D:850:LEU:H	1.69	0.58
3:D:924:MET:O	3:D:927:THR:HB	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:230:LYS:HB2	9:F:771:HOH:O	2.03	0.58
5:F:247:ILE:HG12	9:F:482:HOH:O	2.04	0.58
5:F:264:MET:HB3	9:F:624:HOH:O	2.03	0.58
5:F:79:ASP:HB3	5:F:80:PRO:CD	2.34	0.58
1:L:221:HIS:HA	1:L:224:TYR:HD2	1.68	0.58
2:M:1012:PRO:HB3	9:M:1930:HOH:O	2.03	0.58
2:M:1018:GLN:HG3	2:M:1060:ILE:HD13	1.84	0.58
2:M:233:GLU:HG2	9:M:1408:HOH:O	2.04	0.58
2:M:484:VAL:HA	9:M:1294:HOH:O	2.04	0.58
2:M:882:LEU:HD12	3:N:1061:PHE:HB3	1.86	0.58
3:N:120:ALA:HB1	9:N:9285:HOH:O	2.03	0.58
3:N:1350:GLU:O	3:N:1354:LYS:HG2	2.03	0.58
3:N:149:LYS:HA	9:N:9092:HOH:O	2.03	0.58
3:N:555:LYS:HB3	9:P:6985:HOH:O	2.04	0.58
3:N:52:PRO:HB2	3:N:80:VAL:HG13	1.85	0.58
5:P:205:ARG:HG3	5:P:251:ILE:HD13	1.86	0.58
5:P:317:LEU:O	5:P:329:TYR:HB3	2.04	0.58
1:A:189:ARG:HB2	9:A:371:HOH:O	2.04	0.58
1:B:218:LEU:O	1:B:222:LEU:HG	2.03	0.58
1:B:5:LYS:O	1:B:8:ALA:HB2	2.04	0.58
2:C:208:ALA:O	2:C:218:VAL:HG21	2.04	0.58
3:D:12:LEU:HD13	3:D:511:TRP:HB2	1.84	0.58
3:D:193:PRO:HD3	9:D:9827:HOH:O	2.03	0.58
3:D:89:ARG:O	3:D:521:PRO:HG3	2.04	0.58
1:K:186:LEU:HB3	1:K:192:LEU:HD11	1.86	0.58
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.27	0.58
9:K:4223:HOH:O	1:L:43:ILE:HD11	2.03	0.58
2:M:108:ILE:HD12	2:M:108:ILE:H	1.68	0.58
2:M:227:PHE:HD2	2:M:230:ARG:HH21	1.51	0.58
2:M:889:HIS:CE1	3:N:951:ILE:HB	2.38	0.58
3:N:97:THR:HG21	3:N:571:LYS:HD3	1.85	0.58
4:O:16:LYS:HD3	4:O:17:TYR:HE2	1.69	0.58
1:B:132:LEU:HD13	1:B:138:LEU:HD13	1.86	0.57
1:B:16:GLN:HB3	9:B:447:HOH:O	2.04	0.57
2:C:1031:ARG:HD3	3:D:619:LEU:CD2	2.34	0.57
2:C:397:GLU:HG2	2:C:403:SER:HB3	1.84	0.57
2:C:503:LEU:HD13	2:C:507:ARG:O	2.04	0.57
3:D:1307:LYS:CD	3:D:1307:LYS:H	2.17	0.57
3:D:1472:ILE:HG22	3:D:1474:ALA:H	1.69	0.57
3:D:28:LYS:HG3	3:D:29:PRO:HD2	1.84	0.57
3:D:438:ASP:HB2	9:D:9161:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:527:MET:HB3	9:D:9990:HOH:O	2.04	0.57
3:D:834:THR:HB	3:D:838:ARG:HB3	1.85	0.57
3:D:877:PRO:O	3:D:880:ILE:HG22	2.03	0.57
1:K:209:GLU:O	1:K:213:GLN:HG3	2.03	0.57
2:M:594:ALA:HB1	2:M:654:LEU:HD12	1.86	0.57
3:N:106:LYS:HE2	9:N:9886:HOH:O	2.04	0.57
3:N:131:LYS:HD2	5:P:83:GLN:HE21	1.68	0.57
3:N:1493:LYS:HA	3:N:1496:GLU:OE2	2.04	0.57
3:N:685:ASP:HB3	9:N:9661:HOH:O	2.03	0.57
5:P:120:THR:HG21	5:P:122:LEU:HD22	1.86	0.57
5:P:166:LEU:O	5:P:171:LYS:HB2	2.04	0.57
2:C:139:GLN:OE1	2:C:414:GLY:HA3	2.04	0.57
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.87	0.57
2:C:554:ASP:OD2	2:C:556:ASN:HB3	2.04	0.57
3:D:1047:LYS:NZ	3:D:1053:PHE:HA	2.19	0.57
3:D:1314:LYS:HZ3	3:D:1317:ASP:H	1.50	0.57
3:D:87:ARG:CB	3:D:523:ASP:HB2	2.34	0.57
5:F:282:LEU:HD11	5:F:286:PRO:HG3	1.86	0.57
1:K:88:ARG:HD2	1:K:88:ARG:O	2.04	0.57
2:M:51:THR:OG1	2:M:348:LEU:HD23	2.03	0.57
2:M:629:TYR:HB2	2:M:637:LEU:HG	1.86	0.57
2:M:648:ARG:HG2	9:M:2052:HOH:O	2.03	0.57
2:M:926:PHE:O	2:M:930:LYS:HG3	2.04	0.57
3:N:710:ARG:HH22	3:N:1210:SER:CB	2.17	0.57
3:N:1462:LEU:HD22	3:N:1472:ILE:HG23	1.86	0.57
3:N:424:GLY:HA2	3:N:436:GLU:HA	1.86	0.57
3:N:911:LEU:O	3:N:915:VAL:HG23	2.04	0.57
4:O:23:VAL:HG21	4:O:65:MET:HG2	1.85	0.57
1:A:127:LEU:HD12	1:A:128:HIS:N	2.18	0.57
1:B:205:VAL:HG11	9:B:348:HOH:O	2.03	0.57
2:C:1060:ILE:HG23	2:C:1061:GLU:N	2.20	0.57
2:C:257:VAL:HG12	2:C:263:ASP:OD1	2.04	0.57
2:C:274:ARG:HG3	2:C:285:LEU:HD22	1.85	0.57
2:C:355:VAL:CG2	2:C:372:LEU:HG	2.34	0.57
2:C:666:LEU:HD23	2:C:668:LEU:HD11	1.84	0.57
3:D:1148:VAL:HG13	3:D:1163:GLY:O	2.05	0.57
3:D:1262:LEU:HD23	3:D:1352:ILE:HG13	1.86	0.57
3:D:525:ARG:HB2	3:D:541:ASN:ND2	2.20	0.57
3:D:560:GLN:HB2	9:F:762:HOH:O	2.04	0.57
3:D:871:LYS:HD3	3:D:873:LEU:HD21	1.85	0.57
5:F:198:ILE:HA	9:F:560:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:176:ARG:NH2	3:N:884:ARG:HD3	2.19	0.57
2:M:341:THR:O	2:M:345:ARG:HG2	2.04	0.57
2:M:611:ILE:HD11	2:M:641:PRO:HB3	1.85	0.57
2:M:722:ILE:CD1	2:M:823:VAL:HG21	2.33	0.57
2:M:881:ASN:H	2:M:881:ASN:HD22	1.51	0.57
2:M:861:LEU:HD21	2:M:925:TYR:CE2	2.39	0.57
3:N:131:LYS:HD2	5:P:83:GLN:NE2	2.19	0.57
3:N:197:SER:HA	9:N:9482:HOH:O	2.04	0.57
3:N:642:CYS:SG	3:N:716:PHE:HB2	2.44	0.57
3:N:704:ARG:CG	3:N:736:PHE:HB3	2.35	0.57
5:P:409:LYS:HG3	5:P:410:TYR:N	2.19	0.57
1:A:59:GLU:CD	1:A:139:ASN:HD21	2.07	0.57
2:C:1073:GLY:HA2	9:C:1177:HOH:O	2.04	0.57
2:C:418:LEU:H	2:C:418:LEU:HD22	1.69	0.57
2:C:588:VAL:HG12	2:C:666:LEU:HD12	1.86	0.57
2:C:833:LEU:HD11	2:C:849:VAL:HG21	1.86	0.57
3:D:10:ILE:HG13	3:D:1434:TRP:CZ2	2.40	0.57
3:D:191:LEU:HD22	3:D:195:VAL:HG21	1.87	0.57
3:D:131:LYS:HE3	5:F:83:GLN:HE22	1.69	0.57
1:L:16:GLN:HG3	9:L:6332:HOH:O	2.05	0.57
2:M:999:HIS:HB3	2:M:1003:ASP:OD1	2.05	0.57
2:M:1114:GLY:N	2:M:1115:LEU:HD12	2.07	0.57
2:M:159:ILE:HD11	9:M:1995:HOH:O	2.03	0.57
3:N:141:ILE:HB	9:N:9457:HOH:O	2.04	0.57
3:N:404:GLU:HB3	3:N:414:ARG:CD	2.34	0.57
3:N:712:GLY:C	3:N:713:ILE:HD12	2.24	0.57
3:N:800:LYS:HG2	9:N:9126:HOH:O	2.04	0.57
4:O:41:GLU:O	4:O:45:ARG:HG2	2.05	0.57
2:C:1091:GLU:HG2	3:D:606:ILE:HG21	1.84	0.57
2:C:338:GLU:O	2:C:341:THR:HG22	2.04	0.57
2:C:924:VAL:HG23	9:C:1396:HOH:O	2.03	0.57
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.04	0.57
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.34	0.57
3:D:1394:VAL:HB	3:D:1397:LYS:HD2	1.86	0.57
3:D:476:GLU:HG2	9:D:9334:HOH:O	2.05	0.57
3:D:809:PRO:HB2	3:D:812:ALA:HB2	1.86	0.57
5:F:105:LYS:HE3	9:F:642:HOH:O	2.05	0.57
2:M:1051:GLU:HG3	2:M:1055:LEU:HD12	1.87	0.57
2:M:1085:PHE:CE2	3:N:1468:LEU:HG	2.39	0.57
2:M:864:GLY:HA2	9:M:1403:HOH:O	2.04	0.57
3:N:1033:GLN:NE2	3:N:1036:ARG:HH11	1.90	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:183:GLU:O	3:N:186:VAL:HG12	2.04	0.57
3:N:28:LYS:HG3	3:N:29:PRO:HD2	1.86	0.57
3:N:455:ARG:NH1	3:N:463:GLN:HG3	2.19	0.57
5:P:290:GLU:HG3	9:P:5633:HOH:O	2.03	0.57
2:C:313:LEU:HD13	2:C:321:GLU:O	2.03	0.57
2:C:332:ARG:HE	2:C:464:LEU:CD1	2.17	0.57
2:C:342:ASP:HA	2:C:345:ARG:HG2	1.86	0.57
2:C:524:VAL:HB	9:C:1200:HOH:O	2.02	0.57
2:C:732:ALA:HB3	9:C:1156:HOH:O	2.03	0.57
2:C:89:THR:HA	2:C:129:ILE:O	2.05	0.57
2:C:935:GLY:HA2	9:C:1635:HOH:O	2.04	0.57
3:D:1061:PHE:HE1	3:D:1065:LEU:HD23	1.68	0.57
3:D:1120:VAL:HB	3:D:1144:LEU:HD21	1.85	0.57
3:D:1209:LEU:HD21	4:E:16:LYS:HZ3	1.70	0.57
5:F:403:LYS:HD2	9:F:436:HOH:O	2.05	0.57
1:K:127:LEU:HD12	1:K:128:HIS:N	2.20	0.57
2:M:1018:GLN:NE2	2:M:1063:ARG:HH22	2.03	0.57
2:M:1085:PHE:HD2	3:N:1468:LEU:HA	1.69	0.57
2:M:218:VAL:O	2:M:221:LEU:HG	2.05	0.57
2:M:233:GLU:OE1	2:M:237:ARG:HD3	2.04	0.57
3:N:1262:LEU:CD2	3:N:1351:GLU:HG3	2.28	0.57
3:N:737:ASN:HA	9:N:9235:HOH:O	2.04	0.57
4:O:69:LEU:O	4:O:69:LEU:HD23	2.03	0.57
1:B:190:THR:HG22	9:B:367:HOH:O	2.04	0.57
1:B:30:ARG:HH11	1:B:30:ARG:HB2	1.70	0.57
2:C:1012:PRO:HG2	9:C:2108:HOH:O	2.05	0.57
2:C:264:PRO:HB3	2:C:289:THR:CB	2.34	0.57
2:C:583:LEU:O	2:C:587:VAL:HG23	2.04	0.57
2:C:580:MET:HB3	2:C:584:GLU:OE2	2.05	0.57
2:C:706:GLU:HB3	2:C:708:TYR:CE1	2.39	0.57
2:C:728:HIS:HB3	2:C:729:LEU:HD12	1.87	0.57
3:D:525:ARG:HA	3:D:538:SER:HB3	1.87	0.57
3:D:53:ILE:O	3:D:53:ILE:HG12	2.03	0.57
4:E:26:ARG:HE	4:E:30:LEU:HD11	1.68	0.57
5:F:401:GLU:O	5:F:405:LEU:HB2	2.04	0.57
1:K:102:LYS:HE2	1:K:139:ASN:CG	2.25	0.57
1:K:219:ARG:HH22	1:L:223:THR:CG2	2.11	0.57
1:L:80:LEU:HG	3:N:844:ALA:HB2	1.87	0.57
2:M:1013:TYR:HE1	2:M:1020:PRO:HG3	1.69	0.57
2:M:510:ALA:HB3	2:M:513:VAL:CG2	2.35	0.57
2:M:79:PRO:HG2	2:M:82:GLU:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:861:LEU:HD23	2:M:862:PRO:HD2	1.87	0.57
3:N:1111:ASP:HB2	3:N:1203:LYS:CG	2.32	0.57
3:N:443:VAL:HG12	3:N:445:ARG:HD2	1.87	0.57
3:N:486:ARG:HG2	9:N:2235:HOH:O	2.04	0.57
3:N:564:GLU:HA	3:N:567:ILE:HD12	1.87	0.57
4:O:32:ARG:HA	9:O:4513:HOH:O	2.05	0.57
3:N:760:ARG:HH21	4:O:3:GLU:CD	2.06	0.57
4:O:72:ARG:HA	9:O:5797:HOH:O	2.05	0.57
5:P:361:LEU:HD23	5:P:362:SER:H	1.69	0.57
1:B:86:VAL:HA	9:B:479:HOH:O	2.04	0.57
2:C:395:LYS:HG2	2:C:397:GLU:HG3	1.86	0.57
2:C:661:SER:HB2	9:C:2008:HOH:O	2.04	0.57
2:C:816:LYS:HB2	2:C:819:VAL:HG21	1.85	0.57
3:D:420:VAL:HG23	9:D:9536:HOH:O	2.04	0.57
4:E:47:LYS:HA	4:E:54:LEU:HB3	1.87	0.57
1:L:41:ARG:HG3	1:L:177:VAL:CG2	2.34	0.57
1:K:67:THR:OG1	2:M:609:ASN:ND2	2.37	0.57
3:N:1129:THR:HG23	3:N:1130:ARG:H	1.70	0.57
2:M:1109:VAL:HG11	3:N:5:VAL:HG22	1.86	0.57
5:P:416:ARG:NH1	5:P:419:ARG:HB2	2.20	0.57
1:B:226:SER:HB3	9:B:512:HOH:O	2.04	0.57
2:C:122:THR:HG21	9:C:1356:HOH:O	2.04	0.57
2:C:184:MET:HG2	9:C:1676:HOH:O	2.04	0.57
2:C:859:PRO:O	2:C:867:VAL:HG22	2.05	0.57
3:D:36:THR:C	3:D:38:LYS:H	2.08	0.57
3:D:141:ILE:HG12	3:D:449:SER:HA	1.86	0.57
3:D:574:LEU:O	3:D:578:VAL:HG23	2.05	0.57
5:F:115:LYS:HE2	5:F:118:GLU:OE2	2.04	0.57
5:F:142:ARG:CZ	5:F:150:THR:HG21	2.35	0.57
5:F:321:ILE:HG22	5:F:322:GLY:H	1.69	0.57
2:M:397:GLU:HG3	2:M:633:GLN:NE2	2.20	0.57
2:M:569:VAL:HG11	2:M:996:LYS:NZ	2.19	0.57
2:M:721:ARG:HH22	2:M:785:VAL:HG21	1.70	0.57
3:N:1019:PRO:O	3:N:1023:MET:HG3	2.05	0.57
3:N:820:GLU:HB2	3:N:836:VAL:HG11	1.85	0.57
4:O:39:VAL:HB	4:O:72:ARG:HD2	1.87	0.57
1:A:5:LYS:O	1:A:8:ALA:HB2	2.05	0.57
1:B:73:GLU:HB3	1:B:77:GLU:CG	2.35	0.57
2:C:1067:TYR:O	2:C:1071:ILE:HG12	2.05	0.57
2:C:1085:PHE:O	2:C:1089:VAL:HG23	2.05	0.57
2:C:710:ILE:HD11	2:C:758:ARG:HE	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:906:PHE:HB2	9:C:1288:HOH:O	2.04	0.57
3:D:1107:VAL:HG12	3:D:1217:ILE:HA	1.87	0.57
3:D:1277:ILE:CD1	3:D:1301:LYS:HB2	2.33	0.57
3:D:478:LEU:HD13	3:D:1388:ARG:HH22	1.68	0.57
3:D:598:ARG:HG3	3:D:599:PRO:N	2.20	0.57
3:D:81:THR:HG22	3:D:82:LYS:H	1.70	0.57
1:K:88:ARG:HE	1:K:121:GLU:CG	2.15	0.57
1:K:57:TYR:CE2	1:K:161:ARG:HD2	2.40	0.57
2:M:286:SER:CB	2:M:299:LYS:HE3	2.34	0.57
2:M:513:VAL:HG13	9:M:1395:HOH:O	2.05	0.57
2:M:72:ARG:NH2	2:M:112:GLU:HG3	2.20	0.57
2:M:810:ASP:HB2	9:M:1758:HOH:O	2.05	0.57
5:P:403:LYS:HA	5:P:403:LYS:HZ3	1.70	0.57
1:B:206:THR:CG2	1:B:209:GLU:H	2.18	0.56
2:C:644:VAL:HG11	9:C:1903:HOH:O	2.04	0.56
2:C:773:LEU:O	2:C:777:ILE:HG13	2.05	0.56
2:C:971:LYS:HA	2:C:988:VAL:HA	1.87	0.56
3:D:210:ARG:HG3	3:D:398:ALA:H	1.70	0.56
3:D:714:GLN:HB2	3:D:736:PHE:HZ	1.69	0.56
4:E:48:MET:N	4:E:54:LEU:HB2	2.19	0.56
4:E:73:LEU:HG	9:E:100:HOH:O	2.03	0.56
5:F:171:LYS:HD2	5:F:174:LEU:HD12	1.86	0.56
1:L:112:ARG:HH12	1:L:126:ASP:HA	1.69	0.56
1:L:28:LEU:O	1:L:192:LEU:HD23	2.05	0.56
2:M:162:ILE:O	2:M:164:PRO:HD3	2.04	0.56
2:M:676:ILE:HG23	2:M:676:ILE:O	2.05	0.56
2:M:957:LYS:HG3	9:M:1885:HOH:O	2.05	0.56
2:M:984:GLU:O	3:N:946:GLY:HA3	2.04	0.56
3:N:19:ARG:HB3	9:N:9131:HOH:O	2.04	0.56
3:N:625:TYR:O	3:N:749:VAL:HG23	2.04	0.56
4:O:61:GLU:O	4:O:65:MET:HE2	2.05	0.56
1:B:52:ALA:HB1	9:B:364:HOH:O	2.04	0.56
2:C:146:VAL:HG13	2:C:161:SER:O	2.05	0.56
2:C:172:ILE:H	2:C:172:ILE:HD12	1.70	0.56
3:D:1425:THR:HG23	3:D:1426:LYS:N	2.19	0.56
3:D:116:LEU:HD23	3:D:468:LEU:HD11	1.87	0.56
3:D:49:ILE:HB	3:D:50:PHE:CD1	2.41	0.56
3:D:864:VAL:HG23	3:D:877:PRO:HD3	1.87	0.56
3:D:868:TYR:CG	3:D:869:MET:N	2.72	0.56
5:F:293:GLU:HG2	9:F:663:HOH:O	2.05	0.56
1:L:67:THR:HG23	9:L:5452:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:281:LEU:CD1	2:M:306:THR:HA	2.34	0.56
2:M:534:VAL:H	2:M:538:GLN:NE2	2.03	0.56
2:C:838:LYS:HD2	2:C:846:LYS:NZ	2.21	0.56
3:D:18:ILE:HG21	3:D:516:ALA:O	2.05	0.56
3:D:530:VAL:HB	3:D:534:ARG:CB	2.35	0.56
3:D:86:ARG:HH11	3:D:86:ARG:HG2	1.68	0.56
5:F:136:LEU:HD11	9:F:879:HOH:O	2.05	0.56
1:L:36:LEU:O	1:L:39:PRO:HD2	2.05	0.56
2:M:288:ARG:HB3	9:M:1410:HOH:O	2.05	0.56
2:M:304:LEU:HD23	2:M:305:PRO:HD3	1.88	0.56
2:M:54:ILE:HG22	2:M:66:LEU:HB3	1.86	0.56
3:N:728:LEU:HD22	3:N:745:MET:SD	2.45	0.56
3:N:8:VAL:HG23	9:N:9563:HOH:O	2.04	0.56
1:A:206:THR:CG2	1:A:209:GLU:H	2.18	0.56
1:A:224:TYR:CD2	1:B:9:PRO:HG2	2.40	0.56
2:C:41:ASN:O	2:C:46:ALA:HB2	2.06	0.56
3:D:1314:LYS:HD2	9:D:9848:HOH:O	2.03	0.56
3:D:834:THR:HG22	3:D:838:ARG:HD2	1.87	0.56
5:F:127:ILE:HG12	9:F:445:HOH:O	2.05	0.56
5:F:363:GLU:HG3	9:F:548:HOH:O	2.05	0.56
1:L:74:ASP:OD2	1:L:76:VAL:HG23	2.05	0.56
2:M:879:ARG:NH1	3:N:1029:ARG:HH12	2.02	0.56
3:N:409:VAL:HG23	9:N:9521:HOH:O	2.06	0.56
1:B:139:ASN:HB2	9:B:334:HOH:O	2.06	0.56
2:C:724:ARG:NH1	2:C:734:LEU:HD23	2.21	0.56
3:D:957:PRO:HG2	3:D:1007:VAL:HG12	1.87	0.56
3:D:1093:TYR:O	3:D:1097:LYS:HG2	2.05	0.56
3:D:1280:VAL:HG23	3:D:1295:GLU:O	2.05	0.56
3:D:817:GLU:O	3:D:821:VAL:HG23	2.05	0.56
5:F:260:ILE:HD11	5:F:310:ILE:HG22	1.86	0.56
2:M:89:THR:HA	2:M:129:ILE:O	2.06	0.56
2:M:145:GLY:O	2:M:163:ILE:HG23	2.06	0.56
2:M:52:PHE:CG	2:M:68:PHE:HB2	2.41	0.56
2:M:918:LEU:HD23	2:M:968:LEU:HA	1.87	0.56
5:P:132:ARG:NE	5:P:184:ARG:HH12	2.04	0.56
5:P:292:ALA:HB1	5:P:299:TRP:O	2.06	0.56
1:B:144:VAL:HG12	9:B:467:HOH:O	2.05	0.56
2:C:1055:LEU:HD21	2:C:1079:PRO:HG3	1.87	0.56
2:C:313:LEU:HB2	2:C:321:GLU:HG3	1.87	0.56
2:C:338:GLU:HA	2:C:341:THR:HG22	1.88	0.56
2:C:941:VAL:HG22	9:C:1556:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1277:ILE:HG23	9:D:9898:HOH:O	2.05	0.56
3:D:154:THR:HG22	3:D:157:GLU:OE2	2.05	0.56
3:D:171:LEU:HD22	3:D:390:PRO:HG3	1.87	0.56
3:D:424:GLY:HA2	3:D:435:VAL:O	2.04	0.56
3:D:460:ALA:O	3:D:464:LEU:HG	2.05	0.56
3:D:462:GLN:HG2	9:D:9526:HOH:O	2.06	0.56
3:D:890:VAL:HG22	3:D:926:LYS:HD3	1.87	0.56
3:D:984:THR:HG23	3:D:987:GLU:H	1.70	0.56
1:L:100:LEU:O	1:L:115:LEU:HG	2.05	0.56
2:M:262:ALA:HA	9:M:1860:HOH:O	2.06	0.56
3:N:1000:THR:O	3:N:1003:VAL:HG22	2.06	0.56
3:N:1147:ARG:O	3:N:1165:TYR:HA	2.06	0.56
4:O:31:LEU:HD23	4:O:35:PHE:CE1	2.40	0.56
4:O:61:GLU:H	4:O:61:GLU:CD	2.07	0.56
5:P:152:ASP:HB2	5:P:153:PRO:HD3	1.87	0.56
2:C:95:TYR:CD2	2:C:114:PHE:HB3	2.41	0.56
2:C:949:LYS:HA	3:D:798:GLU:OE1	2.06	0.56
3:D:1036:ARG:HH21	3:D:1042:ARG:HA	1.71	0.56
3:D:996:TRP:HA	3:D:999:THR:HG22	1.86	0.56
5:F:361:LEU:HD23	5:F:362:SER:N	2.16	0.56
5:F:87:GLU:HB3	9:F:725:HOH:O	2.04	0.56
2:M:157:ARG:HB3	9:M:1582:HOH:O	2.04	0.56
2:M:358:ARG:HH22	2:M:374:ASN:HB3	1.71	0.56
2:M:545:ASN:O	2:M:581:THR:HG21	2.06	0.56
3:N:1290:LEU:HA	9:N:9828:HOH:O	2.06	0.56
3:N:562:ALA:HB1	3:N:567:ILE:HD11	1.88	0.56
5:P:292:ALA:HA	5:P:299:TRP:HB3	1.88	0.56
5:P:321:ILE:HB	5:P:327:SER:OG	2.05	0.56
1:A:180:GLN:HB3	9:A:522:HOH:O	2.05	0.56
2:C:70:GLU:HB3	9:C:1380:HOH:O	2.04	0.56
3:D:483:HIS:ND1	3:D:483:HIS:N	2.54	0.56
2:C:889:HIS:HE1	3:D:951:ILE:H	1.53	0.56
2:M:447:ALA:HB2	9:M:1391:HOH:O	2.04	0.56
3:N:75:ARG:HB3	9:N:9139:HOH:O	2.05	0.56
5:P:210:LEU:HA	5:P:213:ILE:HD12	1.88	0.56
5:P:79:ASP:HB3	5:P:80:PRO:CD	2.36	0.56
1:A:42:ARG:HH21	1:B:34:VAL:HB	1.71	0.56
2:C:24:GLU:OE1	2:C:27:ARG:HD3	2.06	0.56
2:C:264:PRO:HB3	2:C:289:THR:CG2	2.35	0.56
2:C:305:PRO:HA	2:C:308:ARG:NE	2.21	0.56
2:C:577:PRO:HG3	2:C:993:PHE:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1000:THR:O	3:D:1003:VAL:HG22	2.05	0.56
3:D:1117:TYR:HE2	3:D:1151:ARG:HH11	1.53	0.56
3:D:111:LYS:CE	3:D:1452:ILE:HG12	2.35	0.56
3:D:427:VAL:CG2	3:D:435:VAL:HB	2.35	0.56
3:D:500:ARG:HH11	3:D:500:ARG:HG3	1.70	0.56
1:L:24:VAL:HG13	9:L:6021:HOH:O	2.05	0.56
2:M:216:GLU:HG2	2:M:217:LEU:HD23	1.88	0.56
2:M:244:PRO:CD	2:M:245:GLY:H	2.18	0.56
3:N:1175:ILE:O	3:N:1179:GLU:HG3	2.04	0.56
3:N:1109:GLU:HG2	3:N:1201:CYS:CA	2.34	0.56
3:N:472:ALA:HA	9:N:9634:HOH:O	2.05	0.56
3:N:62:LYS:HD2	3:N:75:ARG:NH1	2.20	0.56
2:C:1054:THR:HG22	2:C:1059:ASP:CB	2.35	0.56
2:C:195:LEU:HD12	2:C:234:ALA:HB1	1.87	0.56
2:C:521:PRO:HB2	3:D:1055:VAL:HB	1.86	0.56
3:D:523:ASP:O	3:D:526:PRO:HG3	2.06	0.56
3:D:869:MET:HE3	9:D:9791:HOH:O	2.06	0.56
3:D:907:GLU:O	3:D:911:LEU:HD13	2.06	0.56
1:K:104:GLU:HG2	1:K:105:GLY:N	2.21	0.56
1:K:18:ARG:O	1:K:207:PRO:HD3	2.06	0.56
2:M:469:THR:OG1	2:M:470:PRO:HD2	2.05	0.56
2:M:605:LYS:HB2	2:M:610:ARG:HH12	1.71	0.56
3:N:1478:SER:OG	3:N:1480:PHE:HB3	2.04	0.56
3:N:554:LEU:O	3:N:558:LEU:HG	2.06	0.56
3:N:95:LEU:CD2	3:N:574:LEU:HD11	2.35	0.56
2:C:1003:ASP:O	2:C:1005:MET:N	2.39	0.56
2:C:941:VAL:HA	2:C:944:LEU:HD12	1.87	0.56
3:D:1049:SER:HB3	9:D:9373:HOH:O	2.06	0.56
3:D:1379:VAL:HA	3:D:1420:LEU:HB2	1.88	0.56
3:D:560:GLN:HG2	5:F:218:GLN:HE22	1.71	0.56
1:L:73:GLU:HB3	1:L:77:GLU:HG2	1.88	0.56
2:M:154:ARG:NH2	2:M:156:GLY:HA3	2.12	0.56
2:M:173:ASP:HB2	2:M:185:LYS:NZ	2.21	0.56
2:M:368:THR:HB	2:M:369:PRO:HD3	1.88	0.56
2:M:371:LYS:HB2	9:M:1144:HOH:O	2.05	0.56
2:M:620:LEU:HD21	9:M:1351:HOH:O	2.05	0.56
3:N:1314:LYS:HD3	3:N:1314:LYS:N	2.21	0.56
3:N:573:MET:HE3	5:P:210:LEU:HD22	1.87	0.56
5:P:352:GLU:O	5:P:356:LYS:HG3	2.06	0.56
2:C:12:VAL:HG21	9:C:1844:HOH:O	2.05	0.55
2:C:640:ARG:HG3	9:C:1776:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1104:GLU:HA	3:D:1461:GLY:HA2	1.89	0.55
3:D:1232:PRO:HB3	3:D:1361:VAL:CG2	2.30	0.55
3:D:206:ARG:O	3:D:206:ARG:HD3	2.06	0.55
1:K:224:TYR:CD2	1:L:9:PRO:HG2	2.41	0.55
2:M:1039:ALA:O	2:M:1043:TYR:HD1	1.88	0.55
2:M:1085:PHE:O	2:M:1089:VAL:HG23	2.05	0.55
2:M:361:MET:HA	9:M:1201:HOH:O	2.06	0.55
2:M:707:ARG:HG3	2:M:826:TYR:CD2	2.41	0.55
2:M:916:GLU:HG2	9:M:1287:HOH:O	2.06	0.55
3:N:1047:LYS:HB3	3:N:1048:PRO:CD	2.36	0.55
3:N:119:SER:H	3:N:123:LEU:CD1	2.20	0.55
3:N:105:VAL:HG21	3:N:128:TYR:HE2	1.71	0.55
3:N:36:THR:C	3:N:38:LYS:H	2.09	0.55
3:N:853:VAL:HG22	3:N:858:VAL:HG23	1.89	0.55
5:P:113:ILE:HA	5:P:116:LEU:HD12	1.87	0.55
5:P:94:LEU:HB2	5:P:98:GLU:OE2	2.06	0.55
2:C:193:LEU:HD23	2:C:307:LEU:HD11	1.88	0.55
2:C:232:GLU:HB2	9:C:1510:HOH:O	2.06	0.55
2:C:249:LYS:HB3	9:C:1545:HOH:O	2.06	0.55
2:C:250:ARG:HG2	2:C:253:ALA:HB3	1.89	0.55
3:D:1224:VAL:HG11	9:D:2435:HOH:O	2.04	0.55
3:D:148:GLU:HG2	3:D:151:GLN:CD	2.27	0.55
3:D:153:LEU:HD11	3:D:158:TYR:N	2.20	0.55
3:D:211:VAL:CG1	3:D:393:ILE:HG13	2.37	0.55
3:D:27:GLU:O	3:D:28:LYS:HD2	2.06	0.55
3:D:699:VAL:H	3:D:756:GLN:HE22	1.52	0.55
5:F:125:ASP:HA	5:F:128:ARG:CZ	2.37	0.55
5:F:255:ALA:HB3	9:F:662:HOH:O	2.06	0.55
2:M:22:GLN:HE22	2:M:336:VAL:HG21	1.67	0.55
2:M:63:GLY:O	2:M:103:LYS:HE2	2.06	0.55
3:N:1020:LEU:HA	3:N:1023:MET:HE2	1.89	0.55
3:N:1201:CYS:HB3	9:N:9751:HOH:O	2.07	0.55
3:N:1279:GLY:O	3:N:1318:TYR:HA	2.05	0.55
3:N:208:PRO:CB	3:N:395:VAL:HG13	2.33	0.55
4:O:59:ASN:HB2	9:O:3650:HOH:O	2.06	0.55
5:P:287:THR:C	5:P:289:GLU:H	2.10	0.55
1:A:42:ARG:HG2	1:A:42:ARG:HH11	1.71	0.55
2:C:176:VAL:C	2:C:178:PRO:HD3	2.26	0.55
2:C:193:LEU:HA	9:C:1346:HOH:O	2.06	0.55
3:D:1310:ARG:CD	3:D:1310:ARG:H	2.19	0.55
3:D:230:TRP:HA	9:D:9066:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:395:VAL:HG23	9:D:9389:HOH:O	2.06	0.55
3:D:409:VAL:HG21	9:F:551:HOH:O	2.06	0.55
3:D:493:ARG:NE	3:D:1388:ARG:HB3	2.20	0.55
3:D:531:ASP:C	3:D:533:GLY:H	2.07	0.55
3:D:923:GLY:N	9:D:9237:HOH:O	2.38	0.55
1:K:95:GLN:HG3	9:K:3698:HOH:O	2.07	0.55
2:M:136:ILE:HG21	2:M:336:VAL:HG13	1.88	0.55
3:N:16:GLU:HB2	9:N:2292:HOH:O	2.06	0.55
3:N:629:SER:HB3	9:N:9650:HOH:O	2.04	0.55
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.87	0.55
5:P:166:LEU:HA	9:P:3458:HOH:O	2.06	0.55
2:M:1021:LEU:HD22	5:P:331:ASP:O	2.07	0.55
5:P:385:GLU:O	5:P:397:ILE:HD13	2.06	0.55
1:A:19:GLU:HB2	9:A:348:HOH:O	2.05	0.55
1:B:38:ASN:HB3	9:B:384:HOH:O	2.05	0.55
2:C:713:ARG:HD3	9:C:1752:HOH:O	2.06	0.55
3:D:1033:GLN:HE21	3:D:1036:ARG:NH1	2.04	0.55
3:D:1123:PHE:CE2	3:D:1184:GLN:HA	2.41	0.55
3:D:152:LEU:HD21	9:D:2148:HOH:O	2.06	0.55
3:D:152:LEU:HD23	3:D:152:LEU:H	1.70	0.55
3:D:424:GLY:HA2	3:D:436:GLU:HA	1.88	0.55
2:C:983:ILE:HG23	3:D:944:THR:O	2.06	0.55
5:F:151:LEU:HD21	9:F:614:HOH:O	2.06	0.55
5:F:375:LEU:HD13	9:F:731:HOH:O	2.05	0.55
2:M:1102:LEU:HB2	3:N:7:LYS:CG	2.31	0.55
2:M:332:ARG:HG3	9:M:1433:HOH:O	2.04	0.55
2:M:979:THR:HG23	2:M:981:GLU:HB2	1.88	0.55
3:N:1281:VAL:HG23	3:N:1317:ASP:O	2.07	0.55
4:O:33:HIS:CD2	4:O:89:MET:HG2	2.40	0.55
5:P:112:ALA:HA	5:P:173:TYR:HD2	1.70	0.55
5:P:132:ARG:HE	5:P:184:ARG:HH12	1.54	0.55
5:P:272:SER:HB3	9:P:3990:HOH:O	2.06	0.55
5:P:321:ILE:HG22	5:P:322:GLY:N	2.21	0.55
5:P:369:LEU:O	5:P:373:LYS:HB2	2.07	0.55
1:B:19:GLU:HG3	1:B:201:THR:O	2.06	0.55
1:B:211:LEU:O	1:B:215:VAL:HG13	2.06	0.55
2:C:149:THR:HG22	9:C:1612:HOH:O	2.07	0.55
2:C:204:GLN:NE2	2:C:222:MET:HA	2.21	0.55
2:C:285:LEU:HD12	2:C:288:ARG:O	2.06	0.55
2:C:660:ALA:HB1	2:C:667:ALA:O	2.07	0.55
3:D:1008:PHE:HB3	9:D:2325:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1541:HOH:O	3:D:1471:LEU:HA	2.07	0.55
3:D:93:ILE:HD13	3:D:547:LEU:HD23	1.87	0.55
3:D:576:GLU:HA	3:D:579:ASP:OD2	2.07	0.55
5:F:152:ASP:HB2	5:F:153:PRO:HD3	1.89	0.55
3:D:423:ASP:OD2	5:F:174:LEU:HD22	2.07	0.55
2:M:860:HIS:N	9:M:1226:HOH:O	2.39	0.55
3:N:1362:LYS:HD3	9:N:9859:HOH:O	2.07	0.55
3:N:225:LEU:HA	9:N:9604:HOH:O	2.07	0.55
3:N:428:LYS:HB3	3:N:450:TYR:HE1	1.72	0.55
5:P:244:ARG:HG3	5:P:244:ARG:NH1	2.21	0.55
2:C:218:VAL:HA	2:C:221:LEU:HD23	1.88	0.55
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.86	0.55
3:D:1468:LEU:HD23	3:D:1468:LEU:O	2.05	0.55
5:F:94:LEU:HD22	5:F:97:GLU:HG2	1.89	0.55
1:K:150:TYR:CE1	2:M:696:LYS:HA	2.41	0.55
2:M:1106:ASP:HB3	9:M:1439:HOH:O	2.06	0.55
2:M:758:ARG:HB3	2:M:788:THR:O	2.06	0.55
2:M:928:LYS:HB3	9:M:1297:HOH:O	2.06	0.55
3:N:105:VAL:HG13	3:N:124:GLU:OE1	2.07	0.55
3:N:1362:LYS:HE3	9:N:9889:HOH:O	2.06	0.55
3:N:1468:LEU:HD23	3:N:1468:LEU:O	2.06	0.55
3:N:402:PRO:HG2	3:N:444:VAL:HG11	1.89	0.55
5:P:335:ASP:OD1	5:P:338:LEU:HB2	2.07	0.55
5:P:351:SER:O	5:P:355:GLU:HB2	2.07	0.55
1:A:26:GLU:HB3	9:A:331:HOH:O	2.06	0.55
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.40	0.55
2:C:535:SER:H	2:C:538:GLN:NE2	2.04	0.55
3:D:1291:SER:HB2	3:D:1293:PHE:HE1	1.71	0.55
3:D:135:LEU:HD11	3:D:139:GLY:HA3	1.88	0.55
5:F:274:THR:O	5:F:278:LEU:HG	2.06	0.55
5:F:364:ARG:HB3	9:F:765:HOH:O	2.07	0.55
1:L:73:GLU:HB3	1:L:77:GLU:CG	2.36	0.55
2:M:1040:LEU:HG	2:M:1045:ALA:HB3	1.88	0.55
3:N:1038:LEU:O	3:N:1060:SER:HB2	2.07	0.55
3:N:1428:ALA:O	3:N:1431:THR:HG22	2.07	0.55
3:N:422:ALA:H	3:N:427:VAL:CG1	2.19	0.55
3:N:427:VAL:HB	3:N:435:VAL:CG2	2.37	0.55
3:N:543:LEU:HD23	9:N:9308:HOH:O	2.07	0.55
5:P:105:LYS:NZ	5:P:179:GLU:HB3	2.22	0.55
5:P:192:LEU:O	5:P:196:VAL:HG23	2.07	0.55
1:A:198:ARG:HB2	1:A:200:TRP:CH2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HH12	2:C:857:ASP:CB	2.01	0.55
2:C:1101:THR:HB	3:D:5:VAL:HG13	1.87	0.55
2:C:320:HIS:HB3	9:C:2145:HOH:O	2.06	0.55
2:C:437:ARG:HE	2:C:469:THR:N	2.05	0.55
2:C:802:ARG:HG2	9:C:1991:HOH:O	2.07	0.55
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.88	0.55
3:D:380:GLU:O	3:D:382:GLU:N	2.39	0.55
2:M:146:VAL:HG13	2:M:161:SER:O	2.07	0.55
2:M:861:LEU:HD22	2:M:863:ASP:OD1	2.06	0.55
3:N:1045:MET:HB2	9:N:2112:HOH:O	2.06	0.55
3:N:1282:ARG:HD3	3:N:1295:GLU:OE1	2.07	0.55
3:N:380:GLU:O	3:N:382:GLU:N	2.39	0.55
3:N:973:GLN:HA	3:N:976:GLN:NE2	2.18	0.55
5:P:261:PRO:HB3	9:P:5968:HOH:O	2.07	0.55
1:A:9:PRO:HB3	1:A:25:LEU:HD11	1.89	0.55
1:B:184:THR:HB	1:B:194:LYS:NZ	2.22	0.55
2:C:208:ALA:HB1	2:C:218:VAL:HG13	1.88	0.55
2:C:302:VAL:HG12	9:C:1479:HOH:O	2.06	0.55
2:C:347:GLY:HA2	2:C:350:ARG:HD2	1.89	0.55
2:C:360:LEU:HD12	9:C:1422:HOH:O	2.06	0.55
3:D:1164:ARG:HA	9:D:9172:HOH:O	2.06	0.55
3:D:207:PHE:CB	3:D:208:PRO:HD2	2.35	0.55
5:F:107:GLU:HG2	9:F:554:HOH:O	2.07	0.55
1:K:211:LEU:O	1:K:215:VAL:HG22	2.07	0.55
1:L:41:ARG:NH1	1:L:177:VAL:HG23	2.21	0.55
2:M:173:ASP:O	2:M:184:MET:HA	2.06	0.55
2:M:319:GLY:HA3	9:M:1194:HOH:O	2.06	0.55
2:M:607:ASP:HB3	2:M:609:ASN:H	1.71	0.55
2:M:742:VAL:HG12	2:M:743:VAL:N	2.22	0.55
3:N:1058:ARG:HH11	3:N:1058:ARG:HG3	1.72	0.55
3:N:593:ASN:CG	5:P:206:GLY:HA2	2.27	0.55
3:N:68:PHE:O	3:N:71:LYS:HG2	2.07	0.55
1:A:13:VAL:HG12	1:A:15:THR:HG22	1.89	0.55
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.38	0.55
2:C:186:VAL:HG23	9:C:1478:HOH:O	2.06	0.55
2:C:313:LEU:CA	2:C:321:GLU:HG3	2.36	0.55
2:C:351:LEU:HG	9:C:1597:HOH:O	2.07	0.55
2:C:135:VAL:O	2:C:392:SER:HA	2.07	0.55
2:C:697:ARG:HA	9:C:1783:HOH:O	2.07	0.55
3:D:1159:ARG:HB2	9:D:9819:HOH:O	2.07	0.55
3:D:1262:LEU:HD23	3:D:1352:ILE:CG1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1468:LEU:HD22	3:D:1470:ARG:HB2	1.89	0.55
3:D:459:GLU:HG2	9:D:9650:HOH:O	2.07	0.55
3:D:493:ARG:CZ	3:D:1388:ARG:HB3	2.37	0.55
3:D:805:GLU:OE1	3:D:809:PRO:HD2	2.07	0.55
4:E:31:LEU:HD12	4:E:32:ARG:HD3	1.89	0.55
5:F:361:LEU:HD23	5:F:362:SER:OG	2.07	0.55
5:F:393:THR:HG21	9:F:866:HOH:O	2.07	0.55
1:L:137:ARG:HB2	9:L:5311:HOH:O	2.07	0.55
1:L:30:ARG:NH2	2:M:854:PRO:HG3	2.22	0.55
3:N:1267:ARG:NH2	3:N:1271:LYS:HD2	2.22	0.55
3:N:566:ILE:HG12	5:P:217:ASN:ND2	2.21	0.55
3:N:602:SER:O	3:N:606:ILE:HG12	2.07	0.55
1:A:109:VAL:HG23	1:A:132:LEU:HD13	1.88	0.54
1:A:184:THR:HG23	1:A:192:LEU:HD12	1.88	0.54
2:C:1085:PHE:CE2	3:D:1468:LEU:HA	2.42	0.54
2:C:333:ILE:HD11	2:C:467:ILE:HG13	1.89	0.54
2:C:534:VAL:H	2:C:538:GLN:HE22	1.56	0.54
2:C:601:GLY:O	2:C:648:ARG:HA	2.07	0.54
2:C:79:PRO:HD3	9:C:1934:HOH:O	2.07	0.54
2:C:866:PRO:HD2	9:C:1297:HOH:O	2.07	0.54
2:C:86:LYS:HE2	9:C:1713:HOH:O	2.06	0.54
3:D:1086:LEU:N	6:D:8001:STD:H32	2.22	0.54
3:D:209:ARG:HH22	3:D:397:LYS:HG3	1.71	0.54
3:D:584:ASN:ND2	3:D:590:PRO:HD2	2.22	0.54
2:M:1116:ALA:HB3	9:M:1163:HOH:O	2.06	0.54
3:N:105:VAL:HG21	3:N:128:TYR:CE2	2.42	0.54
3:N:211:VAL:HG13	3:N:393:ILE:HA	1.90	0.54
3:N:80:VAL:HG23	9:N:9633:HOH:O	2.06	0.54
3:N:844:ALA:O	3:N:867:ARG:HB3	2.06	0.54
5:P:291:ILE:O	5:P:295:MET:HB2	2.07	0.54
1:A:116:PRO:HD3	9:A:510:HOH:O	2.06	0.54
1:A:26:GLU:HG2	1:A:27:PRO:HG3	1.88	0.54
2:C:418:LEU:HD22	2:C:418:LEU:N	2.23	0.54
2:C:464:LEU:O	2:C:466:PHE:N	2.40	0.54
2:C:405:ARG:NH2	2:C:566:THR:HG21	2.22	0.54
2:C:643:VAL:HG13	2:C:647:GLN:OE1	2.08	0.54
2:C:666:LEU:HD21	9:C:1827:HOH:O	2.07	0.54
3:D:1103:HIS:CD2	3:D:1463:LYS:H	2.25	0.54
3:D:135:LEU:CD1	3:D:147:VAL:HG23	2.35	0.54
3:D:215:TYR:O	3:D:389:GLU:HB2	2.08	0.54
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:965:GLU:HB2	9:D:9143:HOH:O	2.06	0.54
1:L:38:ASN:HB3	1:L:39:PRO:HD3	1.90	0.54
2:M:165:LEU:HD12	2:M:166:PRO:C	2.28	0.54
2:M:170:PRO:HD3	2:M:263:ASP:HB3	1.89	0.54
2:M:231:PRO:HA	9:M:2063:HOH:O	2.06	0.54
3:N:1127:GLU:CB	3:N:1133:ARG:HH12	2.21	0.54
3:N:1182:GLU:HG2	9:N:2291:HOH:O	2.06	0.54
3:N:1396:GLU:O	3:N:1400:VAL:HG23	2.07	0.54
3:N:1502:ALA:HB3	9:N:2086:HOH:O	2.08	0.54
3:N:423:ASP:OD1	5:P:174:LEU:HD13	2.06	0.54
3:N:584:ASN:CG	3:N:590:PRO:HD2	2.27	0.54
3:N:656:PHE:CE2	3:N:698:LYS:HE3	2.42	0.54
3:N:661:MET:CE	3:N:677:LEU:HD11	2.37	0.54
3:N:829:VAL:HA	9:N:9025:HOH:O	2.06	0.54
3:N:996:TRP:HE3	3:N:999:THR:HG21	1.71	0.54
2:C:140:ILE:HD11	9:C:1460:HOH:O	2.06	0.54
2:C:285:LEU:HD23	2:C:285:LEU:O	2.07	0.54
2:C:32:ALA:HB2	2:C:73:LEU:HD21	1.89	0.54
3:D:1063:GLU:HB2	9:D:9009:HOH:O	2.06	0.54
3:D:1090:ASP:O	3:D:1093:TYR:HB3	2.06	0.54
3:D:126:VAL:HG12	3:D:132:TYR:HB2	1.87	0.54
3:D:104:PHE:CD2	3:D:1448:THR:HG23	2.43	0.54
5:F:132:ARG:O	5:F:136:LEU:HG	2.07	0.54
5:F:142:ARG:NH1	5:F:150:THR:HG21	2.23	0.54
1:K:198:ARG:HD3	1:K:200:TRP:HH2	1.72	0.54
1:K:5:LYS:O	1:K:8:ALA:HB2	2.07	0.54
1:L:91:ASN:O	1:L:94:LEU:HD12	2.08	0.54
2:M:176:VAL:HG12	2:M:182:VAL:CG1	2.33	0.54
2:M:276:LYS:O	2:M:280:LYS:HB2	2.08	0.54
2:M:33:ASP:OD1	2:M:34:VAL:HG13	2.07	0.54
2:M:464:LEU:O	2:M:466:PHE:N	2.41	0.54
2:M:839:LEU:HD21	2:M:849:VAL:HG23	1.90	0.54
2:M:674:VAL:HG23	2:M:869:VAL:O	2.07	0.54
2:M:862:PRO:HA	2:M:975:TYR:CE1	2.41	0.54
3:N:104:PHE:CE2	3:N:1448:THR:HG23	2.42	0.54
3:N:399:ARG:HB3	3:N:402:PRO:HG3	1.90	0.54
3:N:416:ALA:HB3	3:N:417:PRO:HD3	1.89	0.54
1:A:198:ARG:C	1:A:199:ILE:HD12	2.27	0.54
1:B:44:LEU:HD21	1:B:199:ILE:HD13	1.88	0.54
2:C:196:LEU:HD13	2:C:303:PHE:CZ	2.41	0.54
2:C:198:ARG:HH21	2:C:204:GLN:H	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:486:MET:SD	2:C:491:GLU:HA	2.46	0.54
2:C:530:GLU:HA	9:C:1437:HOH:O	2.06	0.54
2:C:881:ASN:HD22	2:C:881:ASN:H	1.56	0.54
3:D:130:SER:HB3	3:D:132:TYR:CE1	2.42	0.54
3:D:513:ILE:HA	9:D:2414:HOH:O	2.06	0.54
3:D:571:LYS:HB2	3:D:571:LYS:NZ	2.23	0.54
3:D:583:ASP:HA	3:D:602:SER:OG	2.07	0.54
3:D:679:ARG:HD2	9:D:9184:HOH:O	2.07	0.54
4:E:86:GLN:O	4:E:90:GLU:HG3	2.07	0.54
5:F:152:ASP:HA	9:F:446:HOH:O	2.06	0.54
5:F:260:ILE:CG2	5:F:264:MET:HB2	2.35	0.54
1:K:3:ASP:HB2	9:K:4710:HOH:O	2.07	0.54
1:L:123:MET:O	1:L:125:PRO:HD3	2.08	0.54
1:L:24:VAL:HG23	9:L:5344:HOH:O	2.08	0.54
2:M:798:GLY:H	2:M:827:VAL:CG1	2.20	0.54
3:N:102:ILE:HB	9:N:2184:HOH:O	2.08	0.54
3:N:1104:GLU:O	3:N:1106:VAL:HG23	2.07	0.54
3:N:478:LEU:HD22	3:N:1388:ARG:NH2	2.22	0.54
3:N:134:VAL:HG12	3:N:152:LEU:HB3	1.90	0.54
3:N:430:ASP:HB2	3:N:432:TYR:CE2	2.42	0.54
3:N:464:LEU:HD11	9:N:9332:HOH:O	2.07	0.54
3:N:130:SER:O	3:N:568:ARG:NH2	2.40	0.54
3:N:681:ARG:HG3	3:N:682:ASP:OD1	2.08	0.54
3:N:69:GLU:HA	9:N:9077:HOH:O	2.08	0.54
4:O:33:HIS:HB2	4:O:37:ASN:ND2	2.23	0.54
4:O:54:LEU:O	4:O:54:LEU:HD23	2.08	0.54
5:P:420:ASP:HB2	9:P:5127:HOH:O	2.07	0.54
1:A:24:VAL:HG12	9:A:331:HOH:O	2.07	0.54
2:C:173:ASP:O	2:C:184:MET:HA	2.07	0.54
2:C:182:VAL:HG21	9:C:1151:HOH:O	2.07	0.54
2:C:274:ARG:CD	2:C:285:LEU:HD22	2.36	0.54
2:C:380:ALA:O	2:C:384:GLU:HB2	2.07	0.54
2:C:69:LEU:HD21	2:C:99:GLN:NE2	2.22	0.54
3:D:209:ARG:HE	3:D:210:ARG:HD3	1.72	0.54
9:C:1424:HOH:O	3:D:3:LYS:HE3	2.07	0.54
3:D:767:HIS:NE2	4:E:6:ILE:HG12	2.23	0.54
2:C:423:ALA:HB2	6:D:8001:STD:C10	2.38	0.54
2:M:260:LEU:HG	2:M:261:ILE:HG13	1.88	0.54
2:M:409:ARG:HA	2:M:454:SER:CA	2.35	0.54
2:M:669:GLY:C	2:M:670:GLN:HG3	2.28	0.54
3:N:1335:LEU:HD21	9:N:9791:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:123:LEU:HD21	3:N:152:LEU:HD22	1.89	0.54
3:N:181:ASP:HB3	9:N:9482:HOH:O	2.08	0.54
3:N:428:LYS:HB3	3:N:450:TYR:CE1	2.43	0.54
3:N:52:PRO:HB3	3:N:80:VAL:HG13	1.89	0.54
3:N:560:GLN:HB2	9:P:5398:HOH:O	2.07	0.54
3:N:661:MET:SD	3:N:673:ALA:HB1	2.47	0.54
1:A:92:PRO:HD3	9:A:335:HOH:O	2.07	0.54
2:C:105:THR:HG23	9:C:1683:HOH:O	2.06	0.54
2:C:142:ARG:NH1	2:C:325:ILE:HG12	2.22	0.54
2:C:28:ARG:HG3	2:C:40:GLU:OE1	2.08	0.54
2:C:534:VAL:HB	2:C:538:GLN:CD	2.27	0.54
2:C:577:PRO:HG3	2:C:993:PHE:CE2	2.43	0.54
2:C:604:ALA:HB3	2:C:612:VAL:O	2.08	0.54
3:D:628:ARG:HG2	9:D:9834:HOH:O	2.07	0.54
3:D:774:SER:C	3:D:776:GLU:H	2.11	0.54
3:D:865:THR:HG21	9:D:9950:HOH:O	2.08	0.54
3:D:966:GLU:O	3:D:969:ARG:HG2	2.07	0.54
4:E:33:HIS:CD2	4:E:89:MET:HG2	2.42	0.54
5:F:407:LYS:HD3	9:F:714:HOH:O	2.08	0.54
1:K:100:LEU:HG	9:K:3937:HOH:O	2.08	0.54
2:M:264:PRO:HB3	2:M:289:THR:CB	2.37	0.54
2:M:380:ALA:HB2	9:M:1838:HOH:O	2.08	0.54
2:M:707:ARG:HG3	2:M:826:TYR:CE2	2.42	0.54
2:M:564:MET:HG2	2:M:840:ALA:HB3	1.90	0.54
3:N:1380:GLU:OE2	3:N:1390:LEU:HD22	2.07	0.54
3:N:422:ALA:HB2	9:N:9964:HOH:O	2.07	0.54
3:N:459:GLU:HG3	3:N:460:ALA:N	2.22	0.54
3:N:49:ILE:HB	3:N:50:PHE:CD1	2.43	0.54
3:N:584:ASN:ND2	3:N:590:PRO:HD2	2.23	0.54
3:N:624:ASP:HB3	3:N:625:TYR:CD1	2.42	0.54
3:N:661:MET:HE2	3:N:677:LEU:HD11	1.89	0.54
5:P:135:ILE:HD12	9:P:4903:HOH:O	2.07	0.54
5:P:374:GLY:HA3	9:P:5465:HOH:O	2.08	0.54
1:A:11:PHE:CD1	1:A:25:LEU:HD13	2.41	0.54
2:C:1105:LYS:HA	9:C:2031:HOH:O	2.07	0.54
2:C:233:GLU:HB2	9:C:1569:HOH:O	2.08	0.54
2:C:281:LEU:HD11	2:C:306:THR:HA	1.90	0.54
2:C:325:ILE:HD12	9:C:1988:HOH:O	2.07	0.54
2:C:402:SER:OG	2:C:566:THR:HG22	2.07	0.54
2:C:717:LEU:HD12	9:C:1324:HOH:O	2.07	0.54
2:C:722:ILE:CG2	2:C:805:ARG:HH21	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:793:PRO:HD2	9:C:2039:HOH:O	2.05	0.54
3:D:15:PRO:HA	3:D:18:ILE:CG1	2.38	0.54
2:M:209:ARG:O	2:M:213:ALA:HB2	2.07	0.54
2:M:257:VAL:HG13	9:M:1389:HOH:O	2.08	0.54
2:M:305:PRO:CG	2:M:308:ARG:HH21	2.21	0.54
2:M:143:SER:HB3	2:M:330:ASN:O	2.07	0.54
2:M:41:ASN:HB3	9:M:1869:HOH:O	2.06	0.54
2:M:604:ALA:HB3	2:M:612:VAL:O	2.08	0.54
2:M:717:LEU:HD12	2:M:761:PHE:HB2	1.89	0.54
3:N:1310:ARG:HG3	3:N:1327:ARG:HB2	1.90	0.54
3:N:1395:LEU:HG	9:N:2029:HOH:O	2.08	0.54
2:C:433:THR:HA	9:C:1158:HOH:O	2.06	0.54
2:C:53:PRO:HA	9:C:1326:HOH:O	2.08	0.54
2:C:724:ARG:NE	2:C:737:LEU:O	2.41	0.54
3:D:992:ILE:O	3:D:995:LEU:HB3	2.08	0.54
5:F:100:VAL:HG23	9:F:444:HOH:O	2.07	0.54
5:F:220:LEU:HD21	9:F:598:HOH:O	2.06	0.54
5:F:282:LEU:HD12	5:F:284:ARG:O	2.08	0.54
2:M:1098:ASP:HB2	3:N:21:TRP:HZ2	1.71	0.54
2:M:139:GLN:HE21	2:M:334:ARG:HD2	1.71	0.54
3:N:542:ASP:O	3:N:546:ARG:HG2	2.08	0.54
3:N:863:VAL:HA	9:N:9076:HOH:O	2.07	0.54
5:P:260:ILE:HD11	5:P:310:ILE:CG2	2.36	0.54
1:A:30:ARG:HG2	9:D:2211:HOH:O	2.08	0.54
1:A:29:GLU:HB2	1:A:32:PHE:CD1	2.43	0.54
2:C:290:LEU:HB2	9:C:1479:HOH:O	2.08	0.54
2:C:359:MET:HB2	9:C:1415:HOH:O	2.07	0.54
3:D:1057:VAL:HG13	3:D:1069:GLU:HB3	1.89	0.54
3:D:1487:VAL:CG1	3:D:1492:LEU:HG	2.38	0.54
3:D:465:LEU:HG	9:D:9464:HOH:O	2.08	0.54
3:D:478:LEU:HD13	3:D:1388:ARG:NH2	2.22	0.54
3:D:525:ARG:HB2	3:D:541:ASN:HD21	1.73	0.54
3:D:519:VAL:HA	3:D:544:TYR:OH	2.08	0.54
3:D:668:PRO:HD2	3:D:672:ALA:CB	2.38	0.54
3:D:742:GLY:HA3	9:D:2453:HOH:O	2.07	0.54
1:K:63:HIS:HD2	1:K:65:PHE:H	1.56	0.54
2:M:144:PRO:HA	2:M:163:ILE:CG1	2.37	0.54
2:M:853:LEU:HB3	2:M:858:MET:HE3	1.88	0.54
3:N:1077:ALA:HA	9:N:9068:HOH:O	2.06	0.54
3:N:1459:LEU:HD13	3:N:1465:ASN:ND2	2.23	0.54
3:N:961:LYS:HG3	3:N:962:GLN:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:994:GLN:HA	3:N:994:GLN:HE21	1.72	0.54
2:C:176:VAL:HG12	2:C:182:VAL:HG13	1.89	0.54
2:C:198:ARG:HH21	2:C:204:GLN:CG	2.21	0.54
2:C:410:ILE:HB	9:C:1130:HOH:O	2.08	0.54
2:C:431:HIS:CD2	2:C:433:THR:H	2.25	0.54
2:C:513:VAL:HG23	9:C:1298:HOH:O	2.06	0.54
2:C:682:TYR:HB3	2:C:689:VAL:HG22	1.89	0.54
2:C:630:ARG:HH22	2:C:706:GLU:C	2.12	0.54
2:C:774:LEU:HG	9:C:1519:HOH:O	2.08	0.54
2:C:775:ARG:NH2	2:C:782:ALA:HB1	2.11	0.54
2:C:791:ARG:O	2:C:793:PRO:HD3	2.08	0.54
2:C:91:GLN:OE1	2:C:117:HIS:HB3	2.07	0.54
3:D:391:ALA:HB3	9:D:9395:HOH:O	2.07	0.54
3:D:525:ARG:HA	3:D:538:SER:CB	2.38	0.54
3:D:929:ARG:HH11	3:D:929:ARG:HG3	1.73	0.54
5:F:138:SER:HB2	5:F:140:ARG:HG2	1.90	0.54
1:K:20:TYR:CD2	1:K:21:GLY:N	2.76	0.54
1:L:133:GLU:HB2	9:L:5764:HOH:O	2.08	0.54
1:L:185:ARG:HA	9:L:5714:HOH:O	2.08	0.54
1:L:204:SER:HA	9:L:3964:HOH:O	2.08	0.54
2:M:399:ASN:HB3	2:M:568:ALA:O	2.07	0.54
2:M:601:GLY:O	2:M:648:ARG:HA	2.08	0.54
2:M:650:ARG:CG	2:M:653:ASP:HB2	2.37	0.54
2:M:834:GLN:HG2	9:M:1208:HOH:O	2.07	0.54
2:M:976:ASP:HB2	2:M:979:THR:HG22	1.89	0.54
2:M:998:TYR:CE2	2:M:1000:MET:HG2	2.42	0.54
3:N:1018:ASN:O	3:N:1022:VAL:HG23	2.08	0.54
3:N:1097:LYS:HA	9:N:9338:HOH:O	2.06	0.54
3:N:127:LEU:HD11	3:N:461:ILE:HD11	1.90	0.54
3:N:1291:SER:HB2	9:N:9921:HOH:O	2.07	0.54
3:N:758:GLU:HG2	4:O:20:THR:HG23	1.90	0.54
5:P:264:MET:HA	9:P:5687:HOH:O	2.08	0.54
5:P:299:TRP:HH2	5:P:307:THR:HG21	1.73	0.54
2:C:1086:ARG:HD2	3:D:88:TYR:OH	2.08	0.53
2:C:504:GLU:CD	2:C:509:ALA:HB2	2.29	0.53
1:L:127:LEU:HD11	9:L:4237:HOH:O	2.07	0.53
1:L:143:ARG:HH11	1:L:158:ILE:HG23	1.73	0.53
1:L:88:ARG:HH11	1:L:88:ARG:HG2	1.72	0.53
2:M:998:TYR:CZ	2:M:1000:MET:HA	2.44	0.53
2:M:408:ARG:NH1	2:M:542:VAL:HG22	2.23	0.53
2:M:525:SER:OG	2:M:527:GLU:HG3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:971:LYS:HA	2:M:988:VAL:HA	1.90	0.53
3:N:1065:LEU:HD13	3:N:1069:GLU:HB2	1.89	0.53
3:N:120:ALA:HB2	9:N:9789:HOH:O	2.08	0.53
3:N:131:LYS:HA	3:N:456:MET:HG3	1.89	0.53
3:N:1459:LEU:HD23	3:N:1464:GLU:HG3	1.90	0.53
3:N:969:ARG:O	3:N:972:LEU:HB3	2.07	0.53
5:P:153:PRO:HG2	5:P:154:LYS:H	1.73	0.53
1:B:143:ARG:HD3	1:B:158:ILE:HG21	1.90	0.53
2:C:193:LEU:HD12	9:C:1346:HOH:O	2.08	0.53
2:C:308:ARG:HD2	9:C:1789:HOH:O	2.07	0.53
2:C:430:VAL:HG11	3:D:1074:SER:HB2	1.89	0.53
3:D:1310:ARG:NE	3:D:1310:ARG:H	2.06	0.53
3:D:1434:TRP:CZ3	3:D:1457:ASP:HB2	2.43	0.53
3:D:191:LEU:HB3	3:D:195:VAL:HG21	1.91	0.53
3:D:601:ARG:HD2	5:F:328:PHE:CE1	2.43	0.53
3:D:720:LEU:CD1	3:D:720:LEU:H	2.18	0.53
5:F:396:ARG:HG2	9:F:810:HOH:O	2.08	0.53
1:K:225:PHE:HE1	1:L:25:LEU:HD22	1.72	0.53
2:M:197:LEU:HD22	2:M:202:TYR:HD2	1.72	0.53
2:M:542:VAL:HG23	2:M:543:ASN:H	1.73	0.53
2:M:612:VAL:HG22	2:M:622:GLU:HA	1.89	0.53
2:M:660:ALA:HB1	2:M:667:ALA:O	2.08	0.53
2:M:678:PRO:HA	2:M:683:ASN:HD21	1.73	0.53
2:M:943:VAL:HG11	2:M:973:VAL:HG22	1.90	0.53
2:M:975:TYR:HA	2:M:982:PRO:HA	1.89	0.53
3:N:116:LEU:HD23	9:N:9142:HOH:O	2.08	0.53
3:N:1314:LYS:HE2	3:N:1317:ASP:OD2	2.07	0.53
3:N:1465:ASN:ND2	3:N:1470:ARG:HD3	2.23	0.53
3:N:787:LEU:HD21	3:N:947:ILE:CD1	2.38	0.53
3:N:969:ARG:HD2	9:N:9270:HOH:O	2.08	0.53
5:P:201:LYS:HE2	9:P:5773:HOH:O	2.06	0.53
1:A:95:GLN:CA	1:A:146:ARG:HH12	2.16	0.53
1:A:36:LEU:O	1:A:40:LEU:HG	2.07	0.53
2:C:1060:ILE:HD12	2:C:1063:ARG:NH1	2.23	0.53
2:C:668:LEU:HD12	2:C:668:LEU:N	2.24	0.53
2:C:780:GLU:HG3	2:C:781:LYS:H	1.72	0.53
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.49	0.53
2:C:944:LEU:HD11	2:C:963:LEU:HD21	1.89	0.53
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.39	0.53
3:D:1396:GLU:O	3:D:1400:VAL:HG23	2.08	0.53
3:D:153:LEU:HD12	3:D:154:THR:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:662:GLU:CD	3:D:669:ASN:HA	2.28	0.53
4:E:72:ARG:HH11	4:E:72:ARG:HG2	1.72	0.53
5:F:102:LEU:O	5:F:106:VAL:HG23	2.08	0.53
1:L:20:TYR:HE2	1:L:198:ARG:HB3	1.73	0.53
1:L:227:ASN:H	1:L:227:ASN:ND2	2.06	0.53
3:N:1003:VAL:O	3:N:1007:VAL:HG13	2.07	0.53
3:N:1112:CYS:HB2	3:N:1195:GLN:CD	2.29	0.53
3:N:52:PRO:CG	3:N:80:VAL:HG22	2.39	0.53
3:N:54:LYS:HG3	3:N:57:GLU:HB3	1.90	0.53
3:N:957:PRO:HB3	3:N:959:GLU:OE1	2.08	0.53
3:N:1485:GLN:NE2	4:O:80:VAL:H	2.03	0.53
5:P:256:ARG:HD2	9:P:3830:HOH:O	2.07	0.53
1:A:94:LEU:HD11	1:A:119:ASP:HB3	1.89	0.53
1:B:94:LEU:HD11	1:B:119:ASP:HB3	1.90	0.53
2:C:1031:ARG:HH11	2:C:1031:ARG:HG3	1.74	0.53
2:C:282:GLY:N	2:C:308:ARG:NH2	2.55	0.53
2:C:341:THR:HG23	2:C:345:ARG:HH21	1.74	0.53
3:D:183:GLU:HA	3:D:186:VAL:HG12	1.91	0.53
3:D:181:ASP:O	3:D:185:VAL:HG23	2.09	0.53
3:D:566:ILE:HG22	5:F:214:GLN:HE22	1.74	0.53
1:K:8:ALA:HA	9:K:4167:HOH:O	2.08	0.53
9:K:6352:HOH:O	1:L:155:LYS:HD2	2.07	0.53
2:M:254:VAL:HG11	9:M:1618:HOH:O	2.08	0.53
2:M:815:LEU:HD21	2:M:820:ARG:O	2.07	0.53
2:M:798:GLY:H	2:M:827:VAL:HG11	1.74	0.53
2:M:943:VAL:CG2	2:M:985:GLY:H	2.19	0.53
3:N:957:PRO:HG3	3:N:1007:VAL:HA	1.90	0.53
3:N:1110:ALA:HB1	9:N:9543:HOH:O	2.08	0.53
3:N:1283:ILE:HG23	3:N:1290:LEU:HD21	1.90	0.53
3:N:754:PHE:CZ	4:O:21:VAL:HA	2.43	0.53
5:P:122:LEU:HD23	9:P:4172:HOH:O	2.07	0.53
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.39	0.53
2:C:113:VAL:HG22	9:C:1833:HOH:O	2.07	0.53
3:D:1045:MET:HB3	3:D:1072:ILE:HG22	1.89	0.53
3:D:1147:ARG:O	3:D:1166:LEU:HD23	2.08	0.53
3:D:1310:ARG:HG2	3:D:1327:ARG:HB3	1.90	0.53
3:D:526:PRO:O	3:D:537:THR:HA	2.08	0.53
3:D:551:ASN:O	3:D:555:LYS:HG3	2.09	0.53
3:D:710:ARG:HD2	3:D:772:PRO:HG2	1.89	0.53
5:F:243:ILE:O	5:F:247:ILE:HG13	2.09	0.53
1:K:101:LEU:HD21	1:K:113:ASP:HB3	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:39:PRO:O	1:K:43:ILE:HG12	2.08	0.53
2:M:1034:GLU:HA	2:M:1037:VAL:HG23	1.90	0.53
2:M:266:ARG:HB2	9:M:1427:HOH:O	2.07	0.53
2:M:137:VAL:HG22	2:M:391:LEU:O	2.09	0.53
2:M:723:THR:HG23	2:M:725:ASP:HB2	1.88	0.53
2:M:879:ARG:CZ	3:N:1029:ARG:HH12	2.21	0.53
3:N:12:LEU:HD22	3:N:511:TRP:CB	2.38	0.53
3:N:892:ASP:HB3	3:N:895:VAL:CG2	2.39	0.53
5:P:142:ARG:HG2	9:P:4970:HOH:O	2.07	0.53
5:P:363:GLU:HA	5:P:367:MET:HG2	1.90	0.53
1:B:47:SER:O	1:B:49:PRO:N	2.41	0.53
2:C:369:PRO:HG2	9:F:698:HOH:O	2.09	0.53
2:C:557:ARG:HB2	9:C:1189:HOH:O	2.08	0.53
3:D:1087:ARG:HG2	9:D:9918:HOH:O	2.08	0.53
3:D:168:THR:HA	9:D:9020:HOH:O	2.07	0.53
3:D:473:LEU:HD21	3:D:495:ARG:CZ	2.39	0.53
3:D:744:GLN:HB3	9:D:9834:HOH:O	2.08	0.53
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.08	0.53
5:F:299:TRP:CE3	5:F:303:ARG:HD3	2.44	0.53
1:K:54:THR:CG2	1:K:158:ILE:HG13	2.38	0.53
1:L:57:TYR:CE2	1:L:161:ARG:HG2	2.43	0.53
2:M:380:ALA:O	2:M:384:GLU:HB2	2.09	0.53
2:M:331:ARG:CZ	2:M:427:VAL:HG13	2.39	0.53
2:M:460:ARG:HD2	2:M:485:TYR:CD2	2.43	0.53
2:M:881:ASN:N	2:M:881:ASN:ND2	2.55	0.53
3:N:1235:GLN:HA	9:N:9533:HOH:O	2.08	0.53
3:N:172:PRO:HD2	3:N:389:GLU:O	2.08	0.53
1:L:65:PHE:CD1	3:N:813:LEU:HD22	2.38	0.53
5:P:164:LYS:HG2	9:P:5668:HOH:O	2.08	0.53
1:A:156:HIS:CD2	1:A:157:GLY:H	2.26	0.53
1:A:205:VAL:HG23	1:A:206:THR:N	2.24	0.53
1:B:170:VAL:HG22	9:B:364:HOH:O	2.07	0.53
2:C:141:HIS:HB3	2:C:418:LEU:HB3	1.91	0.53
2:C:663:ASN:N	9:C:2008:HOH:O	2.40	0.53
3:D:1209:LEU:HD23	3:D:1210:SER:N	2.23	0.53
3:D:1239:ARG:HA	9:D:2088:HOH:O	2.08	0.53
3:D:141:ILE:HD13	3:D:450:TYR:H	1.73	0.53
4:E:40:LEU:HD22	4:E:40:LEU:O	2.09	0.53
5:F:226:LYS:HE3	9:F:490:HOH:O	2.07	0.53
5:F:81:VAL:O	5:F:85:LEU:HG	2.09	0.53
1:L:110:LYS:HD2	1:L:112:ARG:HH12	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:59:GLU:HG3	1:L:139:ASN:ND2	2.23	0.53
2:M:163:ILE:HB	2:M:171:TRP:CH2	2.44	0.53
2:M:449:ILE:HG12	9:M:1213:HOH:O	2.09	0.53
2:M:748:GLU:HA	2:M:799:ILE:HG22	1.90	0.53
2:M:874:LEU:HD13	3:N:783:ARG:HB2	1.90	0.53
2:M:881:ASN:ND2	2:M:881:ASN:H	2.06	0.53
2:M:926:PHE:CE2	2:M:960:GLU:HG3	2.41	0.53
3:N:130:SER:HB3	3:N:132:TYR:CE1	2.44	0.53
3:N:18:ILE:HG23	3:N:518:PRO:CG	2.37	0.53
3:N:207:PHE:CB	3:N:208:PRO:HD2	2.34	0.53
3:N:488:ARG:HB3	3:N:488:ARG:NH1	2.24	0.53
3:N:58:CYS:HA	3:N:78:VAL:HG11	1.91	0.53
3:N:822:ALA:HB2	9:N:9137:HOH:O	2.08	0.53
1:B:76:VAL:HA	1:B:79:ILE:HG12	1.90	0.53
2:C:304:LEU:HD23	2:C:305:PRO:HD3	1.90	0.53
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.91	0.53
2:C:842:ARG:HH21	2:C:887:GLU:CD	2.12	0.53
3:D:1175:ILE:O	3:D:1179:GLU:HG3	2.09	0.53
3:D:567:ILE:HG22	3:D:571:LYS:NZ	2.23	0.53
2:C:1020:PRO:O	3:D:622:ARG:HD2	2.09	0.53
3:D:957:PRO:HG3	3:D:1007:VAL:HA	1.91	0.53
4:E:54:LEU:HD23	4:E:54:LEU:O	2.09	0.53
3:D:669:ASN:OD1	5:F:349:LEU:HD11	2.09	0.53
1:L:100:LEU:HB2	1:L:115:LEU:HD11	1.91	0.53
1:L:221:HIS:HA	1:L:224:TYR:CD2	2.44	0.53
1:L:95:GLN:N	1:L:95:GLN:HE21	2.06	0.53
2:M:1059:ASP:CG	2:M:1062:GLY:HA3	2.29	0.53
2:M:241:LEU:HD23	9:M:1478:HOH:O	2.08	0.53
2:M:569:VAL:HG12	2:M:996:LYS:O	2.09	0.53
2:M:773:LEU:HG	2:M:777:ILE:HD11	1.91	0.53
3:N:172:PRO:HB2	9:N:9436:HOH:O	2.08	0.53
3:N:77:GLY:O	3:N:78:VAL:HG23	2.09	0.53
1:L:176:ARG:HH22	3:N:884:ARG:HD3	1.73	0.53
1:A:182:GLU:HB2	9:A:512:HOH:O	2.09	0.53
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.89	0.53
2:C:163:ILE:HD12	9:C:1850:HOH:O	2.09	0.53
2:C:22:GLN:NE2	2:C:336:VAL:HG21	2.24	0.53
2:C:25:SER:HB2	2:C:335:THR:HB	1.90	0.53
2:C:266:ARG:HB2	9:C:1885:HOH:O	2.09	0.53
2:C:302:VAL:O	2:C:306:THR:HG23	2.09	0.53
2:C:41:ASN:HB3	9:C:1171:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:670:GLN:O	2:C:672:VAL:HG12	2.09	0.53
3:D:1192:LEU:HD21	3:D:1372:VAL:HG13	1.90	0.53
3:D:502:PHE:CE1	3:D:509:PRO:HB3	2.44	0.53
3:D:97:THR:CG2	3:D:571:LYS:HD3	2.37	0.53
1:K:216:GLU:O	1:K:220:GLU:HG3	2.09	0.53
2:M:1040:LEU:HG	2:M:1045:ALA:CB	2.39	0.53
2:M:148:PHE:CZ	2:M:281:LEU:HD13	2.44	0.53
2:M:282:GLY:HA2	2:M:308:ARG:HH22	1.73	0.53
2:M:626:ARG:HB2	2:M:639:GLN:NE2	2.12	0.53
2:M:890:LEU:HA	2:M:914:ILE:CD1	2.38	0.53
3:N:1432:LYS:CD	3:N:1433:SER:H	2.20	0.53
3:N:583:ASP:HA	3:N:602:SER:HB2	1.91	0.53
3:N:836:VAL:HA	3:N:839:LEU:HB2	1.91	0.53
2:M:987:ILE:HG23	3:N:948:THR:HG21	1.90	0.53
5:P:117:SER:OG	5:P:124:PRO:HG3	2.09	0.53
1:A:106:PRO:HB3	9:A:500:HOH:O	2.08	0.53
3:D:1044:LEU:HA	9:D:9902:HOH:O	2.09	0.53
3:D:1129:THR:HG23	3:D:1130:ARG:H	1.74	0.53
3:D:1132:LEU:HD23	9:D:2203:HOH:O	2.09	0.53
3:D:1217:ILE:HD12	3:D:1480:PHE:HE2	1.74	0.53
3:D:1333:HIS:O	3:D:1336:LEU:HB3	2.09	0.53
3:D:1361:VAL:HG23	9:D:9147:HOH:O	2.09	0.53
3:D:853:VAL:HG22	3:D:858:VAL:HG23	1.91	0.53
4:E:53:GLY:HA3	9:E:196:HOH:O	2.08	0.53
5:F:163:LEU:HD22	5:F:174:LEU:HG	1.91	0.53
5:F:207:LEU:HB3	5:F:212:LEU:HD12	1.91	0.53
1:K:198:ARG:HB2	1:K:200:TRP:CH2	2.44	0.53
2:M:172:ILE:HG23	2:M:184:MET:CE	2.39	0.53
2:M:144:PRO:HB2	2:M:267:TYR:HE1	1.74	0.53
2:M:428:ARG:HH21	2:M:451:LEU:HD11	1.73	0.53
2:M:52:PHE:HA	9:M:1741:HOH:O	2.09	0.53
2:M:674:VAL:HG21	2:M:871:LEU:CD1	2.39	0.53
2:M:706:GLU:HB3	2:M:708:TYR:CE1	2.43	0.53
2:M:789:SER:O	2:M:791:ARG:HG2	2.09	0.53
3:N:1281:VAL:HG21	3:N:1313:VAL:HG21	1.90	0.53
3:N:30:GLU:HB3	3:N:40:GLU:CB	2.39	0.53
5:P:261:PRO:O	5:P:265:VAL:HG23	2.09	0.53
2:C:137:VAL:O	2:C:391:LEU:HD21	2.09	0.52
2:C:142:ARG:HB2	9:C:1317:HOH:O	2.08	0.52
2:C:534:VAL:HB	2:C:538:GLN:OE1	2.08	0.52
2:C:580:MET:SD	2:C:584:GLU:HG3	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:625:LEU:HD13	2:C:639:GLN:O	2.10	0.52
2:C:6:PHE:CE2	2:C:913:GLU:HB3	2.45	0.52
2:C:679:PHE:CE2	2:C:853:LEU:HD21	2.45	0.52
3:D:1334:GLN:HG2	9:D:9604:HOH:O	2.09	0.52
3:D:18:ILE:HG23	3:D:518:PRO:CG	2.35	0.52
3:D:396:VAL:CG2	3:D:447:VAL:HB	2.38	0.52
3:D:455:ARG:HA	9:D:9353:HOH:O	2.09	0.52
2:C:848:VAL:HG23	3:D:740:PHE:O	2.09	0.52
4:E:63:TRP:O	4:E:67:GLU:HG3	2.08	0.52
5:F:278:LEU:CB	5:F:286:PRO:HG2	2.40	0.52
5:F:94:LEU:HD23	5:F:96:LEU:N	2.24	0.52
2:M:71:TYR:HD2	2:M:71:TYR:H	1.57	0.52
2:M:774:LEU:HB2	9:M:2065:HOH:O	2.08	0.52
2:M:577:PRO:HG3	2:M:993:PHE:CE1	2.44	0.52
3:N:1220:ALA:HB1	3:N:1223:ILE:CD1	2.40	0.52
3:N:149:LYS:HD3	9:N:9623:HOH:O	2.09	0.52
3:N:171:LEU:HD11	9:N:9804:HOH:O	2.08	0.52
3:N:562:ALA:HB1	3:N:567:ILE:CD1	2.38	0.52
3:N:661:MET:HA	3:N:666:ILE:CD1	2.40	0.52
1:A:101:LEU:HD21	1:A:113:ASP:HB3	1.92	0.52
2:C:1004:LYS:HB2	9:C:1264:HOH:O	2.09	0.52
2:C:339:LEU:HB3	2:C:385:PHE:HZ	1.74	0.52
2:C:549:PHE:HB3	2:C:552:HIS:HD2	1.74	0.52
2:C:643:VAL:HG13	2:C:647:GLN:CD	2.29	0.52
2:C:902:ILE:O	2:C:904:PRO:HD3	2.09	0.52
3:D:119:SER:CB	3:D:123:LEU:HB2	2.40	0.52
3:D:1205:TYR:HE1	3:D:1221:VAL:HG13	1.74	0.52
3:D:1295:GLU:HB3	3:D:1300:SER:CB	2.39	0.52
3:D:1367:HIS:O	3:D:1371:VAL:HG23	2.08	0.52
3:D:148:GLU:HA	9:D:9078:HOH:O	2.09	0.52
3:D:434:ARG:HB2	3:D:447:VAL:HG13	1.90	0.52
3:D:699:VAL:HG21	3:D:760:ARG:HB3	1.90	0.52
3:D:781:PRO:HA	3:D:785:ILE:HD12	1.90	0.52
5:F:245:GLN:HA	9:F:471:HOH:O	2.09	0.52
1:K:91:ASN:OD1	1:K:92:PRO:HD2	2.09	0.52
1:L:27:PRO:O	1:L:28:LEU:HD23	2.09	0.52
2:M:198:ARG:HB3	9:M:2063:HOH:O	2.10	0.52
2:M:242:LEU:HB3	9:M:1173:HOH:O	2.10	0.52
2:M:474:VAL:HG23	2:M:478:VAL:O	2.09	0.52
2:M:524:VAL:HG22	2:M:528:GLU:HG3	1.90	0.52
2:M:724:ARG:CG	2:M:740:GLU:HA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:563:PRO:O	3:N:567:ILE:HG13	2.09	0.52
3:N:795:VAL:CG1	3:N:863:VAL:HG13	2.38	0.52
3:N:838:ARG:HD3	3:N:874:GLU:HG2	1.92	0.52
3:N:984:THR:HG23	3:N:986:ARG:H	1.74	0.52
5:P:129:GLU:HB3	5:P:142:ARG:HH21	1.74	0.52
1:A:123:MET:C	1:A:125:PRO:HD3	2.29	0.52
1:A:14:ARG:HH22	1:A:24:VAL:HG23	1.72	0.52
1:A:18:ARG:HH12	1:A:88:ARG:CZ	2.22	0.52
1:A:222:LEU:HD12	1:B:215:VAL:CB	2.36	0.52
2:C:1089:VAL:O	2:C:1093:GLN:HG3	2.09	0.52
2:C:275:TYR:HA	9:C:1202:HOH:O	2.09	0.52
2:C:470:PRO:HB3	2:C:485:TYR:CE1	2.44	0.52
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.10	0.52
3:D:1286:THR:HG22	9:D:9077:HOH:O	2.09	0.52
3:D:197:SER:CB	3:D:203:ALA:HB3	2.27	0.52
3:D:520:LEU:HD23	3:D:540:LEU:HD22	1.90	0.52
3:D:783:ARG:HE	3:D:1029:ARG:NE	2.07	0.52
3:D:809:PRO:O	3:D:812:ALA:HB3	2.09	0.52
3:D:926:LYS:HE2	9:D:9035:HOH:O	2.08	0.52
5:F:102:LEU:HD12	5:F:187:LEU:HG	1.91	0.52
5:F:404:ALA:O	5:F:408:LEU:HD23	2.08	0.52
1:L:115:LEU:O	1:L:115:LEU:HD12	2.10	0.52
1:L:104:GLU:OE1	1:L:137:ARG:HG3	2.09	0.52
2:M:274:ARG:CD	2:M:285:LEU:HD22	2.36	0.52
2:M:18:LEU:HB2	2:M:590:ASP:HB3	1.91	0.52
2:M:666:LEU:HD12	2:M:667:ALA:H	1.74	0.52
2:M:52:PHE:CE1	2:M:66:LEU:HG	2.45	0.52
3:N:1272:ALA:CA	3:N:1326:THR:HB	2.37	0.52
3:N:1489:GLN:O	3:N:1493:LYS:HG2	2.08	0.52
3:N:843:PHE:HE1	3:N:864:VAL:HG11	1.73	0.52
5:P:134:LYS:HG3	5:P:178:ARG:NH2	2.25	0.52
1:A:229:GLN:HG3	9:B:611:HOH:O	2.10	0.52
1:A:41:ARG:O	1:A:45:LEU:HD12	2.10	0.52
1:B:102:LYS:HE2	1:B:104:GLU:CD	2.30	0.52
2:C:1034:GLU:HA	2:C:1037:VAL:HG23	1.91	0.52
2:C:1052:MET:SD	2:C:1056:LYS:HD3	2.49	0.52
2:C:1060:ILE:HG23	2:C:1061:GLU:H	1.74	0.52
2:C:1098:ASP:N	9:C:1791:HOH:O	2.42	0.52
2:C:137:VAL:CG2	2:C:391:LEU:HG	2.38	0.52
2:C:481:ASP:HA	9:C:1844:HOH:O	2.10	0.52
3:D:1234:THR:HG21	9:D:2326:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:444:VAL:HG11	9:D:9854:HOH:O	2.10	0.52
3:D:553:ARG:NH1	5:F:211:ASP:HA	2.24	0.52
3:D:601:ARG:HD2	5:F:328:PHE:HE1	1.75	0.52
3:D:619:LEU:HB2	9:D:9123:HOH:O	2.09	0.52
3:D:697:GLY:HA2	3:D:717:GLN:OE1	2.08	0.52
3:D:724:GLN:HG3	3:D:725:SER:N	2.24	0.52
3:D:880:ILE:O	3:D:883:ALA:HB3	2.09	0.52
5:F:160:ASP:HA	5:F:163:LEU:HD12	1.91	0.52
5:F:192:LEU:O	5:F:192:LEU:HD23	2.09	0.52
5:F:399:GLN:HG3	9:F:772:HOH:O	2.09	0.52
2:M:310:LEU:HD12	2:M:313:LEU:CD2	2.39	0.52
2:M:92:ALA:HB2	2:M:120:LEU:HD21	1.92	0.52
3:N:1147:ARG:CB	3:N:1188:VAL:HG21	2.38	0.52
3:N:161:LEU:HD21	9:N:9457:HOH:O	2.10	0.52
3:N:421:LEU:HD12	3:N:435:VAL:HG11	1.90	0.52
3:N:555:LYS:HA	3:N:558:LEU:HD12	1.92	0.52
3:N:422:ALA:CB	5:P:178:ARG:HH12	2.17	0.52
1:B:29:GLU:HG3	9:B:336:HOH:O	2.08	0.52
2:C:162:ILE:HB	2:C:172:ILE:HB	1.91	0.52
2:C:428:ARG:HG3	2:C:428:ARG:NH1	2.24	0.52
2:C:442:GLU:HB3	2:C:453:THR:OG1	2.08	0.52
2:C:633:GLN:NE2	2:C:633:GLN:H	2.07	0.52
2:C:924:VAL:HG21	9:C:2023:HOH:O	2.09	0.52
3:D:1496:GLU:HA	3:D:1499:ARG:NE	2.24	0.52
3:D:165:LYS:CB	3:D:395:VAL:HG11	2.40	0.52
2:M:154:ARG:HG3	9:M:1568:HOH:O	2.08	0.52
2:M:167:LYS:HD2	2:M:168:ARG:NH1	2.25	0.52
2:M:9:ILE:HD11	2:M:537:LYS:NZ	2.25	0.52
5:P:274:THR:O	5:P:278:LEU:HG	2.09	0.52
5:P:81:VAL:O	5:P:85:LEU:HG	2.10	0.52
1:B:84:GLU:HB3	1:B:127:LEU:HD21	1.92	0.52
2:C:572:ILE:CG2	2:C:703:ILE:HD13	2.39	0.52
2:C:884:GLN:HG2	2:C:885:ILE:N	2.23	0.52
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.10	0.52
3:D:434:ARG:HB2	3:D:447:VAL:CG2	2.40	0.52
3:D:770:LEU:HG	3:D:919:PHE:CE1	2.45	0.52
3:D:984:THR:HG22	3:D:987:GLU:HB2	1.92	0.52
4:E:42:PRO:HG2	9:E:146:HOH:O	2.09	0.52
5:F:88:ILE:HD13	5:F:193:ARG:HD3	1.90	0.52
2:M:932:GLU:HG2	9:M:1541:HOH:O	2.08	0.52
3:N:1129:THR:O	3:N:1130:ARG:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1324:PRO:HG3	3:N:1330:ILE:HD11	1.92	0.52
3:N:422:ALA:O	3:N:427:VAL:HG21	2.10	0.52
3:N:907:GLU:HG2	3:N:908:LYS:H	1.74	0.52
5:P:138:SER:O	5:P:141:VAL:HG12	2.09	0.52
5:P:291:ILE:HG23	5:P:304:VAL:HG21	1.90	0.52
5:P:363:GLU:HA	5:P:367:MET:HE2	1.92	0.52
1:A:216:GLU:O	1:A:220:GLU:HG3	2.09	0.52
1:B:91:ASN:H	1:B:94:LEU:HD12	1.75	0.52
2:C:288:ARG:HD3	9:C:1496:HOH:O	2.09	0.52
2:C:397:GLU:H	2:C:633:GLN:NE2	2.07	0.52
2:C:665:PHE:N	9:C:2008:HOH:O	2.41	0.52
2:C:74:GLY:O	2:C:76:PRO:HD3	2.09	0.52
3:D:1341:PRO:HD2	3:D:1342:GLU:OE2	2.09	0.52
3:D:1463:LYS:O	3:D:1467:ILE:HD12	2.10	0.52
5:F:365:GLU:HG2	5:F:397:ILE:HA	1.92	0.52
5:F:86:HIS:HB3	9:F:802:HOH:O	2.10	0.52
1:L:143:ARG:NH1	1:L:158:ILE:HG23	2.24	0.52
2:M:182:VAL:CG1	2:M:193:LEU:HD13	2.39	0.52
2:M:232:GLU:O	2:M:235:LEU:HB2	2.09	0.52
3:N:1441:GLN:OE1	3:N:1442:ASN:HB2	2.10	0.52
3:N:571:LYS:NZ	3:N:571:LYS:HB2	2.24	0.52
3:N:774:SER:C	3:N:776:GLU:H	2.13	0.52
3:N:787:LEU:HD11	3:N:947:ILE:HG12	1.91	0.52
2:C:63:GLY:HA3	2:C:103:LYS:HE2	1.91	0.52
2:C:838:LYS:HD2	2:C:846:LYS:HZ1	1.74	0.52
2:C:669:GLY:HA3	2:C:995:MET:HA	1.91	0.52
3:D:1109:GLU:HG2	3:D:1202:GLN:H	1.75	0.52
3:D:1385:GLY:HA2	9:D:9072:HOH:O	2.10	0.52
3:D:1443:THR:O	3:D:1447:LEU:HD13	2.10	0.52
3:D:26:VAL:N	9:D:9002:HOH:O	2.42	0.52
3:D:131:LYS:HB3	3:D:456:MET:HE2	1.92	0.52
3:D:704:ARG:NH1	3:D:738:ALA:HA	2.25	0.52
5:F:124:PRO:O	5:F:128:ARG:HB2	2.10	0.52
5:F:190:ALA:HB1	9:F:704:HOH:O	2.10	0.52
5:F:225:GLU:HG3	5:F:226:LYS:HG3	1.91	0.52
2:M:428:ARG:HD3	2:M:449:ILE:CG2	2.40	0.52
2:M:578:VAL:HG13	2:M:671:ASN:ND2	2.25	0.52
2:M:61:LYS:HG2	9:M:1592:HOH:O	2.10	0.52
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.90	0.52
2:M:925:TYR:HE1	2:M:929:ARG:HH11	1.57	0.52
3:N:171:LEU:HD13	3:N:389:GLU:C	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:416:ALA:HA	3:N:442:ASN:ND2	2.24	0.52
3:N:676:MET:CE	3:N:684:LYS:HD2	2.40	0.52
3:N:699:VAL:HB	3:N:716:PHE:O	2.10	0.52
5:P:215:GLU:HA	9:P:6496:HOH:O	2.10	0.52
1:A:136:GLY:HA3	9:A:360:HOH:O	2.08	0.52
1:A:153:ALA:HA	1:A:156:HIS:NE2	2.24	0.52
1:A:181:VAL:HG12	9:A:370:HOH:O	2.08	0.52
1:B:102:LYS:HE2	1:B:104:GLU:OE1	2.10	0.52
1:B:226:SER:O	1:B:228:PRO:HD3	2.09	0.52
1:B:26:GLU:HG2	1:B:27:PRO:HA	1.91	0.52
2:C:56:GLU:OE1	2:C:356:ARG:HD3	2.09	0.52
2:C:504:GLU:HG2	2:C:507:ARG:O	2.09	0.52
2:C:662:GLU:N	9:C:2008:HOH:O	2.42	0.52
2:C:674:VAL:HG23	2:C:869:VAL:O	2.09	0.52
2:C:730:SER:O	2:C:734:LEU:HD13	2.09	0.52
3:D:1369:GLU:O	3:D:1372:VAL:HG12	2.10	0.52
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.92	0.52
4:E:58:PRO:HB2	9:E:102:HOH:O	2.08	0.52
5:F:253:ASP:HB2	9:F:629:HOH:O	2.09	0.52
2:M:5:ARG:CB	2:M:902:ILE:HB	2.40	0.52
3:N:1343:ALA:HB1	9:N:9791:HOH:O	2.09	0.52
3:N:148:GLU:CB	3:N:151:GLN:HB3	2.39	0.52
3:N:438:ASP:HA	9:N:9374:HOH:O	2.10	0.52
3:N:996:TRP:CE3	3:N:999:THR:HG21	2.44	0.52
5:P:111:GLU:O	5:P:115:LYS:HG3	2.08	0.52
1:A:132:LEU:HD12	9:A:328:HOH:O	2.10	0.52
1:B:154:GLU:HB3	9:B:483:HOH:O	2.09	0.52
2:C:1033:GLY:O	2:C:1037:VAL:HG23	2.10	0.52
2:C:1063:ARG:O	2:C:1066:ALA:HB3	2.10	0.52
3:D:1018:ASN:ND2	3:D:1019:PRO:HD2	2.25	0.52
3:D:1283:ILE:N	3:D:1315:ASP:OD1	2.43	0.52
3:D:496:LEU:HD23	3:D:1388:ARG:HG2	1.92	0.52
3:D:796:ARG:HG3	3:D:828:LYS:HD2	1.92	0.52
3:D:55:ASP:O	3:D:82:LYS:HA	2.09	0.52
1:K:227:ASN:HD22	1:K:227:ASN:H	1.57	0.52
2:M:208:ALA:HA	2:M:218:VAL:HG22	1.91	0.52
3:N:12:LEU:HD23	3:N:13:ALA:H	1.75	0.52
3:N:1395:LEU:HD13	3:N:1396:GLU:N	2.25	0.52
3:N:1086:LEU:HD11	6:N:8002:STD:H113	1.92	0.52
3:N:933:ALA:O	3:N:937:TYR:HD1	1.93	0.52
3:N:787:LEU:HD21	3:N:947:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:163:LEU:HB3	5:P:174:LEU:HD11	1.91	0.52
5:P:132:ARG:HE	5:P:184:ARG:NH1	2.07	0.52
1:B:33:GLY:O	1:B:195:LEU:HD22	2.10	0.51
2:C:1008:ARG:NH1	2:C:1011:GLY:HA3	2.25	0.51
2:C:384:GLU:CD	2:C:388:ARG:HH21	2.14	0.51
2:C:564:MET:HE2	2:C:846:LYS:HE2	1.92	0.51
1:A:178:ALA:CB	2:C:864:GLY:H	2.23	0.51
3:D:1326:THR:HA	9:D:9040:HOH:O	2.11	0.51
3:D:1481:VAL:HG11	4:E:18:ARG:CA	2.35	0.51
3:D:530:VAL:HB	3:D:534:ARG:HB2	1.92	0.51
3:D:63:TYR:HB3	3:D:68:PHE:CZ	2.45	0.51
3:D:847:ASP:HA	3:D:850:LEU:CD1	2.40	0.51
1:K:159:LYS:HD3	9:K:3711:HOH:O	2.10	0.51
1:K:227:ASN:N	1:K:227:ASN:HD22	2.06	0.51
1:K:98:THR:HG22	9:K:3937:HOH:O	2.08	0.51
1:L:101:LEU:HB3	1:L:140:MET:SD	2.50	0.51
1:L:59:GLU:HG3	1:L:139:ASN:HD22	1.74	0.51
2:M:267:TYR:CD1	2:M:272:ALA:HB1	2.45	0.51
3:N:132:TYR:HA	9:N:9350:HOH:O	2.09	0.51
3:N:136:ASP:HB3	3:N:137:PRO:HD3	1.92	0.51
9:N:9551:HOH:O	5:P:258:ILE:HD12	2.10	0.51
2:C:204:GLN:HB2	9:C:1650:HOH:O	2.10	0.51
2:C:232:GLU:O	2:C:235:LEU:HB2	2.10	0.51
2:C:441:VAL:CG1	2:C:559:LEU:HA	2.39	0.51
2:C:578:VAL:HG11	2:C:991:GLN:CB	2.33	0.51
3:D:1335:LEU:CD2	3:D:1344:VAL:HA	2.40	0.51
3:D:1476:THR:C	3:D:1478:SER:H	2.13	0.51
5:F:283:GLY:HA2	9:F:586:HOH:O	2.09	0.51
1:L:110:LYS:HD2	1:L:126:ASP:HA	1.90	0.51
2:M:160:ALA:O	2:M:173:ASP:HA	2.10	0.51
2:M:264:PRO:HB3	2:M:289:THR:HG21	1.91	0.51
2:M:335:THR:CG2	2:M:461:VAL:HG11	2.40	0.51
2:M:129:ILE:HD13	2:M:386:PHE:HB3	1.92	0.51
2:M:704:HIS:HB3	2:M:831:ARG:NE	2.25	0.51
3:N:135:LEU:HD11	3:N:139:GLY:HA3	1.92	0.51
3:N:671:LYS:CE	3:N:674:ARG:HH21	2.24	0.51
1:A:161:ARG:HG2	9:A:442:HOH:O	2.11	0.51
1:B:223:THR:HA	9:B:419:HOH:O	2.09	0.51
2:C:141:HIS:CB	2:C:418:LEU:HG	2.40	0.51
2:C:498:GLN:NE2	3:D:1068:LEU:HD12	2.25	0.51
2:C:536:PRO:HB2	2:C:905:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:432:ARG:NH1	3:D:1048:PRO:HD3	2.26	0.51
3:D:12:LEU:HD21	3:D:104:PHE:CE1	2.42	0.51
3:D:116:LEU:CD2	3:D:468:LEU:HD11	2.41	0.51
3:D:1295:GLU:HB3	3:D:1300:SER:OG	2.10	0.51
3:D:1380:GLU:HG3	3:D:1381:VAL:N	2.25	0.51
3:D:543:LEU:CD2	3:D:600:LEU:HD12	2.40	0.51
3:D:639:LEU:N	3:D:639:LEU:HD12	2.26	0.51
2:C:1090:LYS:NZ	3:D:90:MET:HG3	2.22	0.51
5:F:122:LEU:HD12	9:F:488:HOH:O	2.11	0.51
5:F:295:MET:HB3	5:F:299:TRP:CD1	2.46	0.51
5:F:337:HIS:CD2	5:F:337:HIS:N	2.74	0.51
2:M:335:THR:HG21	2:M:461:VAL:HG11	1.92	0.51
2:M:526:PRO:HD2	9:M:1644:HOH:O	2.10	0.51
2:M:720:GLU:HA	2:M:759:THR:O	2.11	0.51
3:N:1237:THR:HB	3:N:1359:GLN:OE1	2.10	0.51
3:N:1492:LEU:HD12	3:N:1493:LYS:NZ	2.24	0.51
3:N:424:GLY:HA2	3:N:435:VAL:O	2.10	0.51
3:N:54:LYS:HB3	9:N:9416:HOH:O	2.09	0.51
3:N:601:ARG:NE	3:N:606:ILE:HD13	2.25	0.51
5:P:325:LYS:HB2	9:P:6651:HOH:O	2.09	0.51
5:P:392:VAL:HG21	9:P:3714:HOH:O	2.09	0.51
2:C:110:GLU:HG2	2:C:369:PRO:CB	2.39	0.51
2:C:140:ILE:HD12	2:C:140:ILE:H	1.76	0.51
3:D:1263:PHE:HD2	3:D:1375:MET:HE2	1.75	0.51
3:D:1354:LYS:HD3	9:D:9764:HOH:O	2.08	0.51
3:D:1432:LYS:HD2	3:D:1433:SER:H	1.75	0.51
2:C:1115:LEU:HD23	3:D:85:VAL:HA	1.92	0.51
5:F:289:GLU:O	5:F:293:GLU:HG3	2.10	0.51
2:M:1016:ILE:HD13	2:M:1016:ILE:N	2.23	0.51
2:M:1073:GLY:HA3	9:M:1801:HOH:O	2.11	0.51
2:M:141:HIS:O	2:M:331:ARG:HA	2.10	0.51
9:K:5022:HOH:O	2:M:608:GLY:HA3	2.11	0.51
2:M:860:HIS:CD2	2:M:975:TYR:HB2	2.45	0.51
2:M:837:ASP:OD1	2:M:996:LYS:HE2	2.10	0.51
2:M:9:ILE:HD11	2:M:537:LYS:HZ3	1.75	0.51
3:N:1365:ASP:O	3:N:1369:GLU:HG3	2.10	0.51
3:N:481:MET:HE1	3:N:493:ARG:NH2	2.25	0.51
3:N:634:GLY:O	3:N:637:LEU:HB3	2.09	0.51
4:O:47:LYS:HA	4:O:54:LEU:HB3	1.92	0.51
4:O:58:PRO:HB2	9:O:3650:HOH:O	2.10	0.51
4:O:84:ARG:HB2	4:O:84:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:144:ILE:HG23	9:P:4405:HOH:O	2.10	0.51
5:P:412:GLU:OE1	5:P:418:LEU:HD13	2.10	0.51
1:A:10:VAL:HG12	1:A:12:THR:HG22	1.92	0.51
1:A:13:VAL:HG21	9:B:442:HOH:O	2.10	0.51
1:A:156:HIS:HD2	1:A:157:GLY:N	2.08	0.51
1:B:18:ARG:O	1:B:207:PRO:HD3	2.11	0.51
2:C:1032:PHE:HZ	2:C:1040:LEU:HD22	1.75	0.51
2:C:541:SER:HB2	9:C:1121:HOH:O	2.10	0.51
3:D:1372:VAL:HA	3:D:1375:MET:CE	2.40	0.51
3:D:1455:LYS:HD3	3:D:1456:LYS:N	2.25	0.51
3:D:704:ARG:CG	3:D:736:PHE:HB3	2.41	0.51
4:E:26:ARG:O	4:E:29:GLN:HG3	2.10	0.51
5:F:238:TYR:HB2	9:F:612:HOH:O	2.10	0.51
2:M:1082:PRO:HG3	9:M:1191:HOH:O	2.10	0.51
2:M:157:ARG:HG2	2:M:157:ARG:HH11	1.74	0.51
2:M:244:PRO:HD3	9:M:1602:HOH:O	2.10	0.51
3:N:1404:ASN:ND2	3:N:1408:ILE:HD12	2.25	0.51
2:M:1009:SER:OG	3:N:654:LYS:HB3	2.09	0.51
3:N:1481:VAL:CG1	4:O:18:ARG:HE	2.12	0.51
4:O:17:TYR:O	4:O:21:VAL:HG23	2.11	0.51
5:P:278:LEU:HB2	5:P:286:PRO:HG2	1.92	0.51
2:C:185:LYS:HG2	2:C:190:LYS:HG2	1.91	0.51
2:C:526:PRO:HB3	9:C:1428:HOH:O	2.11	0.51
2:C:80:GLN:HB3	2:C:84:ARG:HH21	1.75	0.51
2:C:897:LEU:HD23	2:C:899:GLN:NE2	2.26	0.51
2:C:975:TYR:HA	2:C:982:PRO:HA	1.91	0.51
3:D:1031:ASN:HB3	3:D:1034:GLN:CD	2.31	0.51
3:D:1090:ASP:HA	3:D:1093:TYR:HB2	1.91	0.51
3:D:131:LYS:HG3	3:D:568:ARG:HG2	1.93	0.51
3:D:32:ILE:HG12	3:D:38:LYS:O	2.11	0.51
3:D:421:LEU:HD11	3:D:437:VAL:HG22	1.93	0.51
3:D:696:HIS:HB2	4:E:48:MET:HE1	1.93	0.51
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.92	0.51
3:D:955:VAL:HG22	9:D:2109:HOH:O	2.10	0.51
2:M:1000:MET:HE1	9:M:1491:HOH:O	2.10	0.51
2:M:860:HIS:NE2	2:M:975:TYR:HB2	2.26	0.51
3:N:957:PRO:HG2	3:N:1007:VAL:HG12	1.90	0.51
3:N:1112:CYS:HA	3:N:1195:GLN:HE22	1.76	0.51
3:N:146:PRO:HB3	9:N:9665:HOH:O	2.11	0.51
3:N:181:ASP:OD1	3:N:199:LEU:HD12	2.10	0.51
3:N:29:PRO:HA	9:N:9523:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:32:ILE:O	5:P:258:ILE:HG23	2.11	0.51
3:N:809:PRO:O	3:N:812:ALA:HB3	2.11	0.51
4:O:85:LEU:HD23	4:O:86:GLN:N	2.25	0.51
5:P:256:ARG:NH2	5:P:258:ILE:HB	2.25	0.51
1:B:77:GLU:HB2	3:D:872:ARG:HH21	1.75	0.51
2:C:260:LEU:HA	2:C:291:ALA:CB	2.40	0.51
2:C:367:LEU:HA	2:C:371:LYS:CD	2.41	0.51
2:C:704:HIS:HB2	9:C:1879:HOH:O	2.10	0.51
3:D:656:PHE:HB3	3:D:694:VAL:HG11	1.92	0.51
3:D:669:ASN:HB3	9:D:9017:HOH:O	2.10	0.51
3:D:838:ARG:HD3	3:D:874:GLU:HB3	1.92	0.51
4:E:13:VAL:HG23	9:E:108:HOH:O	2.11	0.51
4:E:33:HIS:HB2	4:E:37:ASN:ND2	2.25	0.51
9:C:1234:HOH:O	5:F:335:ASP:HB3	2.10	0.51
5:F:393:THR:HG22	5:F:394:ARG:H	1.74	0.51
1:K:41:ARG:HH11	1:K:177:VAL:HB	1.75	0.51
2:M:1095:LEU:HD23	3:N:582:LEU:HD22	1.93	0.51
2:M:137:VAL:CG2	2:M:391:LEU:HG	2.40	0.51
2:M:176:VAL:C	2:M:178:PRO:HD3	2.31	0.51
2:M:290:LEU:H	2:M:290:LEU:HD23	1.75	0.51
2:M:139:GLN:HB3	2:M:334:ARG:CD	2.41	0.51
2:M:64:LEU:HB2	2:M:359:MET:SD	2.51	0.51
2:M:68:PHE:HE1	2:M:96:ALA:HB1	1.75	0.51
3:N:1105:ILE:HD11	3:N:1374:GLN:CD	2.31	0.51
3:N:154:THR:HG23	3:N:157:GLU:H	1.76	0.51
3:N:112:ILE:HG22	3:N:512:MET:SD	2.51	0.51
3:N:543:LEU:HD21	3:N:600:LEU:HD12	1.91	0.51
3:N:638:LYS:HE3	9:N:9110:HOH:O	2.11	0.51
3:N:770:LEU:HD12	3:N:1210:SER:O	2.11	0.51
3:N:799:LYS:H	3:N:826:PRO:HG2	1.76	0.51
1:A:58:ILE:HB	1:A:61:VAL:HB	1.92	0.51
1:B:101:LEU:HD12	1:B:114:PHE:CE1	2.45	0.51
1:B:46:SER:O	1:B:148:VAL:HB	2.10	0.51
2:C:199:VAL:HG21	9:C:1222:HOH:O	2.09	0.51
2:C:279:GLU:HG3	2:C:280:LYS:N	2.26	0.51
2:C:387:SER:HB2	2:C:388:ARG:HD3	1.93	0.51
2:C:742:VAL:HG12	2:C:743:VAL:N	2.26	0.51
3:D:543:LEU:HD21	3:D:600:LEU:HD12	1.91	0.51
3:D:87:ARG:HB3	3:D:523:ASP:CB	2.38	0.51
3:D:131:LYS:CE	5:F:83:GLN:HE22	2.24	0.51
2:M:208:ALA:HB1	2:M:218:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:749:VAL:HG12	2:M:753:ASP:HB2	1.92	0.51
3:N:1014:ASN:HA	9:N:9833:HOH:O	2.09	0.51
3:N:1093:TYR:HA	3:N:1096:ARG:NH2	2.25	0.51
2:M:1046:ALA:CB	3:N:1476:THR:HB	2.40	0.51
3:N:628:ARG:HG2	3:N:744:GLN:HE21	1.76	0.51
3:N:678:GLU:HG3	3:N:679:ARG:HG3	1.93	0.51
3:N:65:ARG:HB3	5:P:375:LEU:O	2.11	0.51
1:A:161:ARG:HB2	1:A:161:ARG:CZ	2.41	0.51
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.92	0.51
1:A:86:VAL:CG1	1:A:124:ASN:HB2	2.41	0.51
1:B:101:LEU:HG	1:B:114:PHE:HA	1.92	0.51
1:B:105:GLY:O	1:B:132:LEU:HB3	2.11	0.51
2:C:358:ARG:HH12	2:C:374:ASN:HB3	1.76	0.51
2:C:34:VAL:CG1	2:C:38:LYS:HG3	2.41	0.51
2:C:850:ALA:HA	3:D:632:VAL:HG11	1.92	0.51
3:D:1066:THR:HG22	3:D:1069:GLU:HG3	1.93	0.51
3:D:186:VAL:HG23	9:D:9609:HOH:O	2.11	0.51
3:D:528:VAL:HG23	3:D:536:ALA:O	2.10	0.51
3:D:969:ARG:O	3:D:972:LEU:HB3	2.11	0.51
5:F:262:VAL:HG12	5:F:266:GLU:OE2	2.10	0.51
5:F:277:GLN:O	5:F:280:GLN:HB3	2.10	0.51
2:M:1054:THR:CG2	2:M:1079:PRO:HB3	2.26	0.51
2:M:1080:SER:HB2	9:M:1326:HOH:O	2.11	0.51
2:M:283:ILE:HA	9:M:1764:HOH:O	2.10	0.51
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.92	0.51
2:M:479:VAL:HG21	2:M:503:LEU:HD11	1.93	0.51
2:M:516:ARG:HD2	3:N:1068:LEU:HD22	1.92	0.51
3:N:215:TYR:HB3	9:N:9520:HOH:O	2.11	0.51
3:N:524:LEU:HD23	9:N:9039:HOH:O	2.11	0.51
5:P:163:LEU:HB3	5:P:174:LEU:CD1	2.41	0.51
5:P:408:LEU:HA	5:P:411:HIS:CE1	2.45	0.51
5:P:95:THR:HB	5:P:96:LEU:HD23	1.93	0.51
2:C:274:ARG:HD3	9:C:2046:HOH:O	2.09	0.51
2:C:473:ARG:HD3	2:C:531:PHE:HE1	1.75	0.51
2:C:720:GLU:HA	2:C:759:THR:O	2.11	0.51
2:C:769:PRO:O	2:C:772:ARG:HB3	2.11	0.51
3:D:1354:LYS:HA	9:D:9764:HOH:O	2.10	0.51
3:D:1382:THR:CG2	3:D:1418:LYS:HE3	2.39	0.51
3:D:179:VAL:HG22	3:D:389:GLU:CG	2.41	0.51
2:C:1005:MET:CE	3:D:648:MET:HB2	2.41	0.51
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:54:LEU:HA	4:E:58:PRO:HG2	1.93	0.51
5:F:121:GLY:HA3	9:F:650:HOH:O	2.11	0.51
5:F:404:ALA:HA	9:F:428:HOH:O	2.10	0.51
1:K:150:TYR:HE1	2:M:696:LYS:HA	1.76	0.51
1:K:63:HIS:HD2	1:K:65:PHE:N	2.09	0.51
1:L:95:GLN:HA	1:L:146:ARG:HD2	1.92	0.51
2:M:584:GLU:O	2:M:588:VAL:HG13	2.11	0.51
2:M:723:THR:CG2	2:M:725:ASP:HB2	2.41	0.51
3:N:1080:GLY:HA3	9:N:9068:HOH:O	2.10	0.51
3:N:1266:ARG:O	3:N:1268:PRO:HD3	2.11	0.51
3:N:1362:LYS:HD2	9:N:9355:HOH:O	2.11	0.51
3:N:593:ASN:OD1	3:N:594:PRO:HD2	2.11	0.51
3:N:65:ARG:HG3	3:N:66:GLN:N	2.12	0.51
3:N:681:ARG:HD3	9:N:9087:HOH:O	2.10	0.51
3:N:953:ASP:O	3:N:955:VAL:HG23	2.10	0.51
4:O:26:ARG:O	4:O:29:GLN:HG3	2.11	0.51
4:O:62:THR:HA	4:O:65:MET:HE3	1.92	0.51
5:P:226:LYS:HB2	5:P:238:TYR:OH	2.11	0.51
1:A:176:ARG:O	1:A:200:TRP:HE3	1.93	0.50
2:C:1032:PHE:CZ	2:C:1040:LEU:HD22	2.46	0.50
2:C:1115:LEU:HD12	2:C:1115:LEU:N	2.26	0.50
2:C:166:PRO:HD2	9:C:1436:HOH:O	2.11	0.50
2:C:274:ARG:CG	2:C:285:LEU:HD22	2.41	0.50
3:D:137:PRO:HD2	3:D:453:ASP:CB	2.40	0.50
3:D:56:TYR:CE2	3:D:69:GLU:HB2	2.45	0.50
3:D:818:ARG:HD2	9:D:9402:HOH:O	2.10	0.50
3:D:865:THR:CG2	3:D:874:GLU:HG2	2.41	0.50
5:F:134:LYS:HD2	9:F:721:HOH:O	2.11	0.50
5:F:287:THR:C	5:F:289:GLU:H	2.14	0.50
1:L:60:ASP:HB2	9:L:3794:HOH:O	2.10	0.50
2:M:107:LEU:HB2	9:M:1746:HOH:O	2.10	0.50
2:M:288:ARG:HB2	9:M:1581:HOH:O	2.11	0.50
2:M:462:ASP:OD1	2:M:468:ARG:HG2	2.12	0.50
2:M:580:MET:HB3	2:M:584:GLU:CD	2.32	0.50
2:M:396:ASP:HA	2:M:633:GLN:OE1	2.11	0.50
3:N:1144:LEU:HA	3:N:1147:ARG:HG3	1.93	0.50
3:N:173:PRO:HA	9:N:9622:HOH:O	2.11	0.50
2:C:1086:ARG:HB3	2:C:1112:PHE:HE2	1.76	0.50
2:C:208:ALA:HB1	2:C:218:VAL:CG1	2.41	0.50
2:C:610:ARG:C	2:C:611:ILE:HD12	2.32	0.50
2:C:749:VAL:HB	2:C:792:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:ILE:HG12	2:C:907:ASP:CG	2.32	0.50
2:C:94:LEU:HD12	2:C:95:TYR:N	2.26	0.50
3:D:1066:THR:CG2	3:D:1069:GLU:HG3	2.41	0.50
3:D:1109:GLU:HG2	3:D:1201:CYS:CA	2.40	0.50
3:D:1389:LEU:HD12	3:D:1390:LEU:H	1.76	0.50
3:D:496:LEU:HD22	9:D:9267:HOH:O	2.11	0.50
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.93	0.50
5:F:301:ALA:HB2	9:F:684:HOH:O	2.11	0.50
1:K:41:ARG:NH1	1:K:177:VAL:HB	2.26	0.50
1:K:178:ALA:O	1:K:198:ARG:HG3	2.12	0.50
2:M:1018:GLN:HE21	2:M:1063:ARG:HH22	1.57	0.50
2:M:379:GLU:O	2:M:383:ARG:HB3	2.11	0.50
2:M:575:GLN:O	2:M:667:ALA:HB1	2.10	0.50
2:M:726:ILE:O	2:M:726:ILE:HG22	2.11	0.50
2:M:85:GLU:HG3	9:M:1240:HOH:O	2.11	0.50
3:N:1020:LEU:HA	3:N:1023:MET:CE	2.42	0.50
3:N:396:VAL:CG2	3:N:447:VAL:HB	2.39	0.50
3:N:141:ILE:HD13	3:N:450:TYR:H	1.77	0.50
3:N:668:PRO:HD2	3:N:672:ALA:CB	2.41	0.50
3:N:786:ILE:HD13	3:N:908:LYS:HB3	1.92	0.50
3:N:983:LEU:HD13	3:N:991:GLN:OE1	2.12	0.50
3:N:99:ALA:HA	3:N:575:GLN:HE22	1.76	0.50
4:O:29:GLN:HB2	4:O:33:HIS:CD2	2.47	0.50
2:C:49:ARG:HA	9:C:1342:HOH:O	2.10	0.50
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.46	0.50
2:C:969:GLN:HG2	9:C:1454:HOH:O	2.11	0.50
3:D:1137:ARG:HG2	9:D:9554:HOH:O	2.11	0.50
3:D:149:LYS:HE3	9:D:9873:HOH:O	2.12	0.50
3:D:399:ARG:HB3	3:D:402:PRO:HG3	1.93	0.50
3:D:486:ARG:HB3	9:D:9316:HOH:O	2.10	0.50
3:D:81:THR:HG22	3:D:82:LYS:N	2.26	0.50
3:D:829:VAL:HG21	9:D:9008:HOH:O	2.12	0.50
5:F:123:ASP:HB2	5:F:126:LEU:HD22	1.93	0.50
5:F:201:LYS:HG2	9:F:891:HOH:O	2.10	0.50
5:F:291:ILE:O	5:F:295:MET:HB2	2.11	0.50
1:L:219:ARG:HB3	1:L:219:ARG:CZ	2.41	0.50
1:L:5:LYS:HE3	1:L:5:LYS:HA	1.93	0.50
2:M:101:ILE:HG22	2:M:102:HIS:H	1.76	0.50
2:M:669:GLY:HA3	2:M:995:MET:HA	1.93	0.50
2:M:700:TYR:HB2	2:M:833:LEU:HD22	1.93	0.50
2:M:841:ASN:HD22	2:M:841:ASN:C	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:104:PHE:CD2	3:N:1448:THR:HG23	2.46	0.50
3:N:955:VAL:HG11	3:N:1015:TYR:HE2	1.76	0.50
4:O:45:ARG:HB2	4:O:46:PRO:CD	2.41	0.50
5:P:217:ASN:O	5:P:221:ILE:HG13	2.12	0.50
5:P:289:GLU:O	5:P:293:GLU:HG3	2.11	0.50
5:P:361:LEU:HD21	5:P:404:ALA:CB	2.42	0.50
1:A:35:THR:HG21	1:B:43:ILE:HD11	1.92	0.50
2:C:267:TYR:CD1	2:C:272:ALA:HB1	2.47	0.50
2:C:612:VAL:HG22	2:C:622:GLU:HB2	1.93	0.50
2:C:626:ARG:HB2	2:C:639:GLN:HE21	1.77	0.50
2:C:651:LYS:HD2	9:C:1839:HOH:O	2.11	0.50
2:C:806:LEU:HD22	9:C:1461:HOH:O	2.11	0.50
3:D:1045:MET:HB2	9:D:9034:HOH:O	2.11	0.50
3:D:128:TYR:CE1	3:D:461:ILE:HG13	2.47	0.50
3:D:156:GLU:CD	3:D:156:GLU:N	2.64	0.50
3:D:407:VAL:HG21	9:D:2098:HOH:O	2.12	0.50
3:D:502:PHE:CE2	3:D:1452:ILE:HG23	2.46	0.50
3:D:704:ARG:HG3	3:D:736:PHE:HB3	1.93	0.50
3:D:790:TYR:HD2	3:D:906:GLN:O	1.94	0.50
4:E:40:LEU:HB3	9:E:164:HOH:O	2.11	0.50
1:L:110:LYS:HG2	1:L:127:LEU:O	2.11	0.50
2:M:709:GLU:HG3	2:M:824:ARG:HG2	1.93	0.50
3:N:956:ILE:HG12	3:N:1039:CYS:O	2.11	0.50
3:N:1109:GLU:CD	3:N:1202:GLN:H	2.14	0.50
3:N:1267:ARG:HH12	3:N:1331:ASP:CB	2.24	0.50
3:N:1472:ILE:O	3:N:1477:GLY:HA3	2.10	0.50
3:N:180:LYS:HB3	9:N:9334:HOH:O	2.11	0.50
3:N:137:PRO:HD2	3:N:453:ASP:CB	2.41	0.50
3:N:643:GLY:CA	3:N:727:GLN:HB2	2.41	0.50
3:N:788:GLY:O	3:N:792:ILE:HG22	2.11	0.50
2:C:1001:VAL:HG23	9:C:1965:HOH:O	2.10	0.50
2:C:15:LEU:HD12	9:C:1190:HOH:O	2.11	0.50
2:C:376:ARG:HB3	2:C:377:PRO:HD3	1.93	0.50
2:C:439:CYS:SG	2:C:540:PHE:HB3	2.52	0.50
2:C:701:THR:HA	2:C:831:ARG:O	2.11	0.50
2:C:757:GLY:HA2	2:C:789:SER:OG	2.12	0.50
3:D:42:ASP:O	3:D:43:GLY:O	2.29	0.50
3:D:768:ASN:N	3:D:768:ASN:HD22	2.09	0.50
5:F:105:LYS:NZ	5:F:179:GLU:HB3	2.27	0.50
5:F:153:PRO:HG2	5:F:154:LYS:H	1.77	0.50
5:F:202:TYR:HB2	5:F:212:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:392:VAL:CG1	5:F:396:ARG:HE	2.24	0.50
2:M:1000:MET:O	2:M:1003:ASP:HB3	2.12	0.50
2:M:322:VAL:HG12	9:M:1579:HOH:O	2.11	0.50
2:M:626:ARG:CB	2:M:639:GLN:HE22	2.12	0.50
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.93	0.50
3:N:36:THR:HG21	9:N:9656:HOH:O	2.12	0.50
3:N:843:PHE:CE1	3:N:864:VAL:HG11	2.47	0.50
3:N:860:LEU:H	3:N:860:LEU:HD12	1.76	0.50
2:M:775:ARG:HH12	5:P:421:PHE:HD2	1.59	0.50
1:A:19:GLU:O	1:A:200:TRP:HA	2.11	0.50
2:C:212:GLY:HA3	2:C:218:VAL:CG2	2.42	0.50
2:C:194:VAL:HG21	2:C:221:LEU:O	2.11	0.50
2:C:251:ASP:HB3	2:C:252:LYS:CE	2.41	0.50
2:C:396:ASP:HA	2:C:633:GLN:OE1	2.12	0.50
2:C:57:GLU:OE1	2:C:63:GLY:HA2	2.11	0.50
2:C:686:ASP:HB3	9:C:1260:HOH:O	2.11	0.50
3:D:1318:TYR:HD1	3:D:1319:VAL:H	1.59	0.50
3:D:229:ALA:HB1	9:D:9029:HOH:O	2.11	0.50
3:D:135:LEU:HA	3:D:453:ASP:O	2.12	0.50
4:E:25:LYS:HA	4:E:28:GLN:NE2	2.25	0.50
5:F:321:ILE:HG22	5:F:322:GLY:N	2.27	0.50
1:K:26:GLU:CB	1:K:194:LYS:HG3	2.42	0.50
3:N:1000:THR:HG23	3:N:1001:GLU:N	2.27	0.50
3:N:126:VAL:O	3:N:132:TYR:HD1	1.95	0.50
1:B:90:LEU:HD23	9:B:411:HOH:O	2.10	0.50
2:C:362:GLY:HA3	2:C:367:LEU:HD23	1.94	0.50
2:C:688:ILE:CD1	2:C:847:GLY:HA3	2.41	0.50
2:C:975:TYR:CD1	2:C:975:TYR:N	2.79	0.50
3:D:1198:TYR:HE2	3:D:1377:LYS:HE3	1.76	0.50
3:D:1209:LEU:HG	3:D:1219:GLU:OE2	2.11	0.50
3:D:603:LEU:O	3:D:606:ILE:HB	2.11	0.50
5:F:408:LEU:HA	5:F:411:HIS:CE1	2.47	0.50
1:K:218:LEU:O	1:K:222:LEU:HD23	2.12	0.50
1:L:24:VAL:HG22	1:L:196:THR:OG1	2.12	0.50
2:M:717:LEU:HD23	2:M:717:LEU:N	2.27	0.50
2:M:722:ILE:HG21	2:M:821:GLU:OE1	2.12	0.50
3:N:1066:THR:HG22	3:N:1069:GLU:HG3	1.93	0.50
3:N:411:THR:HG21	9:N:9050:HOH:O	2.12	0.50
3:N:487:ALA:HB3	9:N:9145:HOH:O	2.12	0.50
3:N:644:LEU:HD12	3:N:645:PRO:CD	2.38	0.50
3:N:658:LEU:O	3:N:661:MET:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:756:GLN:O	3:N:760:ARG:HG2	2.12	0.50
5:P:126:LEU:HB3	9:P:4172:HOH:O	2.11	0.50
1:B:148:VAL:HA	9:B:597:HOH:O	2.12	0.50
2:C:1019:GLN:HE21	2:C:1019:GLN:H	1.59	0.50
2:C:358:ARG:NH2	2:C:374:ASN:HB3	2.25	0.50
2:C:625:LEU:CD1	2:C:641:PRO:HG3	2.41	0.50
2:C:726:ILE:O	2:C:726:ILE:HG22	2.11	0.50
2:C:732:ALA:O	2:C:735:ARG:HG3	2.12	0.50
2:C:735:ARG:HH11	2:C:735:ARG:HG2	1.77	0.50
2:C:946:ARG:HB3	9:C:1400:HOH:O	2.12	0.50
3:D:12:LEU:HB2	9:D:9124:HOH:O	2.11	0.50
3:D:211:VAL:HG11	9:D:9609:HOH:O	2.12	0.50
3:D:401:TYR:CE2	3:D:415:VAL:HG13	2.47	0.50
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.42	0.50
3:D:629:SER:HB3	3:D:726:ILE:HD11	1.94	0.50
4:E:19:LEU:O	4:E:23:VAL:HG23	2.12	0.50
5:F:273:ARG:HG2	5:F:276:ARG:NH1	2.27	0.50
5:F:385:GLU:O	5:F:397:ILE:HD13	2.12	0.50
1:K:132:LEU:HD12	1:K:132:LEU:N	2.26	0.50
1:L:80:LEU:HD23	3:N:867:ARG:NH2	2.27	0.50
2:M:54:ILE:HG23	2:M:54:ILE:O	2.12	0.50
2:M:676:ILE:HD12	2:M:871:LEU:HB2	1.92	0.50
3:N:1194:CYS:HB3	3:N:1373:ARG:HH22	1.75	0.50
3:N:730:PRO:HA	3:N:733:CYS:SG	2.52	0.50
4:O:48:MET:CB	4:O:54:LEU:HB2	2.42	0.50
5:P:419:ARG:O	5:P:421:PHE:N	2.45	0.50
1:B:39:PRO:O	1:B:43:ILE:HG12	2.12	0.50
2:C:17:PRO:O	2:C:20:GLU:HB3	2.11	0.50
2:C:333:ILE:HD12	2:C:333:ILE:N	2.26	0.50
2:C:513:VAL:HG13	9:C:1221:HOH:O	2.12	0.50
2:C:590:ASP:HB2	9:C:1272:HOH:O	2.11	0.50
1:A:67:THR:HG21	2:C:609:ASN:HD21	1.76	0.50
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.94	0.50
3:D:908:LYS:CG	3:D:1027:GLY:HA3	2.42	0.50
3:D:1318:TYR:HB3	9:D:9944:HOH:O	2.11	0.50
3:D:407:VAL:HG11	9:D:9652:HOH:O	2.11	0.50
3:D:115:LEU:HD21	3:D:465:LEU:HD21	1.94	0.50
3:D:690:ALA:O	3:D:694:VAL:HG23	2.11	0.50
3:D:827:ILE:O	3:D:837:GLY:HA3	2.12	0.50
3:D:892:ASP:HB3	3:D:895:VAL:HB	1.94	0.50
5:F:353:GLU:OE2	5:F:356:LYS:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:159:LYS:HE3	9:L:5309:HOH:O	2.11	0.50
1:L:226:SER:O	1:L:228:PRO:HD3	2.12	0.50
2:M:207:LEU:HD22	2:M:221:LEU:CD2	2.42	0.50
2:M:284:ARG:HB2	9:M:1270:HOH:O	2.12	0.50
2:M:603:VAL:HG23	2:M:647:GLN:O	2.11	0.50
2:M:676:ILE:CG2	2:M:988:VAL:HG22	2.41	0.50
2:M:676:ILE:O	3:N:948:THR:HG23	2.12	0.50
2:M:73:LEU:HD12	2:M:73:LEU:O	2.12	0.50
3:N:1086:LEU:HD12	9:N:9724:HOH:O	2.12	0.50
3:N:1425:THR:HG23	3:N:1426:LYS:H	1.77	0.50
3:N:42:ASP:O	3:N:43:GLY:O	2.30	0.50
3:N:603:LEU:O	3:N:606:ILE:HB	2.11	0.50
4:O:61:GLU:C	4:O:65:MET:HE2	2.32	0.50
5:P:297:PRO:HB3	9:P:5408:HOH:O	2.11	0.50
1:A:216:GLU:HG2	9:A:416:HOH:O	2.12	0.49
1:A:20:TYR:CD2	1:A:21:GLY:N	2.72	0.49
1:A:88:ARG:NH1	1:A:90:LEU:HD21	2.27	0.49
1:B:91:ASN:O	1:B:94:LEU:HD12	2.12	0.49
2:C:395:LYS:HE3	2:C:403:SER:HB2	1.94	0.49
2:C:653:ASP:OD1	2:C:654:LEU:HD23	2.12	0.49
2:C:941:VAL:O	2:C:944:LEU:HB2	2.12	0.49
3:D:29:PRO:HG3	3:D:549:ASN:ND2	2.26	0.49
3:D:590:PRO:HG2	9:D:9991:HOH:O	2.11	0.49
9:C:1814:HOH:O	3:D:630:VAL:HG21	2.12	0.49
3:D:844:ALA:O	3:D:867:ARG:HB3	2.11	0.49
3:D:85:VAL:HG12	3:D:89:ARG:NE	2.27	0.49
5:F:247:ILE:O	5:F:251:ILE:HG13	2.11	0.49
1:K:213:GLN:O	1:K:217:ILE:HG13	2.12	0.49
1:L:127:LEU:HA	9:L:5627:HOH:O	2.11	0.49
1:L:7:LYS:HA	9:L:3817:HOH:O	2.12	0.49
2:M:207:LEU:HD23	2:M:211:LEU:HD23	1.94	0.49
2:M:380:ALA:HA	2:M:383:ARG:HG2	1.93	0.49
2:M:438:ILE:CD1	2:M:467:ILE:HD12	2.42	0.49
2:M:71:TYR:HA	9:M:1826:HOH:O	2.11	0.49
2:M:74:GLY:O	2:M:76:PRO:HD3	2.12	0.49
3:N:1123:PHE:HA	3:N:1135:ARG:H	1.76	0.49
3:N:1262:LEU:HD23	3:N:1352:ILE:CG1	2.42	0.49
3:N:1485:GLN:HE21	4:O:80:VAL:N	2.07	0.49
3:N:448:GLU:HG3	9:N:9605:HOH:O	2.12	0.49
3:N:957:PRO:CG	3:N:1007:VAL:HG12	2.42	0.49
5:P:153:PRO:HG3	9:P:7043:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HB2	9:B:530:HOH:O	2.11	0.49
1:B:41:ARG:HG3	1:B:177:VAL:CG2	2.36	0.49
2:C:159:ILE:HG22	9:C:2004:HOH:O	2.12	0.49
2:C:281:LEU:CD1	2:C:306:THR:HA	2.42	0.49
2:C:364:GLU:HB3	9:C:1329:HOH:O	2.12	0.49
2:C:80:GLN:O	2:C:83:CYS:HB2	2.12	0.49
3:D:60:CYS:HB3	9:D:9088:HOH:O	2.12	0.49
3:D:6:ARG:HG3	3:D:7:LYS:HG3	1.93	0.49
3:D:897:TRP:CZ3	3:D:902:LEU:HD21	2.47	0.49
4:E:43:GLU:HG2	4:E:44:GLU:H	1.77	0.49
1:K:198:ARG:C	1:K:199:ILE:HD12	2.32	0.49
1:L:71:VAL:HG22	1:L:132:LEU:CD1	2.42	0.49
2:M:101:ILE:HG22	2:M:102:HIS:N	2.26	0.49
2:M:139:GLN:HE22	2:M:415:PRO:CG	2.23	0.49
2:M:328:LEU:HD23	2:M:437:ARG:HD3	1.93	0.49
2:M:821:GLU:HB2	9:M:1696:HOH:O	2.13	0.49
3:N:1045:MET:HB3	3:N:1072:ILE:HG22	1.93	0.49
3:N:1429:LEU:HG	3:N:1441:GLN:HB2	1.93	0.49
3:N:185:VAL:HG13	9:N:2296:HOH:O	2.12	0.49
3:N:624:ASP:HB3	3:N:625:TYR:HD1	1.75	0.49
5:P:214:GLN:O	5:P:217:ASN:HB2	2.13	0.49
3:N:388:HIS:H	5:P:97:GLU:HG3	1.77	0.49
1:A:192:LEU:HA	9:A:345:HOH:O	2.12	0.49
1:A:208:LEU:CD1	1:A:212:ASN:HD21	2.24	0.49
1:A:212:ASN:O	1:A:215:VAL:HG22	2.13	0.49
1:A:27:PRO:HG2	1:A:186:LEU:CD2	2.39	0.49
1:B:23:PHE:CD2	1:B:211:LEU:HD22	2.47	0.49
2:C:234:ALA:HA	9:C:1236:HOH:O	2.12	0.49
2:C:498:GLN:O	2:C:501:THR:HG23	2.12	0.49
3:D:1164:ARG:HG3	9:D:9760:HOH:O	2.12	0.49
3:D:584:ASN:OD1	3:D:590:PRO:HD2	2.12	0.49
3:D:1086:LEU:HD11	6:D:8001:STD:H6	1.94	0.49
3:D:971:LEU:HD11	3:D:992:ILE:HD13	1.94	0.49
4:E:26:ARG:HE	4:E:30:LEU:CD1	2.24	0.49
4:E:54:LEU:HG	4:E:58:PRO:CG	2.41	0.49
5:F:295:MET:HG3	9:F:706:HOH:O	2.12	0.49
1:K:197:LEU:HD23	1:K:197:LEU:H	1.76	0.49
1:L:45:LEU:HD12	9:L:5472:HOH:O	2.12	0.49
2:M:199:VAL:HG13	2:M:235:LEU:CG	2.36	0.49
2:M:743:VAL:HG11	2:M:800:VAL:HG21	1.95	0.49
2:M:561:GLY:HA3	2:M:842:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:920:GLN:HG2	9:M:1233:HOH:O	2.11	0.49
3:N:1075:HIS:O	3:N:1079:LYS:HD3	2.12	0.49
3:N:1109:GLU:HG2	3:N:1202:GLN:H	1.77	0.49
3:N:1342:GLU:HB3	9:N:9279:HOH:O	2.11	0.49
3:N:1254:GLN:OE1	3:N:1355:VAL:HG13	2.13	0.49
3:N:1498:ALA:HA	3:N:1501:GLU:OE2	2.12	0.49
3:N:482:LYS:HA	3:N:489:ARG:HH21	1.77	0.49
5:P:278:LEU:CB	5:P:286:PRO:HG2	2.41	0.49
5:P:361:LEU:HD23	5:P:362:SER:N	2.27	0.49
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.47	0.49
2:C:101:ILE:HG22	2:C:102:HIS:N	2.27	0.49
2:C:249:LYS:HE3	9:C:1212:HOH:O	2.11	0.49
2:C:384:GLU:HA	2:C:388:ARG:CZ	2.42	0.49
2:C:767:PRO:HG2	9:C:1376:HOH:O	2.11	0.49
2:C:676:ILE:HG22	2:C:988:VAL:HG22	1.94	0.49
3:D:710:ARG:NH1	3:D:1210:SER:OG	2.46	0.49
3:D:178:LEU:HD11	9:D:9048:HOH:O	2.12	0.49
3:D:393:ILE:HD12	3:D:393:ILE:N	2.28	0.49
3:D:480:GLU:O	3:D:484:PRO:HD2	2.11	0.49
3:D:566:ILE:HD13	5:F:217:ASN:HB3	1.93	0.49
3:D:586:ARG:HG2	9:D:9444:HOH:O	2.11	0.49
3:D:601:ARG:HE	3:D:606:ILE:HA	1.76	0.49
2:C:1071:ILE:O	3:D:659:LYS:HG2	2.11	0.49
4:E:33:HIS:HB2	4:E:37:ASN:HD21	1.77	0.49
2:M:78:PHE:CG	2:M:88:LEU:HD21	2.47	0.49
3:N:27:GLU:N	9:N:9381:HOH:O	2.45	0.49
3:N:161:LEU:HD22	3:N:452:ILE:HG21	1.94	0.49
3:N:616:GLN:HA	9:N:9336:HOH:O	2.12	0.49
3:N:828:LYS:N	3:N:828:LYS:HD3	2.28	0.49
3:N:875:THR:HB	9:N:9245:HOH:O	2.13	0.49
3:N:96:ALA:HB1	3:N:554:LEU:HD12	1.94	0.49
4:O:61:GLU:O	4:O:65:MET:HG3	2.11	0.49
5:P:185:GLN:O	5:P:189:GLU:HG3	2.12	0.49
5:P:93:LEU:HG	5:P:190:ALA:HB1	1.93	0.49
1:A:50:GLY:O	1:A:146:ARG:HA	2.12	0.49
1:A:74:ASP:O	1:A:78:ILE:HG13	2.11	0.49
2:C:195:LEU:CD2	2:C:238:LEU:HG	2.42	0.49
3:D:1206:GLY:HA3	3:D:1366:LYS:NZ	2.27	0.49
3:D:1432:LYS:HB2	9:D:9247:HOH:O	2.12	0.49
3:D:150:ARG:HG3	3:D:150:ARG:NH1	2.27	0.49
9:C:1967:HOH:O	3:D:618:LEU:HD22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:166:LEU:HD22	5:F:170:HIS:HB2	1.94	0.49
5:F:93:LEU:HG	5:F:190:ALA:HB1	1.93	0.49
1:L:99:LEU:HD21	1:L:122:ILE:HD11	1.94	0.49
1:L:50:GLY:O	1:L:146:ARG:HA	2.13	0.49
1:L:26:GLU:CB	1:L:194:LYS:HG3	2.38	0.49
2:M:51:THR:CB	2:M:348:LEU:HD23	2.42	0.49
2:M:589:ARG:CB	2:M:589:ARG:HH11	2.22	0.49
2:M:69:LEU:HB2	2:M:97:ARG:HB2	1.94	0.49
3:N:1059:SER:HB3	9:N:9480:HOH:O	2.11	0.49
3:N:1280:VAL:HG23	3:N:1295:GLU:O	2.13	0.49
3:N:427:VAL:HG21	3:N:435:VAL:HB	1.93	0.49
3:N:633:VAL:HG22	3:N:635:PRO:CD	2.42	0.49
3:N:780:LYS:NZ	3:N:780:LYS:HB2	2.27	0.49
3:N:906:GLN:HA	3:N:906:GLN:OE1	2.11	0.49
1:A:62:LEU:HD23	1:A:163:ASN:HD21	1.77	0.49
2:C:374:ASN:HB2	9:C:1848:HOH:O	2.13	0.49
2:C:516:ARG:CD	2:C:521:PRO:HA	2.43	0.49
2:C:495:THR:HG21	2:C:524:VAL:HG21	1.93	0.49
2:C:641:PRO:HD2	9:C:1276:HOH:O	2.13	0.49
2:C:930:LYS:HA	9:C:1256:HOH:O	2.12	0.49
3:D:404:GLU:HB3	3:D:414:ARG:HD2	1.95	0.49
3:D:93:ILE:HG12	3:D:548:ILE:CD1	2.43	0.49
3:D:664:LYS:HG2	9:D:9879:HOH:O	2.12	0.49
3:D:815:ALA:HA	9:D:9402:HOH:O	2.12	0.49
3:D:962:GLN:HG3	9:D:2033:HOH:O	2.12	0.49
5:F:181:GLU:O	5:F:184:ARG:HB3	2.12	0.49
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.48	0.49
2:M:1032:PHE:CE2	2:M:1052:MET:HG2	2.48	0.49
2:M:218:VAL:HG22	2:M:221:LEU:CD2	2.41	0.49
2:M:227:PHE:HB3	9:M:1419:HOH:O	2.13	0.49
2:M:202:TYR:OH	2:M:304:LEU:HD22	2.13	0.49
2:M:37:GLU:HB2	9:M:2125:HOH:O	2.13	0.49
2:M:517:ARG:HD3	2:M:522:VAL:HG11	1.93	0.49
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.48	0.49
3:N:1211:MET:SD	4:O:16:LYS:HD2	2.52	0.49
3:N:1282:ARG:HA	3:N:1315:ASP:OD1	2.12	0.49
2:M:1042:ALA:CB	3:N:710:ARG:HD3	2.43	0.49
1:A:103:ALA:HB1	1:A:107:LYS:HD3	1.94	0.49
1:A:208:LEU:HD11	1:A:212:ASN:HD21	1.77	0.49
1:A:209:GLU:O	1:A:213:GLN:HG3	2.12	0.49
1:A:14:ARG:CZ	1:A:24:VAL:HG23	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ARG:HH22	3:D:884:ARG:CD	2.23	0.49
1:B:87:VAL:HG21	1:B:144:VAL:CG1	2.36	0.49
2:C:1004:LYS:HE3	2:C:1027:PHE:CE1	2.48	0.49
2:C:161:SER:HB2	9:C:1193:HOH:O	2.13	0.49
2:C:745:ILE:HD11	9:C:1385:HOH:O	2.12	0.49
2:C:893:ALA:HB2	2:C:918:LEU:HD12	1.95	0.49
3:D:169:TYR:N	3:D:170:PRO:CD	2.76	0.49
3:D:473:LEU:HD21	3:D:495:ARG:NE	2.28	0.49
3:D:462:GLN:HA	3:D:513:ILE:CD1	2.42	0.49
3:D:573:MET:SD	5:F:210:LEU:HB3	2.52	0.49
3:D:68:PHE:O	3:D:71:LYS:HG2	2.13	0.49
3:D:986:ARG:HD2	9:D:9742:HOH:O	2.11	0.49
5:F:402:ASN:O	5:F:406:ARG:HG3	2.13	0.49
1:L:161:ARG:HG3	9:L:4789:HOH:O	2.11	0.49
2:M:1107:ASN:HA	9:M:1260:HOH:O	2.13	0.49
2:M:34:VAL:HG12	9:M:1886:HOH:O	2.11	0.49
2:M:571:LEU:HA	2:M:701:THR:O	2.12	0.49
2:M:839:LEU:HD21	2:M:849:VAL:CG2	2.42	0.49
2:M:863:ASP:O	2:M:865:THR:N	2.45	0.49
3:N:128:TYR:HE1	3:N:461:ILE:HG13	1.77	0.49
3:N:703:ASN:ND2	3:N:704:ARG:H	2.10	0.49
3:N:820:GLU:HA	3:N:825:ALA:O	2.12	0.49
3:N:945:SER:OG	3:N:947:ILE:HG23	2.13	0.49
3:N:950:GLY:O	3:N:953:ASP:HB2	2.12	0.49
2:C:160:ALA:O	2:C:173:ASP:HA	2.12	0.49
2:C:254:VAL:HA	2:C:257:VAL:HG23	1.95	0.49
2:C:630:ARG:HH21	2:C:705:ILE:CG2	2.18	0.49
9:C:1210:HOH:O	3:D:1048:PRO:HG2	2.11	0.49
3:D:126:VAL:O	3:D:132:TYR:HD1	1.96	0.49
3:D:190:GLU:HG3	3:D:210:ARG:CD	2.42	0.49
3:D:65:ARG:H	3:D:68:PHE:HZ	1.61	0.49
3:D:706:PRO:HD2	9:D:9170:HOH:O	2.12	0.49
3:D:806:PHE:CZ	3:D:813:LEU:HB3	2.47	0.49
5:F:151:LEU:HB2	5:F:155:THR:H	1.78	0.49
5:F:245:GLN:HB3	9:F:604:HOH:O	2.13	0.49
5:F:282:LEU:CD1	5:F:286:PRO:HG3	2.43	0.49
1:K:210:ALA:HA	1:K:213:GLN:NE2	2.27	0.49
1:K:86:VAL:HG23	9:K:4248:HOH:O	2.13	0.49
1:L:189:ARG:HB3	9:L:3718:HOH:O	2.12	0.49
1:L:207:PRO:HD2	9:L:4122:HOH:O	2.12	0.49
2:M:264:PRO:HB3	2:M:289:THR:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:3:ILE:HB	9:M:2130:HOH:O	2.12	0.49
3:N:1115:THR:C	9:N:9343:HOH:O	2.50	0.49
3:N:1148:VAL:HG13	3:N:1163:GLY:O	2.13	0.49
3:N:1213:ARG:HB2	3:N:1214:PRO:CD	2.43	0.49
3:N:135:LEU:HA	3:N:453:ASP:O	2.13	0.49
3:N:152:LEU:HD23	3:N:152:LEU:N	2.21	0.49
3:N:212:ARG:HD2	9:N:9466:HOH:O	2.13	0.49
3:N:423:ASP:HB2	5:P:178:ARG:CD	2.43	0.49
3:N:57:GLU:HG2	3:N:58:CYS:N	2.27	0.49
3:N:793:THR:HA	9:N:9545:HOH:O	2.12	0.49
1:A:88:ARG:CZ	1:A:90:LEU:HD21	2.43	0.49
2:C:1054:THR:HG22	2:C:1059:ASP:OD2	2.13	0.49
2:C:79:PRO:HD2	2:C:82:GLU:HB2	1.95	0.49
3:D:183:GLU:HA	3:D:186:VAL:CG1	2.43	0.49
3:D:402:PRO:HG2	3:D:444:VAL:HG11	1.94	0.49
3:D:493:ARG:HG2	3:D:493:ARG:HH11	1.77	0.49
3:D:671:LYS:HG3	5:F:422:LEU:HA	1.94	0.49
5:F:131:VAL:HG22	5:F:178:ARG:HG2	1.95	0.49
5:F:365:GLU:OE1	5:F:400:ILE:HD12	2.12	0.49
5:F:387:GLY:HA2	9:F:752:HOH:O	2.12	0.49
1:L:123:MET:HA	9:L:6518:HOH:O	2.12	0.49
1:L:143:ARG:NH1	1:L:158:ILE:HD12	2.28	0.49
2:M:334:ARG:NH1	2:M:415:PRO:HG2	2.28	0.49
2:M:52:PHE:HD2	9:M:1848:HOH:O	1.95	0.49
2:M:601:GLY:HA2	2:M:616:GLU:HG2	1.94	0.49
2:M:710:ILE:HB	2:M:790:LEU:CD1	2.41	0.49
3:N:1402:ALA:HB2	3:N:1415:VAL:HG23	1.95	0.49
3:N:52:PRO:HG2	3:N:79:GLU:O	2.12	0.49
3:N:750:PRO:HB2	3:N:756:GLN:OE1	2.13	0.49
4:O:43:GLU:HG2	4:O:44:GLU:H	1.78	0.49
4:O:48:MET:HB2	4:O:54:LEU:HD12	1.93	0.49
1:A:185:ARG:O	1:A:185:ARG:HD2	2.13	0.49
1:B:208:LEU:HD13	1:B:212:ASN:HD21	1.78	0.49
2:C:113:VAL:HG11	2:C:373:VAL:HB	1.95	0.49
2:C:350:ARG:CB	2:C:350:ARG:HH11	2.19	0.49
3:D:104:PHE:CE2	3:D:1448:THR:HG23	2.48	0.49
2:C:429:ASP:HA	3:D:1078:ARG:HB3	1.94	0.49
3:D:1109:GLU:CD	3:D:1202:GLN:H	2.15	0.49
3:D:1135:ARG:HD3	9:D:2510:HOH:O	2.13	0.49
3:D:1356:TYR:CD2	3:D:1363:LEU:HD23	2.48	0.49
3:D:136:ASP:HB3	9:D:2221:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:185:VAL:CG1	3:D:191:LEU:HD21	2.43	0.49
3:D:19:ARG:NH2	3:D:94:GLU:OE2	2.46	0.49
3:D:440:VAL:HA	9:D:9739:HOH:O	2.13	0.49
3:D:539:ASP:CG	5:F:318:GLU:HB2	2.32	0.49
3:D:793:THR:HG22	3:D:879:ARG:HA	1.95	0.49
5:F:277:GLN:HG3	9:F:492:HOH:O	2.11	0.49
1:K:67:THR:HG23	2:M:627:ARG:HH21	1.78	0.49
2:M:1060:ILE:CG2	2:M:1061:GLU:N	2.75	0.49
2:M:220:GLY:HA3	9:M:1230:HOH:O	2.12	0.49
2:M:368:THR:HG23	9:M:1288:HOH:O	2.12	0.49
2:M:532:MET:HG3	2:M:533:ASP:H	1.76	0.49
2:M:549:PHE:CE2	2:M:886:LEU:HB3	2.48	0.49
3:N:440:VAL:HG12	3:N:441:ARG:N	2.27	0.49
3:N:571:LYS:HB2	3:N:571:LYS:HZ2	1.78	0.49
3:N:702:LEU:HD23	3:N:745:MET:HE1	1.95	0.49
4:O:94:PRO:HA	9:O:3788:HOH:O	2.12	0.49
1:A:86:VAL:HG21	1:A:202:ASP:O	2.13	0.48
1:A:97:VAL:HG23	9:A:513:HOH:O	2.13	0.48
1:B:10:VAL:HA	9:B:434:HOH:O	2.13	0.48
1:B:19:GLU:HB2	9:B:416:HOH:O	2.13	0.48
2:C:1059:ASP:CG	2:C:1062:GLY:HA3	2.32	0.48
2:C:400:PRO:N	9:C:1308:HOH:O	2.45	0.48
2:C:429:ASP:HB3	9:D:9038:HOH:O	2.12	0.48
3:D:960:LYS:HZ1	3:D:1041:LEU:HB3	1.78	0.48
3:D:1056:PRO:HD2	9:D:9713:HOH:O	2.12	0.48
3:D:132:TYR:HD2	9:D:9028:HOH:O	1.95	0.48
3:D:131:LYS:HB3	3:D:456:MET:CE	2.43	0.48
3:D:482:LYS:HD3	9:D:9448:HOH:O	2.12	0.48
3:D:829:VAL:H	3:D:835:SER:HB2	1.78	0.48
3:D:986:ARG:HG3	3:D:990:ASP:OD2	2.12	0.48
5:F:143:HIS:HB2	5:F:152:ASP:OD1	2.13	0.48
2:M:19:THR:O	2:M:23:VAL:HG23	2.13	0.48
2:M:308:ARG:HB3	9:M:1174:HOH:O	2.13	0.48
2:M:66:LEU:HD23	9:M:1162:HOH:O	2.13	0.48
2:M:755:LEU:HD22	2:M:825:VAL:HG11	1.95	0.48
3:N:44:LEU:HG	9:N:9441:HOH:O	2.13	0.48
5:P:392:VAL:HG22	9:P:5677:HOH:O	2.13	0.48
5:P:404:ALA:O	5:P:408:LEU:HD23	2.12	0.48
1:B:173:PRO:HG3	9:B:347:HOH:O	2.13	0.48
1:B:206:THR:HG23	1:B:209:GLU:H	1.78	0.48
1:A:219:ARG:NH2	1:B:223:THR:HG22	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:101:ILE:HG23	2:C:107:LEU:CD2	2.42	0.48
2:C:1051:GLU:HG2	2:C:1056:LYS:HD2	1.94	0.48
2:C:496:ILE:HD12	2:C:496:ILE:H	1.78	0.48
2:C:833:LEU:HD12	2:C:834:GLN:H	1.77	0.48
2:C:683:ASN:HB2	2:C:872:ASN:HB2	1.95	0.48
2:C:950:LEU:HB3	2:C:952:LEU:HD23	1.95	0.48
3:D:1096:ARG:CB	3:D:1096:ARG:HH11	2.24	0.48
3:D:1406:ARG:HH11	3:D:1406:ARG:HG2	1.78	0.48
3:D:200:ASP:HB3	9:D:2480:HOH:O	2.13	0.48
3:D:598:ARG:NH1	5:F:320:PRO:HD3	2.27	0.48
3:D:656:PHE:HB3	3:D:694:VAL:CG1	2.44	0.48
2:C:1115:LEU:HB3	3:D:85:VAL:HG13	1.95	0.48
3:D:890:VAL:HG13	3:D:926:LYS:CD	2.43	0.48
5:F:318:GLU:HA	9:F:522:HOH:O	2.13	0.48
5:F:82:ARG:HA	9:F:440:HOH:O	2.12	0.48
2:M:1017:THR:OG1	2:M:1019:GLN:HG2	2.14	0.48
2:M:192:PRO:HD3	9:M:1291:HOH:O	2.12	0.48
2:M:208:ALA:HA	2:M:221:LEU:HD21	1.95	0.48
2:M:35:PRO:HD2	2:M:38:LYS:CG	2.41	0.48
2:M:401:LEU:HD13	2:M:587:VAL:HG11	1.94	0.48
2:M:433:THR:CG2	2:M:488:ALA:HB1	2.43	0.48
2:M:437:ARG:HH21	2:M:488:ALA:HA	1.74	0.48
2:M:602:GLU:HA	2:M:647:GLN:O	2.13	0.48
3:N:1291:SER:HB3	9:N:9004:HOH:O	2.11	0.48
3:N:169:TYR:N	3:N:170:PRO:CD	2.76	0.48
3:N:28:LYS:HB2	3:N:41:ARG:CZ	2.43	0.48
3:N:637:LEU:CD1	3:N:641:GLN:HB2	2.43	0.48
2:M:1071:ILE:O	3:N:659:LYS:HB2	2.12	0.48
3:N:83:SER:O	3:N:86:ARG:HB3	2.13	0.48
5:P:100:VAL:HG11	9:P:5340:HOH:O	2.12	0.48
1:A:125:PRO:HB2	9:A:439:HOH:O	2.13	0.48
2:C:105:THR:HG21	9:C:1762:HOH:O	2.12	0.48
2:C:22:GLN:O	2:C:121:MET:HE1	2.13	0.48
2:C:182:VAL:HG23	9:C:1307:HOH:O	2.13	0.48
2:C:341:THR:CG2	2:C:345:ARG:HH21	2.27	0.48
3:D:1293:PHE:CE2	3:D:1302:GLU:HB2	2.48	0.48
3:D:535:PHE:HB2	9:F:515:HOH:O	2.12	0.48
3:D:561:GLY:HA3	5:F:184:ARG:NH2	2.19	0.48
5:F:278:LEU:HB2	5:F:286:PRO:HG2	1.94	0.48
5:F:416:ARG:HD2	5:F:419:ARG:HB3	1.95	0.48
1:K:191:ASP:O	1:K:192:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:50:GLY:O	1:K:146:ARG:HA	2.13	0.48
1:L:23:PHE:O	1:L:196:THR:HA	2.14	0.48
2:M:1015:LEU:HA	5:P:335:ASP:CB	2.40	0.48
2:M:131:GLY:N	9:M:1177:HOH:O	2.46	0.48
2:M:568:ALA:HB1	2:M:668:LEU:HB3	1.93	0.48
2:M:911:GLU:O	2:M:915:LYS:HG2	2.14	0.48
3:N:1333:HIS:O	3:N:1336:LEU:HB3	2.13	0.48
3:N:1346:ARG:HA	3:N:1346:ARG:NE	2.28	0.48
3:N:490:ALA:HB2	9:N:2018:HOH:O	2.13	0.48
3:N:777:PRO:HD2	3:N:912:LYS:HG3	1.94	0.48
5:P:256:ARG:CZ	5:P:256:ARG:HB3	2.43	0.48
1:B:71:VAL:HG22	1:B:132:LEU:HD12	1.95	0.48
1:B:50:GLY:O	1:B:146:ARG:HA	2.13	0.48
2:C:44:ILE:O	2:C:48:PHE:HB2	2.13	0.48
2:C:611:ILE:HG22	2:C:613:VAL:HG13	1.95	0.48
2:C:750:LYS:HD2	9:C:1684:HOH:O	2.14	0.48
2:C:756:VAL:HG21	2:C:823:VAL:HG11	1.95	0.48
2:C:928:LYS:HE3	9:C:1852:HOH:O	2.13	0.48
2:C:69:LEU:HB2	2:C:97:ARG:HB2	1.94	0.48
2:C:98:LEU:HA	9:C:1321:HOH:O	2.12	0.48
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.13	0.48
3:D:591:VAL:HG22	9:D:9420:HOH:O	2.11	0.48
3:D:82:LYS:O	3:D:85:VAL:HG23	2.13	0.48
3:D:930:LEU:O	3:D:934:LEU:HG	2.14	0.48
4:E:77:GLU:HG3	9:E:139:HOH:O	2.12	0.48
2:M:193:LEU:HD23	2:M:307:LEU:HD13	1.94	0.48
2:M:31:GLN:HG2	9:M:1193:HOH:O	2.13	0.48
2:M:585:GLU:HG3	2:M:665:PHE:CE2	2.48	0.48
2:M:690:ILE:HG23	2:M:852:ILE:HA	1.95	0.48
2:M:799:ILE:HD13	2:M:799:ILE:N	2.27	0.48
2:M:876:VAL:O	2:M:879:ARG:O	2.31	0.48
3:N:1262:LEU:HD23	3:N:1352:ILE:HG12	1.95	0.48
3:N:427:VAL:HG13	9:N:9964:HOH:O	2.13	0.48
2:M:1007:ALA:HB1	3:N:652:LEU:HD22	1.95	0.48
4:O:84:ARG:HG3	4:O:84:ARG:O	2.13	0.48
5:P:169:GLU:H	5:P:169:GLU:CD	2.17	0.48
2:C:100:LEU:HD12	2:C:101:ILE:O	2.13	0.48
2:C:274:ARG:CB	2:C:285:LEU:HD13	2.43	0.48
2:C:569:VAL:HG12	2:C:996:LYS:O	2.14	0.48
2:C:975:TYR:N	2:C:975:TYR:HD1	2.12	0.48
3:D:1413:THR:HG21	9:D:9072:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:696:HIS:CD2	4:E:59:ASN:HB2	2.48	0.48
3:D:911:LEU:O	3:D:915:VAL:HG23	2.14	0.48
3:D:926:LYS:HG3	9:D:2130:HOH:O	2.14	0.48
3:D:996:TRP:O	3:D:999:THR:HG22	2.13	0.48
5:F:132:ARG:HD3	5:F:181:GLU:OE1	2.14	0.48
5:F:256:ARG:HD3	5:F:260:ILE:HD12	1.95	0.48
5:F:397:ILE:HG21	9:F:553:HOH:O	2.13	0.48
2:M:144:PRO:HB2	2:M:267:TYR:CE1	2.47	0.48
2:M:142:ARG:NH1	2:M:325:ILE:HG12	2.28	0.48
2:M:464:LEU:HB2	9:M:1673:HOH:O	2.12	0.48
2:M:925:TYR:C	2:M:925:TYR:CD1	2.87	0.48
3:N:1086:LEU:HA	6:N:8002:STD:H30	1.96	0.48
3:N:1459:LEU:HD22	3:N:1465:ASN:HD22	1.79	0.48
3:N:434:ARG:HB2	3:N:447:VAL:HG13	1.94	0.48
3:N:523:ASP:O	3:N:526:PRO:HG3	2.13	0.48
3:N:715:ALA:O	3:N:764:LEU:HD12	2.13	0.48
3:N:880:ILE:HD13	3:N:880:ILE:O	2.13	0.48
5:P:113:ILE:HG23	5:P:127:ILE:CG2	2.43	0.48
9:N:9491:HOH:O	5:P:318:GLU:HB3	2.13	0.48
1:A:117:VAL:HG12	9:A:324:HOH:O	2.13	0.48
1:B:101:LEU:HD21	1:B:113:ASP:HB3	1.95	0.48
1:B:199:ILE:CD1	1:B:211:LEU:HD13	2.42	0.48
2:C:203:ASP:OD1	2:C:205:GLU:HG3	2.14	0.48
2:C:242:LEU:HD23	9:C:1166:HOH:O	2.14	0.48
2:C:405:ARG:O	2:C:408:ARG:HG3	2.14	0.48
2:C:52:PHE:HE1	2:C:66:LEU:HG	1.79	0.48
3:D:1057:VAL:HG22	3:D:1069:GLU:HB3	1.95	0.48
3:D:1263:PHE:CZ	3:D:1352:ILE:HD13	2.48	0.48
3:D:1103:HIS:HD2	3:D:1462:LEU:H	1.62	0.48
3:D:412:GLY:O	3:D:421:LEU:HB3	2.14	0.48
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.17	0.48
3:D:141:ILE:CD1	3:D:450:TYR:HB2	2.40	0.48
3:D:475:LYS:O	3:D:479:GLU:HG2	2.13	0.48
4:E:31:LEU:HD12	4:E:32:ARG:CD	2.43	0.48
5:F:154:LYS:HB2	9:F:528:HOH:O	2.13	0.48
5:F:399:GLN:O	5:F:403:LYS:HB2	2.14	0.48
1:L:41:ARG:CZ	1:L:177:VAL:HG23	2.43	0.48
2:M:1014:SER:HB3	2:M:1017:THR:O	2.14	0.48
2:M:333:ILE:O	2:M:465:GLY:HA3	2.12	0.48
2:M:495:THR:CG2	2:M:517:ARG:HE	2.27	0.48
2:M:769:PRO:HB2	9:M:1243:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:949:ILE:HD11	3:N:1023:MET:CE	2.44	0.48
3:N:1252:ILE:HD13	9:N:9875:HOH:O	2.12	0.48
3:N:1103:HIS:CD2	3:N:1463:LYS:H	2.31	0.48
3:N:551:ASN:O	3:N:555:LYS:HG3	2.13	0.48
3:N:651:GLU:HG2	9:N:9511:HOH:O	2.14	0.48
3:N:799:LYS:O	3:N:799:LYS:HD3	2.13	0.48
5:P:141:VAL:O	5:P:145:PRO:HD2	2.13	0.48
5:P:167:PRO:HB2	5:P:169:GLU:OE2	2.13	0.48
5:P:321:ILE:HG13	5:P:329:TYR:CA	2.43	0.48
5:P:403:LYS:NZ	5:P:406:ARG:HB2	2.28	0.48
1:A:26:GLU:HG2	1:A:27:PRO:CA	2.43	0.48
1:A:26:GLU:HG2	1:A:27:PRO:HA	1.96	0.48
2:C:27:ARG:HG3	9:C:1390:HOH:O	2.14	0.48
2:C:26:TYR:HH	2:C:386:PHE:HZ	1.61	0.48
2:C:585:GLU:O	2:C:588:VAL:HG22	2.13	0.48
2:C:712:ALA:CB	2:C:820:ARG:HH11	2.27	0.48
2:C:93:PRO:HD2	9:C:1438:HOH:O	2.14	0.48
3:D:1211:MET:SD	3:D:1213:ARG:HD2	2.53	0.48
3:D:661:MET:HA	3:D:666:ILE:CD1	2.43	0.48
3:D:646:LYS:HZ2	3:D:688:TRP:HE1	1.60	0.48
4:E:50:THR:HG23	9:E:222:HOH:O	2.13	0.48
5:F:141:VAL:HG23	9:F:544:HOH:O	2.13	0.48
5:F:207:LEU:CB	5:F:212:LEU:HD12	2.44	0.48
1:K:58:ILE:HG21	1:K:68:ILE:HD11	1.94	0.48
1:L:80:LEU:HD23	3:N:867:ARG:CZ	2.44	0.48
2:M:129:ILE:HD12	2:M:134:ARG:HD2	1.95	0.48
2:M:395:LYS:HG2	2:M:397:GLU:HG2	1.95	0.48
2:M:643:VAL:HG13	2:M:647:GLN:CD	2.34	0.48
2:M:751:PRO:HB2	3:N:680:GLN:HG3	1.96	0.48
2:M:832:LYS:HG2	9:M:1238:HOH:O	2.13	0.48
3:N:186:VAL:HG13	3:N:187:LYS:N	2.28	0.48
3:N:486:ARG:HA	3:N:489:ARG:HD3	1.95	0.48
3:N:115:LEU:CD1	3:N:499:VAL:HG22	2.43	0.48
5:P:137:GLY:HA2	5:P:140:ARG:HH22	1.78	0.48
5:P:184:ARG:O	5:P:188:ILE:HG13	2.14	0.48
1:A:162:ILE:HA	9:A:494:HOH:O	2.14	0.48
1:A:76:VAL:O	1:A:79:ILE:HG13	2.13	0.48
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.49	0.48
2:C:15:LEU:HD12	2:C:15:LEU:H	1.79	0.48
2:C:171:TRP:HB2	9:C:1835:HOH:O	2.13	0.48
2:C:625:LEU:HD11	2:C:641:PRO:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TYR:HE1	2:C:696:LYS:HA	1.78	0.48
2:C:813:VAL:HG11	9:C:1461:HOH:O	2.13	0.48
2:C:831:ARG:HG2	2:C:831:ARG:HH11	1.77	0.48
3:D:1393:GLN:HB2	3:D:1398:TRP:HZ2	1.77	0.48
3:D:154:THR:HG22	3:D:157:GLU:CD	2.33	0.48
3:D:395:VAL:HG21	9:D:9114:HOH:O	2.14	0.48
2:C:1010:THR:HG21	5:F:341:PRO:HB2	1.94	0.48
5:F:369:LEU:HD11	5:F:401:GLU:HB2	1.94	0.48
5:F:411:HIS:HB2	9:F:455:HOH:O	2.14	0.48
1:K:50:GLY:HA3	1:K:173:PRO:HG3	1.96	0.48
1:L:173:PRO:HA	1:L:202:ASP:OD2	2.14	0.48
2:M:1001:VAL:HA	9:M:1286:HOH:O	2.13	0.48
2:M:132:ALA:HB1	2:M:632:ASN:ND2	2.26	0.48
2:M:248:PRO:HG3	9:M:1752:HOH:O	2.14	0.48
2:M:268:ASP:HB2	9:M:1657:HOH:O	2.13	0.48
2:M:328:LEU:HD23	2:M:437:ARG:CD	2.44	0.48
2:M:460:ARG:HG2	2:M:460:ARG:HH11	1.78	0.48
2:M:752:GLY:O	3:N:679:ARG:HG2	2.13	0.48
2:M:952:LEU:HD12	2:M:969:GLN:NE2	2.29	0.48
3:N:1437:ALA:O	3:N:1446:VAL:HG21	2.13	0.48
3:N:702:LEU:HD22	3:N:716:PHE:CE1	2.49	0.48
4:O:35:PHE:HZ	4:O:60:ALA:HA	1.79	0.48
3:N:64:LYS:HD3	5:P:377:ASP:OD2	2.13	0.48
5:P:85:LEU:HB3	9:P:3605:HOH:O	2.14	0.48
1:A:29:GLU:HB2	1:A:32:PHE:HD1	1.79	0.48
2:C:1098:ASP:HB3	9:C:1791:HOH:O	2.14	0.48
2:C:732:ALA:HA	2:C:735:ARG:CZ	2.43	0.48
3:D:1046:GLN:HG3	9:D:9074:HOH:O	2.14	0.48
3:D:1505:ALA:HB3	9:D:9104:HOH:O	2.12	0.48
3:D:441:ARG:O	3:D:443:VAL:N	2.46	0.48
3:D:83:SER:O	3:D:86:ARG:HB3	2.14	0.48
5:F:154:LYS:HG2	9:F:744:HOH:O	2.14	0.48
1:L:101:LEU:HD12	1:L:114:PHE:CE1	2.48	0.48
2:M:1018:GLN:HE21	2:M:1063:ARG:NH2	2.12	0.48
2:M:1008:ARG:HE	2:M:1028:GLY:CA	2.26	0.48
2:M:163:ILE:HG13	2:M:163:ILE:O	2.14	0.48
2:M:439:CYS:HB2	9:M:1316:HOH:O	2.13	0.48
2:M:513:VAL:HG12	9:M:1155:HOH:O	2.13	0.48
3:N:126:VAL:HG12	3:N:132:TYR:HB2	1.96	0.48
3:N:1397:LYS:HD3	9:N:2162:HOH:O	2.13	0.48
3:N:396:VAL:HG22	9:N:9364:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:583:ASP:HB2	3:N:604:THR:OG1	2.13	0.48
3:N:781:PRO:HB3	3:N:785:ILE:CG2	2.43	0.48
3:N:819:GLY:HA2	9:N:9097:HOH:O	2.13	0.48
2:M:1115:LEU:HD23	3:N:85:VAL:CG1	2.44	0.48
5:P:350:LEU:HD23	5:P:351:SER:H	1.78	0.48
1:A:54:THR:HG23	1:A:156:HIS:CE1	2.47	0.48
1:A:197:LEU:HD23	1:A:197:LEU:N	2.29	0.48
1:B:173:PRO:HA	1:B:202:ASP:OD2	2.14	0.48
1:B:52:ALA:N	9:B:467:HOH:O	2.47	0.48
2:C:139:GLN:HE22	2:C:415:PRO:CD	2.26	0.48
2:C:958:THR:HG21	9:C:1582:HOH:O	2.13	0.48
3:D:1235:GLN:C	3:D:1359:GLN:HE22	2.17	0.48
3:D:175:VAL:HG11	9:D:2479:HOH:O	2.13	0.48
3:D:190:GLU:HG3	3:D:210:ARG:HD3	1.95	0.48
3:D:90:MET:CE	3:D:518:PRO:HB3	2.43	0.48
3:D:867:ARG:HD3	9:D:9106:HOH:O	2.14	0.48
5:F:109:GLY:O	5:F:112:ALA:HB3	2.14	0.48
5:F:122:LEU:HD23	9:F:445:HOH:O	2.13	0.48
5:F:247:ILE:HG22	5:F:251:ILE:CD1	2.43	0.48
1:K:23:PHE:O	1:K:196:THR:HA	2.14	0.48
1:K:90:LEU:HD21	9:K:4206:HOH:O	2.12	0.48
1:L:132:LEU:HG	1:L:136:GLY:HA3	1.95	0.48
2:M:250:ARG:HG2	9:M:2036:HOH:O	2.12	0.48
2:M:495:THR:HG23	2:M:517:ARG:HE	1.78	0.48
2:M:839:LEU:N	2:M:839:LEU:HD23	2.29	0.48
2:M:537:LYS:HG3	2:M:905:ILE:CD1	2.44	0.48
2:M:944:LEU:HD11	2:M:963:LEU:CD2	2.44	0.48
3:N:1319:VAL:HG11	3:N:1325:LEU:HD11	1.95	0.48
3:N:1192:LEU:HD21	3:N:1372:VAL:CG1	2.44	0.48
3:N:1397:LYS:O	3:N:1400:VAL:HB	2.14	0.48
3:N:1379:VAL:HA	3:N:1420:LEU:HB3	1.96	0.48
3:N:9:ARG:HA	3:N:1455:LYS:O	2.12	0.48
3:N:431:VAL:HG13	9:N:9125:HOH:O	2.14	0.48
3:N:58:CYS:SG	3:N:59:ALA:N	2.87	0.48
2:M:1101:THR:HB	3:N:5:VAL:HG11	1.94	0.48
9:M:1452:HOH:O	5:P:423:ASP:HB3	2.14	0.48
5:P:94:LEU:HD22	5:P:97:GLU:CB	2.43	0.48
5:P:94:LEU:H	5:P:98:GLU:CD	2.16	0.48
2:C:1113:GLU:HG3	9:C:1553:HOH:O	2.13	0.47
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.95	0.47
2:C:626:ARG:N	2:C:639:GLN:NE2	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1312:LEU:HD21	3:D:1327:ARG:HG3	1.94	0.47
3:D:493:ARG:HE	3:D:1388:ARG:HB3	1.79	0.47
3:D:439:LEU:HD11	9:F:435:HOH:O	2.14	0.47
3:D:86:ARG:NH1	3:D:86:ARG:HG2	2.28	0.47
5:F:154:LYS:O	5:F:158:GLU:HG3	2.14	0.47
2:M:183:SER:HB3	2:M:190:LYS:HD3	1.95	0.47
2:M:253:ALA:HB3	9:M:2036:HOH:O	2.13	0.47
2:M:34:VAL:HB	2:M:38:LYS:CG	2.44	0.47
2:M:47:ALA:O	2:M:50:GLU:HB3	2.13	0.47
3:N:1114:THR:CG2	3:N:1195:GLN:HB3	2.44	0.47
3:N:1476:THR:HG23	4:O:21:VAL:CG2	2.41	0.47
3:N:591:VAL:CG1	3:N:597:ASP:HA	2.44	0.47
3:N:628:ARG:HH11	3:N:744:GLN:NE2	2.11	0.47
3:N:908:LYS:HD3	3:N:1027:GLY:HA3	1.95	0.47
3:N:785:ILE:HG12	3:N:935:LYS:HA	1.95	0.47
3:N:1476:THR:CG2	4:O:21:VAL:HG22	2.40	0.47
4:O:89:MET:HA	9:O:3549:HOH:O	2.13	0.47
1:A:156:HIS:CD2	1:A:157:GLY:N	2.81	0.47
2:C:165:LEU:HD13	9:C:1871:HOH:O	2.13	0.47
2:C:554:ASP:HB3	9:C:1189:HOH:O	2.14	0.47
2:C:589:ARG:HB2	9:C:1302:HOH:O	2.14	0.47
2:C:863:ASP:O	2:C:865:THR:N	2.47	0.47
3:D:960:LYS:NZ	3:D:1041:LEU:HB3	2.29	0.47
3:D:191:LEU:HD12	9:D:9609:HOH:O	2.13	0.47
1:K:47:SER:HB3	1:K:217:ILE:HD13	1.96	0.47
2:M:1090:LYS:HG2	2:M:1112:PHE:CZ	2.49	0.47
2:M:20:GLU:HG3	9:M:1572:HOH:O	2.14	0.47
2:M:31:GLN:HA	9:M:1193:HOH:O	2.12	0.47
2:M:433:THR:O	2:M:437:ARG:HD2	2.14	0.47
2:M:437:ARG:O	2:M:467:ILE:HG21	2.14	0.47
3:N:1403:LEU:O	3:N:1407:LEU:HB2	2.14	0.47
3:N:814:ALA:O	3:N:818:ARG:HG3	2.14	0.47
3:N:81:THR:HG22	3:N:82:LYS:N	2.29	0.47
3:N:87:ARG:HB3	3:N:523:ASP:HB2	1.95	0.47
9:M:1567:HOH:O	3:N:89:ARG:HG3	2.13	0.47
5:P:142:ARG:HH11	5:P:142:ARG:CB	2.21	0.47
1:B:69:PRO:HB2	9:B:413:HOH:O	2.13	0.47
2:C:1111:ILE:HG13	2:C:1112:PHE:N	2.25	0.47
2:C:690:ILE:HD11	2:C:694:LEU:HB2	1.96	0.47
2:C:815:LEU:HD23	9:C:1733:HOH:O	2.14	0.47
3:D:102:ILE:HD12	9:D:9788:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:10:ILE:HG13	3:D:1434:TRP:CE2	2.49	0.47
3:D:119:SER:H	3:D:123:LEU:HD13	1.79	0.47
3:D:1455:LYS:C	3:D:1455:LYS:HD3	2.35	0.47
3:D:661:MET:HE2	3:D:673:ALA:HB1	1.95	0.47
3:D:799:LYS:H	3:D:826:PRO:HG2	1.79	0.47
3:D:844:ALA:HA	3:D:867:ARG:NH1	2.30	0.47
2:M:1018:GLN:HE21	2:M:1060:ILE:CD1	2.21	0.47
2:M:167:LYS:HD3	2:M:168:ARG:N	2.28	0.47
2:M:211:LEU:HD11	2:M:308:ARG:HA	1.96	0.47
3:N:1120:VAL:HB	3:N:1144:LEU:HD21	1.96	0.47
3:N:1156:LEU:CD1	3:N:1176:LYS:HD2	2.44	0.47
3:N:1314:LYS:HZ1	3:N:1317:ASP:H	1.61	0.47
3:N:15:PRO:HA	3:N:18:ILE:CG1	2.43	0.47
3:N:33:ASN:OD1	5:P:259:ARG:HB3	2.15	0.47
3:N:41:ARG:NH1	3:N:42:ASP:HB2	2.29	0.47
3:N:858:VAL:HA	9:N:9278:HOH:O	2.14	0.47
3:N:880:ILE:HB	9:N:9245:HOH:O	2.14	0.47
2:C:1076:VAL:HG23	3:D:752:SER:HA	1.96	0.47
2:C:140:ILE:HG13	2:C:410:ILE:CG2	2.44	0.47
2:C:173:ASP:HB3	9:C:1237:HOH:O	2.15	0.47
2:C:292:ARG:HD2	2:C:299:LYS:HD3	1.96	0.47
2:C:52:PHE:O	2:C:54:ILE:N	2.47	0.47
2:C:575:GLN:HB2	2:C:670:GLN:OE1	2.14	0.47
2:C:64:LEU:HB2	2:C:359:MET:SD	2.54	0.47
2:C:710:ILE:CB	2:C:790:LEU:HD13	2.40	0.47
3:D:1197:ARG:HH11	3:D:1198:TYR:HD1	1.61	0.47
3:D:1268:PRO:HG2	3:D:1329:ALA:HB1	1.97	0.47
3:D:1397:LYS:HG2	9:D:9862:HOH:O	2.14	0.47
3:D:1468:LEU:HD22	3:D:1470:ARG:CB	2.45	0.47
3:D:1475:GLY:HA2	4:E:17:TYR:HE1	1.80	0.47
5:F:128:ARG:O	5:F:132:ARG:HG2	2.15	0.47
2:M:127:PHE:O	2:M:133:ASP:HA	2.14	0.47
2:M:256:TYR:CE1	2:M:293:PHE:HB2	2.49	0.47
2:M:299:LYS:HB2	9:M:1182:HOH:O	2.15	0.47
2:M:583:LEU:N	2:M:583:LEU:HD12	2.29	0.47
2:M:80:GLN:O	2:M:83:CYS:HB2	2.14	0.47
3:N:1051:GLU:HG3	3:N:1051:GLU:H	1.54	0.47
3:N:1065:LEU:HD12	3:N:1070:TYR:HB2	1.95	0.47
3:N:133:ILE:HG21	3:N:454:ALA:CB	2.41	0.47
3:N:136:ASP:HB2	3:N:137:PRO:HD3	1.97	0.47
3:N:12:LEU:HD11	3:N:512:MET:HG2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:52:PRO:HD2	3:N:79:GLU:O	2.14	0.47
3:N:423:ASP:HB2	5:P:178:ARG:HD2	1.96	0.47
5:P:398:ARG:NH1	9:P:6264:HOH:O	2.47	0.47
1:B:188:GLN:HG3	9:D:9361:HOH:O	2.14	0.47
2:C:199:VAL:HG13	2:C:235:LEU:HG	1.95	0.47
2:C:376:ARG:HG2	9:C:1987:HOH:O	2.14	0.47
2:C:54:ILE:HA	9:C:1626:HOH:O	2.14	0.47
2:C:654:LEU:HD13	2:C:664:GLY:N	2.29	0.47
2:C:776:SER:HA	2:C:780:GLU:HB3	1.96	0.47
2:C:86:LYS:CG	2:C:813:VAL:HG12	2.44	0.47
2:C:897:LEU:HB3	2:C:899:GLN:HG2	1.97	0.47
2:C:915:LYS:O	2:C:968:LEU:HD22	2.15	0.47
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.15	0.47
3:D:1084:THR:HA	3:D:1087:ARG:NH1	2.30	0.47
3:D:1403:LEU:O	3:D:1407:LEU:HD12	2.14	0.47
3:D:454:ALA:C	3:D:455:ARG:HD2	2.35	0.47
3:D:42:ASP:O	3:D:46:ASP:HB2	2.14	0.47
1:B:176:ARG:NH2	3:D:884:ARG:HD3	2.24	0.47
4:E:48:MET:HB3	4:E:54:LEU:HB2	1.95	0.47
5:F:302:LYS:HG3	5:F:303:ARG:N	2.28	0.47
1:K:19:GLU:CD	1:K:19:GLU:H	2.17	0.47
2:M:1103:ASP:OD1	3:N:3:LYS:HB2	2.14	0.47
2:M:217:LEU:HG	9:M:1729:HOH:O	2.13	0.47
2:M:402:SER:HA	2:M:566:THR:HG23	1.95	0.47
2:M:50:GLU:HG3	9:M:1427:HOH:O	2.15	0.47
2:M:643:VAL:HG13	2:M:647:GLN:OE1	2.14	0.47
2:M:751:PRO:HA	2:M:792:VAL:CG1	2.44	0.47
2:M:801:VAL:HG12	9:M:1569:HOH:O	2.13	0.47
2:M:941:VAL:O	2:M:944:LEU:HB2	2.14	0.47
3:N:1119:SER:HA	3:N:1186:VAL:O	2.14	0.47
3:N:1195:GLN:OE1	3:N:1196:THR:N	2.48	0.47
3:N:493:ARG:NH2	3:N:1388:ARG:HB3	2.21	0.47
3:N:1104:GLU:HA	3:N:1461:GLY:HA2	1.95	0.47
3:N:170:PRO:HG2	9:N:2108:HOH:O	2.14	0.47
9:M:1607:HOH:O	3:N:647:ARG:HG3	2.15	0.47
3:N:681:ARG:NH1	3:N:681:ARG:HB3	2.30	0.47
3:N:828:LYS:HB3	9:N:9243:HOH:O	2.15	0.47
5:P:93:LEU:HG	5:P:190:ALA:CB	2.44	0.47
1:A:122:ILE:N	1:A:122:ILE:HD12	2.29	0.47
1:A:128:HIS:HB2	9:A:329:HOH:O	2.14	0.47
2:C:65:VAL:HB	2:C:101:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:117:HIS:HD2	9:C:1136:HOH:O	1.97	0.47
2:C:212:GLY:C	2:C:215:GLY:H	2.18	0.47
2:C:199:VAL:HG13	2:C:235:LEU:CD2	2.44	0.47
2:C:352:ALA:HA	2:C:355:VAL:CG1	2.44	0.47
2:C:426:ASP:HB2	9:C:1138:HOH:O	2.15	0.47
2:C:332:ARG:NE	2:C:464:LEU:HD11	2.25	0.47
2:C:620:LEU:HD13	2:C:620:LEU:N	2.29	0.47
2:C:575:GLN:C	2:C:667:ALA:HB1	2.35	0.47
2:C:679:PHE:C	3:D:943:THR:HG22	2.34	0.47
2:C:918:LEU:HD23	2:C:968:LEU:HA	1.96	0.47
3:D:1123:PHE:HA	3:D:1133:ARG:O	2.15	0.47
3:D:385:VAL:HA	9:D:9728:HOH:O	2.15	0.47
3:D:41:ARG:HD3	3:D:42:ASP:H	1.80	0.47
3:D:795:VAL:CG1	3:D:863:VAL:HG13	2.40	0.47
2:C:987:ILE:CG2	3:D:948:THR:HG21	2.37	0.47
5:F:292:ALA:HB1	5:F:299:TRP:O	2.14	0.47
1:K:186:LEU:CB	1:K:192:LEU:HD11	2.44	0.47
1:L:150:TYR:CE2	3:N:857:ILE:HG13	2.49	0.47
2:M:260:LEU:HD21	9:M:1166:HOH:O	2.15	0.47
2:M:290:LEU:HB2	9:M:2147:HOH:O	2.14	0.47
2:M:44:ILE:HA	2:M:344:PHE:HE1	1.78	0.47
2:M:670:GLN:O	2:M:672:VAL:HG13	2.14	0.47
2:M:890:LEU:HA	2:M:914:ILE:HD11	1.96	0.47
3:N:1223:ILE:HD12	9:N:9798:HOH:O	2.14	0.47
3:N:693:GLU:HA	4:O:48:MET:CE	2.44	0.47
3:N:811:GLU:HA	9:N:9613:HOH:O	2.14	0.47
3:N:861:GLN:H	3:N:861:GLN:CD	2.18	0.47
3:N:861:GLN:N	3:N:861:GLN:CD	2.68	0.47
3:N:930:LEU:O	3:N:934:LEU:HG	2.14	0.47
3:N:696:HIS:HB2	4:O:48:MET:HE1	1.95	0.47
5:P:104:ARG:HA	5:P:229:TYR:CE1	2.48	0.47
5:P:287:THR:O	5:P:289:GLU:N	2.46	0.47
5:P:399:GLN:O	5:P:403:LYS:HB2	2.14	0.47
1:A:14:ARG:HB3	9:A:477:HOH:O	2.13	0.47
1:B:121:GLU:HB2	9:B:567:HOH:O	2.13	0.47
1:B:124:ASN:OD1	1:B:127:LEU:HB2	2.14	0.47
2:C:264:PRO:HB3	2:C:289:THR:HB	1.96	0.47
2:C:328:LEU:HD13	2:C:433:THR:CB	2.40	0.47
3:D:1264:GLU:OE2	3:D:1424:VAL:HG12	2.14	0.47
3:D:1432:LYS:HD2	3:D:1433:SER:N	2.29	0.47
3:D:427:VAL:HA	9:D:9128:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:625:TYR:CD1	3:D:625:TYR:N	2.83	0.47
5:F:141:VAL:O	5:F:145:PRO:HD2	2.15	0.47
5:F:165:SER:HB3	9:F:743:HOH:O	2.14	0.47
5:F:319:THR:N	9:F:522:HOH:O	2.46	0.47
5:F:342:VAL:HG21	9:F:789:HOH:O	2.14	0.47
1:K:19:GLU:O	1:K:200:TRP:HA	2.14	0.47
1:L:109:VAL:HG21	1:L:138:LEU:HD21	1.97	0.47
1:L:173:PRO:HG3	9:L:4500:HOH:O	2.15	0.47
2:M:1090:LYS:HG2	2:M:1112:PHE:HZ	1.80	0.47
2:M:637:LEU:HA	2:M:659:PRO:HG3	1.97	0.47
2:M:721:ARG:NH2	2:M:783:ARG:HH21	2.09	0.47
2:M:926:PHE:HE1	2:M:929:ARG:NH2	2.13	0.47
2:M:500:ASN:HD21	3:N:1067:VAL:CG2	2.28	0.47
3:N:907:GLU:OE1	3:N:909:ASN:HB2	2.14	0.47
4:O:87:LYS:HD2	9:O:4461:HOH:O	2.15	0.47
1:A:106:PRO:HG3	1:A:133:GLU:O	2.15	0.47
1:A:219:ARG:O	1:A:223:THR:HG23	2.14	0.47
2:C:244:PRO:HD3	9:C:1182:HOH:O	2.15	0.47
2:C:29:ALA:HB2	2:C:337:GLY:CA	2.44	0.47
2:C:480:THR:HG22	2:C:481:ASP:N	2.30	0.47
3:D:139:GLY:H	3:D:147:VAL:HG21	1.80	0.47
3:D:496:LEU:HD23	9:D:9266:HOH:O	2.15	0.47
3:D:650:LEU:HD13	3:D:688:TRP:CZ3	2.46	0.47
3:D:699:VAL:HA	3:D:718:PRO:HD3	1.97	0.47
3:D:768:ASN:N	3:D:768:ASN:ND2	2.63	0.47
5:F:112:ALA:O	5:F:116:LEU:HG	2.14	0.47
5:F:129:GLU:HB3	5:F:142:ARG:HH21	1.80	0.47
5:F:270:LYS:HB3	5:F:295:MET:HE3	1.97	0.47
1:K:85:LEU:HA	1:K:124:ASN:HD22	1.80	0.47
1:L:23:PHE:HB2	1:L:197:LEU:HD23	1.95	0.47
2:M:1033:GLY:O	2:M:1037:VAL:HG23	2.15	0.47
2:M:139:GLN:HE22	2:M:415:PRO:CD	2.28	0.47
2:M:148:PHE:CZ	2:M:309:TYR:HB3	2.50	0.47
2:M:606:VAL:CG2	2:M:645:VAL:HG22	2.45	0.47
2:M:52:PHE:HE1	2:M:66:LEU:HG	1.79	0.47
2:M:748:GLU:HB2	9:M:1434:HOH:O	2.14	0.47
2:M:998:TYR:OH	2:M:1000:MET:HA	2.15	0.47
3:N:139:GLY:HA3	3:N:452:ILE:HD12	1.95	0.47
3:N:176:ASP:HA	9:N:9640:HOH:O	2.15	0.47
3:N:181:ASP:O	3:N:185:VAL:HG23	2.15	0.47
3:N:177:ALA:HB1	3:N:199:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:22:SER:HA	3:N:90:MET:O	2.15	0.47
3:N:526:PRO:HB2	5:P:317:LEU:HD11	1.97	0.47
3:N:764:LEU:HD12	3:N:765:SER:N	2.30	0.47
4:O:93:TYR:HA	4:O:94:PRO:HD3	1.71	0.47
5:P:263:HIS:HB2	9:P:3994:HOH:O	2.13	0.47
5:P:291:ILE:HG12	5:P:304:VAL:CG1	2.45	0.47
5:P:375:LEU:HD23	5:P:376:ILE:HG13	1.95	0.47
5:P:414:ARG:HD3	9:P:4633:HOH:O	2.15	0.47
1:A:175:ARG:HB3	9:A:478:HOH:O	2.15	0.47
1:B:23:PHE:O	1:B:196:THR:HA	2.15	0.47
2:C:1013:TYR:C	2:C:1021:LEU:HD23	2.35	0.47
2:C:589:ARG:HG2	9:C:1768:HOH:O	2.14	0.47
1:A:72:LYS:HA	2:C:608:GLY:CA	2.45	0.47
2:C:634:GLY:HA3	9:C:2212:HOH:O	2.14	0.47
3:D:1192:LEU:HD22	3:D:1345:GLU:HG2	1.96	0.47
3:D:1234:THR:HG23	9:D:9918:HOH:O	2.14	0.47
3:D:1237:THR:HG22	3:D:1238:MET:N	2.30	0.47
3:D:1438:ALA:N	3:D:1446:VAL:HG11	2.29	0.47
3:D:44:LEU:O	3:D:525:ARG:NH2	2.47	0.47
3:D:568:ARG:O	3:D:572:ARG:HG3	2.14	0.47
5:F:226:LYS:HA	9:F:842:HOH:O	2.14	0.47
5:F:328:PHE:HA	9:F:522:HOH:O	2.14	0.47
1:L:158:ILE:HD13	9:L:5309:HOH:O	2.14	0.47
1:L:76:VAL:HA	1:L:79:ILE:HG12	1.95	0.47
2:M:1040:LEU:HD21	2:M:1048:THR:HG22	1.96	0.47
2:M:1063:ARG:O	2:M:1066:ALA:HB3	2.14	0.47
2:M:385:PHE:HA	9:M:1703:HOH:O	2.14	0.47
2:M:137:VAL:O	2:M:391:LEU:HD21	2.14	0.47
3:N:1037:GLN:OE1	3:N:1042:ARG:HB3	2.15	0.47
3:N:1059:SER:OG	3:N:1065:LEU:HA	2.15	0.47
3:N:438:ASP:HB2	9:N:2136:HOH:O	2.14	0.47
3:N:452:ILE:HG23	3:N:452:ILE:O	2.14	0.47
3:N:528:VAL:HG12	3:N:529:GLN:N	2.30	0.47
3:N:607:LEU:HA	3:N:613:ARG:HB2	1.97	0.47
3:N:704:ARG:CD	3:N:705:ALA:H	2.19	0.47
3:N:758:GLU:OE1	4:O:20:THR:HG21	2.14	0.47
4:O:52:GLU:HG2	9:O:3988:HOH:O	2.15	0.47
1:A:66:SER:O	1:A:75:VAL:HG23	2.15	0.47
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.49	0.47
1:A:97:VAL:HG12	1:A:99:LEU:HD12	1.97	0.47
2:C:1060:ILE:HB	2:C:1083:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:56:GLU:CG	2:C:64:LEU:HD23	2.44	0.47
2:C:691:SER:HB3	2:C:868:ASP:O	2.15	0.47
3:D:1252:ILE:HD12	3:D:1253:THR:H	1.79	0.47
3:D:1101:VAL:CG2	3:D:1424:VAL:HG22	2.40	0.47
3:D:152:LEU:HG	9:D:2087:HOH:O	2.15	0.47
3:D:601:ARG:NH2	3:D:612:GLY:HA2	2.30	0.47
3:D:637:LEU:HD21	3:D:643:GLY:H	1.80	0.47
3:D:708:LEU:HB2	9:D:9664:HOH:O	2.15	0.47
3:D:729:HIS:CE1	3:D:731:LEU:H	2.33	0.47
3:D:929:ARG:HH11	3:D:929:ARG:CG	2.28	0.47
5:F:270:LYS:HB3	5:F:295:MET:CE	2.44	0.47
9:D:9452:HOH:O	5:F:315:VAL:HB	2.14	0.47
1:L:105:GLY:O	1:L:132:LEU:HB3	2.15	0.47
1:L:52:ALA:HB2	1:L:170:VAL:O	2.14	0.47
2:M:1090:LYS:HA	2:M:1090:LYS:HD2	1.72	0.47
2:M:264:PRO:HB3	2:M:289:THR:CG2	2.45	0.47
2:M:260:LEU:HA	2:M:291:ALA:CB	2.45	0.47
1:K:150:TYR:CD1	2:M:696:LYS:HG2	2.50	0.47
2:M:795:GLY:HA3	2:M:1004:LYS:HD2	1.97	0.47
3:N:1063:GLU:HG2	9:N:9788:HOH:O	2.15	0.47
3:N:1139:ASP:O	3:N:1142:ALA:HB3	2.15	0.47
3:N:1422:MET:HE3	3:N:1427:SER:HA	1.97	0.47
3:N:799:LYS:HE2	3:N:824:ASN:O	2.15	0.47
3:N:864:VAL:HG12	3:N:865:THR:H	1.79	0.47
3:N:897:TRP:HB3	9:N:9323:HOH:O	2.14	0.47
4:O:42:PRO:HB2	9:O:5960:HOH:O	2.13	0.47
5:P:218:GLN:NE2	9:P:5398:HOH:O	2.48	0.47
5:P:358:LEU:CD2	5:P:370:LYS:HE3	2.43	0.47
1:A:48:ILE:HG22	1:A:173:PRO:CD	2.45	0.47
2:C:1088:LEU:HD23	2:C:1089:VAL:N	2.30	0.47
2:C:1090:LYS:HG2	2:C:1112:PHE:CZ	2.50	0.47
2:C:147:TYR:HE2	2:C:280:LYS:HE2	1.79	0.47
2:C:183:SER:HB2	2:C:190:LYS:CG	2.45	0.47
2:C:137:VAL:O	2:C:391:LEU:HD11	2.15	0.47
2:C:433:THR:C	2:C:435:TYR:H	2.18	0.47
2:C:473:ARG:HG3	2:C:474:VAL:N	2.29	0.47
2:C:625:LEU:O	2:C:627:ARG:N	2.48	0.47
2:C:759:THR:HB	2:C:785:VAL:CG2	2.45	0.47
2:C:873:PRO:O	2:C:876:VAL:HG23	2.15	0.47
2:C:950:LEU:HD12	2:C:952:LEU:HD21	1.97	0.47
3:D:1059:SER:HB3	9:D:9310:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:171:LEU:HD13	3:D:389:GLU:C	2.36	0.47
3:D:34:TYR:OH	5:F:261:PRO:HD2	2.15	0.47
1:K:149:GLY:O	1:K:171:PHE:HB2	2.14	0.47
2:M:102:HIS:HB2	2:M:106:GLY:O	2.15	0.47
2:M:184:MET:HB2	2:M:193:LEU:HD12	1.96	0.47
2:M:374:ASN:HD21	2:M:376:ARG:HB2	1.80	0.47
2:M:810:ASP:HA	2:M:811:PRO:HD3	1.73	0.47
9:K:5385:HOH:O	2:M:938:LYS:HE2	2.14	0.47
2:M:953:VAL:HA	2:M:965:GLU:OE1	2.14	0.47
3:N:179:VAL:O	3:N:183:GLU:HB2	2.15	0.47
3:N:470:LEU:HB2	3:N:503:LEU:HD21	1.95	0.47
3:N:502:PHE:CE1	3:N:509:PRO:HB3	2.50	0.47
3:N:693:GLU:HA	4:O:48:MET:HE1	1.97	0.47
3:N:1086:LEU:N	6:N:8002:STD:H32	2.30	0.47
5:P:314:PRO:HD2	9:P:4412:HOH:O	2.15	0.47
5:P:356:LYS:HE3	9:P:5784:HOH:O	2.15	0.47
1:A:115:LEU:O	1:A:115:LEU:HD12	2.15	0.46
1:A:122:ILE:HD12	1:A:122:ILE:H	1.80	0.46
2:C:1031:ARG:HG3	2:C:1031:ARG:NH1	2.29	0.46
2:C:200:LEU:HD13	2:C:300:ASP:CG	2.35	0.46
2:C:216:GLU:OE1	2:C:217:LEU:HG	2.14	0.46
2:C:220:GLY:HA3	9:C:1151:HOH:O	2.16	0.46
2:C:129:ILE:HD11	2:C:386:PHE:HD2	1.79	0.46
2:C:470:PRO:HB3	2:C:485:TYR:CZ	2.50	0.46
2:C:701:THR:HG23	2:C:832:LYS:HA	1.97	0.46
2:C:882:LEU:HD23	2:C:885:ILE:HB	1.96	0.46
3:D:957:PRO:CG	3:D:1007:VAL:HG12	2.44	0.46
3:D:1053:PHE:CE1	3:D:1072:ILE:HG23	2.50	0.46
3:D:1102:THR:HG22	3:D:1222:GLY:CA	2.43	0.46
2:C:886:LEU:CD2	3:D:951:ILE:HG13	2.45	0.46
4:E:17:TYR:O	4:E:21:VAL:HG23	2.14	0.46
5:F:132:ARG:NH2	5:F:184:ARG:HH12	2.13	0.46
1:K:32:PHE:HZ	1:L:47:SER:HG	1.60	0.46
2:M:1038:TRP:HD1	2:M:1041:GLU:OE1	1.98	0.46
2:M:115:LEU:HD22	2:M:373:VAL:CG1	2.34	0.46
2:M:248:PRO:HD2	9:M:1314:HOH:O	2.14	0.46
2:M:428:ARG:NH2	2:M:451:LEU:HD11	2.31	0.46
2:M:625:LEU:O	2:M:627:ARG:N	2.47	0.46
2:M:648:ARG:HB3	9:M:1146:HOH:O	2.14	0.46
2:M:571:LEU:HD21	2:M:700:TYR:CD2	2.50	0.46
2:M:735:ARG:HB2	9:M:1788:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:780:GLU:OE2	2:M:781:LYS:HG3	2.16	0.46
3:N:1084:THR:HA	3:N:1087:ARG:NH2	2.30	0.46
3:N:118:LEU:HB2	9:N:9568:HOH:O	2.15	0.46
3:N:127:LEU:HD12	3:N:128:TYR:HD1	1.80	0.46
3:N:643:GLY:HA2	3:N:719:VAL:HG23	1.97	0.46
2:C:229:MET:HE1	9:C:1650:HOH:O	2.15	0.46
2:C:269:LEU:HG	9:C:1623:HOH:O	2.14	0.46
2:C:55:GLU:HG2	9:C:2078:HOH:O	2.15	0.46
2:C:815:LEU:HD21	2:C:820:ARG:O	2.15	0.46
2:C:876:VAL:HB	3:D:949:ILE:HG13	1.98	0.46
3:D:1274:ILE:HD12	9:D:2452:HOH:O	2.15	0.46
3:D:1362:LYS:HE2	9:D:9177:HOH:O	2.14	0.46
3:D:493:ARG:HH21	3:D:1388:ARG:HB3	1.78	0.46
3:D:1393:GLN:HB2	3:D:1398:TRP:NE1	2.30	0.46
3:D:1462:LEU:HD22	3:D:1472:ILE:CG2	2.44	0.46
3:D:434:ARG:HD2	9:D:2137:HOH:O	2.15	0.46
3:D:54:LYS:HD3	3:D:57:GLU:OE2	2.14	0.46
1:L:14:ARG:HH22	1:L:24:VAL:CG2	2.29	0.46
2:M:12:VAL:HG22	2:M:13:ILE:HG23	1.96	0.46
2:M:139:GLN:HE21	2:M:334:ARG:CD	2.29	0.46
2:M:191:PHE:HE2	2:M:196:LEU:HB2	1.79	0.46
2:M:342:ASP:O	2:M:346:VAL:HG23	2.15	0.46
2:M:708:TYR:N	2:M:708:TYR:CD1	2.82	0.46
3:N:1326:THR:HG22	3:N:1327:ARG:N	2.29	0.46
3:N:441:ARG:O	3:N:443:VAL:N	2.48	0.46
3:N:681:ARG:HA	9:N:2260:HOH:O	2.15	0.46
1:B:23:PHE:HZ	1:B:207:PRO:HB2	1.80	0.46
2:C:305:PRO:HB3	2:C:308:ARG:NH2	2.19	0.46
2:C:549:PHE:CE2	2:C:886:LEU:HB3	2.50	0.46
2:C:569:VAL:O	2:C:571:LEU:HD12	2.14	0.46
2:C:3:ILE:HD13	2:C:900:ARG:O	2.16	0.46
2:C:92:ALA:HB1	9:C:1961:HOH:O	2.15	0.46
2:C:675:ALA:CA	2:C:989:VAL:HG12	2.40	0.46
3:D:1219:GLU:C	9:D:9516:HOH:O	2.53	0.46
2:C:1119:ARG:H	3:D:23:TYR:HE2	1.64	0.46
3:D:410:SER:CB	3:D:414:ARG:HH21	2.29	0.46
3:D:537:THR:HG23	9:D:9070:HOH:O	2.14	0.46
3:D:616:GLN:HE21	3:D:619:LEU:HD13	1.80	0.46
3:D:744:GLN:CD	9:D:9834:HOH:O	2.52	0.46
5:F:75:ILE:HG22	9:F:480:HOH:O	2.14	0.46
1:K:199:ILE:HD12	1:K:199:ILE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:9:PRO:HB3	1:L:25:LEU:HG	1.96	0.46
1:L:30:ARG:HG3	9:L:4517:HOH:O	2.15	0.46
1:L:92:PRO:HD3	9:L:6486:HOH:O	2.16	0.46
2:M:145:GLY:H	2:M:163:ILE:HG13	1.81	0.46
2:M:285:LEU:HD12	2:M:288:ARG:O	2.15	0.46
2:M:403:SER:O	2:M:407:LYS:HG3	2.15	0.46
2:M:817:PRO:C	2:M:819:VAL:H	2.19	0.46
3:N:1004:THR:O	3:N:1007:VAL:HG22	2.16	0.46
3:N:546:ARG:NH2	3:N:550:ARG:HH22	2.12	0.46
3:N:550:ARG:HG3	3:N:550:ARG:NH1	2.29	0.46
3:N:62:LYS:HZ1	3:N:75:ARG:HD2	1.80	0.46
5:P:323:ASP:HB3	5:P:325:LYS:NZ	2.30	0.46
2:C:1034:GLU:HA	2:C:1037:VAL:CG2	2.44	0.46
2:C:249:LYS:HB2	9:C:1212:HOH:O	2.14	0.46
2:C:313:LEU:CB	2:C:321:GLU:HG3	2.46	0.46
2:C:580:MET:HB3	2:C:584:GLU:CD	2.36	0.46
2:C:6:PHE:HE2	2:C:913:GLU:HB3	1.80	0.46
2:C:745:ILE:HG21	9:C:1837:HOH:O	2.15	0.46
2:C:876:VAL:HB	2:C:877:PRO:HD3	1.96	0.46
3:D:116:LEU:HB3	3:D:118:LEU:CD2	2.45	0.46
3:D:572:ARG:HB3	9:F:507:HOH:O	2.16	0.46
3:D:77:GLY:O	3:D:78:VAL:HG23	2.15	0.46
3:D:980:MET:HB3	3:D:982:PHE:CE1	2.51	0.46
5:F:163:LEU:HB3	5:F:174:LEU:CG	2.43	0.46
5:F:370:LYS:HD2	5:F:370:LYS:C	2.35	0.46
1:K:123:MET:C	1:K:125:PRO:HD3	2.35	0.46
1:K:48:ILE:HD13	1:K:210:ALA:HB1	1.96	0.46
1:K:4:SER:HB3	9:K:5976:HOH:O	2.16	0.46
1:L:1:MET:HG2	9:L:4365:HOH:O	2.15	0.46
2:M:433:THR:HG21	2:M:488:ALA:HB1	1.97	0.46
2:M:719:PRO:HD3	9:M:1441:HOH:O	2.14	0.46
2:M:713:ARG:O	2:M:720:GLU:HG3	2.15	0.46
3:N:1336:LEU:HD23	9:N:9785:HOH:O	2.15	0.46
3:N:543:LEU:O	3:N:546:ARG:HB2	2.15	0.46
3:N:615:ARG:HD2	9:N:9404:HOH:O	2.14	0.46
3:N:767:HIS:NE2	4:O:6:ILE:HD13	2.31	0.46
9:N:9220:HOH:O	5:P:140:ARG:HB2	2.14	0.46
3:N:420:VAL:HG13	5:P:164:LYS:HD3	1.98	0.46
1:A:176:ARG:HG3	1:A:200:TRP:CE3	2.50	0.46
1:A:46:SER:HB3	2:C:856:GLU:CG	2.43	0.46
2:C:115:LEU:HD12	2:C:378:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.51	0.46
2:C:525:SER:O	2:C:529:VAL:HG23	2.15	0.46
3:D:952:ASP:HA	3:D:1062:ARG:NH2	2.30	0.46
3:D:1278:ASP:HB2	3:D:1318:TYR:CE1	2.49	0.46
3:D:20:SER:HA	9:D:9314:HOH:O	2.15	0.46
3:D:493:ARG:HA	9:D:9266:HOH:O	2.14	0.46
3:D:596:SER:OG	3:D:598:ARG:HB3	2.15	0.46
3:D:633:VAL:C	3:D:635:PRO:HD3	2.36	0.46
3:D:862:ASP:O	3:D:877:PRO:HD3	2.15	0.46
3:D:890:VAL:HA	9:D:9275:HOH:O	2.16	0.46
4:E:27:ALA:O	4:E:31:LEU:HG	2.16	0.46
2:M:1034:GLU:HA	2:M:1037:VAL:CG2	2.45	0.46
2:M:165:LEU:HA	2:M:166:PRO:O	2.16	0.46
2:M:172:ILE:HG23	2:M:184:MET:HE3	1.97	0.46
2:M:210:GLU:HA	9:M:1714:HOH:O	2.15	0.46
2:M:285:LEU:HB3	9:M:1964:HOH:O	2.15	0.46
2:M:721:ARG:HE	2:M:783:ARG:NH2	2.13	0.46
2:M:848:VAL:HB	3:N:740:PHE:O	2.15	0.46
1:K:46:SER:HB3	2:M:856:GLU:HG2	1.97	0.46
3:N:1189:ARG:HB3	3:N:1204:CYS:HA	1.98	0.46
3:N:1438:ALA:N	3:N:1446:VAL:HG11	2.30	0.46
3:N:183:GLU:HA	3:N:186:VAL:HG12	1.96	0.46
3:N:191:LEU:HD22	3:N:195:VAL:HG21	1.97	0.46
3:N:543:LEU:CD2	3:N:600:LEU:HD12	2.44	0.46
3:N:879:ARG:HD2	9:N:9192:HOH:O	2.14	0.46
5:P:168:LYS:HA	5:P:168:LYS:HE2	1.98	0.46
5:P:395:GLU:HB2	9:P:5193:HOH:O	2.15	0.46
1:A:18:ARG:HH12	1:A:88:ARG:NE	2.14	0.46
1:B:160:ASP:HA	9:B:464:HOH:O	2.16	0.46
2:C:1103:ASP:N	2:C:1107:ASN:O	2.48	0.46
2:C:1090:LYS:HG2	2:C:1112:PHE:HZ	1.80	0.46
2:C:120:LEU:HB2	9:C:1338:HOH:O	2.14	0.46
2:C:305:PRO:CB	2:C:308:ARG:HH21	2.19	0.46
2:C:30:LEU:O	2:C:30:LEU:HD12	2.15	0.46
2:C:520:GLU:O	2:C:522:VAL:HG23	2.16	0.46
2:C:668:LEU:HD12	2:C:668:LEU:H	1.79	0.46
1:A:65:PHE:HE1	2:C:799:ILE:HG12	1.80	0.46
9:A:334:HOH:O	2:C:980:GLY:HA2	2.15	0.46
3:D:1118:ILE:HD11	9:D:2295:HOH:O	2.16	0.46
3:D:1177:ALA:HB3	3:D:1183:ILE:HD11	1.98	0.46
3:D:1211:MET:HG2	3:D:1213:ARG:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1472:ILE:O	3:D:1477:GLY:HA3	2.15	0.46
3:D:178:LEU:HD21	3:D:199:LEU:H	1.81	0.46
3:D:465:LEU:HD12	3:D:513:ILE:HD11	1.97	0.46
3:D:581:LEU:HD12	3:D:582:LEU:N	2.31	0.46
3:D:845:ASN:CB	9:D:2535:HOH:O	2.63	0.46
5:F:321:ILE:HG12	5:F:327:SER:O	2.16	0.46
1:K:10:VAL:HG12	1:K:12:THR:HG22	1.98	0.46
2:M:123:GLU:HB3	9:M:1677:HOH:O	2.16	0.46
2:M:166:PRO:HD3	2:M:265:ARG:CB	2.46	0.46
2:M:172:ILE:N	2:M:172:ILE:HD12	2.31	0.46
2:M:286:SER:OG	2:M:299:LYS:HE3	2.16	0.46
2:M:310:LEU:O	2:M:314:THR:HG23	2.16	0.46
2:M:955:PRO:HA	9:M:1371:HOH:O	2.16	0.46
3:N:1140:ILE:HG21	3:N:1175:ILE:HD11	1.98	0.46
3:N:1189:ARG:NH1	3:N:1201:CYS:SG	2.88	0.46
3:N:1295:GLU:HB3	3:N:1300:SER:CB	2.46	0.46
3:N:1314:LYS:NZ	3:N:1317:ASP:H	2.14	0.46
3:N:1422:MET:CE	3:N:1427:SER:HA	2.46	0.46
3:N:42:ASP:O	3:N:46:ASP:HB2	2.16	0.46
3:N:493:ARG:NH1	3:N:1390:LEU:HB2	2.31	0.46
4:O:8:LYS:HB3	9:O:4335:HOH:O	2.15	0.46
5:P:218:GLN:HA	5:P:221:ILE:HD12	1.96	0.46
1:A:221:HIS:HD1	1:A:224:TYR:HD2	1.62	0.46
1:A:227:ASN:H	1:A:227:ASN:ND2	2.14	0.46
2:C:162:ILE:HD12	2:C:172:ILE:HB	1.96	0.46
2:C:166:PRO:HB2	9:C:1593:HOH:O	2.14	0.46
2:C:55:GLU:HG3	9:C:1573:HOH:O	2.16	0.46
2:C:690:ILE:CG2	2:C:852:ILE:HG13	2.46	0.46
3:D:1103:HIS:HD2	3:D:1462:LEU:N	2.13	0.46
3:D:1342:GLU:HG2	9:D:9397:HOH:O	2.16	0.46
3:D:592:THR:N	3:D:600:LEU:HD21	2.31	0.46
3:D:692:GLU:HG2	3:D:720:LEU:HD22	1.97	0.46
3:D:843:PHE:CD1	3:D:849:ALA:HA	2.51	0.46
3:D:906:GLN:NE2	3:D:910:SER:HB2	2.31	0.46
3:D:974:ILE:HD11	9:D:9959:HOH:O	2.15	0.46
3:D:984:THR:CG2	3:D:987:GLU:H	2.28	0.46
4:E:45:ARG:H	4:E:45:ARG:HD2	1.81	0.46
4:E:84:ARG:HA	4:E:84:ARG:HH11	1.79	0.46
5:F:141:VAL:HA	9:F:544:HOH:O	2.16	0.46
5:F:215:GLU:O	5:F:218:GLN:HB3	2.15	0.46
1:K:25:LEU:HD23	1:K:25:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:30:ARG:NH1	1:L:30:ARG:HG2	2.30	0.46
1:L:89:PHE:CB	1:L:94:LEU:HD13	2.41	0.46
2:M:108:ILE:HG23	9:M:1259:HOH:O	2.16	0.46
2:M:1100:GLN:HG3	2:M:1101:THR:O	2.15	0.46
2:M:12:VAL:CG1	2:M:534:VAL:HG13	2.44	0.46
2:M:144:PRO:HA	2:M:163:ILE:CD1	2.46	0.46
2:M:589:ARG:HD2	9:M:1387:HOH:O	2.15	0.46
2:M:829:GLN:HG2	2:M:831:ARG:HE	1.81	0.46
2:M:928:LYS:HB2	9:M:1588:HOH:O	2.16	0.46
3:N:1152:GLU:HG2	3:N:1160:LEU:O	2.15	0.46
2:M:1046:ALA:HB3	3:N:1476:THR:HB	1.97	0.46
3:N:191:LEU:CB	3:N:195:VAL:HG21	2.44	0.46
2:M:1007:ALA:HB2	3:N:648:MET:HE3	1.98	0.46
4:O:94:PRO:HB2	9:O:4661:HOH:O	2.16	0.46
1:B:110:LYS:NZ	1:B:110:LYS:HB2	2.31	0.46
1:B:112:ARG:HB3	1:B:112:ARG:NH1	2.30	0.46
2:C:1086:ARG:HB3	2:C:1112:PHE:CE2	2.50	0.46
2:C:129:ILE:HG22	2:C:130:ASN:ND2	2.31	0.46
2:C:83:CYS:HA	2:C:88:LEU:HD23	1.97	0.46
3:D:1122:LEU:HD23	3:D:1178:ALA:HB2	1.97	0.46
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.16	0.46
3:D:154:THR:HA	9:D:9028:HOH:O	2.15	0.46
3:D:428:LYS:HD3	3:D:451:ASP:OD1	2.16	0.46
3:D:161:LEU:CD1	3:D:452:ILE:HD12	2.45	0.46
3:D:646:LYS:NZ	3:D:688:TRP:HE1	2.13	0.46
3:D:652:LEU:HB3	3:D:653:PHE:HD1	1.80	0.46
3:D:669:ASN:O	3:D:672:ALA:HB3	2.15	0.46
3:D:998:GLU:HG2	9:D:9130:HOH:O	2.15	0.46
5:F:363:GLU:CA	5:F:367:MET:HG2	2.46	0.46
5:F:406:ARG:HA	5:F:409:LYS:HG2	1.97	0.46
1:L:19:GLU:O	1:L:200:TRP:HA	2.16	0.46
1:L:30:ARG:HH11	1:L:30:ARG:HG2	1.81	0.46
2:M:107:LEU:HG	9:M:1695:HOH:O	2.16	0.46
2:M:195:LEU:CD2	2:M:238:LEU:HG	2.46	0.46
2:M:409:ARG:NE	9:M:1130:HOH:O	2.48	0.46
2:M:432:ARG:NH1	3:N:1048:PRO:HG2	2.29	0.46
3:N:131:LYS:HG2	3:N:568:ARG:CG	2.21	0.46
3:N:1267:ARG:HH22	3:N:1331:ASP:HB3	1.80	0.46
3:N:1444:THR:HG21	9:N:9794:HOH:O	2.16	0.46
3:N:404:GLU:HA	9:N:2182:HOH:O	2.16	0.46
3:N:628:ARG:HD3	3:N:744:GLN:HE22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:785:ILE:HD12	3:N:785:ILE:H	1.81	0.46
5:P:151:LEU:CD2	5:P:153:PRO:HD2	2.45	0.46
1:B:146:ARG:HB2	9:B:513:HOH:O	2.15	0.46
2:C:141:HIS:HB3	2:C:418:LEU:CG	2.46	0.46
2:C:182:VAL:HG11	2:C:193:LEU:HD22	1.97	0.46
2:C:267:TYR:HD1	9:C:1271:HOH:O	1.98	0.46
2:C:462:ASP:CG	2:C:468:ARG:HD2	2.36	0.46
1:A:72:LYS:HA	2:C:608:GLY:N	2.30	0.46
2:C:626:ARG:N	2:C:639:GLN:HE21	2.13	0.46
2:C:808:ARG:HG2	2:C:808:ARG:HH11	1.81	0.46
3:D:1139:ASP:O	3:D:1142:ALA:HB3	2.16	0.46
3:D:1283:ILE:HB	3:D:1315:ASP:OD2	2.16	0.46
3:D:1393:GLN:HB2	3:D:1398:TRP:CE2	2.50	0.46
3:D:608:SER:OG	3:D:609:GLY:N	2.49	0.46
3:D:56:TYR:HE2	3:D:69:GLU:HB2	1.79	0.46
3:D:805:GLU:O	3:D:805:GLU:OE1	2.34	0.46
2:C:882:LEU:HD22	3:D:951:ILE:HG12	1.98	0.46
5:F:164:LYS:HG2	5:F:171:LYS:NZ	2.31	0.46
5:F:179:GLU:HG3	9:F:536:HOH:O	2.16	0.46
3:D:572:ARG:NH2	5:F:83:GLN:NE2	2.59	0.46
1:K:162:ILE:HG13	1:K:163:ASN:OD1	2.16	0.46
1:K:9:PRO:HD2	1:L:224:TYR:CE1	2.51	0.46
2:M:162:ILE:HD11	2:M:306:THR:HG21	1.98	0.46
2:M:254:VAL:HG13	2:M:258:TYR:HE1	1.79	0.46
2:M:273:GLY:HA2	2:M:276:LYS:NZ	2.31	0.46
2:M:141:HIS:HB3	2:M:418:LEU:CG	2.46	0.46
2:M:140:ILE:O	2:M:418:LEU:HD23	2.16	0.46
3:N:34:TYR:HA	9:N:9522:HOH:O	2.16	0.46
3:N:671:LYS:HE2	3:N:674:ARG:HH21	1.81	0.46
5:P:286:PRO:HD2	9:P:5418:HOH:O	2.15	0.46
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.36	0.46
2:C:1004:LYS:O	2:C:1005:MET:C	2.52	0.46
2:C:1053:LEU:HD12	9:D:9467:HOH:O	2.15	0.46
2:C:1105:LYS:HE3	9:C:1173:HOH:O	2.15	0.46
2:C:367:LEU:HA	2:C:371:LYS:HD3	1.98	0.46
2:C:75:GLU:HG3	9:C:1495:HOH:O	2.15	0.46
2:C:892:LEU:HD12	2:C:892:LEU:O	2.16	0.46
2:C:896:PHE:O	2:C:924:VAL:HG11	2.16	0.46
2:C:944:LEU:HD11	2:C:963:LEU:CD2	2.45	0.46
3:D:1319:VAL:HA	3:D:1323:GLN:OE1	2.15	0.46
3:D:132:TYR:HA	9:D:9028:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:133:ILE:HG22	3:D:455:ARG:N	2.30	0.46
3:D:379:ALA:HB3	9:D:9248:HOH:O	2.15	0.46
3:D:957:PRO:CG	3:D:1007:VAL:HA	2.46	0.46
3:D:969:ARG:HD2	9:D:9782:HOH:O	2.15	0.46
5:F:233:PHE:HE1	9:F:456:HOH:O	1.99	0.46
2:M:6:PHE:CD1	2:M:909:ALA:HB2	2.51	0.46
3:N:1209:LEU:HD13	3:N:1211:MET:SD	2.56	0.46
3:N:1264:GLU:HG2	3:N:1266:ARG:NH2	2.31	0.46
3:N:1481:VAL:O	3:N:1481:VAL:HG12	2.16	0.46
3:N:172:PRO:HB3	3:N:178:LEU:HB3	1.96	0.46
3:N:629:SER:OG	3:N:630:VAL:N	2.47	0.46
3:N:671:LYS:HA	3:N:674:ARG:HE	1.81	0.46
3:N:734:GLU:OE1	3:N:782:SER:HB2	2.15	0.46
4:O:13:VAL:HG12	4:O:75:PHE:CE1	2.51	0.46
4:O:62:THR:HG21	9:O:5845:HOH:O	2.15	0.46
1:A:51:THR:HA	1:A:145:ASP:O	2.17	0.45
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.98	0.45
1:A:85:LEU:HD12	1:A:124:ASN:HB3	1.97	0.45
1:B:16:GLN:HA	9:B:370:HOH:O	2.16	0.45
1:B:91:ASN:OD1	1:B:93:SER:HB2	2.16	0.45
2:C:1055:LEU:CD2	2:C:1079:PRO:HG3	2.47	0.45
2:C:165:LEU:HD12	2:C:166:PRO:HA	1.97	0.45
2:C:422:ARG:H	2:C:422:ARG:HG2	1.41	0.45
2:C:54:ILE:HG22	2:C:66:LEU:HB3	1.98	0.45
3:D:1326:THR:HG22	3:D:1327:ARG:N	2.32	0.45
3:D:46:ASP:HB3	3:D:49:ILE:HG13	1.97	0.45
3:D:39:PRO:HG2	3:D:47:GLU:OE2	2.15	0.45
3:D:549:ASN:HB3	9:D:9108:HOH:O	2.15	0.45
2:C:1067:TYR:HE1	3:D:655:PRO:HG3	1.80	0.45
5:F:102:LEU:CD1	5:F:187:LEU:HG	2.46	0.45
2:M:141:HIS:HB3	2:M:418:LEU:CD2	2.47	0.45
2:M:52:PHE:O	2:M:54:ILE:N	2.49	0.45
2:M:893:ALA:O	2:M:897:LEU:HB2	2.16	0.45
3:N:1122:LEU:HD11	3:N:1186:VAL:HG23	1.98	0.45
3:N:1399:ASP:O	3:N:1403:LEU:HD12	2.16	0.45
3:N:1459:LEU:HD13	3:N:1465:ASN:HD21	1.81	0.45
3:N:1503:VAL:HG11	9:N:9426:HOH:O	2.16	0.45
3:N:666:ILE:HG22	3:N:684:LYS:HD3	1.99	0.45
3:N:792:ILE:O	3:N:878:GLY:HA3	2.16	0.45
3:N:7:LYS:HD3	3:N:1456:LYS:NZ	2.31	0.45
3:N:994:GLN:HE21	3:N:994:GLN:CA	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:64:ALA:HA	4:O:67:GLU:OE1	2.16	0.45
4:O:84:ARG:CZ	4:O:84:ARG:HB2	2.46	0.45
5:P:84:TYR:HB2	9:P:5610:HOH:O	2.16	0.45
1:A:170:VAL:HG12	9:A:359:HOH:O	2.14	0.45
2:C:1039:ALA:O	2:C:1043:TYR:HD1	2.00	0.45
2:C:54:ILE:HG12	2:C:56:GLU:HG2	1.98	0.45
2:C:690:ILE:CG1	2:C:694:LEU:HD12	2.47	0.45
2:C:976:ASP:HB3	2:C:979:THR:HG22	1.98	0.45
3:D:1105:ILE:HD11	3:D:1374:GLN:OE1	2.17	0.45
3:D:1403:LEU:O	3:D:1407:LEU:HB2	2.16	0.45
3:D:1432:LYS:CG	3:D:1433:SER:H	2.29	0.45
3:D:389:GLU:HG2	3:D:389:GLU:O	2.16	0.45
3:D:413:ASP:HA	9:D:9536:HOH:O	2.15	0.45
3:D:563:PRO:CG	3:D:566:ILE:HD12	2.46	0.45
3:D:661:MET:CE	3:D:673:ALA:HB1	2.46	0.45
3:D:850:LEU:CD2	3:D:881:LEU:HD13	2.46	0.45
3:D:545:ARG:CZ	5:F:257:THR:HA	2.46	0.45
5:F:360:LYS:HD2	9:F:461:HOH:O	2.15	0.45
1:L:223:THR:HG21	9:L:4720:HOH:O	2.15	0.45
2:M:337:GLY:HA3	9:M:1269:HOH:O	2.16	0.45
2:M:352:ALA:HA	2:M:355:VAL:CG1	2.46	0.45
2:M:448:ASN:ND2	9:M:1423:HOH:O	2.48	0.45
2:M:332:ARG:NH2	2:M:464:LEU:HD11	2.30	0.45
2:M:744:ARG:HG3	2:M:747:ALA:HB2	1.98	0.45
3:N:1045:MET:N	9:N:2112:HOH:O	2.50	0.45
3:N:116:LEU:HD21	3:N:464:LEU:HB3	1.98	0.45
3:N:1281:VAL:HG21	3:N:1313:VAL:CG2	2.46	0.45
3:N:1346:ARG:HD2	9:N:9115:HOH:O	2.15	0.45
5:P:109:GLY:O	5:P:112:ALA:HB3	2.15	0.45
5:P:409:LYS:HE3	5:P:410:TYR:HD1	1.82	0.45
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.99	0.45
1:B:42:ARG:HH11	1:B:42:ARG:HG2	1.82	0.45
1:A:32:PHE:HE2	1:B:43:ILE:CD1	2.29	0.45
2:C:114:PHE:HD1	2:C:114:PHE:H	1.64	0.45
2:C:236:ILE:O	2:C:239:PHE:HB2	2.16	0.45
2:C:428:ARG:HG3	2:C:428:ARG:HH11	1.81	0.45
2:C:831:ARG:NH1	2:C:831:ARG:HG2	2.31	0.45
2:C:841:ASN:HD22	2:C:843:HIS:N	2.08	0.45
2:C:910:LYS:HB2	2:C:913:GLU:OE1	2.17	0.45
2:C:979:THR:HG23	2:C:981:GLU:HB2	1.97	0.45
3:D:1065:LEU:CD1	3:D:1069:GLU:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1192:LEU:CD2	3:D:1345:GLU:HG2	2.45	0.45
3:D:1392:GLY:N	9:D:9363:HOH:O	2.49	0.45
4:E:69:LEU:HD11	9:E:171:HOH:O	2.16	0.45
5:F:184:ARG:HE	5:F:188:ILE:HD11	1.81	0.45
2:M:437:ARG:CZ	2:M:488:ALA:HA	2.46	0.45
2:M:621:VAL:HG13	9:M:1139:HOH:O	2.15	0.45
2:M:627:ARG:HA	9:M:1134:HOH:O	2.16	0.45
2:M:652:GLY:HA2	9:M:1715:HOH:O	2.16	0.45
2:M:752:GLY:C	2:M:791:ARG:HH12	2.19	0.45
3:N:1112:CYS:HA	9:N:9059:HOH:O	2.16	0.45
3:N:1109:GLU:CG	3:N:1202:GLN:H	2.30	0.45
3:N:1493:LYS:HD3	3:N:1496:GLU:OE2	2.16	0.45
3:N:191:LEU:HA	3:N:191:LEU:HD23	1.73	0.45
3:N:637:LEU:HD11	3:N:641:GLN:C	2.36	0.45
3:N:860:LEU:HD13	3:N:861:GLN:HE22	1.81	0.45
5:P:321:ILE:HG13	5:P:329:TYR:HA	1.98	0.45
1:B:89:PHE:CD1	1:B:120:VAL:HG13	2.51	0.45
1:B:187:GLY:HA3	9:B:450:HOH:O	2.17	0.45
1:B:28:LEU:O	1:B:192:LEU:HD23	2.16	0.45
2:C:1097:LEU:HD12	3:D:10:ILE:CG2	2.47	0.45
2:C:29:ALA:HB2	2:C:337:GLY:HA3	1.98	0.45
2:C:435:TYR:C	2:C:437:ARG:H	2.19	0.45
2:C:767:PRO:HA	9:C:1291:HOH:O	2.17	0.45
2:C:833:LEU:HD12	2:C:834:GLN:N	2.30	0.45
3:D:1109:GLU:CG	3:D:1202:GLN:H	2.30	0.45
3:D:213:VAL:HG22	3:D:214:GLU:H	1.81	0.45
3:D:850:LEU:O	3:D:853:VAL:HB	2.16	0.45
5:F:117:SER:HB3	5:F:122:LEU:O	2.16	0.45
5:F:192:LEU:O	5:F:196:VAL:HG23	2.16	0.45
5:F:399:GLN:HG2	9:F:793:HOH:O	2.15	0.45
5:F:82:ARG:HG2	5:F:86:HIS:CD2	2.51	0.45
1:K:181:VAL:O	2:M:938:LYS:HD3	2.16	0.45
1:K:86:VAL:HA	9:K:4248:HOH:O	2.17	0.45
2:M:1105:LYS:O	2:M:1107:ASN:N	2.49	0.45
2:M:191:PHE:O	2:M:192:PRO:C	2.55	0.45
2:M:212:GLY:C	2:M:215:GLY:H	2.20	0.45
2:M:814:GLU:HG3	2:M:814:GLU:O	2.17	0.45
3:N:953:ASP:OD1	3:N:1019:PRO:HG2	2.16	0.45
3:N:1059:SER:HA	9:N:9590:HOH:O	2.17	0.45
3:N:16:GLU:HA	9:N:9730:HOH:O	2.16	0.45
3:N:495:ARG:O	3:N:499:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:675:ARG:O	3:N:678:GLU:HG2	2.17	0.45
3:N:734:GLU:HB2	9:N:9019:HOH:O	2.16	0.45
2:M:685:GLU:CG	3:N:739:ASP:HB2	2.30	0.45
3:N:984:THR:HB	3:N:987:GLU:OE2	2.17	0.45
4:O:26:ARG:NH1	4:O:29:GLN:NE2	2.64	0.45
5:P:335:ASP:CG	5:P:338:LEU:HD12	2.37	0.45
2:C:175:GLU:HB3	2:C:183:SER:OG	2.16	0.45
2:C:282:GLY:H	2:C:308:ARG:NH2	2.13	0.45
2:C:309:TYR:HE2	2:C:321:GLU:HB3	1.81	0.45
2:C:421:GLU:CD	2:C:421:GLU:O	2.55	0.45
2:C:798:GLY:C	2:C:799:ILE:HD13	2.37	0.45
2:C:877:PRO:HG2	3:D:1023:MET:HE1	1.99	0.45
3:D:1320:GLU:O	3:D:1323:GLN:HB2	2.16	0.45
3:D:1496:GLU:OE1	3:D:1500:LYS:HE3	2.16	0.45
3:D:491:LYS:HD3	3:D:492:ALA:N	2.31	0.45
3:D:682:ASP:N	3:D:682:ASP:OD1	2.49	0.45
3:D:649:ALA:CB	3:D:691:LEU:HD21	2.46	0.45
5:F:126:LEU:O	5:F:130:VAL:HG23	2.17	0.45
5:F:335:ASP:OD1	5:F:338:LEU:HB2	2.17	0.45
5:F:401:GLU:HG3	5:F:405:LEU:HD22	1.98	0.45
1:K:61:VAL:HG21	1:K:68:ILE:HD11	1.98	0.45
2:M:794:PRO:HB2	2:M:1027:PHE:CZ	2.51	0.45
2:M:1118:LYS:HD3	3:N:20:SER:O	2.16	0.45
2:M:171:TRP:HB2	9:M:1883:HOH:O	2.17	0.45
2:M:435:TYR:C	2:M:437:ARG:H	2.19	0.45
3:N:1235:GLN:O	3:N:1237:THR:N	2.50	0.45
3:N:183:GLU:HA	3:N:186:VAL:CG1	2.47	0.45
3:N:560:GLN:O	5:P:184:ARG:NH2	2.47	0.45
3:N:673:ALA:O	3:N:677:LEU:HG	2.17	0.45
3:N:696:HIS:HB2	4:O:48:MET:CE	2.47	0.45
5:P:168:LYS:H	5:P:168:LYS:HG2	1.46	0.45
5:P:218:GLN:HA	5:P:221:ILE:CD1	2.47	0.45
2:C:27:ARG:HA	9:C:1366:HOH:O	2.16	0.45
2:C:157:ARG:HD2	2:C:314:THR:HG22	1.99	0.45
2:C:625:LEU:HB3	2:C:639:GLN:HB2	1.98	0.45
2:C:575:GLN:O	2:C:667:ALA:HB1	2.17	0.45
2:C:777:ILE:HG22	2:C:778:PHE:HD1	1.82	0.45
2:C:861:LEU:HG	2:C:862:PRO:HD2	1.98	0.45
2:C:890:LEU:HA	2:C:914:ILE:CD1	2.35	0.45
2:C:943:VAL:HG11	2:C:973:VAL:HG22	1.99	0.45
2:C:956:GLY:HA2	9:C:1808:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1462:LEU:N	3:D:1462:LEU:HD23	2.31	0.45
3:D:208:PRO:HB2	3:D:395:VAL:HG13	1.99	0.45
3:D:42:ASP:HA	3:D:46:ASP:OD1	2.17	0.45
3:D:704:ARG:HE	3:D:705:ALA:N	2.11	0.45
3:D:72:VAL:HG23	3:D:78:VAL:H	1.81	0.45
3:D:813:LEU:O	3:D:839:LEU:HD11	2.16	0.45
3:D:820:GLU:HA	3:D:825:ALA:O	2.16	0.45
3:D:827:ILE:HG23	3:D:837:GLY:HA2	1.98	0.45
3:D:872:ARG:HB3	9:D:9461:HOH:O	2.16	0.45
3:D:916:TYR:HE2	3:D:920:LEU:HD13	1.81	0.45
5:F:202:TYR:OH	5:F:244:ARG:HD2	2.16	0.45
5:F:292:ALA:HA	5:F:299:TRP:HB3	1.99	0.45
5:F:403:LYS:HA	5:F:403:LYS:NZ	2.31	0.45
2:C:778:PHE:HZ	5:F:409:LYS:HB2	1.79	0.45
5:F:85:LEU:HB2	9:F:440:HOH:O	2.16	0.45
1:L:145:ASP:O	1:L:171:PHE:HE1	2.00	0.45
2:M:1006:HIS:ND1	2:M:1006:HIS:N	2.64	0.45
2:M:166:PRO:HD3	2:M:265:ARG:CG	2.46	0.45
2:M:274:ARG:HG3	2:M:285:LEU:HD13	1.98	0.45
2:M:300:ASP:HA	9:M:1823:HOH:O	2.15	0.45
2:M:342:ASP:O	2:M:345:ARG:HG3	2.16	0.45
2:M:89:THR:HG23	2:M:91:GLN:NE2	2.31	0.45
3:N:1003:VAL:O	3:N:1006:ALA:HB3	2.16	0.45
3:N:681:ARG:CB	3:N:681:ARG:HH11	2.29	0.45
3:N:653:PHE:CD1	3:N:695:ILE:HD11	2.51	0.45
3:N:950:GLY:H	3:N:953:ASP:CB	2.29	0.45
5:P:287:THR:N	5:P:290:GLU:OE1	2.49	0.45
5:P:396:ARG:HG2	9:P:3845:HOH:O	2.17	0.45
1:B:156:HIS:CE1	1:B:166:PRO:HB3	2.51	0.45
1:B:19:GLU:O	1:B:200:TRP:HA	2.16	0.45
2:C:115:LEU:HD22	2:C:373:VAL:CG1	2.43	0.45
2:C:183:SER:HB3	9:C:1141:HOH:O	2.15	0.45
2:C:195:LEU:HB3	9:C:1703:HOH:O	2.15	0.45
2:C:267:TYR:N	2:C:267:TYR:HD2	2.15	0.45
2:C:342:ASP:O	2:C:345:ARG:HG2	2.17	0.45
2:C:423:ALA:CB	2:C:428:ARG:HH22	2.29	0.45
2:C:744:ARG:HD3	9:C:1611:HOH:O	2.16	0.45
2:C:993:PHE:CD1	2:C:993:PHE:C	2.90	0.45
3:D:1203:LYS:HE3	9:D:9590:HOH:O	2.16	0.45
3:D:1314:LYS:HD3	3:D:1314:LYS:H	1.82	0.45
3:D:1350:GLU:HG3	9:D:9098:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1192:LEU:HD21	3:D:1372:VAL:CG1	2.47	0.45
3:D:1377:LYS:NZ	9:D:9064:HOH:O	2.50	0.45
3:D:799:LYS:HE2	3:D:801:GLY:HA3	1.99	0.45
1:B:65:PHE:HE1	3:D:806:PHE:HZ	1.64	0.45
3:D:790:TYR:CZ	3:D:905:PRO:HB2	2.52	0.45
3:D:777:PRO:HG2	3:D:915:VAL:HB	1.99	0.45
5:F:148:LYS:HD3	9:F:504:HOH:O	2.16	0.45
5:F:166:LEU:HD22	5:F:170:HIS:CB	2.46	0.45
1:K:220:GLU:HG2	9:K:5302:HOH:O	2.16	0.45
1:L:183:ASP:HB3	9:L:6719:HOH:O	2.16	0.45
1:L:206:THR:CG2	1:L:209:GLU:H	2.23	0.45
2:M:274:ARG:CB	2:M:285:LEU:HD13	2.44	0.45
2:M:603:VAL:H	2:M:647:GLN:H	1.65	0.45
2:M:902:ILE:O	2:M:904:PRO:HD3	2.17	0.45
3:N:1047:LYS:HD2	3:N:1051:GLU:OE2	2.17	0.45
3:N:397:LYS:HE3	9:N:9553:HOH:O	2.14	0.45
3:N:28:LYS:CB	3:N:41:ARG:HD2	2.47	0.45
3:N:480:GLU:O	3:N:484:PRO:HD2	2.17	0.45
3:N:484:PRO:HB2	9:N:9818:HOH:O	2.15	0.45
3:N:594:PRO:HA	9:N:9546:HOH:O	2.16	0.45
3:N:633:VAL:C	3:N:635:PRO:HD3	2.36	0.45
3:N:656:PHE:HB3	3:N:694:VAL:CG1	2.47	0.45
3:N:868:TYR:HB2	3:N:873:LEU:HD12	1.97	0.45
5:P:416:ARG:HD3	5:P:419:ARG:HB3	1.98	0.45
1:A:138:LEU:HD12	1:A:138:LEU:HA	1.86	0.45
1:B:89:PHE:N	1:B:89:PHE:CD1	2.85	0.45
1:B:90:LEU:HD22	9:B:320:HOH:O	2.16	0.45
2:C:191:PHE:CZ	2:C:196:LEU:HD12	2.51	0.45
2:C:208:ALA:HA	2:C:218:VAL:HG22	1.98	0.45
2:C:313:LEU:HD12	9:C:1484:HOH:O	2.16	0.45
2:C:495:THR:H	2:C:530:GLU:CD	2.19	0.45
3:D:1442:ASN:O	3:D:1446:VAL:HG23	2.17	0.45
3:D:210:ARG:HG3	3:D:398:ALA:N	2.30	0.45
3:D:451:ASP:HB3	9:D:2046:HOH:O	2.17	0.45
3:D:114:THR:O	3:D:495:ARG:HG3	2.17	0.45
5:F:289:GLU:HG2	9:F:680:HOH:O	2.17	0.45
5:F:313:GLU:HB3	9:F:481:HOH:O	2.17	0.45
2:M:1050:GLN:HG2	2:M:1079:PRO:HG2	1.98	0.45
2:M:129:ILE:HD13	2:M:386:PHE:O	2.17	0.45
2:M:197:LEU:HD22	2:M:202:TYR:CD2	2.51	0.45
2:M:690:ILE:HG12	2:M:691:SER:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:670:GLN:HE22	2:M:699:PHE:C	2.20	0.45
2:M:802:ARG:HG3	9:M:1172:HOH:O	2.16	0.45
3:N:1026:SER:C	3:N:1028:ALA:H	2.20	0.45
3:N:1209:LEU:CD1	3:N:1216:SER:HB2	2.47	0.45
3:N:1365:ASP:O	3:N:1368:ILE:HG13	2.16	0.45
3:N:1101:VAL:CG1	3:N:1428:ALA:HB2	2.46	0.45
3:N:477:LEU:HD21	3:N:495:ARG:HD3	1.97	0.45
3:N:540:LEU:HA	3:N:543:LEU:HD12	1.99	0.45
3:N:640:HIS:HB3	9:N:9110:HOH:O	2.17	0.45
3:N:637:LEU:HD11	3:N:641:GLN:HB2	1.99	0.45
3:N:769:LEU:HB2	3:N:919:PHE:HE1	1.81	0.45
3:N:806:PHE:CG	3:N:806:PHE:O	2.70	0.45
2:M:1102:LEU:HD11	3:N:9:ARG:HB2	1.98	0.45
5:P:361:LEU:HD13	5:P:366:ALA:HB1	1.98	0.45
5:P:82:ARG:HG2	5:P:86:HIS:NE2	2.30	0.45
1:B:159:LYS:N	1:B:159:LYS:HD3	2.32	0.45
2:C:216:GLU:HB2	9:C:1669:HOH:O	2.15	0.45
2:C:275:TYR:CD2	2:C:276:LYS:HG3	2.52	0.45
2:C:307:LEU:HG	2:C:311:PHE:CZ	2.52	0.45
2:C:367:LEU:HB3	9:C:1983:HOH:O	2.16	0.45
2:C:64:LEU:HD22	2:C:359:MET:CG	2.41	0.45
2:C:798:GLY:H	2:C:827:VAL:CG1	2.30	0.45
3:D:1026:SER:C	3:D:1028:ALA:H	2.19	0.45
3:D:1213:ARG:HB2	3:D:1214:PRO:HD3	1.99	0.45
3:D:1405:GLU:CD	3:D:1413:THR:HB	2.37	0.45
3:D:860:LEU:HD23	3:D:877:PRO:CB	2.46	0.45
1:L:212:ASN:O	1:L:215:VAL:HG22	2.16	0.45
2:M:1013:TYR:CE1	2:M:1020:PRO:HG3	2.50	0.45
2:M:429:ASP:HB3	3:N:1079:LYS:HZ1	1.82	0.45
2:M:979:THR:CG2	2:M:981:GLU:HB2	2.46	0.45
3:N:1389:LEU:CD1	3:N:1390:LEU:HD23	2.47	0.45
3:N:1397:LYS:HB2	9:N:9957:HOH:O	2.17	0.45
3:N:378:ILE:HA	9:N:2123:HOH:O	2.16	0.45
1:A:76:VAL:HA	1:A:79:ILE:HG12	1.99	0.45
2:C:1020:PRO:HD2	2:C:1057:SER:OG	2.17	0.45
2:C:1032:PHE:HE2	2:C:1037:VAL:HA	1.81	0.45
2:C:1091:GLU:HG2	3:D:606:ILE:CG2	2.47	0.45
2:C:218:VAL:HG22	2:C:221:LEU:CD2	2.47	0.45
2:C:602:GLU:HA	2:C:647:GLN:O	2.17	0.45
2:C:893:ALA:O	2:C:897:LEU:HB2	2.16	0.45
3:D:1099:VAL:HG13	3:D:1223:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1393:GLN:HB2	3:D:1398:TRP:HE1	1.82	0.45
3:D:1476:THR:HA	9:E:104:HOH:O	2.17	0.45
3:D:191:LEU:HD11	9:D:9494:HOH:O	2.17	0.45
3:D:393:ILE:HG22	9:D:9389:HOH:O	2.16	0.45
3:D:729:HIS:ND1	3:D:730:PRO:N	2.64	0.45
3:D:819:GLY:HA3	9:D:9206:HOH:O	2.17	0.45
4:E:60:ALA:HB3	9:E:111:HOH:O	2.17	0.45
1:L:149:GLY:O	1:L:171:PHE:HB2	2.17	0.45
2:M:167:LYS:HD3	2:M:168:ARG:HD2	1.99	0.45
2:M:300:ASP:OD2	2:M:303:PHE:HB2	2.17	0.45
2:M:312:ALA:HB2	9:M:1641:HOH:O	2.17	0.45
2:M:472:ARG:HD2	2:M:480:THR:O	2.17	0.45
3:N:137:PRO:HD2	3:N:453:ASP:CG	2.38	0.45
3:N:508:ARG:HG3	9:N:9392:HOH:O	2.17	0.45
3:N:47:GLU:OE1	3:N:53:ILE:HG22	2.17	0.45
3:N:553:ARG:HD3	5:P:214:GLN:HB3	1.99	0.45
3:N:631:ILE:HG21	3:N:745:MET:HG3	1.99	0.45
3:N:669:ASN:O	3:N:672:ALA:HB3	2.16	0.45
3:N:704:ARG:HD2	3:N:705:ALA:N	2.23	0.45
1:B:101:LEU:HD12	1:B:114:PHE:CD1	2.52	0.44
2:C:1078:GLU:HG3	9:C:2012:HOH:O	2.16	0.44
2:C:19:THR:O	2:C:23:VAL:HG23	2.16	0.44
2:C:773:LEU:N	9:C:1403:HOH:O	2.50	0.44
2:C:818:GLY:N	9:C:2148:HOH:O	2.49	0.44
3:D:121:THR:HG23	9:D:9102:HOH:O	2.16	0.44
3:D:1290:LEU:CD2	3:D:1291:SER:H	2.27	0.44
3:D:1487:VAL:HG12	4:E:74:VAL:HB	1.99	0.44
3:D:699:VAL:HG12	3:D:717:GLN:CA	2.43	0.44
5:F:153:PRO:CG	5:F:154:LYS:H	2.30	0.44
5:F:288:TYR:HB2	9:F:819:HOH:O	2.17	0.44
1:L:185:ARG:HA	9:L:4092:HOH:O	2.16	0.44
1:L:75:VAL:O	1:L:79:ILE:HG23	2.17	0.44
1:L:81:ASN:O	1:L:84:GLU:HB3	2.16	0.44
2:M:1088:LEU:HD12	9:N:9389:HOH:O	2.17	0.44
2:M:172:ILE:H	2:M:172:ILE:HD12	1.82	0.44
2:M:176:VAL:O	2:M:178:PRO:HD3	2.16	0.44
2:M:28:ARG:HG3	2:M:40:GLU:OE1	2.16	0.44
2:M:461:VAL:HG13	2:M:465:GLY:HA2	1.99	0.44
2:M:77:PRO:HD3	2:M:93:PRO:HG3	1.97	0.44
2:M:86:LYS:HG2	2:M:813:VAL:HG12	1.99	0.44
2:M:877:PRO:HB3	3:N:1020:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1171:VAL:HG12	3:N:1171:VAL:O	2.17	0.44
3:N:1220:ALA:O	3:N:1224:VAL:HG23	2.17	0.44
3:N:1403:LEU:HD23	3:N:1407:LEU:CD2	2.46	0.44
3:N:1431:THR:OG1	3:N:1432:LYS:N	2.51	0.44
3:N:1493:LYS:HA	3:N:1496:GLU:HG2	1.99	0.44
3:N:28:LYS:O	3:N:43:GLY:HA2	2.17	0.44
3:N:493:ARG:O	3:N:497:GLU:HG3	2.17	0.44
3:N:99:ALA:HA	3:N:575:GLN:NE2	2.32	0.44
3:N:804:LEU:O	3:N:804:LEU:HD12	2.17	0.44
4:O:89:MET:HG3	9:O:5639:HOH:O	2.16	0.44
5:P:142:ARG:HA	9:P:3722:HOH:O	2.17	0.44
5:P:321:ILE:O	5:P:327:SER:HB3	2.17	0.44
2:M:1067:TYR:HE2	5:P:342:VAL:HA	1.82	0.44
5:P:357:ALA:HB2	9:P:3982:HOH:O	2.17	0.44
2:C:150:PRO:HB2	9:C:2194:HOH:O	2.18	0.44
2:C:226:VAL:HG12	9:C:1509:HOH:O	2.16	0.44
2:C:333:ILE:O	2:C:465:GLY:HA3	2.17	0.44
2:C:385:PHE:O	2:C:389:SER:HB3	2.17	0.44
2:C:486:MET:HG2	2:C:487:THR:O	2.16	0.44
2:C:73:LEU:N	2:C:73:LEU:HD23	2.32	0.44
2:C:761:PHE:CD1	2:C:761:PHE:N	2.85	0.44
2:C:817:PRO:C	2:C:819:VAL:H	2.19	0.44
2:C:841:ASN:ND2	2:C:843:HIS:HB2	2.32	0.44
3:D:955:VAL:HG21	3:D:1015:TYR:CE2	2.52	0.44
3:D:1047:LYS:HB2	3:D:1051:GLU:OE2	2.18	0.44
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.99	0.44
3:D:1343:ALA:HA	9:D:9548:HOH:O	2.17	0.44
3:D:1353:GLN:O	3:D:1357:ARG:HD2	2.17	0.44
3:D:161:LEU:CD2	3:D:452:ILE:HG21	2.46	0.44
3:D:510:GLU:HG3	9:D:9443:HOH:O	2.17	0.44
3:D:671:LYS:N	9:D:9017:HOH:O	2.50	0.44
3:D:939:PHE:O	3:D:943:THR:HG23	2.17	0.44
3:D:1481:VAL:HG13	4:E:18:ARG:HE	1.82	0.44
3:D:1476:THR:HG23	4:E:21:VAL:HG22	2.00	0.44
4:E:93:TYR:HA	4:E:94:PRO:HD3	1.74	0.44
5:F:369:LEU:HD22	9:F:840:HOH:O	2.18	0.44
2:M:1052:MET:SD	2:M:1056:LYS:HD2	2.57	0.44
2:M:1102:LEU:N	3:N:7:LYS:O	2.49	0.44
2:M:282:GLY:HA2	2:M:308:ARG:NH2	2.33	0.44
2:M:211:LEU:CD1	2:M:308:ARG:HA	2.47	0.44
3:N:1156:LEU:HG	3:N:1177:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1298:GLY:HA3	9:N:9525:HOH:O	2.17	0.44
3:N:431:VAL:HA	9:N:9353:HOH:O	2.16	0.44
3:N:57:GLU:HG2	3:N:58:CYS:O	2.18	0.44
3:N:585:GLY:HA3	9:N:9488:HOH:O	2.17	0.44
3:N:774:SER:OG	3:N:776:GLU:HB2	2.18	0.44
3:N:813:LEU:HD12	3:N:814:ALA:N	2.31	0.44
5:P:133:ALA:HB1	9:P:3678:HOH:O	2.17	0.44
5:P:249:ARG:HG3	5:P:253:ASP:OD1	2.17	0.44
9:N:9147:HOH:O	5:P:254:GLN:HA	2.17	0.44
1:A:159:LYS:HE3	9:A:341:HOH:O	2.18	0.44
1:B:184:THR:HB	1:B:194:LYS:HZ3	1.83	0.44
2:C:442:GLU:HG2	2:C:454:SER:OG	2.17	0.44
2:C:648:ARG:HG2	9:C:1175:HOH:O	2.16	0.44
2:C:668:LEU:O	2:C:993:PHE:CZ	2.71	0.44
2:C:862:PRO:HG3	2:C:975:TYR:CE1	2.48	0.44
3:D:1445:HIS:HB2	9:D:9269:HOH:O	2.17	0.44
3:D:214:GLU:OE2	3:D:390:PRO:HB2	2.17	0.44
3:D:39:PRO:HB2	9:D:2416:HOH:O	2.17	0.44
2:C:885:ILE:HD12	3:D:949:ILE:HB	1.98	0.44
5:F:295:MET:HE2	5:F:295:MET:HA	1.99	0.44
2:M:101:ILE:HG23	2:M:107:LEU:HD22	1.98	0.44
2:M:212:GLY:HA3	2:M:218:VAL:CG2	2.46	0.44
2:M:267:TYR:HB2	2:M:272:ALA:HB1	1.99	0.44
2:M:358:ARG:HH22	2:M:374:ASN:HB2	1.83	0.44
3:N:1007:VAL:HG23	3:N:1008:PHE:N	2.32	0.44
3:N:1270:ALA:HB3	9:N:9875:HOH:O	2.17	0.44
3:N:1467:ILE:HG13	3:N:1467:ILE:H	1.65	0.44
3:N:442:ASN:HB3	9:N:9550:HOH:O	2.16	0.44
5:P:363:GLU:CA	5:P:367:MET:HG2	2.46	0.44
1:A:9:PRO:HB3	1:A:25:LEU:CD1	2.47	0.44
1:B:101:LEU:HB2	1:B:114:PHE:CD2	2.52	0.44
1:B:109:VAL:HA	9:B:383:HOH:O	2.17	0.44
2:C:155:PRO:HB2	9:C:1303:HOH:O	2.16	0.44
2:C:185:LYS:HD3	2:C:190:LYS:NZ	2.33	0.44
2:C:260:LEU:HA	2:C:291:ALA:HB2	1.98	0.44
2:C:603:VAL:H	2:C:647:GLN:H	1.65	0.44
2:C:810:ASP:HA	2:C:811:PRO:HD3	1.72	0.44
3:D:112:ILE:O	3:D:112:ILE:HD12	2.17	0.44
3:D:1429:LEU:HG	3:D:1441:GLN:OE1	2.17	0.44
3:D:65:ARG:HD3	9:D:2178:HOH:O	2.18	0.44
3:D:860:LEU:O	3:D:877:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:921:ARG:HD2	9:D:9298:HOH:O	2.18	0.44
2:C:773:LEU:HD13	5:F:373:LYS:HG3	1.99	0.44
5:F:403:LYS:HD3	9:F:714:HOH:O	2.17	0.44
1:K:156:HIS:CD2	1:K:157:GLY:N	2.86	0.44
1:L:59:GLU:HG2	1:L:139:ASN:O	2.17	0.44
2:M:241:LEU:HB3	9:M:1577:HOH:O	2.17	0.44
2:M:326:ASP:HA	2:M:331:ARG:HD3	1.99	0.44
2:M:350:ARG:HA	2:M:353:ARG:CZ	2.47	0.44
2:M:599:GLU:HB2	9:M:1325:HOH:O	2.17	0.44
2:M:575:GLN:C	2:M:667:ALA:HB1	2.38	0.44
2:M:817:PRO:HB3	5:P:305:GLU:OE1	2.18	0.44
2:M:835:VAL:HG11	9:N:9423:HOH:O	2.17	0.44
2:M:877:PRO:HG2	2:M:878:SER:H	1.82	0.44
2:M:925:TYR:C	2:M:925:TYR:HD1	2.21	0.44
3:N:1093:TYR:O	3:N:1096:ARG:HB3	2.16	0.44
3:N:1219:GLU:HG3	4:O:17:TYR:OH	2.17	0.44
3:N:1232:PRO:HB3	3:N:1361:VAL:CG2	2.45	0.44
3:N:1399:ASP:HA	9:N:9219:HOH:O	2.16	0.44
3:N:838:ARG:HG2	3:N:865:THR:OG1	2.18	0.44
3:N:960:LYS:HG2	3:N:964:LEU:HD12	1.99	0.44
5:P:102:LEU:HD22	5:P:183:ALA:O	2.17	0.44
5:P:331:ASP:HB2	9:P:5195:HOH:O	2.18	0.44
5:P:361:LEU:HD13	5:P:366:ALA:CB	2.47	0.44
1:B:120:VAL:HB	9:B:441:HOH:O	2.16	0.44
1:B:175:ARG:HD3	1:B:175:ARG:HA	1.73	0.44
1:B:65:PHE:HE1	3:D:806:PHE:CZ	2.35	0.44
2:C:1105:LYS:O	2:C:1107:ASN:N	2.50	0.44
2:C:142:ARG:HD3	2:C:325:ILE:HG23	1.99	0.44
2:C:198:ARG:HH21	2:C:204:GLN:HG3	1.82	0.44
2:C:371:LYS:HE3	9:C:1918:HOH:O	2.17	0.44
2:C:437:ARG:NH2	2:C:486:MET:O	2.50	0.44
2:C:567:GLN:O	2:C:997:LEU:HD22	2.18	0.44
2:C:603:VAL:HG23	2:C:647:GLN:O	2.17	0.44
2:C:688:ILE:N	2:C:688:ILE:HD12	2.32	0.44
2:C:792:VAL:HG23	9:C:1301:HOH:O	2.18	0.44
3:D:1009:LYS:O	3:D:1013:GLU:HG3	2.18	0.44
3:D:1239:ARG:HB2	9:D:9447:HOH:O	2.17	0.44
3:D:80:VAL:HG23	9:D:9031:HOH:O	2.17	0.44
3:D:906:GLN:HE22	3:D:910:SER:HB2	1.82	0.44
3:D:971:LEU:O	3:D:975:GLU:HG3	2.18	0.44
3:D:996:TRP:HE3	3:D:999:THR:CG2	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:372:ARG:HG2	9:F:685:HOH:O	2.17	0.44
5:F:77:THR:O	5:F:81:VAL:HG23	2.17	0.44
1:K:179:PHE:HE2	9:K:3599:HOH:O	2.00	0.44
1:K:227:ASN:ND2	1:K:227:ASN:H	2.16	0.44
2:M:200:LEU:H	2:M:200:LEU:HG	1.59	0.44
3:N:1112:CYS:HA	9:N:9572:HOH:O	2.17	0.44
3:N:10:ILE:O	3:N:1454:GLY:HA2	2.18	0.44
3:N:550:ARG:HH11	3:N:550:ARG:HG3	1.82	0.44
3:N:656:PHE:HB3	3:N:694:VAL:HG11	1.99	0.44
3:N:827:ILE:O	3:N:837:GLY:HA3	2.18	0.44
4:O:54:LEU:HA	4:O:58:PRO:CG	2.47	0.44
5:P:104:ARG:HG2	9:P:4251:HOH:O	2.16	0.44
5:P:370:LYS:HB3	5:P:370:LYS:HZ2	1.82	0.44
1:A:184:THR:HG23	1:A:192:LEU:CB	2.46	0.44
2:C:265:ARG:HB2	9:C:1143:HOH:O	2.16	0.44
2:C:305:PRO:HA	2:C:308:ARG:HE	1.82	0.44
2:C:39:ARG:HG3	9:C:1262:HOH:O	2.18	0.44
2:C:492:ASP:HB3	2:C:518:LYS:HD2	2.00	0.44
2:C:81:ASP:HB2	9:C:1292:HOH:O	2.17	0.44
2:C:672:VAL:CG2	2:C:868:ASP:HB2	2.46	0.44
2:C:876:VAL:O	2:C:879:ARG:O	2.36	0.44
2:C:918:LEU:HD23	2:C:967:PHE:O	2.17	0.44
1:A:182:GLU:OE1	2:C:934:PHE:HB3	2.18	0.44
3:D:105:VAL:HG13	3:D:124:GLU:OE1	2.18	0.44
3:D:1114:THR:O	3:D:1114:THR:HG23	2.17	0.44
3:D:1369:GLU:HA	3:D:1372:VAL:HG12	1.99	0.44
3:D:1468:LEU:HD22	3:D:1470:ARG:HG3	2.00	0.44
3:D:186:VAL:HG13	3:D:187:LYS:N	2.31	0.44
3:D:600:LEU:HD23	3:D:600:LEU:N	2.32	0.44
3:D:617:ASN:HA	3:D:617:ASN:HD22	1.62	0.44
3:D:794:GLN:HG2	3:D:905:PRO:HB3	1.98	0.44
4:E:87:LYS:HB2	9:E:127:HOH:O	2.17	0.44
3:D:566:ILE:HG23	5:F:214:GLN:OE1	2.18	0.44
5:F:319:THR:HG22	5:F:320:PRO:HD2	2.00	0.44
5:F:366:ALA:HB3	5:F:367:MET:HE2	1.99	0.44
5:F:401:GLU:O	5:F:405:LEU:HD13	2.17	0.44
5:F:407:LYS:HB3	9:F:453:HOH:O	2.18	0.44
1:K:175:ARG:NH2	1:K:202:ASP:HA	2.33	0.44
1:K:225:PHE:CE1	1:L:25:LEU:HD22	2.52	0.44
2:M:164:PRO:HD2	2:M:170:PRO:O	2.17	0.44
2:M:332:ARG:HB2	2:M:466:PHE:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:18:LEU:HD13	2:M:590:ASP:CG	2.38	0.44
2:M:747:ALA:O	2:M:799:ILE:HA	2.18	0.44
3:N:1312:LEU:HG	3:N:1327:ARG:HG3	1.98	0.44
3:N:1364:HIS:ND1	3:N:1365:ASP:N	2.65	0.44
3:N:1385:GLY:HA3	9:N:9569:HOH:O	2.16	0.44
3:N:1391:GLU:HB3	3:N:1393:GLN:OE1	2.18	0.44
3:N:1491:THR:O	3:N:1495:ILE:HD13	2.17	0.44
3:N:34:TYR:OH	5:P:264:MET:HG3	2.18	0.44
3:N:535:PHE:O	5:P:314:PRO:HA	2.17	0.44
3:N:866:VAL:HG12	3:N:867:ARG:N	2.31	0.44
3:N:905:PRO:HD3	9:N:9581:HOH:O	2.17	0.44
3:N:928:ALA:O	3:N:931:LEU:HB2	2.18	0.44
1:A:52:ALA:HB2	1:A:170:VAL:O	2.18	0.44
1:B:143:ARG:NH1	1:B:158:ILE:HG23	2.33	0.44
1:B:51:THR:HB	9:B:467:HOH:O	2.17	0.44
2:C:198:ARG:CZ	2:C:228:ALA:O	2.65	0.44
2:C:194:VAL:HG21	2:C:221:LEU:HA	2.00	0.44
2:C:437:ARG:HA	2:C:467:ILE:HG21	2.00	0.44
2:C:599:GLU:HB3	9:C:1560:HOH:O	2.17	0.44
2:C:611:ILE:HD11	2:C:641:PRO:HG3	1.98	0.44
3:D:1044:LEU:HD23	9:D:9902:HOH:O	2.18	0.44
3:D:1065:LEU:HD13	3:D:1069:GLU:HB2	2.00	0.44
3:D:1164:ARG:HH21	3:D:1170:ASP:CG	2.21	0.44
3:D:1465:ASN:HD21	3:D:1470:ARG:NE	2.16	0.44
3:D:558:LEU:HD13	5:F:145:PRO:HB3	2.00	0.44
3:D:775:GLY:HA3	3:D:1145:TYR:CE1	2.53	0.44
3:D:781:PRO:HB3	3:D:785:ILE:HB	2.00	0.44
3:D:794:GLN:HE21	3:D:794:GLN:HB3	1.58	0.44
4:E:37:ASN:HD22	4:E:89:MET:CE	2.31	0.44
5:F:361:LEU:HD21	5:F:404:ALA:HB1	1.99	0.44
1:K:19:GLU:CD	1:K:19:GLU:N	2.71	0.44
1:K:20:TYR:CE2	1:K:22:GLU:HG3	2.52	0.44
2:M:262:ALA:O	2:M:264:PRO:O	2.36	0.44
2:M:290:LEU:HA	9:M:1823:HOH:O	2.18	0.44
2:M:442:GLU:CG	2:M:454:SER:H	2.31	0.44
2:M:428:ARG:HH21	2:M:451:LEU:CD1	2.30	0.44
2:M:780:GLU:HG3	2:M:781:LYS:N	2.31	0.44
3:N:172:PRO:HG3	3:N:178:LEU:HD13	2.00	0.44
3:N:185:VAL:HG22	9:N:2180:HOH:O	2.18	0.44
3:N:674:ARG:HH11	3:N:674:ARG:HG2	1.82	0.44
3:N:75:ARG:HB2	9:N:9306:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:783:ARG:HG2	3:N:783:ARG:HH11	1.82	0.44
3:N:87:ARG:HD2	3:N:88:TYR:CE2	2.53	0.44
5:P:159:ILE:O	5:P:163:LEU:HG	2.18	0.44
5:P:291:ILE:HG12	5:P:304:VAL:HG11	2.00	0.44
5:P:391:GLY:HA3	9:P:3841:HOH:O	2.18	0.44
1:B:98:THR:HG22	1:B:100:LEU:CD2	2.48	0.44
1:B:83:LYS:HE3	1:B:167:VAL:CG1	2.46	0.44
2:C:1056:LYS:HD3	3:D:623:VAL:HG13	2.00	0.44
2:C:269:LEU:HD12	2:C:288:ARG:HG3	1.99	0.44
2:C:420:ARG:CD	2:C:420:ARG:H	2.29	0.44
2:C:437:ARG:HE	2:C:469:THR:H	1.65	0.44
2:C:504:GLU:CG	2:C:507:ARG:HB2	2.48	0.44
2:C:430:VAL:O	3:D:1075:HIS:ND1	2.51	0.44
3:D:122:GLU:HG3	9:D:9582:HOH:O	2.18	0.44
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.99	0.44
3:D:148:GLU:HG3	9:D:9078:HOH:O	2.18	0.44
3:D:171:LEU:C	3:D:171:LEU:HD12	2.38	0.44
3:D:444:VAL:O	3:D:446:VAL:HG23	2.17	0.44
3:D:545:ARG:HD2	9:D:9153:HOH:O	2.18	0.44
3:D:810:GLU:HA	3:D:813:LEU:CD2	2.47	0.44
3:D:844:ALA:HB3	3:D:848:GLU:OE2	2.17	0.44
5:F:287:THR:O	5:F:289:GLU:N	2.50	0.44
1:K:12:THR:HG21	9:K:5148:HOH:O	2.17	0.44
2:M:1012:PRO:HD2	2:M:1021:LEU:O	2.18	0.44
2:M:218:VAL:HG22	2:M:221:LEU:HD21	1.99	0.44
2:M:356:ARG:HD3	9:M:1999:HOH:O	2.17	0.44
3:N:1042:ARG:O	3:N:1057:VAL:HB	2.18	0.44
3:N:1108:ARG:HH21	3:N:1198:TYR:C	2.21	0.44
3:N:1481:VAL:HA	4:O:18:ARG:HH21	1.83	0.44
3:N:161:LEU:HD13	9:N:9313:HOH:O	2.17	0.44
3:N:112:ILE:HD13	3:N:461:ILE:HG21	2.00	0.44
3:N:950:GLY:O	3:N:953:ASP:N	2.41	0.44
5:P:129:GLU:HB3	5:P:142:ARG:NH2	2.33	0.44
1:A:89:PHE:HB2	1:A:94:LEU:HD13	2.00	0.44
1:A:9:PRO:HG2	1:B:224:TYR:CD2	2.52	0.44
1:B:182:GLU:N	9:B:579:HOH:O	2.50	0.44
2:C:185:LYS:HG2	2:C:190:LYS:CG	2.47	0.44
2:C:208:ALA:HA	2:C:221:LEU:HD21	1.99	0.44
2:C:267:TYR:N	2:C:267:TYR:CD2	2.85	0.44
2:C:339:LEU:HB3	2:C:385:PHE:CZ	2.53	0.44
2:C:547:ILE:HA	2:C:548:PRO:HD3	1.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1318:TYR:CD1	3:D:1319:VAL:N	2.84	0.44
3:D:1442:ASN:HA	9:D:9032:HOH:O	2.17	0.44
3:D:500:ARG:NH1	3:D:500:ARG:HG3	2.33	0.44
2:C:1042:ALA:CB	3:D:710:ARG:HB3	2.45	0.44
3:D:925:GLU:HA	9:D:9129:HOH:O	2.17	0.44
5:F:291:ILE:HG23	5:F:304:VAL:HG21	1.99	0.44
5:F:321:ILE:O	5:F:327:SER:HB3	2.18	0.44
2:M:252:LYS:NZ	2:M:296:GLY:HA3	2.33	0.44
2:M:56:GLU:HG2	2:M:64:LEU:HD23	2.00	0.44
2:M:642:ARG:HG3	2:M:654:LEU:HD21	2.00	0.44
2:M:835:VAL:HG13	3:N:725:SER:OG	2.18	0.44
2:M:893:ALA:HB2	2:M:918:LEU:HD12	2.00	0.44
3:N:1123:PHE:HA	3:N:1135:ARG:N	2.33	0.44
3:N:117:ASP:HB2	3:N:495:ARG:HH21	1.79	0.44
3:N:438:ASP:OD2	3:N:440:VAL:HB	2.18	0.44
5:P:231:ARG:HD3	9:P:4958:HOH:O	2.17	0.44
2:C:1060:ILE:CG2	2:C:1061:GLU:H	2.30	0.43
2:C:185:LYS:HB3	2:C:188:LYS:O	2.17	0.43
2:C:267:TYR:H	2:C:267:TYR:HD2	1.65	0.43
3:D:1087:ARG:C	9:D:9918:HOH:O	2.57	0.43
3:D:1258:ARG:NH2	3:D:1262:LEU:HD11	2.33	0.43
3:D:1366:LYS:O	3:D:1369:GLU:HB2	2.18	0.43
3:D:1459:LEU:HD12	3:D:1470:ARG:NH1	2.33	0.43
3:D:169:TYR:N	3:D:170:PRO:HD2	2.33	0.43
3:D:397:LYS:NZ	3:D:399:ARG:HH21	2.15	0.43
3:D:695:ILE:HG21	3:D:720:LEU:HD11	1.99	0.43
3:D:762:GLN:HE21	4:E:20:THR:HG21	1.83	0.43
3:D:80:VAL:HG12	3:D:81:THR:O	2.18	0.43
1:L:206:THR:HG23	1:L:208:LEU:N	2.33	0.43
1:L:63:HIS:HB3	9:L:3555:HOH:O	2.18	0.43
2:M:1019:GLN:HE22	3:N:621:LYS:HG2	1.83	0.43
2:M:108:ILE:HD12	2:M:108:ILE:N	2.33	0.43
2:M:196:LEU:O	2:M:199:VAL:HB	2.18	0.43
2:M:413:LEU:HD13	2:M:448:ASN:OD1	2.18	0.43
2:M:554:ASP:HB3	2:M:880:MET:O	2.18	0.43
2:M:586:ARG:NH1	2:M:590:ASP:OD2	2.51	0.43
2:M:594:ALA:HB3	2:M:596:TYR:HE1	1.83	0.43
2:M:9:ILE:HD13	2:M:536:PRO:HD2	1.99	0.43
3:N:1035:ILE:HG22	3:N:1039:CYS:SG	2.58	0.43
3:N:1337:GLU:HB3	9:N:9327:HOH:O	2.17	0.43
3:N:178:LEU:HG	3:N:200:ASP:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:215:TYR:O	3:N:389:GLU:HB3	2.18	0.43
3:N:513:ILE:HB	9:N:9876:HOH:O	2.18	0.43
3:N:534:ARG:HG2	9:P:3569:HOH:O	2.17	0.43
3:N:614:PHE:O	3:N:617:ASN:HB2	2.17	0.43
3:N:729:HIS:ND1	3:N:730:PRO:HD2	2.34	0.43
3:N:787:LEU:O	3:N:787:LEU:HD12	2.18	0.43
5:P:226:LYS:HG3	5:P:242:TRP:CH2	2.53	0.43
5:P:414:ARG:HG3	9:P:4806:HOH:O	2.18	0.43
2:C:101:ILE:HD12	2:C:107:LEU:HD22	2.00	0.43
2:C:165:LEU:HA	2:C:166:PRO:O	2.18	0.43
2:C:19:THR:HG21	2:C:124:ASP:O	2.18	0.43
2:C:262:ALA:O	2:C:264:PRO:O	2.36	0.43
2:C:289:THR:O	2:C:291:ALA:N	2.51	0.43
2:C:479:VAL:HG22	2:C:508:ILE:CD1	2.48	0.43
2:C:722:ILE:HG21	2:C:805:ARG:HH21	1.82	0.43
3:D:1007:VAL:HG23	3:D:1008:PHE:N	2.33	0.43
2:C:1039:ALA:HB2	3:D:707:THR:HG21	2.00	0.43
3:D:900:ILE:CD1	3:D:902:LEU:HD23	2.48	0.43
3:D:903:ASP:HB3	9:D:9214:HOH:O	2.17	0.43
3:D:928:ALA:HA	3:D:931:LEU:HD12	1.99	0.43
3:D:947:ILE:H	3:D:947:ILE:HG13	1.57	0.43
5:F:360:LYS:HA	9:F:621:HOH:O	2.17	0.43
1:K:217:ILE:HG23	9:K:6003:HOH:O	2.18	0.43
1:K:41:ARG:HH11	1:K:41:ARG:HG3	1.83	0.43
1:K:44:LEU:O	1:K:174:VAL:HG21	2.18	0.43
2:M:1104:GLU:H	2:M:1104:GLU:CD	2.21	0.43
2:M:292:ARG:CD	2:M:299:LYS:HD3	2.45	0.43
2:M:383:ARG:HB2	2:M:383:ARG:CZ	2.47	0.43
2:M:571:LEU:HD21	2:M:700:TYR:HD2	1.83	0.43
2:M:577:PRO:HD2	2:M:580:MET:HG2	1.99	0.43
2:M:708:TYR:HD1	2:M:708:TYR:H	1.64	0.43
2:M:917:LEU:HD23	2:M:920:GLN:NE2	2.32	0.43
3:N:1209:LEU:HD12	3:N:1216:SER:HB2	1.99	0.43
3:N:1406:ARG:HG3	3:N:1412:LYS:HG2	2.00	0.43
3:N:30:GLU:HB3	3:N:40:GLU:CG	2.48	0.43
3:N:684:LYS:H	3:N:684:LYS:HG3	1.59	0.43
3:N:880:ILE:O	3:N:883:ALA:HB3	2.18	0.43
1:A:163:ASN:HD22	1:A:163:ASN:HA	1.65	0.43
1:A:9:PRO:HB3	1:A:25:LEU:CG	2.48	0.43
1:B:106:PRO:HG3	1:B:133:GLU:O	2.19	0.43
2:C:1007:ALA:HB2	9:C:1170:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1012:PRO:HD2	2:C:1021:LEU:O	2.18	0.43
2:C:1060:ILE:CG2	2:C:1061:GLU:N	2.81	0.43
2:C:141:HIS:HB2	2:C:418:LEU:HD12	2.00	0.43
2:C:244:PRO:CD	2:C:245:GLY:N	2.81	0.43
2:C:455:LEU:H	2:C:455:LEU:HD23	1.82	0.43
2:C:619:ARG:HA	9:C:1206:HOH:O	2.18	0.43
2:C:759:THR:HB	2:C:785:VAL:HG21	2.00	0.43
3:D:1045:MET:N	9:D:9034:HOH:O	2.51	0.43
3:D:1119:SER:HA	3:D:1186:VAL:O	2.18	0.43
3:D:1209:LEU:HD23	3:D:1210:SER:H	1.82	0.43
3:D:1235:GLN:O	3:D:1237:THR:N	2.51	0.43
3:D:186:VAL:HG11	3:D:213:VAL:HB	2.00	0.43
3:D:414:ARG:HB3	9:D:9281:HOH:O	2.19	0.43
3:D:416:ALA:H	3:D:417:PRO:CD	2.30	0.43
3:D:486:ARG:HA	3:D:489:ARG:HG2	1.99	0.43
3:D:618:LEU:HG	9:D:9956:HOH:O	2.18	0.43
2:C:1036:GLU:HG3	3:D:707:THR:OG1	2.18	0.43
3:D:847:ASP:O	3:D:851:LEU:HG	2.19	0.43
3:D:45:PHE:CD1	3:D:86:ARG:NH2	2.86	0.43
3:D:912:LYS:O	3:D:915:VAL:HG23	2.19	0.43
3:D:928:ALA:O	3:D:931:LEU:HB2	2.18	0.43
3:D:988:ARG:O	3:D:992:ILE:HG13	2.19	0.43
5:F:282:LEU:HB2	5:F:284:ARG:H	1.83	0.43
5:F:361:LEU:CD2	5:F:362:SER:H	2.22	0.43
5:F:421:PHE:C	5:F:423:ASP:H	2.22	0.43
1:K:189:ARG:HD2	1:K:191:ASP:OD1	2.18	0.43
2:M:1019:GLN:NE2	3:N:621:LYS:HG2	2.33	0.43
2:M:1043:TYR:HE2	3:N:768:ASN:ND2	2.17	0.43
2:M:301:GLU:O	2:M:305:PRO:HG2	2.19	0.43
2:M:304:LEU:HD21	9:M:1857:HOH:O	2.17	0.43
2:M:897:LEU:HB3	2:M:899:GLN:HG2	2.00	0.43
2:M:77:PRO:HD2	2:M:91:GLN:O	2.18	0.43
3:N:1390:LEU:HD11	9:N:9190:HOH:O	2.17	0.43
3:N:456:MET:HE3	3:N:568:ARG:HD3	2.00	0.43
3:N:567:ILE:HG22	3:N:571:LYS:CE	2.47	0.43
3:N:829:VAL:H	3:N:835:SER:HB2	1.82	0.43
3:N:957:PRO:CD	3:N:1007:VAL:HG12	2.48	0.43
5:P:214:GLN:HA	5:P:214:GLN:OE1	2.16	0.43
5:P:409:LYS:HE3	5:P:410:TYR:CD1	2.53	0.43
1:A:132:LEU:HD12	1:A:132:LEU:N	2.33	0.43
2:C:1011:GLY:HA3	2:C:1026:GLN:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:203:ASP:OD1	2:C:206:THR:HG22	2.19	0.43
2:C:534:VAL:H	2:C:538:GLN:NE2	2.15	0.43
2:C:57:GLU:HG2	9:C:1767:HOH:O	2.18	0.43
2:C:892:LEU:HD21	2:C:967:PHE:CE1	2.54	0.43
3:D:1065:LEU:HD12	3:D:1065:LEU:C	2.38	0.43
3:D:190:GLU:HB3	9:D:9431:HOH:O	2.18	0.43
3:D:374:GLU:HA	9:D:2147:HOH:O	2.17	0.43
3:D:543:LEU:O	3:D:546:ARG:HB2	2.19	0.43
3:D:621:LYS:NZ	9:D:9787:HOH:O	2.51	0.43
3:D:654:LYS:HB3	3:D:655:PRO:CD	2.38	0.43
3:D:804:LEU:HD23	3:D:804:LEU:H	1.83	0.43
3:D:423:ASP:OD1	5:F:174:LEU:HD13	2.18	0.43
5:F:320:PRO:HB2	5:F:324:GLU:HG3	2.00	0.43
1:L:94:LEU:HD11	1:L:119:ASP:HB3	2.00	0.43
2:M:1103:ASP:N	2:M:1107:ASN:O	2.51	0.43
2:M:433:THR:C	2:M:435:TYR:H	2.22	0.43
2:M:95:TYR:CD1	2:M:95:TYR:N	2.87	0.43
3:N:1123:PHE:HE2	3:N:1184:GLN:HA	1.81	0.43
3:N:1267:ARG:NH1	3:N:1331:ASP:HB2	2.29	0.43
3:N:169:TYR:HA	3:N:392:SER:HA	2.00	0.43
3:N:520:LEU:HD12	3:N:521:PRO:CD	2.47	0.43
3:N:764:LEU:HD12	3:N:765:SER:H	1.83	0.43
3:N:938:GLY:O	3:N:942:SER:HB3	2.18	0.43
5:P:225:GLU:HB2	9:P:3558:HOH:O	2.17	0.43
1:A:29:GLU:HB3	1:A:30:ARG:H	1.69	0.43
1:B:182:GLU:O	1:B:194:LYS:HB3	2.19	0.43
2:C:15:LEU:HD13	2:C:583:LEU:HD11	1.99	0.43
2:C:197:LEU:HD22	2:C:202:TYR:HD2	1.83	0.43
2:C:352:ALA:O	2:C:355:VAL:HG12	2.19	0.43
2:C:47:ALA:HB1	2:C:345:ARG:HB3	2.00	0.43
2:C:501:THR:HG22	2:C:513:VAL:CG2	2.49	0.43
2:C:704:HIS:HB2	2:C:831:ARG:NE	2.34	0.43
2:C:78:PHE:HB3	2:C:79:PRO:HD2	2.00	0.43
2:C:91:GLN:HE21	2:C:119:PRO:HD3	1.83	0.43
3:D:1068:LEU:C	3:D:1070:TYR:N	2.71	0.43
3:D:1120:VAL:HA	3:D:1121:PRO:HD3	1.74	0.43
3:D:1264:GLU:HB3	3:D:1266:ARG:NE	2.33	0.43
3:D:1402:ALA:HB2	3:D:1415:VAL:HG23	1.99	0.43
3:D:34:TYR:CD2	3:D:34:TYR:N	2.87	0.43
3:D:396:VAL:HG13	3:D:446:VAL:O	2.19	0.43
2:C:1071:ILE:HD13	3:D:655:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:894:LYS:HD3	9:D:9911:HOH:O	2.17	0.43
3:D:914:LEU:O	3:D:914:LEU:HD23	2.19	0.43
3:D:972:LEU:CD2	3:D:973:GLN:HE21	2.31	0.43
4:E:45:ARG:HB2	4:E:46:PRO:CD	2.49	0.43
1:K:101:LEU:HD12	1:K:114:PHE:CD1	2.53	0.43
2:M:1108:PRO:HD3	9:M:1260:HOH:O	2.18	0.43
2:M:148:PHE:CE1	2:M:309:TYR:HB3	2.54	0.43
2:M:260:LEU:HA	2:M:291:ALA:HB2	2.00	0.43
2:M:421:GLU:HB3	9:M:2092:HOH:O	2.18	0.43
2:M:438:ILE:HG12	9:M:1460:HOH:O	2.17	0.43
2:M:496:ILE:HD12	2:M:496:ILE:H	1.83	0.43
2:M:575:GLN:HA	2:M:662:GLU:CD	2.39	0.43
2:M:654:LEU:HD11	2:M:657:ASP:HA	2.00	0.43
3:N:1097:LYS:O	3:N:1101:VAL:HG22	2.19	0.43
3:N:1136:LYS:O	3:N:1140:ILE:HG13	2.17	0.43
3:N:127:LEU:HD23	3:N:134:VAL:HG11	1.99	0.43
3:N:41:ARG:HD3	3:N:42:ASP:N	2.34	0.43
3:N:396:VAL:HG13	3:N:446:VAL:O	2.18	0.43
9:N:9213:HOH:O	5:P:136:LEU:HD21	2.19	0.43
5:P:131:VAL:HG13	5:P:178:ARG:HG2	2.01	0.43
5:P:232:ARG:HA	5:P:232:ARG:HD2	1.89	0.43
1:A:38:ASN:ND2	9:A:334:HOH:O	2.52	0.43
1:B:184:THR:O	1:B:192:LEU:HB2	2.18	0.43
2:C:1004:LYS:HE3	2:C:1027:PHE:HE1	1.83	0.43
2:C:1097:LEU:HD21	3:D:103:TRP:CZ3	2.53	0.43
2:C:172:ILE:N	2:C:172:ILE:HD12	2.32	0.43
2:C:328:LEU:HB2	2:C:488:ALA:CB	2.38	0.43
2:C:347:GLY:HA2	2:C:350:ARG:CD	2.48	0.43
2:C:393:GLN:HG2	9:C:1727:HOH:O	2.17	0.43
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.54	0.43
1:A:150:TYR:OH	2:C:832:LYS:HE3	2.18	0.43
2:C:837:ASP:O	2:C:849:VAL:HG23	2.19	0.43
2:C:944:LEU:HD22	2:C:962:GLN:OE1	2.18	0.43
3:D:1237:THR:HG21	9:D:9202:HOH:O	2.19	0.43
3:D:1408:ILE:HG12	9:D:9641:HOH:O	2.18	0.43
3:D:1437:ALA:O	3:D:1446:VAL:HG21	2.19	0.43
3:D:1495:ILE:O	3:D:1499:ARG:HG3	2.19	0.43
3:D:185:VAL:HG12	3:D:191:LEU:HD21	2.01	0.43
3:D:131:LYS:HE2	3:D:568:ARG:CB	2.48	0.43
3:D:850:LEU:HD22	3:D:884:ARG:NH2	2.33	0.43
4:E:49:GLN:HA	4:E:51:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:SER:HA	9:K:4719:HOH:O	2.18	0.43
1:K:76:VAL:O	1:K:79:ILE:HG13	2.18	0.43
1:L:206:THR:HG23	1:L:208:LEU:H	1.83	0.43
1:L:74:ASP:HB3	9:N:9057:HOH:O	2.19	0.43
2:M:394:PHE:HB3	9:M:1953:HOH:O	2.18	0.43
2:M:939:ARG:HG3	9:M:1198:HOH:O	2.18	0.43
2:M:937:ASP:HB2	2:M:940:GLU:HB2	2.01	0.43
3:N:1459:LEU:HD22	3:N:1465:ASN:ND2	2.33	0.43
3:N:399:ARG:HB2	3:N:444:VAL:HG13	1.99	0.43
3:N:410:SER:CB	3:N:414:ARG:HH21	2.32	0.43
3:N:606:ILE:O	3:N:613:ARG:HB2	2.18	0.43
2:M:1076:VAL:CG2	3:N:752:SER:HB3	2.49	0.43
3:N:965:GLU:O	3:N:968:ASP:HB3	2.19	0.43
4:O:23:VAL:CG2	4:O:65:MET:HG2	2.49	0.43
5:P:213:ILE:HG22	5:P:217:ASN:OD1	2.19	0.43
5:P:247:ILE:O	5:P:251:ILE:HG13	2.19	0.43
5:P:358:LEU:CD1	5:P:370:LYS:HG3	2.43	0.43
5:P:392:VAL:HG12	5:P:396:ARG:HG3	2.00	0.43
1:A:122:ILE:HD11	9:A:394:HOH:O	2.18	0.43
1:A:23:PHE:O	1:A:196:THR:HA	2.19	0.43
1:B:109:VAL:HG22	9:B:383:HOH:O	2.18	0.43
1:B:211:LEU:O	1:B:214:ALA:HB3	2.19	0.43
1:A:221:HIS:HB3	1:B:36:LEU:HD21	1.99	0.43
2:C:213:ALA:N	9:C:1550:HOH:O	2.51	0.43
2:C:317:VAL:HG12	9:C:1216:HOH:O	2.19	0.43
2:C:358:ARG:HH12	2:C:374:ASN:CG	2.22	0.43
2:C:549:PHE:HB3	2:C:552:HIS:CD2	2.54	0.43
2:C:721:ARG:HH21	2:C:783:ARG:NH2	2.04	0.43
2:C:774:LEU:HA	2:C:777:ILE:HD12	2.00	0.43
3:D:1397:LYS:NZ	3:D:1432:LYS:HB3	2.33	0.43
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.84	0.43
3:D:565:ILE:HD12	3:D:565:ILE:H	1.84	0.43
3:D:57:GLU:OE1	3:D:64:LYS:HE2	2.19	0.43
9:B:529:HOH:O	3:D:851:LEU:HD21	2.16	0.43
3:D:969:ARG:HB3	3:D:969:ARG:HE	1.63	0.43
5:F:119:ILE:HD11	9:F:580:HOH:O	2.18	0.43
5:F:188:ILE:HA	9:F:598:HOH:O	2.18	0.43
5:F:271:LEU:HD11	5:F:307:THR:HB	2.01	0.43
1:K:38:ASN:HB3	1:K:39:PRO:HD3	2.00	0.43
2:M:1045:ALA:HB1	2:M:1048:THR:HB	2.00	0.43
2:M:141:HIS:NE2	2:M:332:ARG:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:147:TYR:HB3	2:M:323:ASP:OD2	2.19	0.43
2:M:283:ILE:HG22	2:M:284:ARG:HG3	2.01	0.43
2:M:63:GLY:HA3	2:M:103:LYS:CG	2.48	0.43
2:M:771:GLU:HA	9:M:1452:HOH:O	2.18	0.43
2:M:775:ARG:N	2:M:775:ARG:HD2	2.33	0.43
2:M:674:VAL:O	2:M:989:VAL:HA	2.18	0.43
3:N:1023:MET:O	3:N:1028:ALA:HB3	2.19	0.43
3:N:1353:GLN:HG2	3:N:1368:ILE:CD1	2.48	0.43
3:N:21:TRP:HZ3	3:N:518:PRO:HG2	1.84	0.43
3:N:591:VAL:HG11	3:N:597:ASP:HA	2.01	0.43
2:M:1020:PRO:HD2	3:N:622:ARG:O	2.19	0.43
4:O:36:LYS:HD3	4:O:36:LYS:HA	1.87	0.43
5:P:211:ASP:N	5:P:211:ASP:OD1	2.51	0.43
5:P:294:ALA:HB2	9:P:3652:HOH:O	2.19	0.43
5:P:410:TYR:O	5:P:413:SER:HB2	2.18	0.43
1:A:85:LEU:HA	1:A:124:ASN:HD22	1.83	0.43
2:C:165:LEU:HD12	2:C:166:PRO:C	2.38	0.43
2:C:286:SER:CB	2:C:299:LYS:HE3	2.48	0.43
2:C:374:ASN:ND2	2:C:377:PRO:HD3	2.34	0.43
2:C:437:ARG:HG2	2:C:467:ILE:CG2	2.47	0.43
2:C:436:GLY:O	2:C:459:ALA:HB2	2.19	0.43
2:C:332:ARG:HB2	2:C:466:PHE:CE1	2.54	0.43
2:C:773:LEU:HG	2:C:777:ILE:HD11	1.99	0.43
2:C:881:ASN:HD22	2:C:881:ASN:N	2.14	0.43
3:D:112:ILE:HG13	3:D:124:GLU:OE2	2.19	0.43
3:D:1183:ILE:HG22	9:D:9139:HOH:O	2.17	0.43
3:D:1148:VAL:HG21	3:D:1203:LYS:HA	2.01	0.43
3:D:141:ILE:HD13	3:D:450:TYR:N	2.34	0.43
3:D:521:PRO:O	3:D:525:ARG:HG2	2.19	0.43
3:D:696:HIS:HD2	4:E:59:ASN:HB2	1.83	0.43
3:D:882:PHE:O	3:D:886:VAL:HG23	2.18	0.43
3:D:902:LEU:HG	9:D:9056:HOH:O	2.18	0.43
3:D:953:ASP:O	3:D:955:VAL:HG23	2.19	0.43
3:D:960:LYS:HB3	9:D:9060:HOH:O	2.18	0.43
4:E:9:LEU:HD22	4:E:19:LEU:HD11	2.01	0.43
4:E:35:PHE:HZ	4:E:60:ALA:HA	1.83	0.43
1:L:81:ASN:ND2	1:L:128:HIS:O	2.52	0.43
1:L:54:THR:HG22	1:L:158:ILE:HG13	2.01	0.43
2:M:1089:VAL:O	2:M:1093:GLN:HG3	2.19	0.43
2:M:183:SER:C	2:M:193:LEU:HD11	2.38	0.43
2:M:342:ASP:HA	2:M:345:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:405:ARG:HD2	2:M:442:GLU:OE2	2.19	0.43
2:M:9:ILE:HD13	2:M:536:PRO:CD	2.49	0.43
2:M:546:LEU:HA	2:M:581:THR:HG1	1.82	0.43
2:M:582:GLY:N	2:M:584:GLU:OE2	2.44	0.43
2:M:585:GLU:HG2	9:M:1469:HOH:O	2.18	0.43
2:M:81:ASP:HB3	9:M:2035:HOH:O	2.19	0.43
3:N:1153:VAL:HG12	3:N:1155:VAL:HG23	2.00	0.43
3:N:112:ILE:HG13	3:N:124:GLU:OE2	2.19	0.43
3:N:1260:ILE:HA	3:N:1260:ILE:HD13	1.86	0.43
3:N:1492:LEU:HD12	3:N:1493:LYS:CE	2.48	0.43
3:N:443:VAL:HG11	3:N:445:ARG:HE	1.82	0.43
3:N:473:LEU:HD21	3:N:495:ARG:CZ	2.48	0.43
3:N:66:GLN:O	3:N:69:GLU:HB3	2.19	0.43
3:N:775:GLY:HA2	9:N:9022:HOH:O	2.19	0.43
3:N:799:LYS:N	3:N:826:PRO:HG2	2.34	0.43
3:N:834:THR:HB	3:N:838:ARG:HB3	2.00	0.43
5:P:115:LYS:O	5:P:119:ILE:HG13	2.19	0.43
5:P:262:VAL:N	9:P:4345:HOH:O	2.51	0.43
5:P:358:LEU:HD11	5:P:367:MET:SD	2.59	0.43
5:P:74:LYS:HG2	9:P:4226:HOH:O	2.19	0.43
1:A:61:VAL:HG11	1:A:75:VAL:HG21	2.01	0.43
1:B:44:LEU:HD11	1:B:199:ILE:HD11	1.99	0.43
1:B:213:GLN:HG3	9:B:515:HOH:O	2.17	0.43
1:B:2:LEU:HD12	1:B:3:ASP:HB2	2.01	0.43
2:C:127:PHE:O	2:C:133:ASP:HA	2.19	0.43
2:C:218:VAL:HG22	2:C:221:LEU:HD23	2.01	0.43
2:C:352:ALA:C	2:C:355:VAL:HG12	2.39	0.43
2:C:355:VAL:HB	9:C:1597:HOH:O	2.17	0.43
2:C:110:GLU:H	2:C:368:THR:HG21	1.83	0.43
2:C:409:ARG:HA	2:C:454:SER:HA	2.01	0.43
2:C:438:ILE:HG22	2:C:439:CYS:O	2.19	0.43
2:C:564:MET:CE	2:C:846:LYS:HE2	2.49	0.43
3:D:126:VAL:CG1	3:D:132:TYR:HB2	2.48	0.43
3:D:1403:LEU:HD12	9:D:9824:HOH:O	2.19	0.43
3:D:1405:GLU:OE2	3:D:1413:THR:HB	2.19	0.43
3:D:545:ARG:HH21	5:F:257:THR:HG23	1.83	0.43
3:D:591:VAL:HG12	3:D:592:THR:O	2.19	0.43
3:D:64:LYS:N	3:D:68:PHE:HZ	2.16	0.43
3:D:829:VAL:HG11	9:D:9455:HOH:O	2.18	0.43
3:D:918:ALA:O	3:D:922:LEU:HG	2.18	0.43
3:D:947:ILE:HD12	3:D:947:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1475:GLY:HA2	4:E:17:TYR:CE1	2.54	0.43
5:F:88:ILE:CD1	5:F:193:ARG:HB2	2.44	0.43
1:L:12:THR:OG1	1:L:24:VAL:HB	2.18	0.43
1:L:133:GLU:N	9:L:4988:HOH:O	2.51	0.43
1:L:23:PHE:CE1	1:L:208:LEU:HD22	2.54	0.43
2:M:166:PRO:HD3	2:M:265:ARG:HG3	2.01	0.43
2:M:358:ARG:HB3	2:M:371:LYS:O	2.19	0.43
2:M:420:ARG:NE	2:M:420:ARG:H	2.17	0.43
2:M:42:VAL:HG12	2:M:43:GLY:N	2.29	0.43
2:M:691:SER:HB2	2:M:858:MET:SD	2.59	0.43
2:M:93:PRO:HG3	2:M:117:HIS:HE1	1.84	0.43
3:N:1353:GLN:HE21	3:N:1353:GLN:HB3	1.64	0.43
3:N:625:TYR:N	3:N:625:TYR:CD1	2.87	0.43
3:N:749:VAL:HA	3:N:750:PRO:HD3	1.91	0.43
3:N:765:SER:O	3:N:767:HIS:N	2.51	0.43
3:N:85:VAL:HB	3:N:89:ARG:NH1	2.33	0.43
5:P:185:GLN:HG3	9:P:4903:HOH:O	2.19	0.43
5:P:243:ILE:O	5:P:247:ILE:HG13	2.18	0.43
1:A:38:ASN:ND2	9:C:1607:HOH:O	2.52	0.43
1:A:1:MET:O	1:A:6:LEU:HB2	2.19	0.43
1:B:162:ILE:HG13	1:B:163:ASN:N	2.34	0.43
1:B:165:ILE:O	1:B:165:ILE:HG13	2.19	0.43
2:C:183:SER:HB2	2:C:190:LYS:HG2	2.01	0.43
2:C:25:SER:CB	2:C:335:THR:HB	2.49	0.43
2:C:708:TYR:CE2	2:C:793:PRO:HD2	2.54	0.43
2:C:777:ILE:HD13	9:C:1214:HOH:O	2.18	0.43
2:C:816:LYS:O	2:C:819:VAL:HB	2.19	0.43
2:C:579:VAL:HG11	2:C:887:GLU:HG3	2.01	0.43
3:D:1013:GLU:HA	9:D:9714:HOH:O	2.18	0.43
3:D:1496:GLU:HA	3:D:1499:ARG:HG3	2.01	0.43
3:D:154:THR:CG2	3:D:156:GLU:HG2	2.48	0.43
3:D:164:GLY:HA2	9:D:9007:HOH:O	2.18	0.43
3:D:36:THR:O	3:D:38:LYS:N	2.51	0.43
3:D:422:ALA:O	3:D:427:VAL:HG21	2.19	0.43
3:D:657:LEU:HD21	3:D:687:VAL:HG13	2.00	0.43
3:D:702:LEU:HB3	3:D:745:MET:CE	2.49	0.43
3:D:761:ILE:HD13	4:E:20:THR:HA	2.00	0.43
3:D:806:PHE:O	3:D:807:ALA:C	2.56	0.43
3:D:972:LEU:HD23	9:D:2386:HOH:O	2.19	0.43
4:E:13:VAL:HG12	4:E:75:PHE:CE1	2.53	0.43
5:F:226:LYS:HD2	5:F:242:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1036:GLU:O	2:M:1039:ALA:HB3	2.19	0.43
2:M:134:ARG:HH12	2:M:387:SER:HA	1.82	0.43
2:M:148:PHE:HD2	2:M:160:ALA:HA	1.84	0.43
2:M:217:LEU:HD12	2:M:311:PHE:CD2	2.54	0.43
2:M:324:ASP:CG	2:M:431:HIS:HE1	2.22	0.43
2:M:495:THR:HG21	2:M:524:VAL:HG21	2.00	0.43
2:M:686:ASP:HB2	3:N:739:ASP:OD2	2.18	0.43
2:M:721:ARG:O	2:M:758:ARG:HA	2.19	0.43
2:M:808:ARG:HD2	2:M:808:ARG:HA	1.89	0.43
2:M:876:VAL:HG22	2:M:884:GLN:NE2	2.33	0.43
2:M:69:LEU:HD11	2:M:99:GLN:HE21	1.84	0.43
3:N:445:ARG:HG2	3:N:445:ARG:HH11	1.84	0.43
3:N:482:LYS:HA	3:N:489:ARG:NH2	2.34	0.43
3:N:729:HIS:CE1	3:N:935:LYS:HD3	2.54	0.43
5:P:273:ARG:O	5:P:276:ARG:HB2	2.19	0.43
1:A:176:ARG:NH1	2:C:863:ASP:OD2	2.52	0.42
1:A:97:VAL:HG23	9:A:368:HOH:O	2.18	0.42
1:B:142:VAL:HG23	1:B:142:VAL:O	2.19	0.42
2:C:159:ILE:HD12	9:C:1237:HOH:O	2.19	0.42
2:C:184:MET:HB2	2:C:193:LEU:HD12	2.01	0.42
2:C:189:ARG:HG2	2:C:189:ARG:HH11	1.84	0.42
2:C:299:LYS:HB2	9:C:1862:HOH:O	2.19	0.42
2:C:321:GLU:HG2	2:C:321:GLU:H	1.57	0.42
2:C:841:ASN:ND2	2:C:843:HIS:H	2.13	0.42
1:A:34:VAL:HG21	2:C:939:ARG:NE	2.34	0.42
3:D:396:VAL:HG22	9:D:9055:HOH:O	2.18	0.42
3:D:583:ASP:OD2	3:D:586:ARG:HD2	2.19	0.42
3:D:616:GLN:HG2	3:D:616:GLN:O	2.19	0.42
3:D:667:ALA:HB3	9:D:9062:HOH:O	2.20	0.42
4:E:87:LYS:HG2	9:E:103:HOH:O	2.19	0.42
5:F:419:ARG:O	5:F:421:PHE:N	2.52	0.42
1:K:133:GLU:OE2	2:M:605:LYS:HB3	2.19	0.42
2:M:184:MET:SD	2:M:303:PHE:HE2	2.42	0.42
2:M:470:PRO:HD3	2:M:485:TYR:CE2	2.54	0.42
2:M:516:ARG:NE	3:N:1068:LEU:HD13	2.32	0.42
2:M:535:SER:O	2:M:538:GLN:HG2	2.19	0.42
2:M:569:VAL:HG11	2:M:996:LYS:HZ2	1.83	0.42
2:M:605:LYS:HB2	2:M:610:ARG:NH1	2.33	0.42
2:M:565:GLN:OE1	2:M:842:ARG:HG2	2.19	0.42
3:N:102:ILE:N	9:N:2184:HOH:O	2.51	0.42
3:N:1112:CYS:HB3	9:N:9751:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1311:LEU:H	3:N:1311:LEU:HD23	1.83	0.42
3:N:1275:SER:HB3	3:N:1325:LEU:HD22	2.00	0.42
3:N:1364:HIS:CE1	3:N:1366:LYS:H	2.35	0.42
3:N:1376:MET:HB2	9:N:9599:HOH:O	2.18	0.42
3:N:135:LEU:CD1	3:N:147:VAL:HG23	2.46	0.42
3:N:153:LEU:HD12	3:N:154:THR:N	2.34	0.42
3:N:516:ALA:O	3:N:518:PRO:HD3	2.19	0.42
3:N:563:PRO:HG2	3:N:566:ILE:HB	2.01	0.42
2:M:1115:LEU:CB	3:N:85:VAL:HG12	2.46	0.42
3:N:964:LEU:HB3	9:N:2215:HOH:O	2.18	0.42
3:N:760:ARG:NE	4:O:3:GLU:OE2	2.48	0.42
5:P:203:THR:HG22	5:P:204:GLY:N	2.34	0.42
1:A:180:GLN:HE22	2:C:929:ARG:NH2	2.17	0.42
1:A:206:THR:HG22	1:A:209:GLU:H	1.83	0.42
1:A:20:TYR:HE2	1:A:22:GLU:HG3	1.84	0.42
2:C:174:LEU:CD2	2:C:184:MET:HG3	2.49	0.42
2:C:197:LEU:HD22	2:C:202:TYR:CD2	2.54	0.42
2:C:802:ARG:HB2	9:C:2027:HOH:O	2.19	0.42
2:C:983:ILE:HG21	2:C:987:ILE:CD1	2.47	0.42
3:D:1059:SER:OG	3:D:1065:LEU:HA	2.19	0.42
3:D:1128:VAL:O	3:D:1129:THR:C	2.56	0.42
3:D:1155:VAL:CG1	3:D:1177:ALA:HB1	2.49	0.42
3:D:1425:THR:CG2	3:D:1426:LYS:N	2.82	0.42
3:D:153:LEU:HD13	3:D:157:GLU:HB2	1.99	0.42
3:D:32:ILE:HG22	5:F:258:ILE:HD12	2.02	0.42
3:D:209:ARG:NH1	3:D:397:LYS:HG3	2.34	0.42
3:D:399:ARG:HB2	3:D:444:VAL:HG13	2.00	0.42
3:D:567:ILE:HG22	3:D:571:LYS:HZ2	1.84	0.42
3:D:574:LEU:O	3:D:577:ALA:HB3	2.19	0.42
3:D:704:ARG:CD	3:D:705:ALA:H	2.32	0.42
3:D:804:LEU:HB3	9:D:9141:HOH:O	2.18	0.42
3:D:86:ARG:HG2	3:D:523:ASP:OD2	2.19	0.42
4:E:17:TYR:CD2	4:E:17:TYR:N	2.87	0.42
1:K:52:ALA:HB2	1:K:170:VAL:O	2.19	0.42
2:M:1002:GLU:HG3	2:M:1002:GLU:H	1.52	0.42
2:M:114:PHE:HE1	9:P:4182:HOH:O	2.01	0.42
2:M:414:GLY:HA3	2:M:415:PRO:HD3	1.91	0.42
2:M:464:LEU:HA	2:M:464:LEU:HD12	1.82	0.42
2:M:603:VAL:O	2:M:646:GLY:HA2	2.19	0.42
2:M:811:PRO:HA	9:M:1349:HOH:O	2.18	0.42
3:N:1139:ASP:HB3	3:N:1357:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:149:LYS:HG3	3:N:149:LYS:H	1.53	0.42
3:N:983:LEU:HD23	9:N:9324:HOH:O	2.19	0.42
4:O:49:GLN:HA	4:O:51:LEU:O	2.19	0.42
3:N:1495:ILE:HG21	4:O:80:VAL:HG13	2.01	0.42
5:P:195:VAL:HG12	5:P:213:ILE:HG23	2.00	0.42
5:P:370:LYS:C	5:P:370:LYS:HD2	2.39	0.42
1:B:26:GLU:HG2	1:B:27:PRO:CA	2.49	0.42
1:B:69:PRO:O	1:B:71:VAL:HG23	2.20	0.42
2:C:122:THR:HG22	2:C:123:GLU:N	2.34	0.42
2:C:474:VAL:HG13	2:C:530:GLU:C	2.40	0.42
2:C:689:VAL:HB	2:C:870:ILE:HG13	2.01	0.42
3:D:1269:LYS:O	3:D:1269:LYS:HE2	2.18	0.42
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.19	0.42
3:D:1377:LYS:O	3:D:1394:VAL:HA	2.18	0.42
3:D:180:LYS:HG2	9:D:9440:HOH:O	2.19	0.42
3:D:427:VAL:HG21	3:D:435:VAL:HB	2.01	0.42
5:F:367:MET:HE1	9:F:519:HOH:O	2.19	0.42
1:K:10:VAL:HG12	1:K:12:THR:CG2	2.49	0.42
1:K:56:VAL:HG21	1:K:82:LEU:CD1	2.49	0.42
1:L:140:MET:HB2	9:L:3859:HOH:O	2.18	0.42
1:L:191:ASP:O	1:L:192:LEU:HG	2.19	0.42
1:L:24:VAL:HG11	1:L:194:LYS:HE2	2.01	0.42
2:M:287:GLY:O	2:M:288:ARG:C	2.58	0.42
2:M:326:ASP:HB2	2:M:431:HIS:CG	2.53	0.42
2:M:514:VAL:HG11	2:M:516:ARG:CZ	2.49	0.42
2:M:752:GLY:N	2:M:792:VAL:HB	2.23	0.42
2:M:676:ILE:HG21	2:M:988:VAL:HG22	2.01	0.42
3:N:744:GLN:HE21	3:N:744:GLN:HB3	1.62	0.42
2:M:971:LYS:HE2	3:N:950:GLY:HA3	2.01	0.42
4:O:13:VAL:HG23	9:O:3506:HOH:O	2.18	0.42
5:P:361:LEU:CD2	5:P:366:ALA:HB2	2.41	0.42
1:A:112:ARG:HA	9:A:459:HOH:O	2.20	0.42
1:B:180:GLN:HB3	9:B:579:HOH:O	2.19	0.42
2:C:404:LEU:O	2:C:408:ARG:HG2	2.19	0.42
2:C:479:VAL:HG23	2:C:506:ASN:C	2.40	0.42
2:C:52:PHE:HB2	9:C:1342:HOH:O	2.18	0.42
2:C:551:GLU:O	3:D:1065:LEU:HB3	2.19	0.42
2:C:717:LEU:HB2	9:C:1324:HOH:O	2.19	0.42
2:C:798:GLY:HA2	9:C:1154:HOH:O	2.19	0.42
2:C:722:ILE:HG23	2:C:805:ARG:HH21	1.83	0.42
2:C:979:THR:CG2	2:C:981:GLU:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1138:ALA:HB3	9:D:9318:HOH:O	2.20	0.42
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	2.00	0.42
3:D:1274:ILE:HB	3:D:1322:GLY:HA2	2.02	0.42
3:D:1331:ASP:OD1	3:D:1333:HIS:HB2	2.20	0.42
3:D:152:LEU:HD23	3:D:152:LEU:N	2.34	0.42
3:D:528:VAL:O	3:D:535:PHE:CA	2.65	0.42
3:D:762:GLN:NE2	4:E:20:THR:HG21	2.34	0.42
3:D:800:LYS:HD3	3:D:804:LEU:HD22	2.01	0.42
3:D:900:ILE:HD11	3:D:902:LEU:HD23	2.01	0.42
1:K:184:THR:O	1:K:192:LEU:HD12	2.20	0.42
1:L:89:PHE:HE2	1:L:146:ARG:NE	2.17	0.42
1:L:48:ILE:HA	1:L:49:PRO:HD3	1.87	0.42
2:M:1098:ASP:HB2	3:N:21:TRP:CZ2	2.53	0.42
2:M:140:ILE:HD12	9:M:1151:HOH:O	2.18	0.42
2:M:174:LEU:HD23	2:M:184:MET:HG2	2.02	0.42
2:M:203:ASP:OD1	2:M:205:GLU:HG3	2.19	0.42
2:M:412:ALA:O	2:M:414:GLY:N	2.53	0.42
2:M:976:ASP:OD1	2:M:978:ARG:HD3	2.20	0.42
3:N:1344:VAL:HG12	3:N:1348:LEU:CD2	2.50	0.42
3:N:1262:LEU:HD11	3:N:1351:GLU:CG	2.49	0.42
3:N:493:ARG:CZ	3:N:493:ARG:HB2	2.49	0.42
3:N:494:LYS:HA	3:N:497:GLU:OE1	2.19	0.42
3:N:628:ARG:HD3	3:N:744:GLN:NE2	2.35	0.42
3:N:879:ARG:HD3	9:N:9187:HOH:O	2.18	0.42
4:O:74:VAL:HB	4:O:79:LEU:HD21	2.01	0.42
5:P:131:VAL:CG1	5:P:181:GLU:HG3	2.41	0.42
2:M:1016:ILE:HD12	5:P:317:LEU:HD21	2.01	0.42
1:A:68:ILE:HG21	1:A:138:LEU:HD13	2.02	0.42
1:B:151:VAL:HB	1:B:169:ALA:HB3	2.00	0.42
2:C:1002:GLU:HA	2:C:1006:HIS:HE1	1.85	0.42
2:C:1013:TYR:CZ	2:C:1063:ARG:NE	2.88	0.42
2:C:138:SER:HB2	2:C:410:ILE:HG13	2.01	0.42
2:C:19:THR:HG22	2:C:22:GLN:HB2	2.01	0.42
2:C:147:TYR:CE2	2:C:280:LYS:HE2	2.54	0.42
2:C:480:THR:HG22	2:C:482:GLU:H	1.85	0.42
2:C:543:ASN:HD22	2:C:543:ASN:C	2.23	0.42
2:C:987:ILE:HG22	2:C:988:VAL:O	2.18	0.42
3:D:1149:LEU:HD12	3:D:1161:GLU:O	2.19	0.42
3:D:1264:GLU:CD	3:D:1425:THR:HG22	2.40	0.42
3:D:1280:VAL:O	3:D:1294:VAL:HA	2.19	0.42
3:D:1281:VAL:HG21	3:D:1313:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1311:LEU:CD2	3:D:1311:LEU:H	2.25	0.42
3:D:8:VAL:O	3:D:1434:TRP:HH2	2.02	0.42
3:D:422:ALA:H	3:D:427:VAL:CG1	2.31	0.42
3:D:495:ARG:O	3:D:495:ARG:HG2	2.20	0.42
2:C:678:PRO:CG	3:D:947:ILE:HD11	2.45	0.42
5:F:80:PRO:O	5:F:83:GLN:HB2	2.20	0.42
1:L:91:ASN:H	1:L:94:LEU:CD1	2.32	0.42
2:M:1012:PRO:HA	9:M:1524:HOH:O	2.19	0.42
2:M:115:LEU:HB3	2:M:375:SER:OG	2.20	0.42
2:M:208:ALA:HB1	2:M:218:VAL:CG1	2.49	0.42
2:M:273:GLY:HA2	2:M:276:LYS:HD3	2.00	0.42
2:M:475:VAL:O	2:M:475:VAL:HG23	2.19	0.42
2:M:44:ILE:O	2:M:48:PHE:HB2	2.19	0.42
2:M:742:VAL:HB	9:M:1733:HOH:O	2.17	0.42
3:N:957:PRO:CG	3:N:1007:VAL:HA	2.50	0.42
3:N:1108:ARG:HG2	9:N:9360:HOH:O	2.18	0.42
3:N:1124:GLN:HA	3:N:1125:PRO:HD3	1.51	0.42
3:N:1493:LYS:O	3:N:1496:GLU:HG2	2.20	0.42
3:N:171:LEU:HD13	3:N:389:GLU:O	2.19	0.42
2:M:1006:HIS:C	3:N:648:MET:HE2	2.40	0.42
3:N:850:LEU:O	3:N:853:VAL:HB	2.20	0.42
5:P:241:TRP:CZ3	5:P:245:GLN:HG2	2.54	0.42
1:B:86:VAL:HG12	1:B:124:ASN:HB2	2.01	0.42
2:C:1054:THR:HB	2:C:1055:LEU:H	1.57	0.42
2:C:207:LEU:HD13	2:C:221:LEU:CD1	2.50	0.42
2:C:571:LEU:HD13	2:C:669:GLY:H	1.84	0.42
2:C:837:ASP:O	2:C:848:VAL:HG13	2.20	0.42
2:C:929:ARG:HH11	2:C:929:ARG:HG3	1.84	0.42
3:D:1000:THR:HG23	3:D:1001:GLU:N	2.35	0.42
3:D:1139:ASP:CB	9:D:2265:HOH:O	2.62	0.42
3:D:895:VAL:O	3:D:899:LEU:HG	2.19	0.42
5:F:167:PRO:HB2	5:F:169:GLU:OE1	2.20	0.42
5:F:88:ILE:O	5:F:92:PRO:HG3	2.20	0.42
1:K:58:ILE:HD12	1:K:138:LEU:CD1	2.47	0.42
1:K:9:PRO:HB3	1:K:25:LEU:HG	2.01	0.42
1:L:69:PRO:HG3	9:L:7028:HOH:O	2.18	0.42
2:M:473:ARG:HG3	2:M:474:VAL:N	2.35	0.42
3:N:1485:GLN:HG2	3:N:1485:GLN:H	1.69	0.42
3:N:186:VAL:HG23	3:N:211:VAL:CG1	2.50	0.42
3:N:30:GLU:N	9:N:9441:HOH:O	2.52	0.42
3:N:36:THR:O	3:N:38:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:397:LYS:HD3	9:N:9346:HOH:O	2.18	0.42
3:N:610:LYS:C	3:N:611:GLN:HG2	2.39	0.42
3:N:78:VAL:HG12	3:N:78:VAL:O	2.20	0.42
3:N:937:TYR:HB3	3:N:941:PHE:CE1	2.55	0.42
3:N:955:VAL:HB	3:N:1011:PHE:CE1	2.53	0.42
4:O:26:ARG:HH11	4:O:29:GLN:CD	2.23	0.42
5:P:119:ILE:HD13	5:P:170:HIS:CG	2.54	0.42
2:C:1104:GLU:HB3	9:C:1420:HOH:O	2.18	0.42
2:C:165:LEU:HD12	2:C:166:PRO:CA	2.49	0.42
2:C:196:LEU:HB3	9:C:1668:HOH:O	2.19	0.42
2:C:221:LEU:HG	2:C:222:MET:N	2.35	0.42
2:C:358:ARG:HB3	2:C:371:LYS:O	2.19	0.42
2:C:492:ASP:HB3	2:C:518:LYS:CD	2.49	0.42
2:C:496:ILE:N	2:C:496:ILE:HD12	2.34	0.42
2:C:527:GLU:HG2	2:C:527:GLU:H	1.54	0.42
2:C:5:ARG:HG2	2:C:5:ARG:HH11	1.85	0.42
2:C:905:ILE:N	2:C:905:ILE:HD12	2.34	0.42
3:D:1045:MET:HA	3:D:1045:MET:CE	2.49	0.42
3:D:1103:HIS:N	9:D:9090:HOH:O	2.53	0.42
3:D:1129:THR:HB	9:D:9663:HOH:O	2.19	0.42
3:D:1164:ARG:HG3	3:D:1164:ARG:NH1	2.34	0.42
3:D:1209:LEU:CD2	3:D:1211:MET:HB3	2.49	0.42
3:D:1275:SER:HB3	3:D:1325:LEU:HD13	2.01	0.42
3:D:175:VAL:HG13	3:D:217:LYS:CB	2.50	0.42
3:D:520:LEU:CD2	3:D:540:LEU:HD22	2.50	0.42
5:F:136:LEU:HD12	5:F:137:GLY:N	2.35	0.42
3:D:601:ARG:NH1	5:F:328:PHE:HD1	2.18	0.42
1:K:5:LYS:HE3	9:L:6423:HOH:O	2.18	0.42
1:L:219:ARG:O	1:L:223:THR:HG23	2.18	0.42
2:M:1042:ALA:HB1	3:N:710:ARG:HD3	2.02	0.42
2:M:1100:GLN:HB2	2:M:1100:GLN:HE21	1.59	0.42
2:M:136:ILE:CG2	2:M:336:VAL:HG13	2.50	0.42
2:M:170:PRO:HG2	2:M:258:TYR:CD2	2.55	0.42
2:M:242:LEU:HD22	9:M:1173:HOH:O	2.19	0.42
2:M:291:ALA:O	2:M:299:LYS:HE2	2.19	0.42
2:M:771:GLU:HG3	9:M:1452:HOH:O	2.19	0.42
2:M:782:ALA:HB1	9:M:2039:HOH:O	2.19	0.42
2:M:816:LYS:HB2	2:M:819:VAL:HG21	2.01	0.42
2:M:958:THR:HG23	2:M:961:GLU:H	1.84	0.42
3:N:963:TYR:CE2	3:N:1002:LYS:HB3	2.55	0.42
3:N:1209:LEU:CD2	3:N:1210:SER:H	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1285:GLU:H	3:N:1285:GLU:CD	2.23	0.42
3:N:775:GLY:HA3	3:N:1145:TYR:CE1	2.54	0.42
3:N:809:PRO:HG2	9:N:9787:HOH:O	2.19	0.42
3:N:786:ILE:CD1	3:N:908:LYS:HB3	2.50	0.42
4:O:25:LYS:HG2	4:O:28:GLN:HE22	1.85	0.42
1:A:177:VAL:HG12	1:A:178:ALA:N	2.35	0.42
2:C:1014:SER:HB3	2:C:1017:THR:O	2.20	0.42
2:C:129:ILE:CG1	2:C:386:PHE:HB3	2.49	0.42
2:C:394:PHE:HE1	9:C:2065:HOH:O	2.02	0.42
2:C:420:ARG:HG2	2:C:422:ARG:HG2	2.02	0.42
2:C:443:THR:HA	2:C:444:PRO:HD3	1.72	0.42
2:C:462:ASP:CG	2:C:463:GLU:H	2.23	0.42
3:D:1107:VAL:O	3:D:1218:GLY:N	2.43	0.42
3:D:1112:CYS:HA	9:D:9558:HOH:O	2.20	0.42
3:D:122:GLU:HA	3:D:122:GLU:OE1	2.18	0.42
3:D:1489:GLN:OE1	3:D:1492:LEU:HD12	2.19	0.42
3:D:188:GLY:HA3	9:D:2377:HOH:O	2.19	0.42
3:D:169:TYR:HA	3:D:392:SER:HA	2.02	0.42
3:D:439:LEU:HD21	9:F:435:HOH:O	2.20	0.42
3:D:550:ARG:NH1	3:D:573:MET:HB3	2.35	0.42
3:D:684:LYS:HG3	9:D:9754:HOH:O	2.18	0.42
5:F:194:LEU:HD23	9:F:591:HOH:O	2.20	0.42
5:F:300:ASP:CG	5:F:301:ALA:N	2.73	0.42
5:F:363:GLU:HA	5:F:367:MET:HG2	2.02	0.42
1:L:147:GLY:N	1:L:171:PHE:CE1	2.87	0.42
2:M:244:PRO:CD	2:M:245:GLY:N	2.83	0.42
2:M:290:LEU:HB3	2:M:302:VAL:HG12	2.01	0.42
2:M:397:GLU:H	2:M:633:GLN:CD	2.23	0.42
2:M:419:THR:N	9:M:2102:HOH:O	2.52	0.42
2:M:409:ARG:HG3	2:M:454:SER:HB3	2.01	0.42
2:M:925:TYR:HE1	2:M:929:ARG:NH1	2.18	0.42
3:N:196:VAL:HG13	3:N:202:VAL:CG1	2.49	0.42
3:N:197:SER:CB	3:N:203:ALA:HB3	2.27	0.42
3:N:462:GLN:HA	3:N:513:ILE:CD1	2.49	0.42
3:N:93:ILE:CD1	3:N:548:ILE:HD11	2.49	0.42
4:O:86:GLN:HE21	4:O:86:GLN:HB3	1.72	0.42
5:P:157:GLU:HG2	9:P:3795:HOH:O	2.20	0.42
5:P:321:ILE:HG12	5:P:327:SER:O	2.20	0.42
5:P:94:LEU:HD23	5:P:96:LEU:H	1.85	0.42
1:A:180:GLN:HE21	1:A:180:GLN:HB3	1.61	0.42
1:A:96:THR:N	9:A:513:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:CD1	1:B:212:ASN:HD21	2.33	0.42
1:B:38:ASN:HD22	1:B:38:ASN:HA	1.62	0.42
1:B:48:ILE:HD13	1:B:210:ALA:HB1	2.01	0.42
2:C:127:PHE:HA	9:C:1619:HOH:O	2.19	0.42
2:C:199:VAL:HG13	2:C:235:LEU:CG	2.50	0.42
2:C:395:LYS:HE3	2:C:407:LYS:HE3	2.02	0.42
2:C:420:ARG:HG2	2:C:422:ARG:CG	2.50	0.42
2:C:447:ALA:O	2:C:449:ILE:N	2.53	0.42
2:C:611:ILE:HD11	2:C:641:PRO:CG	2.50	0.42
2:C:674:VAL:O	2:C:989:VAL:HA	2.19	0.42
2:C:31:GLN:HB3	2:C:71:TYR:OH	2.19	0.42
3:D:1059:SER:HB2	9:D:9027:HOH:O	2.20	0.42
3:D:1379:VAL:CG1	3:D:1395:LEU:HD23	2.48	0.42
3:D:178:LEU:CD2	3:D:199:LEU:H	2.32	0.42
3:D:249:TYR:HA	9:D:2084:HOH:O	2.18	0.42
3:D:30:GLU:HG3	3:D:41:ARG:HG2	2.00	0.42
3:D:395:VAL:HG12	9:D:9458:HOH:O	2.19	0.42
3:D:397:LYS:HE2	9:D:2321:HOH:O	2.20	0.42
3:D:66:GLN:O	3:D:69:GLU:HB3	2.20	0.42
3:D:792:ILE:O	3:D:878:GLY:HA3	2.20	0.42
4:E:37:ASN:HA	4:E:93:TYR:CE2	2.54	0.42
5:F:378:GLY:HA2	9:F:832:HOH:O	2.20	0.42
1:K:210:ALA:HA	1:K:213:GLN:HE21	1.83	0.42
1:L:101:LEU:HD21	1:L:113:ASP:HB3	2.00	0.42
1:L:211:LEU:O	1:L:214:ALA:HB3	2.19	0.42
1:L:73:GLU:HB3	1:L:77:GLU:HG3	2.02	0.42
2:M:1060:ILE:HG22	2:M:1061:GLU:H	1.83	0.42
2:M:157:ARG:NH1	2:M:157:ARG:HG2	2.33	0.42
2:M:48:PHE:HD1	9:M:1409:HOH:O	2.03	0.42
2:M:776:SER:HB3	9:M:1271:HOH:O	2.19	0.42
3:N:1156:LEU:HD11	3:N:1176:LYS:HD2	2.02	0.42
3:N:152:LEU:CD2	3:N:152:LEU:H	2.24	0.42
3:N:196:VAL:HG21	9:N:2241:HOH:O	2.19	0.42
3:N:441:ARG:HG3	9:N:2261:HOH:O	2.19	0.42
3:N:703:ASN:ND2	3:N:704:ARG:N	2.66	0.42
9:M:1524:HOH:O	5:P:340:SER:HB2	2.18	0.42
1:A:26:GLU:HG3	1:A:184:THR:HG21	2.02	0.42
2:C:191:PHE:CE2	2:C:196:LEU:HD12	2.55	0.42
2:C:56:GLU:HB3	9:C:1339:HOH:O	2.19	0.42
2:C:78:PHE:HB3	2:C:79:PRO:CD	2.50	0.42
2:C:838:LYS:HE2	2:C:997:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:LYS:HG3	2:C:813:VAL:HG12	2.02	0.42
3:D:1007:VAL:O	3:D:1010:ASN:HB3	2.20	0.42
3:D:34:TYR:N	3:D:34:TYR:HD2	2.18	0.42
3:D:565:ILE:HD12	3:D:565:ILE:N	2.35	0.42
3:D:658:LEU:HD11	3:D:674:ARG:HH11	1.85	0.42
2:C:1051:GLU:OE2	3:D:751:LEU:HB2	2.20	0.42
5:F:262:VAL:HG23	9:F:670:HOH:O	2.19	0.42
2:M:1109:VAL:HG12	2:M:1110:ASP:N	2.35	0.42
2:M:252:LYS:HB3	2:M:298:PHE:HZ	1.85	0.42
2:M:423:ALA:HB3	9:M:1712:HOH:O	2.18	0.42
3:N:1004:THR:HG22	9:N:9321:HOH:O	2.20	0.42
3:N:1065:LEU:HD11	3:N:1069:GLU:C	2.41	0.42
3:N:1065:LEU:HD11	3:N:1070:TYR:N	2.35	0.42
3:N:1084:THR:HG23	3:N:1087:ARG:NH1	2.35	0.42
3:N:1128:VAL:O	3:N:1129:THR:C	2.58	0.42
3:N:1305:LEU:HD22	3:N:1309:ALA:CB	2.50	0.42
3:N:1462:LEU:O	3:N:1466:VAL:HB	2.20	0.42
3:N:186:VAL:HG11	3:N:213:VAL:HB	2.02	0.42
3:N:759:ALA:HA	3:N:763:MET:HB3	2.02	0.42
3:N:81:THR:HG22	3:N:82:LYS:H	1.85	0.42
4:O:62:THR:HA	4:O:65:MET:CE	2.50	0.42
5:P:260:ILE:HG23	5:P:264:MET:CB	2.46	0.42
1:A:227:ASN:N	1:A:227:ASN:HD22	2.18	0.41
2:C:146:VAL:HG23	9:C:1227:HOH:O	2.19	0.41
2:C:198:ARG:CZ	2:C:203:ASP:HA	2.50	0.41
2:C:357:GLU:HB2	9:C:1268:HOH:O	2.20	0.41
2:C:129:ILE:HG12	2:C:386:PHE:HB3	2.02	0.41
2:C:428:ARG:HD3	2:C:450:GLY:N	2.31	0.41
2:C:864:GLY:O	2:C:866:PRO:HD3	2.19	0.41
2:C:99:GLN:HB2	9:C:1802:HOH:O	2.18	0.41
3:D:1004:THR:O	3:D:1007:VAL:HG22	2.21	0.41
3:D:1105:ILE:HD11	3:D:1374:GLN:CD	2.40	0.41
3:D:1196:THR:HG22	9:D:9004:HOH:O	2.20	0.41
3:D:131:LYS:HE3	5:F:83:GLN:NE2	2.34	0.41
3:D:1394:VAL:HB	3:D:1397:LYS:CD	2.48	0.41
3:D:1472:ILE:HG22	3:D:1474:ALA:O	2.20	0.41
3:D:28:LYS:O	3:D:43:GLY:HA2	2.20	0.41
3:D:527:MET:CE	5:F:258:ILE:HD11	2.50	0.41
3:D:29:PRO:CB	3:D:545:ARG:HG2	2.49	0.41
3:D:613:ARG:HA	3:D:613:ARG:HD3	1.78	0.41
3:D:868:TYR:HB3	3:D:873:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:113:ILE:HG23	5:F:127:ILE:CG2	2.49	0.41
1:K:140:MET:HG3	1:K:142:VAL:HG12	2.02	0.41
1:K:218:LEU:HG	1:L:222:LEU:HD11	2.02	0.41
1:K:79:ILE:HA	1:K:82:LEU:HD12	2.02	0.41
1:L:111:ALA:HB3	1:L:124:ASN:O	2.20	0.41
1:L:13:VAL:HG11	1:L:208:LEU:HD11	2.02	0.41
1:L:88:ARG:NH1	1:L:88:ARG:HG2	2.34	0.41
2:M:100:LEU:HD12	2:M:101:ILE:O	2.20	0.41
2:M:1103:ASP:HB3	2:M:1105:LYS:O	2.20	0.41
2:M:289:THR:O	2:M:291:ALA:N	2.53	0.41
2:M:393:GLN:HB2	2:M:393:GLN:HE21	1.69	0.41
2:M:503:LEU:HD13	2:M:507:ARG:O	2.20	0.41
2:M:497:ALA:HA	2:M:515:ALA:HA	2.01	0.41
2:M:626:ARG:HB2	2:M:626:ARG:HH11	1.84	0.41
2:M:783:ARG:HD3	9:M:1522:HOH:O	2.19	0.41
2:M:537:LYS:CG	2:M:905:ILE:HD11	2.50	0.41
3:N:1122:LEU:HD12	9:N:9340:HOH:O	2.19	0.41
3:N:112:ILE:O	3:N:116:LEU:HB2	2.20	0.41
3:N:1155:VAL:HG11	3:N:1177:ALA:CB	2.50	0.41
3:N:1165:TYR:HD1	9:N:2038:HOH:O	2.02	0.41
3:N:1236:LEU:HD11	3:N:1356:TYR:CE1	2.54	0.41
3:N:1269:LYS:HD3	3:N:1269:LYS:C	2.40	0.41
3:N:1389:LEU:HD12	3:N:1390:LEU:HD23	2.02	0.41
3:N:892:ASP:HB3	3:N:895:VAL:HG23	2.02	0.41
4:O:40:LEU:CD2	4:O:67:GLU:HA	2.49	0.41
4:O:45:ARG:HB2	4:O:46:PRO:HD2	2.01	0.41
5:P:417:LYS:HD3	9:P:5784:HOH:O	2.20	0.41
5:P:85:LEU:HD22	9:P:4990:HOH:O	2.20	0.41
1:B:117:VAL:HB	9:B:441:HOH:O	2.20	0.41
1:B:219:ARG:O	1:B:223:THR:HG23	2.20	0.41
1:B:68:ILE:HD12	1:B:71:VAL:HG21	2.02	0.41
1:B:75:VAL:O	1:B:79:ILE:HG23	2.19	0.41
2:C:140:ILE:HD12	2:C:140:ILE:N	2.35	0.41
2:C:244:PRO:HG2	2:C:246:ASP:CG	2.41	0.41
2:C:290:LEU:HB3	2:C:302:VAL:CG1	2.50	0.41
2:C:525:SER:OG	2:C:528:GLU:HG3	2.19	0.41
2:C:546:LEU:HB2	2:C:565:GLN:HE22	1.85	0.41
2:C:86:LYS:HG2	2:C:813:VAL:HG12	2.01	0.41
2:C:91:GLN:HA	2:C:119:PRO:HA	2.02	0.41
2:C:945:ARG:HG3	2:C:946:ARG:H	1.84	0.41
3:D:1041:LEU:HD12	3:D:1058:ARG:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1286:THR:HG21	9:D:9432:HOH:O	2.20	0.41
3:D:1101:VAL:HG12	3:D:1374:GLN:HB3	2.02	0.41
3:D:1463:LYS:HA	3:D:1463:LYS:HD3	1.97	0.41
3:D:490:ALA:HA	9:D:9772:HOH:O	2.20	0.41
3:D:591:VAL:CG1	3:D:597:ASP:HA	2.50	0.41
3:D:598:ARG:CG	3:D:598:ARG:HH11	2.28	0.41
3:D:729:HIS:ND1	3:D:731:LEU:N	2.66	0.41
5:F:122:LEU:HD21	9:F:541:HOH:O	2.19	0.41
2:M:205:GLU:OE1	2:M:206:THR:N	2.53	0.41
2:M:256:TYR:HA	9:M:2103:HOH:O	2.19	0.41
2:M:411:SER:CA	2:M:452:ILE:HG23	2.46	0.41
2:M:525:SER:OG	2:M:528:GLU:HG2	2.20	0.41
2:M:598:GLU:O	2:M:651:LYS:HG3	2.20	0.41
2:M:663:ASN:HD22	2:M:663:ASN:HA	1.53	0.41
2:M:717:LEU:HB2	2:M:761:PHE:HB2	2.01	0.41
2:M:690:ILE:HD12	2:M:833:LEU:HD23	2.02	0.41
2:M:557:ARG:NH1	2:M:879:ARG:HG2	2.35	0.41
3:N:1389:LEU:HD12	3:N:1390:LEU:H	1.84	0.41
3:N:704:ARG:CZ	3:N:737:ASN:O	2.69	0.41
3:N:73:CYS:HB3	3:N:76:CYS:O	2.20	0.41
3:N:74:GLU:HG3	9:N:9879:HOH:O	2.19	0.41
5:P:202:TYR:OH	5:P:244:ARG:HD2	2.19	0.41
5:P:293:GLU:HB3	9:P:4691:HOH:O	2.20	0.41
1:A:124:ASN:OD1	1:A:127:LEU:HB3	2.20	0.41
1:A:149:GLY:O	1:A:171:PHE:HB2	2.20	0.41
1:A:211:LEU:O	1:A:214:ALA:HB3	2.20	0.41
1:B:194:LYS:HZ2	1:B:194:LYS:HB2	1.84	0.41
1:B:24:VAL:HG13	1:B:196:THR:CG2	2.45	0.41
1:B:86:VAL:HG12	1:B:124:ASN:ND2	2.22	0.41
1:B:86:VAL:HG13	1:B:86:VAL:O	2.20	0.41
2:C:147:TYR:HD1	9:C:1799:HOH:O	2.01	0.41
2:C:163:ILE:HB	2:C:171:TRP:CZ2	2.56	0.41
2:C:36:PRO:HB2	2:C:70:GLU:OE2	2.20	0.41
2:C:584:GLU:H	2:C:584:GLU:CD	2.23	0.41
2:C:687:ALA:C	2:C:688:ILE:HD12	2.40	0.41
2:C:722:ILE:O	2:C:722:ILE:HD13	2.20	0.41
2:C:705:ILE:HA	2:C:827:VAL:O	2.20	0.41
2:C:831:ARG:NH1	9:C:2048:HOH:O	2.52	0.41
2:C:858:MET:SD	2:C:867:VAL:O	2.78	0.41
2:C:552:HIS:CD2	2:C:886:LEU:HD12	2.55	0.41
3:D:124:GLU:HG2	3:D:128:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:178:LEU:CD1	3:D:200:ASP:H	2.34	0.41
3:D:90:MET:HE1	3:D:518:PRO:HB3	2.02	0.41
3:D:633:VAL:HG22	3:D:635:PRO:CD	2.47	0.41
3:D:689:ASP:O	3:D:693:GLU:HB2	2.20	0.41
3:D:925:GLU:OE1	4:E:6:ILE:HG22	2.21	0.41
5:F:410:TYR:O	5:F:413:SER:HB2	2.19	0.41
5:F:74:LYS:HD3	5:F:74:LYS:HA	1.88	0.41
1:K:100:LEU:O	1:K:115:LEU:HG	2.20	0.41
1:K:58:ILE:HG21	1:K:68:ILE:CD1	2.50	0.41
1:L:26:GLU:CD	1:L:194:LYS:HE3	2.40	0.41
2:M:102:HIS:HB3	2:M:104:ASP:O	2.20	0.41
2:M:1083:GLU:O	2:M:1087:VAL:HB	2.20	0.41
2:M:1104:GLU:HA	3:N:6:ARG:HH11	1.86	0.41
2:M:1105:LYS:HB2	2:M:1107:ASN:HD22	1.85	0.41
2:M:22:GLN:O	2:M:121:MET:HE1	2.20	0.41
2:M:158:TYR:CE1	2:M:313:LEU:HG	2.55	0.41
2:M:601:GLY:HA3	2:M:615:TYR:HA	2.01	0.41
2:M:695:LEU:HD21	2:M:833:LEU:HB3	2.02	0.41
2:M:516:ARG:CZ	3:N:1068:LEU:HD22	2.49	0.41
3:N:1290:LEU:CD2	3:N:1291:SER:H	2.20	0.41
3:N:1397:LYS:NZ	3:N:1432:LYS:HB3	2.35	0.41
3:N:166:GLN:HG2	3:N:207:PHE:CG	2.55	0.41
2:M:1034:GLU:HB3	3:N:618:LEU:O	2.19	0.41
3:N:708:LEU:HD23	3:N:708:LEU:HA	1.85	0.41
4:O:45:ARG:HD2	4:O:47:LYS:CE	2.50	0.41
5:P:234:LYS:HD3	5:P:236:SER:HB3	2.02	0.41
1:B:99:LEU:HD12	1:B:114:PHE:CD2	2.54	0.41
2:C:277:ALA:HB1	9:C:1539:HOH:O	2.21	0.41
2:C:287:GLY:O	2:C:288:ARG:C	2.58	0.41
2:C:305:PRO:HG2	9:C:1198:HOH:O	2.19	0.41
2:C:45:GLN:HG2	9:C:2162:HOH:O	2.20	0.41
2:C:598:GLU:HG3	2:C:623:TYR:OH	2.21	0.41
2:C:666:LEU:CD2	2:C:668:LEU:HD11	2.49	0.41
2:C:878:SER:HA	9:D:9975:HOH:O	2.20	0.41
2:C:952:LEU:HD12	2:C:969:GLN:OE1	2.19	0.41
3:D:1042:ARG:O	3:D:1057:VAL:HB	2.20	0.41
3:D:1065:LEU:HD11	3:D:1070:TYR:N	2.35	0.41
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.20	0.41
3:D:1130:ARG:CB	3:D:1130:ARG:HH11	2.33	0.41
3:D:124:GLU:HG2	3:D:128:TYR:CE1	2.56	0.41
3:D:1363:LEU:HD12	3:D:1364:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:150:ARG:HH11	3:D:150:ARG:CG	2.30	0.41
3:D:187:LYS:HA	3:D:187:LYS:HD3	1.86	0.41
3:D:475:LYS:HA	3:D:478:LEU:HG	2.01	0.41
3:D:516:ALA:O	3:D:518:PRO:HD3	2.21	0.41
3:D:65:ARG:N	3:D:68:PHE:HZ	2.18	0.41
3:D:781:PRO:HG2	3:D:911:LEU:HD23	2.03	0.41
3:D:796:ARG:HA	3:D:797:LYS:HE2	2.02	0.41
3:D:799:LYS:HB3	3:D:826:PRO:HG2	2.03	0.41
2:C:1115:LEU:CG	3:D:85:VAL:HG13	2.50	0.41
2:C:889:HIS:CE1	3:D:951:ILE:H	2.36	0.41
4:E:70:THR:HG22	4:E:71:GLY:N	2.35	0.41
5:F:134:LYS:NZ	9:F:799:HOH:O	2.53	0.41
5:F:208:SER:HB3	9:F:450:HOH:O	2.19	0.41
5:F:396:ARG:NH1	9:F:512:HOH:O	2.53	0.41
1:K:18:ARG:HH11	1:K:123:MET:CE	2.33	0.41
1:K:181:VAL:HG11	1:K:193:ASP:OD2	2.20	0.41
1:L:18:ARG:O	1:L:207:PRO:HD3	2.20	0.41
1:L:62:LEU:HD12	1:L:62:LEU:N	2.35	0.41
2:M:352:ALA:O	2:M:355:VAL:HG12	2.20	0.41
2:M:654:LEU:HD21	2:M:657:ASP:OD2	2.21	0.41
2:M:748:GLU:CA	2:M:799:ILE:HG22	2.50	0.41
2:M:86:LYS:CE	2:M:813:VAL:HG12	2.51	0.41
2:M:691:SER:CB	2:M:858:MET:SD	3.09	0.41
2:M:890:LEU:HA	2:M:914:ILE:HD13	2.01	0.41
3:N:1047:LYS:HB3	3:N:1048:PRO:HD2	2.01	0.41
2:M:516:ARG:NH1	3:N:1068:LEU:HD22	2.36	0.41
3:N:1048:PRO:O	3:N:1079:LYS:HE2	2.20	0.41
3:N:115:LEU:HD22	3:N:502:PHE:CE1	2.55	0.41
3:N:119:SER:H	3:N:123:LEU:CB	2.30	0.41
3:N:1290:LEU:HD11	3:N:1311:LEU:HD22	2.02	0.41
3:N:1476:THR:C	3:N:1478:SER:H	2.24	0.41
3:N:450:TYR:HD1	3:N:450:TYR:HA	1.67	0.41
3:N:502:PHE:CZ	3:N:509:PRO:HB3	2.55	0.41
3:N:462:GLN:CA	3:N:513:ILE:HD13	2.49	0.41
3:N:525:ARG:N	3:N:526:PRO:HD3	2.35	0.41
3:N:674:ARG:HB3	9:N:2271:HOH:O	2.20	0.41
3:N:679:ARG:HH21	3:N:681:ARG:HE	1.68	0.41
3:N:717:GLN:N	3:N:717:GLN:HE21	2.18	0.41
4:O:41:GLU:HB3	9:O:5925:HOH:O	2.19	0.41
5:P:392:VAL:CG1	5:P:396:ARG:HG3	2.50	0.41
1:A:111:ALA:HB3	1:A:124:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:MET:O	1:B:125:PRO:HD3	2.20	0.41
2:C:1036:GLU:O	2:C:1039:ALA:HB3	2.20	0.41
2:C:1060:ILE:HD12	2:C:1063:ARG:CZ	2.50	0.41
2:C:129:ILE:N	9:C:1435:HOH:O	2.54	0.41
2:C:129:ILE:HG22	2:C:130:ASN:N	2.34	0.41
2:C:456:ALA:HB1	2:C:538:GLN:O	2.20	0.41
2:C:591:SER:HB2	9:C:2055:HOH:O	2.20	0.41
2:C:611:ILE:HD13	2:C:625:LEU:HD11	2.02	0.41
2:C:911:GLU:O	2:C:914:ILE:HG22	2.21	0.41
2:C:9:ILE:HG12	2:C:907:ASP:OD2	2.21	0.41
3:D:1217:ILE:HD12	3:D:1480:PHE:CE2	2.53	0.41
3:D:1236:LEU:HD11	3:D:1356:TYR:CE1	2.56	0.41
3:D:209:ARG:HB2	3:D:395:VAL:O	2.20	0.41
3:D:553:ARG:HD2	3:D:570:GLU:OE2	2.20	0.41
3:D:661:MET:HA	3:D:666:ILE:HD12	2.02	0.41
3:D:6:ARG:HH11	3:D:6:ARG:HB2	1.85	0.41
3:D:793:THR:O	3:D:879:ARG:NH1	2.50	0.41
3:D:806:PHE:O	3:D:806:PHE:CG	2.72	0.41
3:D:811:GLU:HG3	9:D:9257:HOH:O	2.20	0.41
3:D:852:ALA:HB1	3:D:857:ILE:HB	2.02	0.41
4:E:15:SER:O	4:E:18:ARG:HB3	2.21	0.41
1:K:119:ASP:HA	9:K:4192:HOH:O	2.20	0.41
1:K:2:LEU:O	1:K:6:LEU:HB3	2.21	0.41
2:M:1016:ILE:HG23	3:N:526:PRO:HG2	2.03	0.41
2:M:1081:VAL:HA	9:N:9064:HOH:O	2.20	0.41
2:M:442:GLU:HB3	2:M:453:THR:OG1	2.20	0.41
2:M:575:GLN:OE1	2:M:670:GLN:HB3	2.21	0.41
2:M:577:PRO:HA	2:M:993:PHE:CD2	2.55	0.41
3:N:1346:ARG:HG2	9:N:2202:HOH:O	2.19	0.41
3:N:1346:ARG:HB2	3:N:1346:ARG:NH1	2.36	0.41
3:N:1478:SER:O	3:N:1482:ARG:HG3	2.20	0.41
3:N:172:PRO:HA	3:N:173:PRO:HD3	1.64	0.41
3:N:399:ARG:HH21	3:N:432:TYR:HE2	1.66	0.41
3:N:413:ASP:OD1	3:N:419:ASP:HA	2.21	0.41
3:N:484:PRO:O	3:N:489:ARG:HD2	2.20	0.41
3:N:502:PHE:CZ	3:N:1452:ILE:HG13	2.55	0.41
3:N:639:LEU:HD21	3:N:931:LEU:HD13	2.02	0.41
5:P:108:GLU:OE1	5:P:108:GLU:HA	2.19	0.41
5:P:113:ILE:HG23	5:P:127:ILE:HG22	2.03	0.41
5:P:328:PHE:HA	5:P:328:PHE:HD2	1.73	0.41
5:P:338:LEU:HA	5:P:339:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:O	1:A:215:VAL:HG13	2.20	0.41
1:B:173:PRO:HB2	1:B:205:VAL:HG22	2.03	0.41
1:B:72:LYS:HE2	1:B:131:THR:OG1	2.20	0.41
2:C:1012:PRO:HD3	2:C:1026:GLN:HG2	2.03	0.41
2:C:1098:ASP:HB2	3:D:21:TRP:CZ2	2.45	0.41
2:C:19:THR:HG22	2:C:19:THR:O	2.21	0.41
2:C:43:GLY:O	2:C:46:ALA:HB3	2.21	0.41
2:C:460:ARG:HD2	2:C:485:TYR:CE2	2.56	0.41
2:C:860:HIS:CE1	2:C:975:TYR:HB2	2.56	0.41
3:D:1164:ARG:HH11	3:D:1164:ARG:HG3	1.85	0.41
3:D:1168:MET:HE3	3:D:1171:VAL:HB	2.02	0.41
3:D:1310:ARG:HG3	3:D:1327:ARG:CZ	2.51	0.41
3:D:1356:TYR:N	3:D:1356:TYR:CD1	2.88	0.41
3:D:1447:LEU:O	3:D:1448:THR:C	2.59	0.41
3:D:1498:ALA:HB2	4:E:88:GLU:OE1	2.21	0.41
3:D:197:SER:HB2	3:D:205:TYR:CZ	2.56	0.41
3:D:212:ARG:NH2	9:D:2090:HOH:O	2.54	0.41
3:D:127:LEU:HD21	3:D:461:ILE:CD1	2.47	0.41
3:D:65:ARG:N	3:D:68:PHE:CZ	2.87	0.41
3:D:838:ARG:HH11	3:D:874:GLU:CB	2.30	0.41
1:L:212:ASN:HA	1:L:212:ASN:HD22	1.70	0.41
2:M:158:TYR:CD1	2:M:313:LEU:HD21	2.55	0.41
2:M:203:ASP:HB2	9:M:1152:HOH:O	2.20	0.41
2:M:254:VAL:HA	2:M:257:VAL:HG23	2.02	0.41
2:M:302:VAL:C	2:M:305:PRO:HD2	2.41	0.41
2:M:31:GLN:HB2	9:M:2110:HOH:O	2.20	0.41
2:M:425:PHE:HA	9:M:1180:HOH:O	2.18	0.41
2:M:580:MET:SD	2:M:584:GLU:HG3	2.60	0.41
2:M:615:TYR:HB2	2:M:617:ASP:OD1	2.20	0.41
2:M:677:MET:HG2	2:M:987:ILE:HG21	2.02	0.41
3:N:1276:GLU:HG3	3:N:1303:TYR:OH	2.20	0.41
3:N:1341:PRO:O	3:N:1344:VAL:N	2.54	0.41
3:N:43:GLY:HA2	9:N:9381:HOH:O	2.20	0.41
3:N:584:ASN:HB3	9:N:9185:HOH:O	2.19	0.41
3:N:702:LEU:HD23	3:N:745:MET:CE	2.50	0.41
3:N:789:LEU:O	3:N:792:ILE:HG23	2.21	0.41
3:N:799:LYS:N	9:N:9025:HOH:O	2.53	0.41
3:N:806:PHE:O	3:N:807:ALA:C	2.58	0.41
1:L:150:TYR:HE2	3:N:857:ILE:HG13	1.85	0.41
3:N:853:VAL:CG2	3:N:858:VAL:HG23	2.51	0.41
4:O:54:LEU:HD23	4:O:58:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:151:LEU:HB3	5:P:155:THR:H	1.86	0.41
5:P:209:PHE:O	5:P:213:ILE:HG13	2.20	0.41
3:N:573:MET:SD	5:P:210:LEU:HD22	2.61	0.41
5:P:306:GLU:O	5:P:310:ILE:HG13	2.21	0.41
1:A:101:LEU:HB2	1:A:114:PHE:CD2	2.56	0.41
1:B:67:THR:HB	1:B:74:ASP:OD1	2.20	0.41
2:C:1098:ASP:OD1	2:C:1098:ASP:C	2.58	0.41
2:C:189:ARG:HD2	9:C:1870:HOH:O	2.19	0.41
2:C:569:VAL:HG23	2:C:635:THR:HG22	2.02	0.41
2:C:640:ARG:CB	2:C:642:ARG:HH12	2.33	0.41
2:C:70:GLU:O	2:C:97:ARG:HG3	2.20	0.41
2:C:861:LEU:HD23	2:C:862:PRO:N	2.35	0.41
2:C:874:LEU:O	3:D:1029:ARG:HD2	2.20	0.41
2:C:882:LEU:HD12	3:D:1038:LEU:HD22	2.03	0.41
2:C:78:PHE:CB	2:C:88:LEU:HD21	2.50	0.41
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	2.02	0.41
3:D:1303:TYR:HD1	3:D:1325:LEU:HD22	1.85	0.41
3:D:1258:ARG:HH21	3:D:1351:GLU:CG	2.34	0.41
3:D:1353:GLN:HE21	3:D:1353:GLN:HB3	1.49	0.41
5:F:85:LEU:HD22	5:F:193:ARG:HD3	2.02	0.41
5:F:253:ASP:HA	5:F:259:ARG:NH1	2.35	0.41
1:L:2:LEU:HD12	1:L:3:ASP:H	1.84	0.41
2:M:1007:ALA:HB2	3:N:648:MET:CE	2.50	0.41
2:M:176:VAL:HB	9:M:1185:HOH:O	2.20	0.41
2:M:352:ALA:C	2:M:355:VAL:HG12	2.41	0.41
2:M:59:LYS:HD2	9:M:1438:HOH:O	2.19	0.41
2:M:803:THR:N	9:M:1993:HOH:O	2.53	0.41
2:M:930:LYS:HA	9:M:1237:HOH:O	2.20	0.41
3:N:1299:PHE:HD2	9:N:9049:HOH:O	2.03	0.41
3:N:1311:LEU:HD12	3:N:1313:VAL:O	2.19	0.41
3:N:1462:LEU:CD2	3:N:1473:PRO:HD2	2.51	0.41
3:N:1489:GLN:HB3	9:N:9105:HOH:O	2.20	0.41
3:N:219:GLU:CB	9:N:9640:HOH:O	2.69	0.41
3:N:535:PHE:N	9:P:6169:HOH:O	2.52	0.41
3:N:568:ARG:O	3:N:569:ASN:C	2.59	0.41
3:N:852:ALA:HB1	3:N:857:ILE:HB	2.03	0.41
3:N:882:PHE:CE1	3:N:906:GLN:HG3	2.56	0.41
4:O:72:ARG:NH2	9:O:5523:HOH:O	2.54	0.41
4:O:8:LYS:NZ	9:O:6477:HOH:O	2.52	0.41
5:P:140:ARG:O	5:P:144:ILE:HG13	2.21	0.41
5:P:171:LYS:HG3	5:P:175:HIS:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:370:LYS:HB3	5:P:370:LYS:NZ	2.36	0.41
1:A:151:VAL:HB	1:A:169:ALA:HB3	2.02	0.41
2:C:1083:GLU:O	2:C:1087:VAL:HB	2.21	0.41
2:C:8:ARG:HH11	2:C:10:ARG:HH21	1.67	0.41
2:C:280:LYS:HG2	9:C:1148:HOH:O	2.21	0.41
2:C:66:LEU:CD2	2:C:372:LEU:HD23	2.41	0.41
2:C:811:PRO:HD2	2:C:813:VAL:HG13	2.02	0.41
2:C:831:ARG:HA	9:C:1793:HOH:O	2.20	0.41
3:D:501:ALA:HB1	3:D:1453:ALA:CB	2.51	0.41
3:D:1491:THR:HG22	3:D:1491:THR:O	2.21	0.41
3:D:629:SER:CA	9:D:9834:HOH:O	2.68	0.41
3:D:83:SER:HA	9:D:9087:HOH:O	2.20	0.41
9:C:1126:HOH:O	3:D:943:THR:HG21	2.20	0.41
3:D:982:PHE:CD1	3:D:982:PHE:N	2.88	0.41
4:E:51:LEU:HB3	9:E:196:HOH:O	2.20	0.41
5:F:163:LEU:HD13	5:F:174:LEU:HD21	2.03	0.41
5:F:256:ARG:NH2	5:F:310:ILE:O	2.53	0.41
5:F:423:ASP:HB2	9:F:809:HOH:O	2.20	0.41
1:K:215:VAL:HG12	1:L:222:LEU:HD22	2.03	0.41
1:K:88:ARG:HB3	9:K:4125:HOH:O	2.19	0.41
1:L:56:VAL:HG13	9:L:3859:HOH:O	2.20	0.41
2:M:305:PRO:CB	2:M:308:ARG:HH21	2.33	0.41
2:M:30:LEU:HD12	2:M:30:LEU:O	2.20	0.41
2:M:713:ARG:HB2	9:M:1832:HOH:O	2.19	0.41
2:M:897:LEU:CD2	2:M:920:GLN:HE21	2.27	0.41
2:M:999:HIS:HD2	9:M:1959:HOH:O	2.03	0.41
3:N:1004:THR:HG21	9:N:9020:HOH:O	2.21	0.41
3:N:1195:GLN:HG3	9:N:2044:HOH:O	2.21	0.41
3:N:1328:GLY:HA3	9:N:9396:HOH:O	2.20	0.41
3:N:178:LEU:HA	3:N:181:ASP:OD2	2.21	0.41
3:N:39:PRO:HD2	9:N:9418:HOH:O	2.19	0.41
3:N:448:GLU:HG2	9:N:9364:HOH:O	2.19	0.41
3:N:570:GLU:OE2	5:P:214:GLN:HG3	2.21	0.41
3:N:601:ARG:HG2	3:N:606:ILE:HD13	2.01	0.41
3:N:60:CYS:HB2	9:N:9577:HOH:O	2.21	0.41
2:M:1044:GLY:N	3:N:762:GLN:OE1	2.53	0.41
3:N:893:GLU:O	3:N:896:ALA:HB3	2.21	0.41
4:O:26:ARG:CZ	4:O:73:LEU:HD21	2.50	0.41
5:P:218:GLN:HB3	9:P:6496:HOH:O	2.19	0.41
5:P:278:LEU:O	5:P:282:LEU:HD12	2.21	0.41
1:B:164:ALA:HB3	9:B:393:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ASN:O	1:B:84:GLU:HB3	2.20	0.41
2:C:1094:ALA:HB1	3:D:603:LEU:HD13	2.02	0.41
2:C:186:VAL:HG23	2:C:187:ASN:N	2.27	0.41
2:C:267:TYR:HB2	2:C:272:ALA:HB1	2.03	0.41
2:C:438:ILE:HD11	2:C:467:ILE:HD12	2.02	0.41
2:C:474:VAL:HG13	2:C:530:GLU:O	2.21	0.41
2:C:586:ARG:HG2	9:C:1254:HOH:O	2.21	0.41
2:C:607:ASP:HB3	2:C:609:ASN:H	1.84	0.41
2:C:708:TYR:N	2:C:708:TYR:CD1	2.87	0.41
2:C:769:PRO:HG3	9:F:775:HOH:O	2.20	0.41
2:C:834:GLN:HE21	2:C:834:GLN:HB2	1.66	0.41
3:D:1231:GLU:HG2	3:D:1232:PRO:N	2.35	0.41
3:D:1380:GLU:HB2	3:D:1420:LEU:HD23	2.03	0.41
3:D:159:ARG:NH1	3:D:159:ARG:HB2	2.35	0.41
3:D:661:MET:HE1	3:D:677:LEU:CD1	2.37	0.41
3:D:74:GLU:HB3	9:D:9568:HOH:O	2.21	0.41
5:F:123:ASP:H	5:F:126:LEU:HD22	1.85	0.41
5:F:117:SER:CB	5:F:124:PRO:HG3	2.51	0.41
5:F:385:GLU:HA	9:F:553:HOH:O	2.21	0.41
1:L:2:LEU:HD13	1:L:3:ASP:CG	2.40	0.41
2:M:1008:ARG:NH1	2:M:1020:PRO:HB3	2.35	0.41
2:M:1075:ASP:OD1	3:N:753:SER:HB2	2.21	0.41
2:M:200:LEU:HD13	2:M:300:ASP:OD2	2.19	0.41
2:M:139:GLN:HB3	2:M:334:ARG:HD3	2.03	0.41
2:M:441:VAL:O	2:M:559:LEU:HD12	2.20	0.41
2:M:578:VAL:HG22	2:M:671:ASN:HD21	1.86	0.41
2:M:83:CYS:SG	2:M:88:LEU:HD23	2.61	0.41
3:N:1263:PHE:CE2	3:N:1371:VAL:HG11	2.56	0.41
3:N:1278:ASP:HA	3:N:1319:VAL:O	2.21	0.41
3:N:129:PHE:HB3	3:N:587:ARG:NH2	2.36	0.41
3:N:1398:TRP:HZ3	3:N:1401:GLU:OE2	2.04	0.41
3:N:1425:THR:CG2	3:N:1426:LYS:N	2.83	0.41
3:N:133:ILE:HD12	3:N:454:ALA:HB1	2.02	0.41
3:N:462:GLN:CB	3:N:513:ILE:HD13	2.51	0.41
3:N:482:LYS:HG2	9:N:9544:HOH:O	2.21	0.41
3:N:676:MET:HG3	9:N:9565:HOH:O	2.20	0.41
3:N:924:MET:N	4:O:7:ASP:OD2	2.54	0.41
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.55	0.41
4:O:72:ARG:HG2	4:O:72:ARG:HH11	1.85	0.41
1:A:127:LEU:HD11	1:A:129:ILE:HD13	2.03	0.41
2:C:1036:GLU:HG2	3:D:703:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1045:ALA:HB1	2:C:1048:THR:HB	2.03	0.41
2:C:1109:VAL:HG23	3:D:3:LYS:CG	2.43	0.41
2:C:212:GLY:O	2:C:215:GLY:O	2.38	0.41
2:C:437:ARG:C	2:C:438:ILE:HD12	2.42	0.41
2:C:854:PRO:C	2:C:856:GLU:N	2.74	0.41
2:C:943:VAL:HG11	2:C:973:VAL:CG2	2.51	0.41
3:D:1124:GLN:HA	3:D:1125:PRO:HD3	1.72	0.41
3:D:122:GLU:O	3:D:126:VAL:HG23	2.21	0.41
3:D:1503:VAL:HA	9:D:2114:HOH:O	2.21	0.41
3:D:179:VAL:HG13	3:D:389:GLU:HG3	2.03	0.41
3:D:465:LEU:CD1	3:D:513:ILE:HD11	2.51	0.41
3:D:115:LEU:HD22	3:D:502:PHE:HE1	1.86	0.41
3:D:517:VAL:N	9:D:9427:HOH:O	2.53	0.41
3:D:824:ASN:HD22	3:D:824:ASN:HA	1.63	0.41
3:D:838:ARG:HE	3:D:838:ARG:HB2	1.62	0.41
3:D:844:ALA:O	3:D:867:ARG:HD2	2.20	0.41
3:D:989:TYR:CE2	3:D:993:LEU:HD11	2.55	0.41
4:E:54:LEU:HG	4:E:58:PRO:HD2	2.03	0.41
5:F:291:ILE:HG23	5:F:292:ALA:N	2.36	0.41
1:K:37:GLY:HA3	1:K:179:PHE:CD1	2.56	0.41
2:M:164:PRO:HG2	9:M:1133:HOH:O	2.21	0.41
2:M:264:PRO:HD2	9:M:1477:HOH:O	2.19	0.41
2:M:400:PRO:O	2:M:401:LEU:C	2.59	0.41
2:M:537:LYS:CB	2:M:545:ASN:HD21	2.33	0.41
2:M:565:GLN:HG2	2:M:995:MET:HE1	2.02	0.41
2:M:626:ARG:CB	2:M:626:ARG:HH11	2.34	0.41
2:M:771:GLU:O	2:M:775:ARG:HG2	2.21	0.41
2:M:816:LYS:O	2:M:819:VAL:HB	2.21	0.41
2:M:9:ILE:HG12	2:M:907:ASP:OD2	2.21	0.41
2:M:943:VAL:HG11	2:M:973:VAL:CG2	2.51	0.41
3:N:1012:GLU:HG3	9:N:9072:HOH:O	2.21	0.41
9:M:1261:HOH:O	3:N:1079:LYS:HG3	2.21	0.41
3:N:116:LEU:HB3	3:N:118:LEU:HG	2.03	0.41
3:N:1237:THR:HG22	3:N:1238:MET:N	2.35	0.41
3:N:1290:LEU:HD23	3:N:1291:SER:N	2.22	0.41
3:N:44:LEU:HB3	3:N:525:ARG:NH2	2.36	0.41
3:N:462:GLN:CG	3:N:513:ILE:HD13	2.50	0.41
3:N:93:ILE:HD13	3:N:548:ILE:HD11	2.03	0.41
3:N:780:LYS:HD2	9:N:9812:HOH:O	2.20	0.41
3:N:89:ARG:O	3:N:521:PRO:HG3	2.20	0.41
3:N:924:MET:HB2	4:O:7:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:566:ILE:CG1	5:P:217:ASN:HD22	2.34	0.41
1:A:76:VAL:HA	1:A:79:ILE:CG1	2.50	0.41
1:B:13:VAL:HG12	1:B:14:ARG:N	2.35	0.41
2:C:1067:TYR:CE2	5:F:345:ALA:HB2	2.56	0.41
2:C:269:LEU:HD11	9:C:1386:HOH:O	2.19	0.41
2:C:302:VAL:C	2:C:305:PRO:HD2	2.42	0.41
2:C:328:LEU:C	2:C:330:ASN:H	2.24	0.41
2:C:358:ARG:HH12	2:C:374:ASN:CB	2.34	0.41
2:C:515:ALA:C	2:C:516:ARG:HG2	2.42	0.41
2:C:777:ILE:HG22	2:C:778:PHE:CD1	2.56	0.41
3:D:1045:MET:O	3:D:1053:PHE:HD1	2.03	0.41
3:D:1167:SER:O	3:D:1171:VAL:HG23	2.21	0.41
3:D:126:VAL:O	3:D:132:TYR:CD1	2.73	0.41
3:D:1326:THR:CA	9:D:9040:HOH:O	2.69	0.41
3:D:1420:LEU:HD13	3:D:1421:LEU:N	2.36	0.41
3:D:1483:PHE:CD1	3:D:1483:PHE:N	2.87	0.41
3:D:47:GLU:OE1	3:D:53:ILE:HG22	2.21	0.41
3:D:93:ILE:HG22	3:D:551:ASN:ND2	2.36	0.41
3:D:95:LEU:CD2	3:D:574:LEU:HD11	2.51	0.41
3:D:658:LEU:O	3:D:661:MET:HB2	2.21	0.41
3:D:696:HIS:HB3	9:D:9044:HOH:O	2.21	0.41
5:F:123:ASP:HB3	5:F:125:ASP:OD1	2.21	0.41
1:K:98:THR:N	9:K:3519:HOH:O	2.54	0.41
1:L:143:ARG:HH11	1:L:158:ILE:CG2	2.32	0.41
2:M:1065:ALA:HB3	2:M:1077:PRO:HG2	2.02	0.41
2:M:1101:THR:HB	3:N:5:VAL:HG13	2.01	0.41
2:M:141:HIS:O	2:M:332:ARG:N	2.40	0.41
2:M:321:GLU:HG3	9:M:1256:HOH:O	2.22	0.41
2:M:546:LEU:HA	2:M:581:THR:OG1	2.20	0.41
2:M:544:THR:O	2:M:547:ILE:HG13	2.20	0.41
2:M:571:LEU:CD2	2:M:669:GLY:HA2	2.50	0.41
2:M:571:LEU:HD12	2:M:701:THR:N	2.36	0.41
3:N:1066:THR:HG22	3:N:1069:GLU:CG	2.50	0.41
3:N:1112:CYS:HB2	3:N:1195:GLN:NE2	2.36	0.41
3:N:1465:ASN:OD1	3:N:1473:PRO:HG3	2.21	0.41
3:N:196:VAL:HG13	3:N:202:VAL:HG11	2.02	0.41
3:N:177:ALA:HB1	3:N:199:LEU:HD22	2.03	0.41
3:N:214:GLU:HB3	9:N:9687:HOH:O	2.21	0.41
3:N:408:GLU:H	3:N:408:GLU:HG3	1.59	0.41
3:N:430:ASP:HB2	3:N:432:TYR:CZ	2.56	0.41
3:N:827:ILE:HG23	3:N:837:GLY:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:881:LEU:HD21	3:N:941:PHE:CZ	2.56	0.41
5:P:79:ASP:HB3	5:P:80:PRO:HD2	2.03	0.41
3:N:572:ARG:HH11	5:P:80:PRO:HD3	1.83	0.41
1:A:206:THR:HG23	1:A:209:GLU:H	1.84	0.40
1:A:42:ARG:HG2	1:A:42:ARG:NH1	2.35	0.40
1:B:59:GLU:HG3	1:B:139:ASN:ND2	2.35	0.40
2:C:193:LEU:HD23	2:C:307:LEU:CD1	2.51	0.40
2:C:504:GLU:HG2	2:C:507:ARG:HB2	2.02	0.40
2:C:603:VAL:O	2:C:646:GLY:HA2	2.21	0.40
2:C:669:GLY:C	2:C:670:GLN:HG2	2.41	0.40
2:C:671:ASN:H	2:C:671:ASN:ND2	2.16	0.40
2:C:793:PRO:O	2:C:794:PRO:C	2.60	0.40
2:C:863:ASP:OD1	2:C:865:THR:HG22	2.22	0.40
3:D:1061:PHE:CE1	3:D:1065:LEU:HD23	2.53	0.40
3:D:1197:ARG:CG	3:D:1198:TYR:H	2.35	0.40
3:D:174:GLY:HA3	9:D:9151:HOH:O	2.21	0.40
3:D:17:LYS:HA	9:D:9899:HOH:O	2.21	0.40
3:D:28:LYS:HD2	3:D:552:ASN:HD21	1.86	0.40
3:D:475:LYS:HG3	9:D:9720:HOH:O	2.21	0.40
3:D:55:ASP:HA	3:D:82:LYS:CG	2.45	0.40
3:D:584:ASN:HB3	9:D:9910:HOH:O	2.20	0.40
3:D:68:PHE:HA	3:D:71:LYS:NZ	2.36	0.40
3:D:764:LEU:HG	3:D:765:SER:N	2.36	0.40
3:D:786:ILE:HD13	3:D:908:LYS:HB3	2.02	0.40
5:F:119:ILE:HA	9:F:584:HOH:O	2.20	0.40
5:F:79:ASP:HB3	5:F:80:PRO:HD3	2.04	0.40
1:K:34:VAL:HB	1:L:42:ARG:HH21	1.85	0.40
1:K:94:LEU:HD21	1:K:119:ASP:HB2	2.03	0.40
2:M:144:PRO:HA	2:M:163:ILE:HD11	2.02	0.40
2:M:253:ALA:N	9:M:2036:HOH:O	2.51	0.40
2:M:352:ALA:CA	2:M:355:VAL:HG12	2.50	0.40
2:M:430:VAL:HG13	2:M:430:VAL:O	2.21	0.40
2:M:462:ASP:HB3	2:M:468:ARG:CD	2.47	0.40
2:M:564:MET:SD	2:M:846:LYS:HD2	2.60	0.40
2:M:897:LEU:CD1	2:M:921:ALA:HA	2.51	0.40
2:M:676:ILE:HG22	2:M:988:VAL:HG22	2.03	0.40
3:N:1000:THR:HB	9:N:9990:HOH:O	2.20	0.40
3:N:1209:LEU:HD23	3:N:1210:SER:N	2.29	0.40
3:N:1301:LYS:HD2	3:N:1301:LYS:HA	1.79	0.40
3:N:470:LEU:HD11	3:N:509:PRO:HG3	2.04	0.40
3:N:742:GLY:HA3	9:N:9339:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:87:ARG:CB	3:N:523:ASP:HB2	2.51	0.40
5:P:225:GLU:OE1	5:P:226:LYS:HE2	2.21	0.40
1:A:117:VAL:HB	1:A:120:VAL:CG1	2.50	0.40
1:B:10:VAL:HG11	9:B:492:HOH:O	2.20	0.40
2:C:1085:PHE:HE1	2:C:1111:ILE:HG21	1.86	0.40
2:C:169:GLY:HA3	9:C:1751:HOH:O	2.20	0.40
2:C:243:ARG:HB3	9:C:1299:HOH:O	2.22	0.40
2:C:244:PRO:HD2	2:C:245:GLY:N	2.24	0.40
2:C:47:ALA:O	2:C:50:GLU:HB3	2.21	0.40
2:C:691:SER:HB3	2:C:868:ASP:HA	2.04	0.40
2:C:707:ARG:HD2	9:C:1247:HOH:O	2.20	0.40
2:C:8:ARG:HB3	9:C:2005:HOH:O	2.20	0.40
2:C:8:ARG:N	9:C:1239:HOH:O	2.55	0.40
3:D:1147:ARG:HD2	3:D:1188:VAL:CG2	2.51	0.40
3:D:1306:PRO:HG3	9:D:9022:HOH:O	2.20	0.40
3:D:1420:LEU:HD13	3:D:1421:LEU:H	1.85	0.40
3:D:177:ALA:HB1	3:D:199:LEU:HB3	2.04	0.40
2:C:1093:GLN:HB3	3:D:21:TRP:CZ3	2.56	0.40
3:D:601:ARG:NH1	5:F:328:PHE:CD1	2.89	0.40
3:D:814:ALA:HB3	9:D:9257:HOH:O	2.21	0.40
3:D:799:LYS:N	3:D:826:PRO:HG2	2.35	0.40
3:D:860:LEU:HD22	3:D:878:GLY:HA2	2.02	0.40
5:F:109:GLY:O	5:F:113:ILE:HG13	2.21	0.40
5:F:273:ARG:O	5:F:276:ARG:HB2	2.21	0.40
1:K:23:PHE:CD1	1:K:211:LEU:HD23	2.57	0.40
1:K:91:ASN:CG	1:K:92:PRO:HD2	2.42	0.40
2:M:1060:ILE:HG22	2:M:1061:GLU:N	2.36	0.40
2:M:305:PRO:HB3	2:M:308:ARG:NH2	2.36	0.40
2:M:51:THR:HB	2:M:348:LEU:HD23	2.03	0.40
2:M:682:TYR:HB3	2:M:689:VAL:HG22	2.02	0.40
3:N:27:GLU:O	3:N:28:LYS:HD3	2.21	0.40
3:N:950:GLY:C	3:N:953:ASP:H	2.22	0.40
5:P:235:PHE:HB2	9:P:4703:HOH:O	2.21	0.40
5:P:366:ALA:HB3	5:P:367:MET:CE	2.49	0.40
1:A:69:PRO:O	1:A:71:VAL:HG23	2.21	0.40
1:A:81:ASN:HA	9:A:321:HOH:O	2.20	0.40
2:C:34:VAL:HG22	9:C:1963:HOH:O	2.22	0.40
2:C:663:ASN:HB3	9:C:1567:HOH:O	2.21	0.40
3:D:996:TRP:HB2	3:D:1044:LEU:HD11	2.02	0.40
3:D:1057:VAL:HG23	9:D:9034:HOH:O	2.21	0.40
3:D:1123:PHE:CZ	3:D:1178:ALA:HB1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:112:ILE:HG12	3:D:128:TYR:OH	2.21	0.40
3:D:1254:GLN:OE1	3:D:1254:GLN:HA	2.21	0.40
3:D:138:LYS:HG2	9:D:9491:HOH:O	2.21	0.40
3:D:36:THR:HA	9:D:9305:HOH:O	2.21	0.40
3:D:491:LYS:HB2	9:D:2025:HOH:O	2.21	0.40
3:D:601:ARG:CD	3:D:606:ILE:HD13	2.52	0.40
3:D:704:ARG:HA	3:D:704:ARG:HD2	1.90	0.40
3:D:984:THR:HG22	3:D:987:GLU:OE2	2.21	0.40
5:F:279:GLN:NE2	9:F:586:HOH:O	2.53	0.40
1:K:198:ARG:HD3	1:K:200:TRP:CH2	2.54	0.40
1:K:206:THR:HG22	1:K:209:GLU:OE1	2.22	0.40
1:L:31:GLY:HA3	9:L:4517:HOH:O	2.20	0.40
1:L:41:ARG:HD3	9:L:3689:HOH:O	2.20	0.40
2:M:1092:LEU:HD21	3:N:1447:LEU:HD21	2.04	0.40
2:M:196:LEU:HD22	2:M:303:PHE:CD2	2.55	0.40
2:M:433:THR:HA	9:M:1375:HOH:O	2.21	0.40
2:M:596:TYR:HB2	9:M:1449:HOH:O	2.22	0.40
2:M:720:GLU:HG2	2:M:760:SER:HB3	2.03	0.40
2:M:811:PRO:HD3	9:M:1239:HOH:O	2.22	0.40
2:M:92:ALA:HA	2:M:93:PRO:HD3	1.95	0.40
3:N:1155:VAL:CG1	3:N:1177:ALA:HB1	2.51	0.40
3:N:1282:ARG:CZ	3:N:1282:ARG:HB3	2.52	0.40
3:N:168:THR:OG1	3:N:393:ILE:HB	2.22	0.40
3:N:213:VAL:HG22	3:N:214:GLU:H	1.86	0.40
3:N:37:LEU:HD23	9:N:9522:HOH:O	2.22	0.40
3:N:411:THR:HG23	3:N:429:SER:OG	2.21	0.40
3:N:427:VAL:HB	3:N:435:VAL:HG23	2.04	0.40
3:N:551:ASN:O	3:N:554:LEU:HB3	2.21	0.40
3:N:782:SER:O	3:N:786:ILE:HG13	2.22	0.40
3:N:847:ASP:HA	3:N:850:LEU:CD1	2.50	0.40
3:N:90:MET:HE3	3:N:518:PRO:HB3	2.03	0.40
3:N:992:ILE:O	3:N:995:LEU:HB3	2.21	0.40
9:N:2191:HOH:O	5:P:225:GLU:HB2	2.21	0.40
5:P:234:LYS:H	5:P:234:LYS:HG3	1.64	0.40
1:A:184:THR:O	1:A:192:LEU:HG	2.21	0.40
1:B:111:ALA:HB3	1:B:124:ASN:O	2.21	0.40
1:B:92:PRO:HA	1:B:146:ARG:CZ	2.51	0.40
1:B:1:MET:HE2	9:B:365:HOH:O	2.20	0.40
1:B:95:GLN:HB2	1:B:95:GLN:HE21	1.63	0.40
2:C:327:HIS:O	2:C:330:ASN:HB2	2.22	0.40
2:C:136:ILE:HG12	2:C:392:SER:OG	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:397:GLU:H	2:C:633:GLN:CD	2.25	0.40
3:D:1273:VAL:O	3:D:1273:VAL:HG23	2.22	0.40
3:D:1139:ASP:OD1	3:D:1357:ARG:NE	2.54	0.40
9:C:1791:HOH:O	3:D:13:ALA:N	2.53	0.40
3:D:170:PRO:HG3	9:D:9689:HOH:O	2.20	0.40
3:D:178:LEU:CG	3:D:200:ASP:H	2.31	0.40
3:D:501:ALA:HB1	3:D:1453:ALA:HA	2.03	0.40
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.84	0.40
3:D:131:LYS:CG	3:D:568:ARG:HG2	2.52	0.40
3:D:570:GLU:HG2	9:D:9564:HOH:O	2.21	0.40
4:E:61:GLU:OE2	4:E:62:THR:N	2.54	0.40
5:F:217:ASN:O	5:F:221:ILE:HG13	2.21	0.40
5:F:266:GLU:O	5:F:270:LYS:HG2	2.21	0.40
5:F:325:LYS:HA	9:F:599:HOH:O	2.21	0.40
5:F:408:LEU:HD13	5:F:411:HIS:HE1	1.86	0.40
1:K:114:PHE:HE2	1:K:142:VAL:HG13	1.87	0.40
1:K:42:ARG:HG2	1:K:42:ARG:HH11	1.87	0.40
2:M:1081:VAL:HG22	9:M:1596:HOH:O	2.21	0.40
2:M:212:GLY:O	2:M:215:GLY:O	2.39	0.40
2:M:26:TYR:HD2	2:M:121:MET:HB2	1.87	0.40
2:M:313:LEU:HD23	2:M:314:THR:HG23	2.03	0.40
2:M:372:LEU:HD22	9:M:1901:HOH:O	2.21	0.40
2:M:487:THR:HG22	2:M:488:ALA:N	2.37	0.40
2:M:53:PRO:HG2	9:M:1765:HOH:O	2.21	0.40
2:M:544:THR:HA	2:M:562:SER:OG	2.21	0.40
2:M:601:GLY:HA2	2:M:616:GLU:CD	2.42	0.40
2:M:78:PHE:HB3	2:M:79:PRO:HD2	2.03	0.40
3:N:1123:PHE:CD1	3:N:1134:LEU:HA	2.56	0.40
3:N:1319:VAL:O	3:N:1319:VAL:HG23	2.21	0.40
3:N:1470:ARG:NE	9:N:9305:HOH:O	2.54	0.40
3:N:1472:ILE:HA	3:N:1473:PRO:HD3	1.85	0.40
3:N:1475:GLY:O	3:N:1478:SER:HB3	2.21	0.40
3:N:553:ARG:HD2	3:N:570:GLU:CD	2.42	0.40
3:N:796:ARG:HD3	3:N:861:GLN:HB2	2.02	0.40
3:N:867:ARG:NH1	9:N:9385:HOH:O	2.47	0.40
3:N:754:PHE:CG	4:O:24:ALA:HB1	2.56	0.40
1:A:191:ASP:O	1:A:191:ASP:CG	2.60	0.40
1:A:29:GLU:O	1:A:193:ASP:OD1	2.40	0.40
2:C:282:GLY:HA3	9:C:1198:HOH:O	2.21	0.40
2:C:376:ARG:HG3	9:C:2017:HOH:O	2.21	0.40
2:C:520:GLU:HA	2:C:521:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:639:GLN:HA	2:C:657:ASP:O	2.22	0.40
2:C:976:ASP:HB2	2:C:979:THR:HG22	2.02	0.40
3:D:1156:LEU:CD1	3:D:1176:LYS:HD2	2.52	0.40
3:D:1293:PHE:HD2	9:D:2310:HOH:O	2.05	0.40
3:D:1480:PHE:O	3:D:1480:PHE:CD1	2.75	0.40
3:D:148:GLU:HG2	3:D:151:GLN:HB2	2.02	0.40
3:D:178:LEU:HD12	3:D:200:ASP:HB2	2.03	0.40
3:D:26:VAL:HG23	9:D:9002:HOH:O	2.22	0.40
3:D:522:PRO:HA	3:D:525:ARG:NH1	2.36	0.40
3:D:601:ARG:NE	3:D:606:ILE:HD13	2.37	0.40
3:D:699:VAL:HB	3:D:716:PHE:O	2.22	0.40
5:F:148:LYS:HG2	9:F:557:HOH:O	2.21	0.40
5:F:418:LEU:N	5:F:418:LEU:HD12	2.36	0.40
1:K:184:THR:HG23	1:K:192:LEU:CB	2.52	0.40
1:K:18:ARG:HG3	1:K:123:MET:CE	2.51	0.40
1:K:68:ILE:HA	1:K:69:PRO:HD3	1.95	0.40
1:L:103:ALA:O	1:L:138:LEU:HD23	2.21	0.40
1:L:89:PHE:CZ	1:L:146:ARG:HB3	2.56	0.40
1:K:219:ARG:NH2	1:L:223:THR:HG22	2.17	0.40
2:M:201:GLY:HA2	9:M:1944:HOH:O	2.20	0.40
2:M:214:TYR:HB2	9:M:1137:HOH:O	2.20	0.40
2:M:195:LEU:CD1	2:M:234:ALA:HB1	2.50	0.40
2:M:304:LEU:O	2:M:308:ARG:HB2	2.21	0.40
2:M:517:ARG:HD2	2:M:517:ARG:N	2.36	0.40
2:M:553:ASP:O	3:N:1070:TYR:CE2	2.74	0.40
2:M:620:LEU:HD22	2:M:620:LEU:H	1.85	0.40
2:M:760:SER:O	2:M:785:VAL:HG22	2.21	0.40
3:N:1280:VAL:O	3:N:1294:VAL:HA	2.21	0.40
3:N:540:LEU:HG	3:N:544:TYR:CE2	2.57	0.40
3:N:885:ILE:HG13	9:N:9120:HOH:O	2.20	0.40
3:N:983:LEU:N	9:N:2283:HOH:O	2.53	0.40
4:O:81:PRO:HB3	9:O:3838:HOH:O	2.22	0.40
5:P:287:THR:C	5:P:289:GLU:N	2.74	0.40
5:P:294:ALA:HA	9:P:5719:HOH:O	2.20	0.40
5:P:77:THR:O	5:P:81:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/315 (72%)	201 (88%)	21 (9%)	5 (2%)	6	7
1	B	227/315 (72%)	200 (88%)	21 (9%)	6 (3%)	5	5
1	K	227/315 (72%)	200 (88%)	24 (11%)	3 (1%)	12	17
1	L	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	8	10
2	C	1117/1119 (100%)	924 (83%)	143 (13%)	50 (4%)	2	2
2	M	1117/1119 (100%)	920 (82%)	149 (13%)	48 (4%)	2	2
3	D	1375/1524 (90%)	1129 (82%)	186 (14%)	60 (4%)	2	2
3	N	1375/1524 (90%)	1129 (82%)	181 (13%)	65 (5%)	2	1
4	E	93/99 (94%)	73 (78%)	16 (17%)	4 (4%)	2	2
4	O	93/99 (94%)	73 (78%)	16 (17%)	4 (4%)	2	2
5	F	341/423 (81%)	288 (84%)	42 (12%)	11 (3%)	4	3
5	P	341/423 (81%)	291 (85%)	37 (11%)	13 (4%)	3	2
All	All	6760/7590 (89%)	5632 (83%)	855 (13%)	273 (4%)	3	2

All (273) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	178	PRO
2	C	231	PRO
2	C	244	PRO
2	C	288	ARG
2	C	369	PRO
2	C	442	GLU
2	C	447	ALA
2	C	462	ASP

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Mol	Chain	Res	Type
2	C	465	GLY
2	C	548	PRO
2	C	908	GLY
3	D	40	GLU
3	D	43	GLY
3	D	55	ASP
3	D	82	LYS
3	D	137	PRO
3	D	208	PRO
3	D	209	ARG
3	D	238	PRO
3	D	246	PRO
3	D	370	ALA
3	D	373	PRO
3	D	385	VAL
3	D	440	VAL
3	D	705	ALA
3	D	832	ARG
3	D	844	ALA
3	D	1028	ALA
3	D	1066	THR
3	D	1129	THR
3	D	1208	ASP
3	D	1236	LEU
3	D	1441	GLN
4	E	42	PRO
4	E	58	PRO
5	F	147	LEU
5	F	153	PRO
5	F	390	PHE
1	K	29	GLU
1	L	29	GLU
2	M	152	PRO
2	M	178	PRO
2	M	231	PRO
2	M	244	PRO
2	M	288	ARG
2	M	290	LEU
2	M	369	PRO
2	M	442	GLU
2	M	447	ALA
2	M	462	ASP

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Mol	Chain	Res	Type
2	M	465	GLY
2	M	548	PRO
2	M	864	GLY
2	M	908	GLY
2	M	1106	ASP
3	N	40	GLU
3	N	43	GLY
3	N	55	ASP
3	N	137	PRO
3	N	208	PRO
3	N	209	ARG
3	N	238	PRO
3	N	246	PRO
3	N	370	ALA
3	N	373	PRO
3	N	385	VAL
3	N	440	VAL
3	N	832	ARG
3	N	844	ALA
3	N	1028	ALA
3	N	1125	PRO
3	N	1129	THR
3	N	1208	ASP
3	N	1441	GLN
4	O	42	PRO
4	O	58	PRO
5	P	147	LEU
5	P	153	PRO
5	P	390	PHE
1	A	187	GLY
1	B	187	GLY
2	C	59	LYS
2	C	156	GLY
2	C	164	PRO
2	C	261	ILE
2	C	290	LEU
2	C	400	PRO
2	C	413	LEU
2	C	425	PHE
2	C	448	ASN
2	C	626	ARG
2	C	627	ARG

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Mol	Chain	Res	Type
2	C	680	ASP
2	C	864	GLY
2	C	1106	ASP
3	D	31	THR
3	D	98	PRO
3	D	231	VAL
3	D	381	ALA
3	D	417	PRO
3	D	504	ASP
3	D	594	PRO
3	D	609	GLY
3	D	803	GLY
3	D	822	ALA
3	D	1213	ARG
4	E	53	GLY
5	F	324	GLU
5	F	325	LYS
5	F	341	PRO
1	K	187	GLY
1	L	187	GLY
2	M	59	LYS
2	M	156	GLY
2	M	413	LEU
2	M	425	PHE
2	M	626	ARG
2	M	680	ASP
3	N	31	THR
3	N	96	ALA
3	N	231	VAL
3	N	381	ALA
3	N	417	PRO
3	N	504	ASP
3	N	594	PRO
3	N	609	GLY
3	N	705	ALA
3	N	766	ALA
3	N	803	GLY
3	N	822	ALA
3	N	1066	THR
3	N	1213	ARG
3	N	1236	LEU
4	O	53	GLY

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Mol	Chain	Res	Type
5	P	288	TYR
5	P	324	GLU
5	P	325	LYS
5	P	341	PRO
2	C	74	GLY
2	C	144	PRO
2	C	170	PRO
2	C	363	SER
2	C	517	ARG
2	C	727	PRO
2	C	781	LYS
2	C	1004	LYS
3	D	37	LEU
3	D	96	ALA
3	D	170	PRO
3	D	424	GLY
3	D	782	SER
3	D	1286	THR
5	F	286	PRO
5	F	288	TYR
5	F	420	ASP
2	M	74	GLY
2	M	164	PRO
2	M	251	ASP
2	M	261	ILE
2	M	282	GLY
2	M	363	SER
2	M	448	ASN
2	M	517	ARG
2	M	627	ARG
2	M	727	PRO
2	M	781	LYS
3	N	37	LEU
3	N	82	LYS
3	N	98	PRO
3	N	170	PRO
3	N	424	GLY
3	N	782	SER
3	N	1286	THR
3	N	1342	GLU
3	N	1385	GLY
5	P	286	PRO

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Mol	Chain	Res	Type
1	A	106	PRO
2	C	180	GLY
2	C	251	ASP
2	C	457	ALA
2	C	598	GLU
2	C	1097	LEU
3	D	120	ALA
3	D	387	LEU
3	D	415	VAL
3	D	416	ALA
3	D	451	ASP
3	D	522	PRO
3	D	530	VAL
3	D	766	ALA
3	D	808	THR
3	D	1385	GLY
3	D	1432	LYS
1	K	106	PRO
1	L	106	PRO
2	M	170	PRO
2	M	180	GLY
2	M	223	ASP
2	M	457	ALA
3	N	120	ALA
3	N	415	VAL
3	N	416	ALA
3	N	522	PRO
3	N	533	GLY
3	N	808	THR
5	P	232	ARG
5	P	416	ARG
1	A	188	GLN
1	B	106	PRO
1	B	188	GLN
2	C	1059	ASP
2	C	1079	PRO
3	D	69	GLU
5	F	167	PRO
2	M	529	VAL
2	M	1079	PRO
3	N	387	LEU
3	N	526	PRO

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Mol	Chain	Res	Type
3	N	530	VAL
3	N	1389	LEU
3	N	1432	LYS
5	P	420	ASP
2	C	415	PRO
2	C	434	HIS
2	C	529	VAL
2	M	40	GLU
2	M	453	THR
2	M	1059	ASP
2	M	1097	LEU
3	N	110	SER
3	N	136	ASP
3	N	173	PRO
3	N	1064	GLY
3	N	1341	PRO
3	N	1349	VAL
5	P	167	PRO
1	A	9	PRO
2	C	282	GLY
2	C	779	GLY
3	D	136	ASP
3	D	526	PRO
3	D	1267	ARG
2	M	779	GLY
2	C	79	PRO
3	D	368	VAL
3	D	509	PRO
3	D	1306	PRO
5	F	297	PRO
2	M	400	PRO
3	N	368	VAL
3	N	1306	PRO
1	B	9	PRO
3	D	521	PRO
4	E	5	GLY
2	M	415	PRO
4	O	5	GLY
5	P	297	PRO
2	C	53	PRO
3	D	173	PRO
3	D	670	VAL

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Mol	Chain	Res	Type
2	M	79	PRO
2	M	317	VAL
2	M	444	PRO
3	N	509	PRO
3	N	1413	THR
2	C	377	PRO
2	C	767	PRO
1	L	9	PRO
3	N	169	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/273 (74%)	154 (76%)	48 (24%)	0	0
1	B	202/273 (74%)	162 (80%)	40 (20%)	1	1
1	K	202/273 (74%)	165 (82%)	37 (18%)	1	2
1	L	202/273 (74%)	156 (77%)	46 (23%)	1	1
2	C	941/941 (100%)	720 (76%)	221 (24%)	1	1
2	M	941/941 (100%)	722 (77%)	219 (23%)	1	1
3	D	1118/1279 (87%)	848 (76%)	270 (24%)	0	0
3	N	1118/1279 (87%)	860 (77%)	258 (23%)	1	1
4	E	83/87 (95%)	65 (78%)	18 (22%)	1	1
4	O	83/87 (95%)	67 (81%)	16 (19%)	1	1
5	F	295/370 (80%)	237 (80%)	58 (20%)	1	1
5	P	295/370 (80%)	245 (83%)	50 (17%)	2	2
All	All	5682/6446 (88%)	4401 (78%)	1281 (22%)	1	1

All (1281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	5	LYS
1	A	9	PRO
1	A	12	THR
1	A	15	THR
1	A	16	GLN
1	A	20	TYR
1	A	26	GLU
1	A	44	LEU
1	A	45	LEU
1	A	47	SER
1	A	60	ASP
1	A	73	GLU
1	A	74	ASP
1	A	89	PHE
1	A	92	PRO
1	A	94	LEU
1	A	96	THR
1	A	100	LEU
1	A	101	LEU
1	A	104	GLU
1	A	113	ASP
1	A	120	VAL
1	A	126	ASP
1	A	127	LEU
1	A	137	ARG
1	A	138	LEU
1	A	139	ASN
1	A	142	VAL
1	A	143	ARG
1	A	145	ASP
1	A	156	HIS
1	A	163	ASN
1	A	167	VAL
1	A	170	VAL
1	A	179	PHE
1	A	180	GLN
1	A	184	THR
1	A	188	GLN
1	A	191	ASP
1	A	196	THR
1	A	197	LEU
1	A	198	ARG

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Mol	Chain	Res	Type
1	A	205	VAL
1	A	211	LEU
1	A	216	GLU
1	A	227	ASN
1	A	229	GLN
1	B	1	MET
1	B	25	LEU
1	B	26	GLU
1	B	30	ARG
1	B	38	ASN
1	B	60	ASP
1	B	62	LEU
1	B	65	PHE
1	B	68	ILE
1	B	73	GLU
1	B	77	GLU
1	B	81	ASN
1	B	88	ARG
1	B	89	PHE
1	B	92	PRO
1	B	94	LEU
1	B	95	GLN
1	B	96	THR
1	B	99	LEU
1	B	101	LEU
1	B	112	ARG
1	B	113	ASP
1	B	124	ASN
1	B	126	ASP
1	B	138	LEU
1	B	140	MET
1	B	141	GLU
1	B	159	LYS
1	B	162	ILE
1	B	176	ARG
1	B	185	ARG
1	B	193	ASP
1	B	196	THR
1	B	200	TRP
1	B	201	THR
1	B	202	ASP
1	B	208	LEU

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Mol	Chain	Res	Type
1	B	209	GLU
1	B	221	HIS
1	B	224	TYR
2	C	5	ARG
2	C	10	ARG
2	C	15	LEU
2	C	20	GLU
2	C	22	GLN
2	C	26	TYR
2	C	27	ARG
2	C	30	LEU
2	C	31	GLN
2	C	34	VAL
2	C	41	ASN
2	C	48	PHE
2	C	49	ARG
2	C	52	PHE
2	C	71	TYR
2	C	73	LEU
2	C	79	PRO
2	C	81	ASP
2	C	89	THR
2	C	95	TYR
2	C	98	LEU
2	C	100	LEU
2	C	104	ASP
2	C	108	ILE
2	C	110	GLU
2	C	114	PHE
2	C	115	LEU
2	C	133	ASP
2	C	140	ILE
2	C	141	HIS
2	C	152	PRO
2	C	157	ARG
2	C	158	TYR
2	C	163	ILE
2	C	168	ARG
2	C	177	GLU
2	C	178	PRO
2	C	194	VAL
2	C	196	LEU

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Mol	Chain	Res	Type
2	C	205	GLU
2	C	209	ARG
2	C	216	GLU
2	C	218	VAL
2	C	221	LEU
2	C	229	MET
2	C	235	LEU
2	C	237	ARG
2	C	238	LEU
2	C	243	ARG
2	C	250	ARG
2	C	252	LYS
2	C	254	VAL
2	C	257	VAL
2	C	267	TYR
2	C	268	ASP
2	C	275	TYR
2	C	279	GLU
2	C	281	LEU
2	C	285	LEU
2	C	288	ARG
2	C	289	THR
2	C	290	LEU
2	C	293	PHE
2	C	297	GLU
2	C	301	GLU
2	C	303	PHE
2	C	304	LEU
2	C	309	TYR
2	C	321	GLU
2	C	327	HIS
2	C	331	ARG
2	C	339	LEU
2	C	343	GLN
2	C	350	ARG
2	C	359	MET
2	C	360	LEU
2	C	365	ASP
2	C	367	LEU
2	C	379	GLU
2	C	384	GLU
2	C	387	SER

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Mol	Chain	Res	Type
2	C	388	ARG
2	C	392	SER
2	C	393	GLN
2	C	396	ASP
2	C	399	ASN
2	C	400	PRO
2	C	402	SER
2	C	408	ARG
2	C	415	PRO
2	C	418	LEU
2	C	419	THR
2	C	420	ARG
2	C	421	GLU
2	C	422	ARG
2	C	425	PHE
2	C	428	ARG
2	C	432	ARG
2	C	442	GLU
2	C	443	THR
2	C	445	GLU
2	C	452	ILE
2	C	455	LEU
2	C	469	THR
2	C	473	ARG
2	C	474	VAL
2	C	479	VAL
2	C	482	GLU
2	C	487	THR
2	C	492	ASP
2	C	500	ASN
2	C	503	LEU
2	C	504	GLU
2	C	524	VAL
2	C	530	GLU
2	C	533	ASP
2	C	543	ASN
2	C	556	ASN
2	C	559	LEU
2	C	564	MET
2	C	566	THR
2	C	584	GLU
2	C	605	LYS

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Mol	Chain	Res	Type
2	C	606	VAL
2	C	607	ASP
2	C	620	LEU
2	C	622	GLU
2	C	633	GLN
2	C	637	LEU
2	C	640	ARG
2	C	645	VAL
2	C	650	ARG
2	C	668	LEU
2	C	671	ASN
2	C	672	VAL
2	C	673	LEU
2	C	679	PHE
2	C	690	ILE
2	C	691	SER
2	C	693	GLU
2	C	697	ARG
2	C	698	ASP
2	C	699	PHE
2	C	701	THR
2	C	702	SER
2	C	715	THR
2	C	716	LYS
2	C	722	ILE
2	C	723	THR
2	C	725	ASP
2	C	727	PRO
2	C	730	SER
2	C	737	LEU
2	C	740	GLU
2	C	744	ARG
2	C	760	SER
2	C	768	THR
2	C	780	GLU
2	C	785	VAL
2	C	799	ILE
2	C	804	VAL
2	C	808	ARG
2	C	821	GLU
2	C	829	GLN
2	C	834	GLN

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Mol	Chain	Res	Type
2	C	839	LEU
2	C	841	ASN
2	C	858	MET
2	C	863	ASP
2	C	870	ILE
2	C	878	SER
2	C	879	ARG
2	C	881	ASN
2	C	882	LEU
2	C	900	ARG
2	C	904	PRO
2	C	905	ILE
2	C	923	GLU
2	C	925	TYR
2	C	934	PHE
2	C	937	ASP
2	C	939	ARG
2	C	945	ARG
2	C	950	LEU
2	C	953	VAL
2	C	958	THR
2	C	960	GLU
2	C	962	GLN
2	C	975	TYR
2	C	978	ARG
2	C	981	GLU
2	C	982	PRO
2	C	984	GLU
2	C	995	MET
2	C	997	LEU
2	C	999	HIS
2	C	1000	MET
2	C	1002	GLU
2	C	1008	ARG
2	C	1016	ILE
2	C	1017	THR
2	C	1018	GLN
2	C	1019	GLN
2	C	1020	PRO
2	C	1021	LEU
2	C	1034	GLU
2	C	1040	LEU

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Mol	Chain	Res	Type
2	C	1052	MET
2	C	1054	THR
2	C	1058	ASP
2	C	1076	VAL
2	C	1079	PRO
2	C	1083	GLU
2	C	1088	LEU
2	C	1091	GLU
2	C	1092	LEU
2	C	1095	LEU
2	C	1098	ASP
2	C	1104	GLU
2	C	1106	ASP
2	C	1113	GLU
3	D	3	LYS
3	D	6	ARG
3	D	9	ARG
3	D	12	LEU
3	D	14	SER
3	D	25	GLU
3	D	27	GLU
3	D	32	ILE
3	D	33	ASN
3	D	34	TYR
3	D	35	ARG
3	D	41	ARG
3	D	42	ASP
3	D	48	ARG
3	D	56	TYR
3	D	69	GLU
3	D	71	LYS
3	D	80	VAL
3	D	82	LYS
3	D	84	ILE
3	D	85	VAL
3	D	86	ARG
3	D	103	TRP
3	D	107	ASP
3	D	112	ILE
3	D	117	ASP
3	D	118	LEU
3	D	127	LEU

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Mol	Chain	Res	Type
3	D	133	ILE
3	D	145	VAL
3	D	147	VAL
3	D	152	LEU
3	D	153	LEU
3	D	155	ASP
3	D	156	GLU
3	D	162	ARG
3	D	166	GLN
3	D	170	PRO
3	D	171	LEU
3	D	185	VAL
3	D	199	LEU
3	D	205	TYR
3	D	206	ARG
3	D	208	PRO
3	D	209	ARG
3	D	210	ARG
3	D	389	GLU
3	D	394	LEU
3	D	395	VAL
3	D	406	ASP
3	D	411	THR
3	D	413	ASP
3	D	430	ASP
3	D	432	TYR
3	D	441	ARG
3	D	444	VAL
3	D	445	ARG
3	D	447	VAL
3	D	450	TYR
3	D	452	ILE
3	D	456	MET
3	D	465	LEU
3	D	475	LYS
3	D	481	MET
3	D	483	HIS
3	D	486	ARG
3	D	503	LEU
3	D	505	SER
3	D	507	ASN
3	D	521	PRO

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Mol	Chain	Res	Type
3	D	528	VAL
3	D	529	GLN
3	D	540	LEU
3	D	542	ASP
3	D	549	ASN
3	D	554	LEU
3	D	565	ILE
3	D	569	ASN
3	D	573	MET
3	D	590	PRO
3	D	594	PRO
3	D	596	SER
3	D	597	ASP
3	D	598	ARG
3	D	605	ASP
3	D	608	SER
3	D	614	PHE
3	D	617	ASN
3	D	624	ASP
3	D	628	ARG
3	D	636	GLN
3	D	639	LEU
3	D	641	GLN
3	D	651	GLU
3	D	659	LYS
3	D	666	ILE
3	D	675	ARG
3	D	676	MET
3	D	679	ARG
3	D	682	ASP
3	D	685	ASP
3	D	688	TRP
3	D	695	ILE
3	D	702	LEU
3	D	704	ARG
3	D	709	HIS
3	D	710	ARG
3	D	713	ILE
3	D	716	PHE
3	D	717	GLN
3	D	720	LEU
3	D	724	GLN

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Mol	Chain	Res	Type
3	D	734	GLU
3	D	752	SER
3	D	754	PHE
3	D	762	GLN
3	D	764	LEU
3	D	767	HIS
3	D	784	ASP
3	D	794	GLN
3	D	797	LYS
3	D	799	LYS
3	D	800	LYS
3	D	804	LEU
3	D	805	GLU
3	D	813	LEU
3	D	824	ASN
3	D	828	LYS
3	D	829	VAL
3	D	833	GLU
3	D	838	ARG
3	D	839	LEU
3	D	847	ASP
3	D	858	VAL
3	D	859	ASP
3	D	862	ASP
3	D	863	VAL
3	D	864	VAL
3	D	865	THR
3	D	867	ARG
3	D	869	MET
3	D	875	THR
3	D	879	ARG
3	D	880	ILE
3	D	888	GLU
3	D	893	GLU
3	D	898	GLU
3	D	901	GLN
3	D	904	VAL
3	D	910	SER
3	D	916	TYR
3	D	922	LEU
3	D	927	THR
3	D	929	ARG

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Mol	Chain	Res	Type
3	D	944	THR
3	D	951	ILE
3	D	952	ASP
3	D	962	GLN
3	D	972	LEU
3	D	973	GLN
3	D	982	PHE
3	D	985	ASP
3	D	987	GLU
3	D	988	ARG
3	D	999	THR
3	D	1001	GLU
3	D	1026	SER
3	D	1032	PRO
3	D	1033	GLN
3	D	1042	ARG
3	D	1045	MET
3	D	1049	SER
3	D	1051	GLU
3	D	1058	ARG
3	D	1060	SER
3	D	1062	ARG
3	D	1065	LEU
3	D	1068	LEU
3	D	1074	SER
3	D	1084	THR
3	D	1086	LEU
3	D	1095	THR
3	D	1096	ARG
3	D	1109	GLU
3	D	1112	CYS
3	D	1127	GLU
3	D	1129	THR
3	D	1130	ARG
3	D	1131	SER
3	D	1133	ARG
3	D	1135	ARG
3	D	1151	ARG
3	D	1152	GLU
3	D	1160	LEU
3	D	1161	GLU
3	D	1162	GLU

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Mol	Chain	Res	Type
3	D	1164	ARG
3	D	1166	LEU
3	D	1167	SER
3	D	1173	LEU
3	D	1176	LYS
3	D	1182	GLU
3	D	1183	ILE
3	D	1191	PRO
3	D	1195	GLN
3	D	1196	THR
3	D	1197	ARG
3	D	1207	TYR
3	D	1213	ARG
3	D	1219	GLU
3	D	1238	MET
3	D	1239	ARG
3	D	1253	THR
3	D	1260	ILE
3	D	1264	GLU
3	D	1267	ARG
3	D	1269	LYS
3	D	1280	VAL
3	D	1285	GLU
3	D	1290	LEU
3	D	1295	GLU
3	D	1299	PHE
3	D	1306	PRO
3	D	1307	LYS
3	D	1310	ARG
3	D	1314	LYS
3	D	1318	TYR
3	D	1323	GLN
3	D	1325	LEU
3	D	1337	GLU
3	D	1344	VAL
3	D	1345	GLU
3	D	1346	ARG
3	D	1348	LEU
3	D	1350	GLU
3	D	1353	GLN
3	D	1359	GLN
3	D	1363	LEU

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Mol	Chain	Res	Type
3	D	1365	ASP
3	D	1374	GLN
3	D	1382	THR
3	D	1383	ASP
3	D	1386	ASP
3	D	1387	SER
3	D	1389	LEU
3	D	1401	GLU
3	D	1403	LEU
3	D	1407	LEU
3	D	1410	GLU
3	D	1415	VAL
3	D	1419	PRO
3	D	1420	LEU
3	D	1421	LEU
3	D	1424	VAL
3	D	1432	LYS
3	D	1433	SER
3	D	1435	LEU
3	D	1439	SER
3	D	1440	PHE
3	D	1455	LYS
3	D	1460	ILE
3	D	1462	LEU
3	D	1480	PHE
3	D	1481	VAL
3	D	1483	PHE
3	D	1485	GLN
3	D	1487	VAL
3	D	1488	ASP
3	D	1496	GLU
3	D	1501	GLU
4	E	7	ASP
4	E	14	ASP
4	E	15	SER
4	E	28	GLN
4	E	29	GLN
4	E	31	LEU
4	E	32	ARG
4	E	40	LEU
4	E	42	PRO
4	E	45	ARG

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Mol	Chain	Res	Type
4	E	57	ASP
4	E	59	ASN
4	E	61	GLU
4	E	67	GLU
4	E	75	PHE
4	E	81	PRO
4	E	84	ARG
4	E	89	MET
5	F	83	GLN
5	F	84	TYR
5	F	87	GLU
5	F	90	GLN
5	F	91	VAL
5	F	115	LYS
5	F	117	SER
5	F	125	ASP
5	F	126	LEU
5	F	135	ILE
5	F	136	LEU
5	F	142	ARG
5	F	149	GLU
5	F	150	THR
5	F	164	LYS
5	F	172	ARG
5	F	174	LEU
5	F	181	GLU
5	F	187	LEU
5	F	192	LEU
5	F	194	LEU
5	F	209	PHE
5	F	212	LEU
5	F	220	LEU
5	F	225	GLU
5	F	233	PHE
5	F	240	THR
5	F	245	GLN
5	F	249	ARG
5	F	266	GLU
5	F	269	ASN
5	F	281	GLU
5	F	282	LEU
5	F	285	GLU

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Mol	Chain	Res	Type
5	F	295	MET
5	F	297	PRO
5	F	302	LYS
5	F	306	GLU
5	F	316	SER
5	F	317	LEU
5	F	319	THR
5	F	324	GLU
5	F	328	PHE
5	F	337	HIS
5	F	340	SER
5	F	341	PRO
5	F	343	ASP
5	F	349	LEU
5	F	353	GLU
5	F	362	SER
5	F	370	LYS
5	F	393	THR
5	F	398	ARG
5	F	399	GLN
5	F	403	LYS
5	F	410	TYR
5	F	419	ARG
5	F	420	ASP
1	K	1	MET
1	K	9	PRO
1	K	18	ARG
1	K	25	LEU
1	K	44	LEU
1	K	45	LEU
1	K	55	SER
1	K	62	LEU
1	K	73	GLU
1	K	80	LEU
1	K	89	PHE
1	K	92	PRO
1	K	95	GLN
1	K	101	LEU
1	K	112	ARG
1	K	113	ASP
1	K	115	LEU
1	K	121	GLU

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Mol	Chain	Res	Type
1	K	127	LEU
1	K	131	THR
1	K	138	LEU
1	K	161	ARG
1	K	167	VAL
1	K	176	ARG
1	K	184	THR
1	K	189	ARG
1	K	190	THR
1	K	193	ASP
1	K	196	THR
1	K	198	ARG
1	K	206	THR
1	K	211	LEU
1	K	215	VAL
1	K	222	LEU
1	K	223	THR
1	K	227	ASN
1	K	229	GLN
1	L	1	MET
1	L	2	LEU
1	L	5	LYS
1	L	7	LYS
1	L	9	PRO
1	L	20	TYR
1	L	25	LEU
1	L	29	GLU
1	L	38	ASN
1	L	47	SER
1	L	62	LEU
1	L	65	PHE
1	L	73	GLU
1	L	77	GLU
1	L	81	ASN
1	L	89	PHE
1	L	94	LEU
1	L	95	GLN
1	L	101	LEU
1	L	104	GLU
1	L	110	LYS
1	L	113	ASP
1	L	124	ASN

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Mol	Chain	Res	Type
1	L	128	HIS
1	L	134	GLU
1	L	138	LEU
1	L	141	GLU
1	L	146	ARG
1	L	159	LYS
1	L	161	ARG
1	L	162	ILE
1	L	172	SER
1	L	176	ARG
1	L	177	VAL
1	L	180	GLN
1	L	181	VAL
1	L	182	GLU
1	L	184	THR
1	L	197	LEU
1	L	200	TRP
1	L	201	THR
1	L	206	THR
1	L	212	ASN
1	L	213	GLN
1	L	216	GLU
1	L	227	ASN
2	M	3	ILE
2	M	9	ILE
2	M	10	ARG
2	M	26	TYR
2	M	30	LEU
2	M	31	GLN
2	M	34	VAL
2	M	39	ARG
2	M	48	PHE
2	M	49	ARG
2	M	51	THR
2	M	71	TYR
2	M	77	PRO
2	M	81	ASP
2	M	82	GLU
2	M	91	GLN
2	M	95	TYR
2	M	98	LEU
2	M	100	LEU

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Mol	Chain	Res	Type
2	M	102	HIS
2	M	104	ASP
2	M	105	THR
2	M	107	LEU
2	M	111	ASP
2	M	114	PHE
2	M	115	LEU
2	M	140	ILE
2	M	141	HIS
2	M	143	SER
2	M	150	PRO
2	M	158	TYR
2	M	163	ILE
2	M	175	GLU
2	M	178	PRO
2	M	184	MET
2	M	198	ARG
2	M	203	ASP
2	M	205	GLU
2	M	221	LEU
2	M	222	MET
2	M	223	ASP
2	M	229	MET
2	M	230	ARG
2	M	233	GLU
2	M	235	LEU
2	M	237	ARG
2	M	238	LEU
2	M	239	PHE
2	M	241	LEU
2	M	242	LEU
2	M	243	ARG
2	M	246	ASP
2	M	252	LYS
2	M	254	VAL
2	M	257	VAL
2	M	260	LEU
2	M	266	ARG
2	M	267	TYR
2	M	268	ASP
2	M	276	LYS
2	M	281	LEU

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Mol	Chain	Res	Type
2	M	285	LEU
2	M	290	LEU
2	M	293	PHE
2	M	295	ASP
2	M	297	GLU
2	M	303	PHE
2	M	304	LEU
2	M	309	TYR
2	M	313	LEU
2	M	321	GLU
2	M	322	VAL
2	M	328	LEU
2	M	339	LEU
2	M	359	MET
2	M	360	LEU
2	M	365	ASP
2	M	366	SER
2	M	367	LEU
2	M	371	LYS
2	M	376	ARG
2	M	379	GLU
2	M	383	ARG
2	M	387	SER
2	M	393	GLN
2	M	394	PHE
2	M	396	ASP
2	M	397	GLU
2	M	399	ASN
2	M	400	PRO
2	M	402	SER
2	M	419	THR
2	M	420	ARG
2	M	421	GLU
2	M	425	PHE
2	M	432	ARG
2	M	443	THR
2	M	445	GLU
2	M	455	LEU
2	M	460	ARG
2	M	462	ASP
2	M	468	ARG
2	M	472	ARG

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Mol	Chain	Res	Type
2	M	480	THR
2	M	481	ASP
2	M	482	GLU
2	M	486	MET
2	M	496	ILE
2	M	500	ASN
2	M	502	PRO
2	M	503	LEU
2	M	507	ARG
2	M	511	GLU
2	M	517	ARG
2	M	524	VAL
2	M	527	GLU
2	M	528	GLU
2	M	533	ASP
2	M	542	VAL
2	M	543	ASN
2	M	544	THR
2	M	545	ASN
2	M	548	PRO
2	M	554	ASP
2	M	562	SER
2	M	563	ASN
2	M	564	MET
2	M	565	GLN
2	M	571	LEU
2	M	579	VAL
2	M	586	ARG
2	M	588	VAL
2	M	589	ARG
2	M	599	GLU
2	M	600	ASP
2	M	607	ASP
2	M	617	ASP
2	M	620	LEU
2	M	626	ARG
2	M	633	GLN
2	M	635	THR
2	M	637	LEU
2	M	639	GLN
2	M	640	ARG
2	M	645	VAL

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Mol	Chain	Res	Type
2	M	648	ARG
2	M	654	LEU
2	M	657	ASP
2	M	659	PRO
2	M	663	ASN
2	M	668	LEU
2	M	676	ILE
2	M	677	MET
2	M	686	ASP
2	M	697	ARG
2	M	699	PHE
2	M	701	THR
2	M	713	ARG
2	M	714	ASP
2	M	715	THR
2	M	717	LEU
2	M	727	PRO
2	M	729	LEU
2	M	737	LEU
2	M	744	ARG
2	M	748	GLU
2	M	749	VAL
2	M	750	LYS
2	M	775	ARG
2	M	785	VAL
2	M	790	LEU
2	M	799	ILE
2	M	808	ARG
2	M	821	GLU
2	M	829	GLN
2	M	839	LEU
2	M	841	ASN
2	M	860	HIS
2	M	862	PRO
2	M	865	THR
2	M	870	ILE
2	M	879	ARG
2	M	881	ASN
2	M	886	LEU
2	M	890	LEU
2	M	900	ARG
2	M	905	ILE

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Mol	Chain	Res	Type
2	M	907	ASP
2	M	911	GLU
2	M	925	TYR
2	M	928	LYS
2	M	937	ASP
2	M	940	GLU
2	M	950	LEU
2	M	976	ASP
2	M	978	ARG
2	M	981	GLU
2	M	984	GLU
2	M	988	VAL
2	M	1000	MET
2	M	1002	GLU
2	M	1004	LYS
2	M	1006	HIS
2	M	1008	ARG
2	M	1009	SER
2	M	1016	ILE
2	M	1017	THR
2	M	1035	MET
2	M	1052	MET
2	M	1054	THR
2	M	1074	GLU
2	M	1079	PRO
2	M	1080	SER
2	M	1088	LEU
2	M	1091	GLU
2	M	1092	LEU
2	M	1097	LEU
2	M	1098	ASP
2	M	1100	GLN
3	N	3	LYS
3	N	7	LYS
3	N	12	LEU
3	N	14	SER
3	N	15	PRO
3	N	27	GLU
3	N	28	LYS
3	N	31	THR
3	N	33	ASN
3	N	34	TYR

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Mol	Chain	Res	Type
3	N	41	ARG
3	N	52	PRO
3	N	55	ASP
3	N	56	TYR
3	N	68	PHE
3	N	71	LYS
3	N	76	CYS
3	N	82	LYS
3	N	85	VAL
3	N	86	ARG
3	N	87	ARG
3	N	95	LEU
3	N	97	THR
3	N	101	HIS
3	N	103	TRP
3	N	107	ASP
3	N	108	VAL
3	N	111	LYS
3	N	112	ILE
3	N	123	LEU
3	N	128	TYR
3	N	131	LYS
3	N	133	ILE
3	N	142	LEU
3	N	145	VAL
3	N	147	VAL
3	N	153	LEU
3	N	162	ARG
3	N	165	LYS
3	N	166	GLN
3	N	169	TYR
3	N	170	PRO
3	N	171	LEU
3	N	172	PRO
3	N	176	ASP
3	N	185	VAL
3	N	199	LEU
3	N	204	LEU
3	N	205	TYR
3	N	206	ARG
3	N	208	PRO
3	N	389	GLU

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Mol	Chain	Res	Type
3	N	394	LEU
3	N	405	ASP
3	N	408	GLU
3	N	411	THR
3	N	413	ASP
3	N	417	PRO
3	N	419	ASP
3	N	421	LEU
3	N	430	ASP
3	N	432	TYR
3	N	441	ARG
3	N	444	VAL
3	N	445	ARG
3	N	447	VAL
3	N	450	TYR
3	N	452	ILE
3	N	453	ASP
3	N	455	ARG
3	N	456	MET
3	N	459	GLU
3	N	465	LEU
3	N	483	HIS
3	N	488	ARG
3	N	493	ARG
3	N	502	PHE
3	N	513	ILE
3	N	518	PRO
3	N	523	ASP
3	N	530	VAL
3	N	531	ASP
3	N	535	PHE
3	N	571	LYS
3	N	576	GLU
3	N	586	ARG
3	N	590	PRO
3	N	593	ASN
3	N	594	PRO
3	N	598	ARG
3	N	600	LEU
3	N	601	ARG
3	N	602	SER
3	N	613	ARG

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Mol	Chain	Res	Type
3	N	614	PHE
3	N	617	ASN
3	N	624	ASP
3	N	625	TYR
3	N	628	ARG
3	N	636	GLN
3	N	639	LEU
3	N	641	GLN
3	N	652	LEU
3	N	664	LYS
3	N	666	ILE
3	N	676	MET
3	N	681	ARG
3	N	684	LYS
3	N	688	TRP
3	N	692	GLU
3	N	695	ILE
3	N	701	LEU
3	N	704	ARG
3	N	716	PHE
3	N	717	GLN
3	N	724	GLN
3	N	725	SER
3	N	732	VAL
3	N	736	PHE
3	N	739	ASP
3	N	749	VAL
3	N	754	PHE
3	N	770	LEU
3	N	781	PRO
3	N	783	ARG
3	N	787	LEU
3	N	792	ILE
3	N	794	GLN
3	N	796	ARG
3	N	797	LYS
3	N	799	LYS
3	N	800	LYS
3	N	805	GLU
3	N	823	LEU
3	N	824	ASN
3	N	828	LYS

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Mol	Chain	Res	Type
3	N	829	VAL
3	N	832	ARG
3	N	833	GLU
3	N	839	LEU
3	N	840	LYS
3	N	846	PRO
3	N	847	ASP
3	N	863	VAL
3	N	865	THR
3	N	875	THR
3	N	880	ILE
3	N	888	GLU
3	N	892	ASP
3	N	897	TRP
3	N	914	LEU
3	N	917	GLN
3	N	926	LYS
3	N	944	THR
3	N	951	ILE
3	N	959	GLU
3	N	970	LYS
3	N	984	THR
3	N	987	GLU
3	N	994	GLN
3	N	999	THR
3	N	1005	GLN
3	N	1019	PRO
3	N	1034	GLN
3	N	1039	CYS
3	N	1042	ARG
3	N	1045	MET
3	N	1051	GLU
3	N	1058	ARG
3	N	1060	SER
3	N	1062	ARG
3	N	1063	GLU
3	N	1065	LEU
3	N	1068	LEU
3	N	1074	SER
3	N	1084	THR
3	N	1086	LEU
3	N	1093	TYR

Continued on next page...

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Mol	Chain	Res	Type
3	N	1101	VAL
3	N	1104	GLU
3	N	1109	GLU
3	N	1111	ASP
3	N	1112	CYS
3	N	1114	THR
3	N	1119	SER
3	N	1127	GLU
3	N	1129	THR
3	N	1135	ARG
3	N	1151	ARG
3	N	1158	VAL
3	N	1161	GLU
3	N	1166	LEU
3	N	1176	LYS
3	N	1183	ILE
3	N	1184	GLN
3	N	1195	GLN
3	N	1197	ARG
3	N	1202	GLN
3	N	1207	TYR
3	N	1210	SER
3	N	1216	SER
3	N	1254	GLN
3	N	1262	LEU
3	N	1264	GLU
3	N	1267	ARG
3	N	1278	ASP
3	N	1280	VAL
3	N	1284	GLU
3	N	1285	GLU
3	N	1286	THR
3	N	1297	GLU
3	N	1299	PHE
3	N	1305	LEU
3	N	1307	LYS
3	N	1312	LEU
3	N	1314	LYS
3	N	1315	ASP
3	N	1325	LEU
3	N	1331	ASP
3	N	1337	GLU

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Mol	Chain	Res	Type
3	N	1346	ARG
3	N	1348	LEU
3	N	1353	GLN
3	N	1359	GLN
3	N	1363	LEU
3	N	1368	ILE
3	N	1372	VAL
3	N	1378	TYR
3	N	1380	GLU
3	N	1381	VAL
3	N	1382	THR
3	N	1387	SER
3	N	1390	LEU
3	N	1395	LEU
3	N	1396	GLU
3	N	1401	GLU
3	N	1403	LEU
3	N	1404	ASN
3	N	1415	VAL
3	N	1419	PRO
3	N	1424	VAL
3	N	1431	THR
3	N	1432	LYS
3	N	1433	SER
3	N	1435	LEU
3	N	1439	SER
3	N	1440	PHE
3	N	1442	ASN
3	N	1447	LEU
3	N	1452	ILE
3	N	1460	ILE
3	N	1463	LYS
3	N	1465	ASN
3	N	1466	VAL
3	N	1478	SER
3	N	1488	ASP
3	N	1499	ARG
3	N	1501	GLU
4	O	6	ILE
4	O	12	MET
4	O	15	SER
4	O	17	TYR

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Mol	Chain	Res	Type
4	O	29	GLN
4	O	32	ARG
4	O	45	ARG
4	O	47	LYS
4	O	48	MET
4	O	57	ASP
4	O	59	ASN
4	O	61	GLU
4	O	70	THR
4	O	84	ARG
4	O	85	LEU
4	O	86	GLN
5	P	77	THR
5	P	83	GLN
5	P	84	TYR
5	P	90	GLN
5	P	91	VAL
5	P	96	LEU
5	P	117	SER
5	P	125	ASP
5	P	135	ILE
5	P	136	LEU
5	P	142	ARG
5	P	143	HIS
5	P	144	ILE
5	P	145	PRO
5	P	150	THR
5	P	151	LEU
5	P	174	LEU
5	P	176	ILE
5	P	185	GLN
5	P	187	LEU
5	P	200	LYS
5	P	211	ASP
5	P	218	GLN
5	P	234	LYS
5	P	249	ARG
5	P	266	GLU
5	P	289	GLU
5	P	295	MET
5	P	306	GLU
5	P	313	GLU

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Mol	Chain	Res	Type
5	P	316	SER
5	P	318	GLU
5	P	328	PHE
5	P	335	ASP
5	P	336	GLU
5	P	341	PRO
5	P	342	VAL
5	P	347	GLN
5	P	349	LEU
5	P	350	LEU
5	P	353	GLU
5	P	363	GLU
5	P	370	LYS
5	P	392	VAL
5	P	393	THR
5	P	399	GLN
5	P	403	LYS
5	P	408	LEU
5	P	410	TYR
5	P	419	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (166) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	81	ASN
1	A	128	HIS
1	A	139	ASN
1	A	156	HIS
1	A	163	ASN
1	A	180	GLN
1	A	227	ASN
1	A	229	GLN
1	B	95	GLN
1	B	124	ASN
1	B	227	ASN
2	C	22	GLN
2	C	31	GLN
2	C	41	ASN
2	C	91	GLN
2	C	99	GLN
2	C	117	HIS

Continued on next page...

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Mol	Chain	Res	Type
2	C	204	GLN
2	C	343	GLN
2	C	374	ASN
2	C	393	GLN
2	C	431	HIS
2	C	448	ASN
2	C	500	ASN
2	C	506	ASN
2	C	538	GLN
2	C	563	ASN
2	C	565	GLN
2	C	633	GLN
2	C	639	GLN
2	C	663	ASN
2	C	728	HIS
2	C	834	GLN
2	C	841	ASN
2	C	881	ASN
2	C	884	GLN
2	C	889	HIS
2	C	899	GLN
2	C	1019	GLN
2	C	1047	HIS
2	C	1107	ASN
3	D	507	ASN
3	D	569	ASN
3	D	616	GLN
3	D	617	ASN
3	D	636	GLN
3	D	724	GLN
3	D	727	GLN
3	D	748	HIS
3	D	756	GLN
3	D	768	ASN
3	D	794	GLN
3	D	824	ASN
3	D	917	GLN
3	D	973	GLN
3	D	1018	ASN
3	D	1033	GLN
3	D	1046	GLN
3	D	1116	ASN

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Mol	Chain	Res	Type
3	D	1124	GLN
3	D	1184	GLN
3	D	1254	GLN
3	D	1359	GLN
3	D	1374	GLN
3	D	1465	ASN
3	D	1485	GLN
4	E	28	GLN
4	E	37	ASN
4	E	86	GLN
5	F	83	GLN
5	F	90	GLN
5	F	217	ASN
5	F	218	GLN
5	F	312	GLN
5	F	337	HIS
5	F	402	ASN
1	K	38	ASN
1	K	63	HIS
1	K	81	ASN
1	K	156	HIS
1	K	180	GLN
1	K	212	ASN
1	K	213	GLN
1	K	227	ASN
1	K	229	GLN
1	L	63	HIS
1	L	81	ASN
1	L	95	GLN
1	L	124	ASN
1	L	139	ASN
1	L	212	ASN
1	L	227	ASN
2	M	22	GLN
2	M	31	GLN
2	M	91	GLN
2	M	99	GLN
2	M	102	HIS
2	M	117	HIS
2	M	139	GLN
2	M	327	HIS
2	M	343	GLN

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Mol	Chain	Res	Type
2	M	374	ASN
2	M	393	GLN
2	M	431	HIS
2	M	545	ASN
2	M	565	GLN
2	M	567	GLN
2	M	609	ASN
2	M	632	ASN
2	M	633	GLN
2	M	639	GLN
2	M	663	ASN
2	M	834	GLN
2	M	841	ASN
2	M	860	HIS
2	M	881	ASN
2	M	889	HIS
2	M	920	GLN
2	M	969	GLN
2	M	1018	GLN
2	M	1019	GLN
2	M	1107	ASN
3	N	125	GLN
3	N	151	GLN
3	N	166	GLN
3	N	442	ASN
3	N	462	GLN
3	N	549	ASN
3	N	560	GLN
3	N	640	HIS
3	N	703	ASN
3	N	717	GLN
3	N	744	GLN
3	N	756	GLN
3	N	768	ASN
3	N	824	ASN
3	N	976	GLN
3	N	994	GLN
3	N	1005	GLN
3	N	1033	GLN
3	N	1034	GLN
3	N	1103	HIS
3	N	1172	HIS

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Mol	Chain	Res	Type
3	N	1184	GLN
3	N	1202	GLN
3	N	1323	GLN
3	N	1333	HIS
3	N	1334	GLN
3	N	1353	GLN
3	N	1374	GLN
3	N	1465	ASN
3	N	1485	GLN
4	O	28	GLN
4	O	33	HIS
4	O	59	ASN
4	O	78	ASN
4	O	86	GLN
5	P	83	GLN
5	P	90	GLN
5	P	170	HIS
5	P	185	GLN
5	P	217	ASN
5	P	245	GLN
5	P	312	GLN
5	P	337	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 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
6	STD	N	8002	-	42,47,47	7.09	24 (57%)	47,73,73	2.35	10 (21%)
6	STD	D	8001	-	42,47,47	7.16	24 (57%)	47,73,73	2.24	10 (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
6	STD	N	8002	-	-	15/31/101/101	0/5/5/5
6	STD	D	8001	-	-	13/31/101/101	0/5/5/5

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	8001	STD	O5-C19	-28.16	1.18	1.43
6	N	8002	STD	O5-C19	-27.26	1.18	1.43
6	N	8002	STD	C23-C21	-14.56	1.21	1.53
6	D	8001	STD	C23-C21	-14.50	1.22	1.53
6	D	8001	STD	C18-C16	-13.42	1.25	1.53
6	N	8002	STD	C18-C16	-13.16	1.25	1.53
6	N	8002	STD	C15-C12	-12.47	1.21	1.52
6	D	8001	STD	C15-C12	-12.12	1.22	1.52
6	N	8002	STD	O8-C19	11.93	1.53	1.43
6	D	8001	STD	O5-C13	11.63	1.62	1.44
6	D	8001	STD	O8-C19	11.25	1.53	1.43
6	N	8002	STD	O5-C13	11.18	1.61	1.44
6	D	8001	STD	C17-C30	9.98	1.66	1.49
6	N	8002	STD	C17-C30	8.99	1.64	1.49
6	D	8001	STD	O8-C17	7.15	1.52	1.44
6	N	8002	STD	C22-N2	7.10	1.43	1.33
6	D	8001	STD	C15-C26	7.08	1.62	1.52
6	N	8002	STD	O8-C17	7.07	1.52	1.44
6	D	8001	STD	C20-C3	7.05	1.61	1.53
6	N	8002	STD	C15-C26	6.94	1.62	1.52
6	D	8001	STD	C22-N2	6.91	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	8001	STD	C16-C13	6.87	1.67	1.53
6	N	8002	STD	C16-C13	6.71	1.67	1.53
6	N	8002	STD	C21-C22	6.59	1.62	1.52
6	D	8001	STD	C26-C25	5.92	1.63	1.52
6	N	8002	STD	C6-C5	-5.72	1.36	1.45
6	N	8002	STD	C26-C25	5.39	1.62	1.52
6	N	8002	STD	O4-C4	5.29	1.48	1.42
6	N	8002	STD	C30-C32	5.25	1.40	1.32
6	N	8002	STD	C7-C8	-5.22	1.34	1.45
6	D	8001	STD	C21-C22	5.11	1.60	1.52
6	D	8001	STD	C30-C32	4.97	1.40	1.32
6	N	8002	STD	C20-C3	4.67	1.59	1.53
6	D	8001	STD	C4-N1	4.29	1.51	1.45
6	D	8001	STD	C7-C8	-4.24	1.36	1.45
6	D	8001	STD	C6-C5	-4.16	1.38	1.45
6	D	8001	STD	O4-C4	3.66	1.46	1.42
6	N	8002	STD	O9-C31	3.35	1.53	1.44
6	N	8002	STD	C4-N1	3.28	1.50	1.45
6	D	8001	STD	O9-C31	3.23	1.52	1.44
6	D	8001	STD	C12-C4	3.00	1.62	1.50
6	D	8001	STD	C29-C19	2.81	1.55	1.51
6	N	8002	STD	C29-C19	2.70	1.55	1.51
6	N	8002	STD	O4-C25	2.62	1.50	1.44
6	D	8001	STD	C28-C32	2.55	1.54	1.50
6	N	8002	STD	C12-C4	2.45	1.60	1.50
6	N	8002	STD	C27-C25	2.27	1.57	1.51
6	D	8001	STD	C11-C8	2.16	1.55	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	8002	STD	C19-O5-C13	9.36	122.91	112.80
6	D	8001	STD	C19-O5-C13	7.86	121.29	112.80
6	D	8001	STD	O8-C17-C30	-6.73	105.06	111.68
6	N	8002	STD	O8-C17-C30	-6.54	105.26	111.68
6	N	8002	STD	C2-C1-C3	-4.87	102.67	107.80
6	D	8001	STD	C10-C13-C16	4.34	122.69	115.55
6	D	8001	STD	C2-C1-C3	-4.32	103.25	107.80
6	D	8001	STD	O2-C2-N1	-3.67	118.39	126.47
6	N	8002	STD	O2-C2-N1	-3.60	118.56	126.47
6	D	8001	STD	O4-C4-N1	3.58	109.83	105.92
6	N	8002	STD	O4-C4-N1	3.41	109.64	105.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	8001	STD	O2-C2-C1	-3.26	122.49	130.61
6	D	8001	STD	C12-C15-C26	3.26	116.53	111.76
6	N	8002	STD	C10-C13-C16	3.19	120.80	115.55
6	D	8001	STD	C7-C6-C5	3.19	127.77	122.45
6	N	8002	STD	O2-C2-C1	-3.06	123.01	130.61
6	N	8002	STD	C12-C15-C26	2.81	115.87	111.76
6	N	8002	STD	O5-C19-C29	2.78	107.99	105.64
6	N	8002	STD	C7-C6-C5	2.73	127.01	122.45
6	D	8001	STD	O5-C19-C29	2.17	107.47	105.64

There are no chirality outliers.

All (28) torsion outliers are listed below:

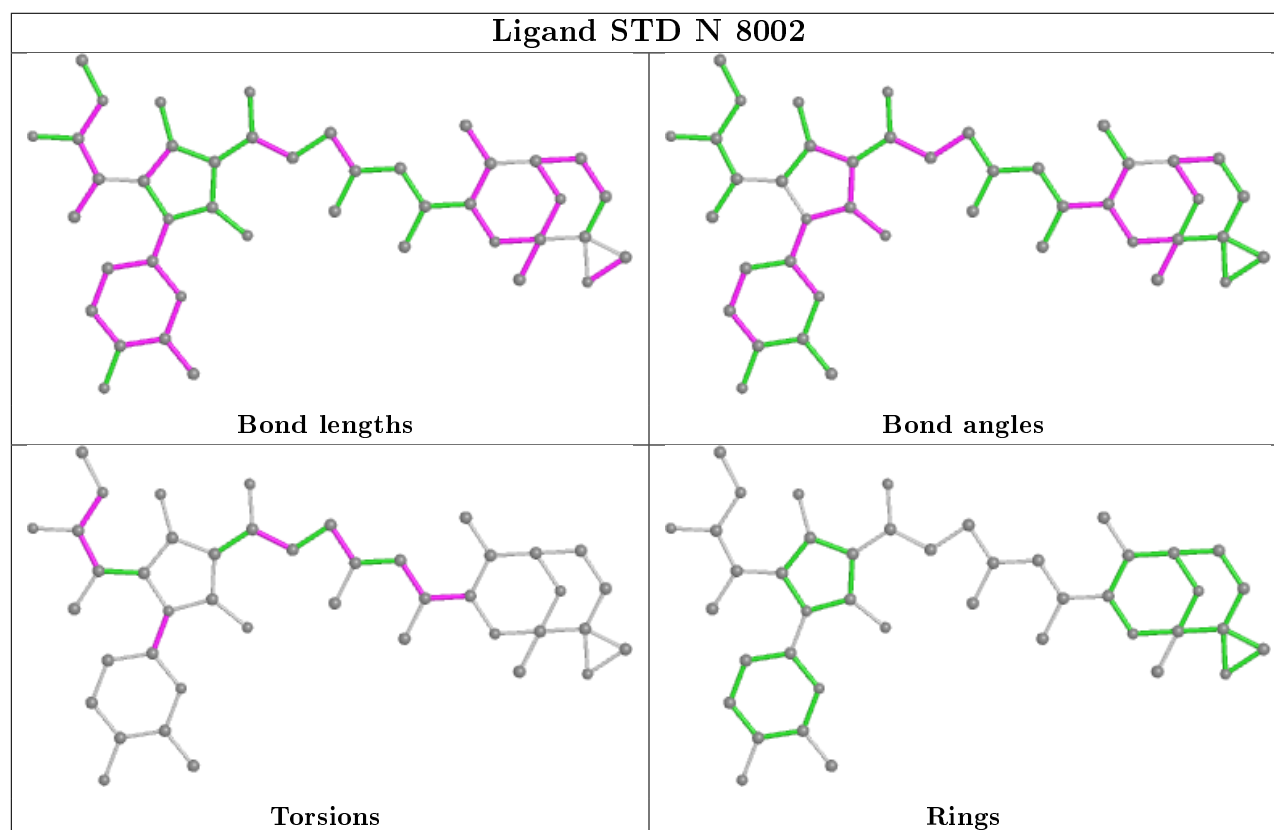
Mol	Chain	Res	Type	Atoms
6	D	8001	STD	O4-C4-N1-C20
6	D	8001	STD	C1-C5-C6-C7
6	D	8001	STD	O3-C5-C6-C7
6	D	8001	STD	C9-C10-C13-C16
6	D	8001	STD	C9-C10-C13-O5
6	D	8001	STD	C14-C10-C13-C16
6	D	8001	STD	C14-C10-C13-O5
6	D	8001	STD	C21-C22-N2-C24
6	D	8001	STD	O6-C22-N2-C24
6	N	8002	STD	O4-C4-N1-C20
6	N	8002	STD	C1-C5-C6-C7
6	N	8002	STD	O3-C5-C6-C7
6	N	8002	STD	C9-C10-C13-C16
6	N	8002	STD	C9-C10-C13-O5
6	N	8002	STD	C14-C10-C13-C16
6	N	8002	STD	C14-C10-C13-O5
6	N	8002	STD	C21-C22-N2-C24
6	N	8002	STD	O6-C22-N2-C24
6	D	8001	STD	C6-C7-C8-C11
6	N	8002	STD	C6-C7-C8-C9
6	N	8002	STD	C6-C7-C8-C11
6	D	8001	STD	C6-C7-C8-C9
6	N	8002	STD	C14-C10-C9-C8
6	N	8002	STD	C13-C10-C9-C8
6	N	8002	STD	C23-C21-C22-O6
6	D	8001	STD	C13-C10-C9-C8
6	D	8001	STD	C14-C10-C9-C8
6	N	8002	STD	C12-C4-N1-C2

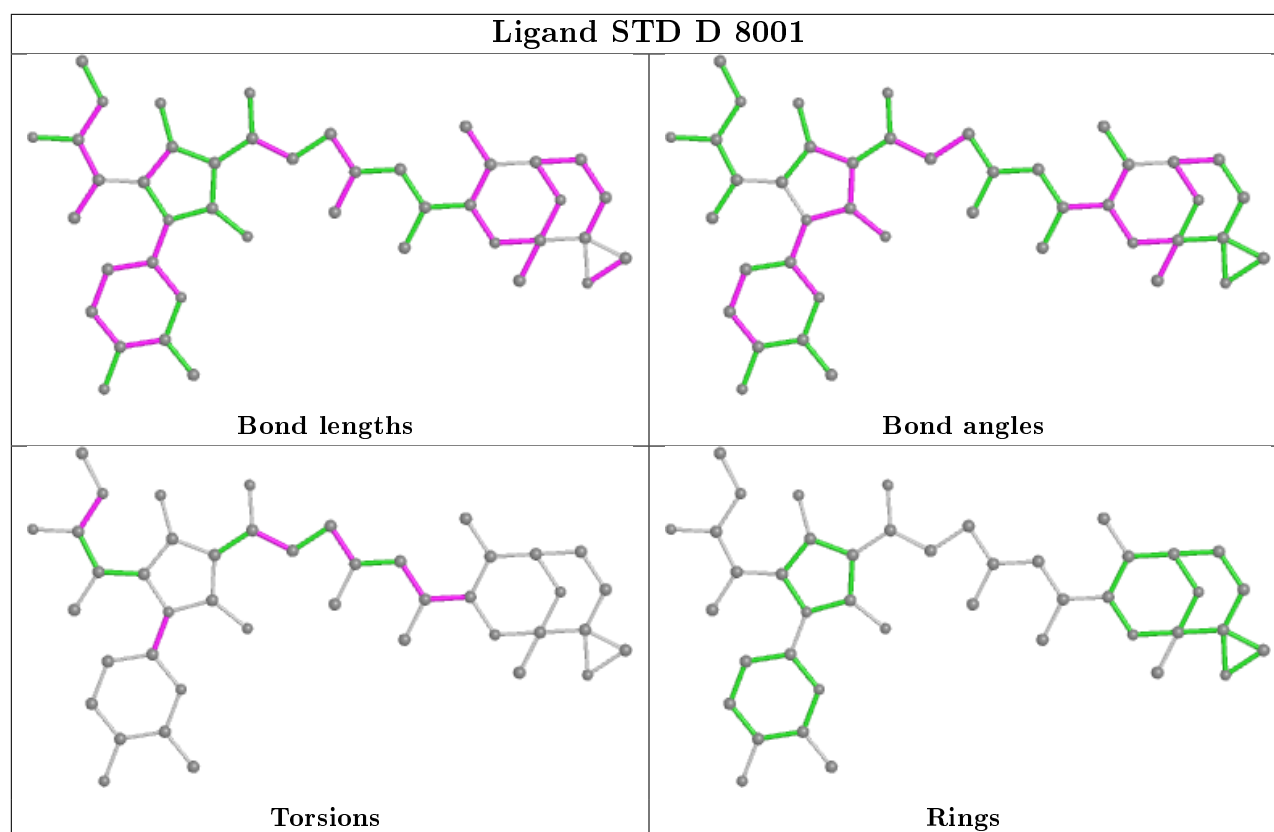
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	8002	STD	6	0
6	D	8001	STD	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	229/315 (72%)	2.28	66 (28%) 0 0	31, 63, 90, 117	0
1	B	229/315 (72%)	2.69	74 (32%) 0 0	53, 90, 112, 118	0
1	K	229/315 (72%)	1.53	59 (25%) 0 0	33, 62, 87, 122	0
1	L	229/315 (72%)	3.11	82 (35%) 0 0	50, 87, 110, 125	0
2	C	1119/1119 (100%)	3.16	424 (37%) 0 0	25, 78, 104, 116	0
2	M	1119/1119 (100%)	2.82	396 (35%) 0 0	23, 72, 104, 115	0
3	D	1381/1524 (90%)	1.84	357 (25%) 0 0	27, 67, 107, 119	0
3	N	1381/1524 (90%)	1.85	373 (27%) 0 0	27, 68, 108, 120	0
4	E	95/99 (95%)	1.87	28 (29%) 0 0	44, 81, 108, 128	0
4	O	95/99 (95%)	1.95	32 (33%) 0 0	44, 75, 93, 105	0
5	F	345/423 (81%)	3.54	146 (42%) 0 0	55, 84, 107, 122	0
5	P	345/423 (81%)	3.06	129 (37%) 0 0	62, 84, 108, 116	0
All	All	6796/7590 (89%)	2.45	2166 (31%) 0 0	23, 73, 106, 128	0

All (2166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	405	ASP	71.3
3	N	406	ASP	57.5
1	A	1	MET	54.5
3	D	853	VAL	52.8
3	N	407	VAL	49.0
3	D	854	ALA	48.9
2	M	729	LEU	48.4
2	C	729	LEU	47.3
5	F	359	SER	47.0
3	N	408	GLU	45.9
2	M	227	PHE	45.8

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Mol	Chain	Res	Type	RSRZ
2	C	1001	VAL	44.3
1	A	2	LEU	43.1
2	C	513	VAL	42.2
3	D	852	ALA	41.9
3	D	855	HIS	41.2
2	C	510	ALA	41.0
5	P	414	ARG	39.3
4	E	49	GLN	38.2
2	M	115	LEU	37.5
2	C	1023	GLY	37.3
2	C	181	VAL	37.0
3	N	404	GLU	36.9
2	C	1000	MET	35.9
3	D	407	VAL	35.7
5	P	415	THR	35.7
1	L	94	LEU	34.8
2	C	194	VAL	34.5
1	L	96	THR	34.1
1	B	118	ALA	34.1
2	C	182	VAL	33.3
2	M	195	LEU	33.2
2	M	152	PRO	32.7
2	C	512	ARG	32.4
3	N	870	GLY	32.2
2	M	1001	VAL	31.9
2	M	1023	GLY	31.9
5	P	182	ALA	31.1
2	C	192	PRO	30.9
1	B	150	TYR	30.8
2	C	509	ALA	30.8
2	C	180	GLY	30.7
2	C	1024	LYS	30.7
1	L	189	ARG	30.6
2	M	223	ASP	30.1
1	L	188	GLN	30.0
5	F	182	ALA	29.6
2	M	228	ALA	29.5
2	C	153	ALA	29.4
3	D	851	LEU	29.3
5	F	386	VAL	29.2
2	C	730	SER	29.0
2	M	1	MET	29.0

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Mol	Chain	Res	Type	RSRZ
2	M	1024	LYS	28.7
3	N	238	PRO	28.6
2	M	18	LEU	28.5
5	F	423	ASP	28.3
5	F	186	HIS	28.2
5	P	186	HIS	28.2
3	D	530	VAL	28.1
4	E	2	ALA	28.1
2	C	223	ASP	27.9
5	F	90	GLN	27.8
3	N	403	PHE	27.5
1	L	93	SER	27.2
3	D	67	ARG	27.1
2	C	763	GLY	27.0
2	M	192	PRO	26.9
3	N	235	ALA	26.7
2	M	17	PRO	26.6
2	C	1	MET	26.5
1	A	157	GLY	26.5
2	M	224	GLU	26.4
1	A	155	LYS	26.2
2	C	224	GLU	26.2
1	A	6	LEU	26.0
2	C	195	LEU	25.9
2	M	226	VAL	25.8
5	P	183	ALA	25.4
3	D	850	LEU	25.4
3	N	530	VAL	25.4
1	B	126	ASP	25.2
5	F	421	PHE	25.1
2	M	116	GLY	24.8
3	D	403	PHE	24.6
2	M	114	PHE	24.5
3	N	1070	TYR	24.5
3	D	440	VAL	24.4
2	C	556	ASN	24.3
5	F	394	ARG	24.2
5	F	360	LYS	24.1
1	L	118	ALA	23.9
3	D	401	TYR	23.8
2	M	730	SER	23.8
2	M	180	GLY	23.8

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Mol	Chain	Res	Type	RSRZ
4	O	49	GLN	23.7
1	K	155	LYS	23.5
5	F	419	ARG	23.3
2	M	153	ALA	23.3
5	P	394	ARG	23.2
5	F	387	GLY	23.2
2	C	728	HIS	23.0
5	P	416	ARG	23.0
2	M	171	TRP	22.9
1	B	149	GLY	22.8
2	M	377	PRO	22.8
2	M	1000	MET	22.7
2	M	230	ARG	22.7
2	C	1077	PRO	22.7
5	P	102	LEU	22.6
2	C	17	PRO	22.3
3	N	531	ASP	22.2
3	D	849	ALA	22.1
3	D	531	ASP	22.1
2	M	231	PRO	22.0
5	P	386	VAL	22.0
2	C	511	GLU	21.9
1	L	157	GLY	21.6
5	F	91	VAL	21.6
3	D	416	ALA	21.5
2	C	21	ILE	21.5
2	M	182	VAL	21.4
2	C	20	GLU	21.4
3	D	1505	ALA	21.4
3	N	1251	ASP	21.3
3	N	853	VAL	21.3
3	D	159	ARG	21.3
5	F	183	ALA	21.0
2	M	194	VAL	21.0
3	N	409	VAL	21.0
1	L	185	ARG	21.0
5	F	415	THR	21.0
2	C	152	PRO	21.0
1	L	159	LYS	20.9
1	A	156	HIS	20.8
3	N	239	GLY	20.8
2	C	196	LEU	20.6

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Mol	Chain	Res	Type	RSRZ
2	M	375	SER	20.6
2	M	191	PHE	20.5
1	B	159	LYS	20.5
3	D	588	GLY	20.5
2	C	1002	GLU	20.4
1	L	190	THR	20.4
5	P	419	ARG	20.3
3	N	871	LYS	20.2
1	B	148	VAL	20.1
2	M	590	ASP	20.0
2	M	513	VAL	19.9
2	M	1077	PRO	19.7
3	D	417	PRO	19.7
3	D	640	HIS	19.6
2	C	16	PRO	19.6
2	M	95	TYR	19.5
3	N	640	HIS	19.5
2	M	19	THR	19.4
4	O	2	ALA	19.4
2	M	1118	LYS	19.4
5	P	180	GLY	19.4
2	M	234	ALA	19.3
2	C	82	GLU	19.2
3	D	156	GLU	19.1
3	N	944	THR	19.1
5	P	105	LYS	19.0
3	D	1342	GLU	18.9
5	P	421	PHE	18.9
2	M	510	ALA	18.9
2	M	181	VAL	18.8
5	F	121	GLY	18.5
2	M	199	VAL	18.5
3	N	534	ARG	18.5
2	C	376	ARG	18.3
2	M	728	HIS	18.2
3	D	364	GLY	18.2
3	D	532	GLY	18.1
1	B	46	SER	18.1
2	C	220	GLY	18.1
2	M	1002	GLU	18.0
2	M	558	ALA	18.0
2	M	512	ARG	18.0

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Mol	Chain	Res	Type	RSRZ
2	C	553	ASP	17.9
2	C	525	SER	17.8
5	F	393	THR	17.8
3	D	856	GLY	17.7
2	M	198	ARG	17.6
1	L	158	ILE	17.6
1	B	188	GLN	17.4
3	N	137	PRO	17.3
2	M	94	LEU	17.3
1	B	119	ASP	17.3
2	C	555	ALA	17.3
2	C	524	VAL	17.2
3	D	1070	TYR	17.2
2	C	764	GLU	17.2
2	M	983	ILE	17.2
1	L	119	ASP	17.2
3	D	441	ARG	17.1
1	B	157	GLY	17.0
3	N	1316	GLY	17.0
1	L	91	ASN	17.0
5	F	391	GLY	17.0
2	M	560	MET	16.9
5	F	102	LEU	16.9
1	K	31	GLY	16.8
3	D	1504	GLU	16.7
3	N	163	TYR	16.7
2	C	514	VAL	16.7
3	D	405	ASP	16.7
3	D	505	SER	16.6
3	D	400	VAL	16.6
3	N	236	TYR	16.6
2	C	504	GLU	16.6
2	C	1118	LYS	16.5
2	C	379	GLU	16.5
2	C	18	LEU	16.5
3	D	585	GLY	16.5
3	N	1073	SER	16.4
5	P	101	GLU	16.4
1	A	126	ASP	16.3
3	D	1341	PRO	16.2
2	C	559	LEU	16.2
2	C	375	SER	16.2

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Mol	Chain	Res	Type	RSRZ
2	C	560	MET	16.2
3	N	696	HIS	16.1
3	D	442	ASN	16.0
3	D	1251	ASP	15.9
2	C	19	THR	15.9
1	L	160	ASP	15.8
5	P	359	SER	15.8
2	C	193	LEU	15.8
2	C	169	GLY	15.8
3	N	595	GLY	15.8
5	F	390	PHE	15.8
2	M	1065	ALA	15.8
2	C	663	ASN	15.7
3	D	534	ARG	15.7
3	N	854	ALA	15.7
3	N	594	PRO	15.7
5	P	90	GLN	15.6
2	M	555	ALA	15.6
2	C	165	LEU	15.6
2	C	15	LEU	15.6
1	K	128	HIS	15.6
2	M	16	PRO	15.5
2	M	1025	ALA	15.5
2	C	981	GLU	15.4
1	L	184	THR	15.4
2	M	219	GLN	15.4
2	C	191	PHE	15.4
5	F	136	LEU	15.4
1	L	95	GLN	15.3
3	D	1408	ILE	15.3
1	B	125	PRO	15.2
3	D	586	ARG	15.2
1	B	151	VAL	15.2
5	F	414	ARG	15.2
3	D	439	LEU	15.2
3	D	1340	GLY	15.1
2	C	586	ARG	15.1
2	M	229	MET	15.0
3	D	1316	GLY	15.0
5	P	334	PRO	15.0
2	C	168	ARG	15.0
1	K	126	ASP	14.8

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Mol	Chain	Res	Type	RSRZ
3	N	717	GLN	14.8
1	K	30	ARG	14.7
3	N	237	LYS	14.7
2	M	1062	GLY	14.6
3	N	533	GLY	14.5
1	L	92	PRO	14.5
2	C	114	PHE	14.5
5	P	179	GLU	14.4
2	C	380	ALA	14.3
2	C	589	ARG	14.3
3	N	1066	THR	14.2
3	D	857	ILE	14.2
2	M	984	GLU	14.2
3	N	225	LEU	14.2
1	B	190	THR	14.2
2	M	21	ILE	14.1
2	C	590	ASP	14.1
2	C	221	LEU	14.1
1	L	90	LEU	14.1
3	D	415	VAL	14.1
1	L	126	ASP	14.0
2	C	116	GLY	14.0
2	C	931	GLY	14.0
2	C	155	PRO	14.0
3	N	1408	ILE	14.0
2	M	380	ALA	14.0
3	N	641	GLN	14.0
1	A	159	LYS	13.9
3	D	1503	VAL	13.9
3	D	717	GLN	13.9
2	C	171	TRP	13.9
5	P	135	ILE	13.8
2	M	233	GLU	13.8
5	P	413	SER	13.8
3	D	696	HIS	13.8
2	M	522	VAL	13.8
2	C	1075	ASP	13.8
5	F	145	PRO	13.7
5	P	333	ILE	13.7
5	F	336	GLU	13.6
2	M	225	SER	13.5
5	F	334	PRO	13.5

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Mol	Chain	Res	Type	RSRZ
2	M	559	LEU	13.4
5	F	245	GLN	13.4
3	N	869	MET	13.4
3	D	858	VAL	13.3
3	N	532	GLY	13.3
2	M	23	VAL	13.3
2	C	881	ASN	13.2
5	F	95	THR	13.2
2	M	523	ILE	13.2
2	C	558	ALA	13.1
2	C	166	PRO	13.1
1	K	156	HIS	13.1
3	D	235	ALA	13.1
2	M	931	GLY	13.0
3	D	533	GLY	13.0
5	F	185	GLN	13.0
1	K	32	PHE	13.0
3	D	233	LYS	13.0
2	C	732	ALA	12.9
2	M	379	GLU	12.9
1	B	189	ARG	12.9
5	F	94	LEU	12.9
2	C	983	ILE	12.9
2	M	981	GLU	12.9
3	D	238	PRO	12.9
2	C	79	PRO	12.8
3	N	852	ALA	12.8
2	C	765	SER	12.8
5	F	93	LEU	12.8
5	F	181	GLU	12.8
2	C	507	ARG	12.8
2	C	523	ILE	12.8
3	D	157	GLU	12.8
2	C	461	VAL	12.7
1	B	158	ILE	12.7
1	L	161	ARG	12.7
2	M	179	ASN	12.6
2	C	554	ASP	12.6
2	M	221	LEU	12.6
3	D	1073	SER	12.6
2	C	183	SER	12.6
2	M	220	GLY	12.6

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Mol	Chain	Res	Type	RSRZ
1	L	191	ASP	12.5
2	C	762	LYS	12.5
2	M	196	LEU	12.5
2	M	155	PRO	12.5
3	N	1437	ALA	12.5
1	B	162	ILE	12.5
3	D	408	GLU	12.4
2	C	464	LEU	12.4
5	P	245	GLN	12.4
3	N	1442	ASN	12.3
2	C	23	VAL	12.3
1	A	128	HIS	12.3
2	M	113	VAL	12.3
3	D	594	PRO	12.2
1	A	158	ILE	12.2
2	M	235	LEU	12.2
1	B	185	ARG	12.2
3	N	855	HIS	12.2
2	C	234	ALA	12.1
5	P	94	LEU	12.1
3	N	159	ARG	12.1
2	C	164	PRO	12.1
1	L	162	ILE	12.0
2	C	251	ASP	12.0
1	A	153	ALA	12.0
3	N	1285	GLU	12.0
1	B	184	THR	12.0
2	M	186	VAL	12.0
5	F	283	GLY	11.9
5	P	75	ILE	11.7
5	P	423	ASP	11.7
3	N	867	ARG	11.7
2	M	553	ASP	11.6
2	M	982	PRO	11.6
2	C	557	ARG	11.6
5	F	358	LEU	11.5
5	P	145	PRO	11.5
3	N	1441	GLN	11.5
2	C	1022	GLY	11.5
3	D	562	ALA	11.5
2	M	979	THR	11.5
3	N	588	GLY	11.5

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Mol	Chain	Res	Type	RSRZ
2	M	48	PHE	11.4
1	B	155	LYS	11.4
2	M	511	GLU	11.4
2	M	589	ARG	11.3
3	N	505	SER	11.3
3	N	156	GLU	11.3
3	D	843	PHE	11.3
1	A	16	GLN	11.3
3	D	154	THR	11.2
4	O	3	GLU	11.2
4	E	48	MET	11.2
3	D	860	LEU	11.2
2	C	1025	ALA	11.2
2	M	232	GLU	11.2
3	N	552	ASN	11.2
3	D	1409	ALA	11.2
3	N	597	ASP	11.1
2	C	227	PHE	11.1
2	C	198	ARG	11.1
2	C	731	GLU	11.1
2	M	554	ASP	11.1
3	N	1317	ASP	11.1
2	C	1078	GLU	11.1
3	N	415	VAL	11.0
3	N	364	GLY	11.0
2	M	172	ILE	11.0
1	L	187	GLY	10.9
1	A	154	GLU	10.8
2	M	1075	ASP	10.8
2	C	37	GLU	10.8
3	D	1337	GLU	10.7
2	M	378	LEU	10.7
5	F	413	SER	10.7
2	C	1076	VAL	10.7
3	D	1404	ASN	10.7
5	F	146	GLY	10.7
1	A	151	VAL	10.6
2	C	335	THR	10.6
5	F	180	GLY	10.6
1	B	117	VAL	10.6
2	M	627	ARG	10.6
2	C	43	GLY	10.6

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Mol	Chain	Res	Type	RSRZ
4	E	3	GLU	10.6
3	N	1341	PRO	10.6
5	P	103	ALA	10.6
3	N	697	GLY	10.5
2	C	1074	GLU	10.5
3	N	858	VAL	10.5
2	M	178	PRO	10.5
2	M	417	GLY	10.5
3	D	638	LYS	10.5
2	C	170	PRO	10.5
2	M	184	MET	10.5
3	N	945	SER	10.4
2	C	377	PRO	10.4
1	B	156	HIS	10.4
3	D	641	GLN	10.3
2	M	164	PRO	10.3
2	C	167	LYS	10.3
3	N	872	ARG	10.3
2	C	85	GLU	10.2
2	M	1022	GLY	10.2
5	P	136	LEU	10.2
2	M	556	ASN	10.2
2	C	1117	SER	10.2
2	M	933	GLY	10.2
2	M	163	ILE	10.2
1	A	152	PRO	10.1
2	M	15	LEU	10.1
3	N	1342	GLU	10.1
1	A	5	LYS	10.1
2	C	81	ASP	10.0
3	N	868	TYR	10.0
5	F	74	LYS	10.0
1	B	182	GLU	10.0
1	K	157	GLY	10.0
3	N	1050	GLY	10.0
5	F	355	GLU	10.0
2	C	717	LEU	10.0
5	F	241	TRP	9.9
5	P	91	VAL	9.9
5	F	120	THR	9.9
2	C	222	MET	9.9
3	D	1049	SER	9.9

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Mol	Chain	Res	Type	RSRZ
2	C	24	GLU	9.9
2	M	347	GLY	9.9
3	N	1358	ALA	9.9
3	N	1340	GLY	9.8
2	M	93	PRO	9.8
2	C	522	VAL	9.8
3	N	844	ALA	9.8
3	D	697	GLY	9.8
2	M	1076	VAL	9.8
2	C	47	ALA	9.7
2	C	979	THR	9.7
5	F	179	GLU	9.7
2	C	984	GLU	9.7
5	F	285	GLU	9.7
2	M	732	ALA	9.7
5	P	332	PHE	9.7
3	D	944	THR	9.7
3	D	1129	THR	9.7
5	P	89	GLY	9.7
5	P	335	ASP	9.7
2	M	557	ARG	9.6
3	N	230	TRP	9.6
2	C	184	MET	9.6
4	O	47	LYS	9.6
2	M	20	GLU	9.6
2	C	782	ALA	9.6
3	N	1343	ALA	9.6
3	D	365	ASP	9.5
5	F	184	ARG	9.5
4	O	94	PRO	9.5
2	M	170	PRO	9.5
3	D	402	PRO	9.5
3	D	1419	PRO	9.5
2	C	219	GLN	9.5
3	N	859	ASP	9.5
2	C	885	ILE	9.5
5	P	181	GLU	9.5
2	M	1061	GLU	9.4
2	M	49	ARG	9.4
2	C	14	PRO	9.4
2	M	183	SER	9.4
1	B	42	ARG	9.4

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Mol	Chain	Res	Type	RSRZ
2	M	169	GLY	9.4
3	N	160	GLU	9.4
3	D	155	ASP	9.4
2	C	338	GLU	9.4
4	O	48	MET	9.4
1	A	108	GLU	9.3
5	P	144	ILE	9.3
1	L	97	VAL	9.3
5	P	385	GLU	9.3
2	M	950	LEU	9.2
3	D	589	ALA	9.2
2	M	167	LYS	9.2
2	C	441	VAL	9.2
2	M	441	VAL	9.2
5	F	135	ILE	9.2
2	M	173	ASP	9.2
5	F	119	ILE	9.1
1	K	127	LEU	9.1
5	F	363	GLU	9.1
5	F	416	ARG	9.1
3	N	1072	ILE	9.0
3	N	528	VAL	9.0
3	D	418	GLY	9.0
2	C	508	ILE	9.0
2	M	238	LEU	9.0
2	M	550	LEU	9.0
3	N	227	LEU	9.0
2	M	350	ARG	9.0
2	M	675	ALA	9.0
3	N	1074	SER	9.0
3	D	108	VAL	9.0
5	F	105	LYS	8.9
3	D	808	THR	8.9
3	N	638	LYS	8.9
1	L	183	ASP	8.9
2	C	172	ILE	8.9
5	P	315	VAL	8.9
3	D	1336	LEU	8.9
1	K	159	LYS	8.9
5	F	335	ASP	8.9
2	C	115	LEU	8.8
3	N	1315	ASP	8.8

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Mol	Chain	Res	Type	RSRZ
2	C	225	SER	8.8
2	C	46	ALA	8.8
2	M	1066	ALA	8.8
1	B	187	GLY	8.8
1	B	152	PRO	8.8
3	D	1065	LEU	8.8
5	P	344	ALA	8.8
1	B	191	ASP	8.8
2	C	25	SER	8.8
5	P	241	TRP	8.8
2	M	586	ARG	8.7
3	N	1051	GLU	8.7
3	N	240	GLU	8.7
3	N	1337	GLU	8.7
5	P	393	THR	8.7
2	C	675	ALA	8.7
3	D	1442	ASN	8.6
3	D	1418	LYS	8.6
3	D	438	ASP	8.6
2	M	222	MET	8.6
3	D	946	GLY	8.6
2	C	1065	ALA	8.6
3	D	1400	VAL	8.5
5	P	363	GLU	8.5
5	P	121	GLY	8.5
3	D	859	ASP	8.5
1	A	31	GLY	8.5
2	C	1003	ASP	8.4
3	D	561	GLY	8.4
2	C	502	PRO	8.4
2	M	946	ARG	8.4
2	C	381	ALA	8.4
2	M	731	GLU	8.3
3	D	234	GLU	8.3
2	C	228	ALA	8.3
3	N	849	ALA	8.3
1	B	127	LEU	8.3
5	P	93	LEU	8.3
3	D	230	TRP	8.3
3	N	873	LEU	8.3
3	N	1286	THR	8.2
3	N	1014	ASN	8.2

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Mol	Chain	Res	Type	RSRZ
5	P	106	VAL	8.2
2	M	1064	ASN	8.2
2	M	778	PHE	8.2
3	D	867	ARG	8.2
3	D	719	VAL	8.2
3	N	856	GLY	8.2
2	M	376	ARG	8.1
2	M	117	HIS	8.1
1	K	77	GLU	8.1
3	D	163	TYR	8.1
3	D	1317	ASP	8.1
2	M	193	LEU	8.1
3	N	226	PRO	8.1
3	D	1360	GLY	8.1
3	D	548	ILE	8.1
1	B	47	SER	8.1
3	D	66	GLN	8.1
5	P	98	GLU	8.1
5	P	104	ARG	8.0
1	L	125	PRO	8.0
5	F	89	GLY	8.0
3	N	555	LYS	8.0
1	A	216	GLU	8.0
2	C	283	ILE	8.0
2	C	378	LEU	8.0
3	D	945	SER	8.0
3	D	552	ASN	7.9
4	E	95	GLY	7.9
5	P	283	GLY	7.9
1	L	186	LEU	7.9
2	M	151	ASP	7.9
5	P	185	GLN	7.9
3	D	20	SER	7.9
5	P	184	ARG	7.8
3	N	1069	GLU	7.8
2	C	238	LEU	7.8
2	C	1004	LYS	7.8
3	N	1239	ARG	7.8
5	F	204	GLY	7.8
3	D	223	LEU	7.8
3	D	430	ASP	7.8
1	L	117	VAL	7.8

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Mol	Chain	Res	Type	RSRZ
3	D	1074	SER	7.8
3	N	167	GLU	7.8
3	D	529	GLN	7.7
4	E	51	LEU	7.7
3	D	504	ASP	7.7
2	C	208	ALA	7.7
3	N	20	SER	7.7
3	D	1362	LYS	7.7
1	L	42	ARG	7.7
1	B	43	ILE	7.7
2	M	1117	SER	7.7
1	K	151	VAL	7.7
2	M	344	PHE	7.7
2	M	677	MET	7.7
2	M	976	ASP	7.7
2	M	351	LEU	7.6
2	M	251	ASP	7.6
2	C	350	ARG	7.6
3	N	241	ILE	7.6
5	P	384	GLU	7.6
3	N	705	ALA	7.6
3	D	240	GLU	7.6
2	C	624	PRO	7.6
2	M	1038	TRP	7.6
5	F	75	ILE	7.6
1	A	213	GLN	7.6
2	C	515	ALA	7.5
5	P	387	GLY	7.5
5	F	144	ILE	7.5
3	D	236	TYR	7.5
3	N	535	PHE	7.5
3	N	946	GLY	7.5
3	D	587	ARG	7.5
2	C	197	LEU	7.5
2	C	231	PRO	7.5
2	C	817	PRO	7.4
2	C	884	GLN	7.4
2	C	150	PRO	7.4
3	N	1068	LEU	7.4
2	M	203	ASP	7.4
3	N	410	SER	7.4
2	M	775	ARG	7.3

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Mol	Chain	Res	Type	RSRZ
5	F	122	LEU	7.3
2	C	252	LYS	7.3
1	K	110	LYS	7.3
2	M	319	GLY	7.3
2	C	263	ASP	7.3
3	N	845	ASN	7.3
1	A	4	SER	7.3
3	N	1065	LEU	7.3
2	M	514	VAL	7.3
3	D	766	ALA	7.3
2	C	179	ASN	7.3
3	D	1441	GLN	7.3
2	C	561	GLY	7.2
2	M	1078	GLU	7.2
3	N	94	GLU	7.2
3	D	229	ALA	7.2
2	M	782	ALA	7.2
3	D	188	GLY	7.2
3	N	561	GLY	7.2
2	C	674	VAL	7.2
3	D	1072	ILE	7.2
3	D	558	LEU	7.2
3	N	1404	ASN	7.2
5	P	339	PRO	7.2
3	D	237	LYS	7.1
1	K	148	VAL	7.1
1	L	46	SER	7.1
2	C	207	LEU	7.1
2	C	460	ARG	7.1
2	M	793	PRO	7.1
2	M	881	ASN	7.1
3	D	699	VAL	7.1
2	C	173	ASP	7.1
2	M	96	ALA	7.1
5	P	141	VAL	7.1
3	N	504	ASP	7.1
5	F	98	GLU	7.0
3	D	404	GLU	7.0
4	O	52	GLU	7.0
1	A	148	VAL	7.0
3	N	108	VAL	7.0
1	K	216	GLU	6.9

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Mol	Chain	Res	Type	RSRZ
5	P	343	ASP	6.9
2	C	349	ALA	6.9
3	D	1502	ALA	6.9
3	N	157	GLU	6.9
1	L	155	LYS	6.9
3	N	1443	THR	6.9
2	M	72	ARG	6.9
2	M	267	TYR	6.9
2	C	988	VAL	6.9
3	N	857	ILE	6.9
3	N	1252	ILE	6.8
3	D	406	ASP	6.8
3	N	414	ARG	6.8
3	D	870	GLY	6.8
3	D	979	GLU	6.8
2	C	716	LYS	6.8
5	F	361	LEU	6.8
3	N	1049	SER	6.8
2	C	232	GLU	6.7
2	C	775	ARG	6.7
2	C	844	GLY	6.7
3	N	1344	VAL	6.7
2	M	980	GLY	6.7
3	N	791	TYR	6.7
2	C	796	GLU	6.7
3	N	850	LEU	6.6
3	N	860	LEU	6.6
1	L	216	GLU	6.6
2	M	165	LEU	6.6
5	F	86	HIS	6.6
3	N	1360	GLY	6.6
2	M	252	LYS	6.6
3	N	947	ILE	6.6
3	D	1128	VAL	6.6
5	F	147	LEU	6.6
5	F	356	LYS	6.6
2	M	14	PRO	6.6
1	A	107	LYS	6.6
1	A	110	LYS	6.6
2	M	185	LYS	6.5
3	D	877	PRO	6.5
3	N	1440	PHE	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	45	LEU	6.5
2	C	618	GLY	6.5
2	C	784	ASP	6.5
2	C	235	LEU	6.5
4	O	77	GLU	6.5
3	N	138	LYS	6.5
2	M	374	ASN	6.5
3	N	1409	ALA	6.5
1	K	152	PRO	6.5
2	M	123	GLU	6.5
5	F	332	PHE	6.5
5	F	177	ALA	6.5
1	B	120	VAL	6.5
2	C	982	PRO	6.5
5	P	336	GLU	6.5
1	L	156	HIS	6.5
2	M	618	GLY	6.5
5	P	329	TYR	6.5
3	N	851	LEU	6.5
3	D	1343	ALA	6.5
3	D	583	ASP	6.5
2	M	461	VAL	6.5
4	O	95	GLY	6.5
1	K	29	GLU	6.5
1	L	192	LEU	6.5
3	N	1129	THR	6.5
3	D	1315	ASP	6.5
5	F	420	ASP	6.5
2	C	226	VAL	6.4
5	F	141	VAL	6.4
2	C	199	VAL	6.4
1	K	67	THR	6.4
3	D	639	LEU	6.4
3	N	430	ASP	6.4
3	N	1434	TRP	6.4
3	N	586	ARG	6.4
2	M	144	PRO	6.4
2	M	175	GLU	6.4
3	D	69	GLU	6.4
2	M	348	LEU	6.3
3	D	137	PRO	6.3
5	F	357	ALA	6.3

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Mol	Chain	Res	Type	RSRZ
3	N	18	ILE	6.3
3	N	556	LYS	6.3
5	F	101	GLU	6.3
5	P	348	SER	6.3
2	C	665	PHE	6.3
2	C	706	GLU	6.3
5	P	360	LYS	6.3
2	M	79	PRO	6.3
5	P	355	GLU	6.3
3	N	154	THR	6.3
3	N	1336	LEU	6.3
4	E	94	PRO	6.3
5	F	338	LEU	6.3
2	C	933	GLY	6.3
3	N	1444	THR	6.2
2	C	999	HIS	6.2
3	D	773	ALA	6.2
3	N	96	ALA	6.2
1	B	116	PRO	6.2
1	L	123	MET	6.2
2	C	781	LYS	6.2
3	D	848	GLU	6.2
2	M	561	GLY	6.2
2	C	42	VAL	6.2
2	C	342	ASP	6.2
2	M	268	ASP	6.2
2	C	255	ALA	6.2
3	N	585	GLY	6.2
5	P	410	TYR	6.2
3	D	980	MET	6.2
2	C	676	ILE	6.1
3	N	224	ARG	6.1
3	N	229	ALA	6.1
3	D	1050	GLY	6.1
5	F	249	ARG	6.1
3	D	845	ASN	6.1
5	P	74	LYS	6.1
3	N	846	PRO	6.1
2	C	880	MET	6.1
1	B	183	ASP	6.1
5	F	389	PHE	6.1
2	M	1074	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
2	C	550	LEU	6.0
1	A	118	ALA	6.0
1	A	3	ASP	6.0
5	P	411	HIS	6.0
1	B	112	ARG	6.0
5	F	248	ASN	6.0
2	M	166	PRO	6.0
3	N	1013	GLU	6.0
3	D	755	ALA	6.0
2	M	112	GLU	5.9
2	M	1079	PRO	5.9
2	M	1026	GLN	5.9
2	C	811	PRO	5.9
1	A	130	ALA	5.9
2	C	250	ARG	5.9
1	B	90	LEU	5.9
2	M	844	GLY	5.9
1	B	124	ASN	5.9
3	D	556	LYS	5.9
3	D	695	ILE	5.9
2	M	92	ALA	5.9
5	F	281	GLU	5.9
1	K	81	ASN	5.9
2	C	333	ILE	5.9
2	C	932	GLU	5.9
3	D	167	GLU	5.9
3	D	1239	ARG	5.8
2	M	75	GLU	5.8
2	M	46	ALA	5.8
3	D	241	ILE	5.8
2	C	795	GLY	5.8
3	N	719	VAL	5.8
3	D	861	GLN	5.8
1	B	161	ARG	5.8
3	N	122	GLU	5.8
2	C	673	LEU	5.8
2	M	47	ALA	5.8
1	A	217	ILE	5.8
2	C	345	ARG	5.8
2	C	465	GLY	5.8
2	M	74	GLY	5.8
2	C	526	PRO	5.8

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Mol	Chain	Res	Type	RSRZ
2	C	463	GLU	5.8
3	D	160	GLU	5.8
5	F	422	LEU	5.8
1	L	219	ARG	5.8
2	C	233	GLU	5.8
2	C	1066	ALA	5.8
1	K	35	THR	5.8
2	C	204	GLN	5.7
2	M	381	ALA	5.7
3	N	1438	ALA	5.7
1	B	160	ASP	5.7
3	D	1252	ILE	5.7
3	D	443	VAL	5.7
1	A	214	ALA	5.7
1	B	186	LEU	5.7
1	K	80	LEU	5.7
2	C	100	LEU	5.7
1	A	189	ARG	5.7
2	C	163	ILE	5.7
5	P	338	LEU	5.7
3	D	595	GLY	5.7
2	M	187	ASN	5.7
2	M	283	ILE	5.7
5	P	140	ARG	5.6
2	C	445	GLU	5.6
2	C	627	ARG	5.6
1	A	109	VAL	5.6
3	N	1446	VAL	5.6
3	D	1288	GLU	5.6
3	D	551	ASN	5.6
3	D	1480	PHE	5.6
5	F	87	GLU	5.6
3	D	756	GLN	5.6
5	P	340	SER	5.6
2	C	664	GLY	5.6
1	L	88	ARG	5.6
2	M	464	LEU	5.6
2	M	674	VAL	5.6
2	M	1004	LYS	5.6
3	D	1314	LYS	5.6
2	M	353	ARG	5.5
3	D	753	SER	5.5

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Mol	Chain	Res	Type	RSRZ
3	N	551	ASN	5.5
1	K	219	ARG	5.5
2	C	462	ASP	5.5
2	C	552	HIS	5.5
2	M	77	PRO	5.5
2	C	786	LYS	5.5
3	D	847	ASP	5.5
3	N	1287	GLU	5.5
5	F	384	GLU	5.5
1	A	106	PRO	5.5
2	C	793	PRO	5.5
3	D	1066	THR	5.4
3	N	121	THR	5.4
1	L	217	ILE	5.4
2	C	987	ILE	5.4
1	K	34	VAL	5.4
3	N	752	SER	5.4
1	K	33	GLY	5.4
2	C	185	LYS	5.4
1	K	154	GLU	5.4
2	M	265	ARG	5.4
5	P	95	THR	5.4
2	C	64	LEU	5.4
5	P	86	HIS	5.4
5	P	281	GLU	5.4
2	C	625	LEU	5.4
3	D	844	ALA	5.4
3	D	1361	VAL	5.4
5	P	302	LYS	5.4
3	N	695	ILE	5.4
2	C	662	GLU	5.3
3	D	615	ARG	5.3
3	N	562	ALA	5.3
3	N	1159	ARG	5.3
2	M	44	ILE	5.3
2	M	987	ILE	5.3
3	D	1444	THR	5.3
2	M	349	ALA	5.3
5	F	103	ALA	5.3
2	C	202	TYR	5.3
2	C	69	LEU	5.3
3	D	752	SER	5.3

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Mol	Chain	Res	Type	RSRZ
2	C	843	HIS	5.3
3	N	19	ARG	5.3
2	M	541	SER	5.3
2	C	603	VAL	5.2
1	L	47	SER	5.2
2	C	86	LYS	5.2
1	A	116	PRO	5.2
5	F	395	GLU	5.2
3	D	225	LEU	5.2
4	O	51	LEU	5.2
2	C	417	GLY	5.2
2	M	346	VAL	5.2
2	M	876	VAL	5.2
3	N	516	ALA	5.2
3	N	1138	ALA	5.2
3	N	980	MET	5.2
5	F	123	ASP	5.2
4	O	78	ASN	5.2
2	M	24	GLU	5.2
5	F	411	HIS	5.2
2	C	359	MET	5.2
3	N	948	THR	5.1
2	C	989	VAL	5.1
1	A	30	ARG	5.1
2	C	950	LEU	5.1
2	C	883	GLY	5.1
3	N	21	TRP	5.1
2	C	346	VAL	5.1
2	M	509	ALA	5.1
3	D	810	GLU	5.1
2	M	168	ARG	5.1
2	M	100	LEU	5.1
2	M	540	PHE	5.1
3	D	1119	SER	5.1
3	N	1445	HIS	5.1
1	L	120	VAL	5.1
2	C	151	ASP	5.1
2	M	591	SER	5.1
4	O	11	GLY	5.1
2	M	949	LYS	5.1
2	M	1042	ALA	5.1
2	M	603	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
3	N	969	ARG	5.1
5	P	322	GLY	5.1
2	C	876	VAL	5.0
3	N	1325	LEU	5.0
3	N	1314	LYS	5.0
2	C	77	PRO	5.0
3	D	776	GLU	5.0
4	E	50	THR	5.0
2	C	175	GLU	5.0
3	D	772	PRO	5.0
3	D	904	VAL	5.0
2	M	542	VAL	5.0
2	M	617	ASP	5.0
3	N	440	VAL	5.0
2	C	766	GLU	5.0
3	D	965	GLU	5.0
2	C	722	ILE	5.0
2	C	41	ASN	5.0
1	B	216	GLU	5.0
5	F	385	GLU	5.0
3	N	1480	PHE	5.0
5	P	420	ASP	4.9
2	C	49	ARG	4.9
3	D	158	TYR	4.9
3	D	547	LEU	4.9
2	M	676	ILE	4.9
3	N	1362	LYS	4.9
3	N	1099	VAL	4.9
3	N	943	THR	4.9
2	M	145	GLY	4.9
2	C	946	ARG	4.9
3	N	675	ARG	4.9
4	E	77	GLU	4.9
2	C	649	VAL	4.9
3	N	1003	VAL	4.9
3	N	1361	VAL	4.9
3	D	958	GLU	4.8
2	C	1012	PRO	4.8
2	M	176	VAL	4.8
3	N	22	SER	4.8
2	M	460	ARG	4.8
3	N	810	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
2	C	727	PRO	4.8
3	D	1003	VAL	4.8
3	N	1158	VAL	4.8
2	C	882	LEU	4.8
3	D	765	SER	4.8
5	P	120	THR	4.8
3	N	93	ILE	4.8
5	F	405	LEU	4.8
3	D	675	ARG	4.8
3	D	70	GLY	4.8
2	C	1027	PHE	4.8
2	M	706	GLU	4.8
3	N	401	TYR	4.8
3	D	698	LYS	4.8
2	M	354	GLY	4.8
3	D	1014	ASN	4.8
2	C	28	ARG	4.8
2	C	267	TYR	4.8
3	D	764	LEU	4.8
5	F	92	PRO	4.8
3	N	1071	PHE	4.8
2	M	64	LEU	4.7
3	N	1210	SER	4.7
2	C	334	ARG	4.7
5	P	92	PRO	4.7
3	N	233	LYS	4.7
3	N	1439	SER	4.7
5	F	300	ASP	4.7
2	C	319	GLY	4.7
2	M	1119	ARG	4.7
2	M	445	GLU	4.7
3	N	1345	GLU	4.7
3	N	1007	VAL	4.7
5	P	249	ARG	4.7
2	C	66	LEU	4.7
2	C	149	THR	4.7
3	N	1067	VAL	4.7
2	C	50	GLU	4.7
2	M	442	GLU	4.7
3	D	239	GLY	4.7
5	F	167	PRO	4.7
2	M	507	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
2	C	123	GLU	4.7
4	O	50	THR	4.7
2	C	761	PHE	4.7
5	F	117	SER	4.7
3	N	1064	GLY	4.6
2	C	1079	PRO	4.6
3	D	909	ASN	4.6
1	L	121	GLU	4.6
2	C	517	ARG	4.6
1	K	66	SER	4.6
2	C	6	PHE	4.6
2	C	249	LYS	4.6
3	D	1345	GLU	4.6
5	P	248	ASN	4.6
2	M	317	VAL	4.6
2	M	932	GLU	4.6
4	E	96	GLU	4.6
5	F	187	LEU	4.6
3	N	1039	CYS	4.6
5	F	312	GLN	4.6
2	M	73	LEU	4.6
2	M	1113	GLU	4.5
4	E	52	GLU	4.5
2	C	1113	GLU	4.5
2	M	985	GLY	4.5
3	N	1128	VAL	4.5
2	M	9	ILE	4.5
3	D	232	GLU	4.5
1	K	130	ALA	4.5
2	M	320	HIS	4.5
3	D	472	ALA	4.5
3	N	536	ALA	4.5
2	C	265	ARG	4.5
1	L	127	LEU	4.5
2	M	455	LEU	4.5
2	C	1080	SER	4.5
2	C	823	VAL	4.5
5	F	262	VAL	4.5
1	A	127	LEU	4.5
3	N	558	LEU	4.5
5	F	96	LEU	4.5
3	N	1017	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
3	D	121	THR	4.5
3	D	379	ALA	4.5
3	N	149	LYS	4.5
3	D	1127	GLU	4.5
3	N	773	ALA	4.4
3	D	864	VAL	4.4
5	F	392	VAL	4.4
5	P	100	VAL	4.4
1	L	138	LEU	4.4
3	D	138	LYS	4.4
3	N	58	CYS	4.4
1	B	192	LEU	4.4
3	N	1223	ILE	4.4
2	M	763	GLY	4.4
3	N	909	ASN	4.4
3	D	1363	LEU	4.4
2	M	177	GLU	4.4
1	K	47	SER	4.4
2	C	1021	LEU	4.4
1	K	14	ARG	4.4
2	C	341	THR	4.4
3	D	1004	THR	4.4
5	P	119	ILE	4.4
3	N	979	GLU	4.4
2	C	841	ASN	4.4
2	M	845	ASN	4.4
3	D	1210	SER	4.4
2	C	629	TYR	4.3
3	N	1346	ARG	4.3
3	D	1325	LEU	4.3
5	F	203	THR	4.3
1	B	142	VAL	4.3
2	M	988	VAL	4.3
3	N	1455	LYS	4.3
1	B	123	MET	4.3
2	C	80	GLN	4.3
3	N	416	ALA	4.3
3	N	1227	GLN	4.3
1	L	150	TYR	4.3
3	D	579	ASP	4.3
2	C	101	ILE	4.3
2	M	101	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
3	D	760	ARG	4.3
3	N	223	LEU	4.3
5	F	137	GLY	4.3
5	P	187	LEU	4.3
3	D	1007	VAL	4.3
3	N	78	VAL	4.3
3	D	1051	GLU	4.3
1	B	41	ARG	4.2
3	N	861	GLN	4.2
3	D	869	MET	4.2
2	M	947	ALA	4.2
1	L	199	ILE	4.2
3	N	548	ILE	4.2
2	C	506	ASN	4.2
2	C	372	LEU	4.2
3	N	799	LYS	4.2
1	B	92	PRO	4.2
2	C	528	GLU	4.2
2	C	1116	ALA	4.2
2	C	812	GLY	4.2
4	O	4	PRO	4.2
2	M	237	ARG	4.2
3	D	475	LYS	4.2
3	N	529	GLN	4.2
3	D	106	LYS	4.2
1	K	108	GLU	4.2
3	D	1501	GLU	4.2
2	C	974	LEU	4.2
2	M	197	LEU	4.2
3	N	365	ASP	4.2
2	C	742	VAL	4.2
5	F	106	VAL	4.2
3	N	1505	ALA	4.2
1	B	128	HIS	4.1
3	D	878	GLY	4.1
2	C	374	ASN	4.1
3	D	1069	GLU	4.1
3	N	706	PRO	4.1
2	C	1069	ALA	4.1
2	C	733	ALA	4.1
4	O	14	ASP	4.1
2	C	177	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
2	C	446	GLY	4.1
3	D	554	LEU	4.1
1	K	112	ARG	4.1
2	M	1069	ALA	4.1
2	C	596	TYR	4.1
5	P	147	LEU	4.1
1	B	121	GLU	4.1
3	N	16	GLU	4.1
5	F	196	VAL	4.1
1	L	43	ILE	4.1
2	C	154	ARG	4.1
3	D	969	ARG	4.1
2	M	2	GLU	4.1
3	N	203	ALA	4.1
1	A	32	PHE	4.1
3	N	1363	LEU	4.1
3	D	871	LYS	4.1
3	D	948	THR	4.1
3	N	1326	THR	4.1
2	C	505	GLY	4.1
2	C	613	VAL	4.1
2	C	756	VAL	4.1
3	N	67	ARG	4.1
2	C	998	TYR	4.0
3	N	596	SER	4.0
3	N	1339	LYS	4.0
3	D	1077	ALA	4.0
2	M	200	LEU	4.0
3	D	1287	GLU	4.0
2	M	154	ARG	4.0
2	C	253	ALA	4.0
2	M	604	ALA	4.0
3	N	506	GLY	4.0
5	F	139	ALA	4.0
2	M	1080	SER	4.0
2	C	186	VAL	4.0
3	D	633	VAL	4.0
2	C	440	PRO	4.0
3	N	1433	SER	4.0
1	K	150	TYR	4.0
2	M	459	ALA	4.0
2	C	936	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
3	N	1273	VAL	4.0
2	C	144	PRO	4.0
3	N	95	LEU	4.0
2	C	347	GLY	4.0
5	P	97	GLU	4.0
2	M	359	MET	4.0
2	C	332	ARG	4.0
2	M	204	GLN	4.0
2	C	320	HIS	4.0
5	F	192	LEU	4.0
2	M	716	LYS	4.0
3	N	718	PRO	4.0
1	A	14	ARG	3.9
2	C	723	THR	3.9
2	C	447	ALA	3.9
1	K	125	PRO	3.9
2	C	845	ASN	3.9
2	M	236	ILE	3.9
2	M	884	GLN	3.9
3	N	1274	ILE	3.9
2	M	59	LYS	3.9
2	M	867	VAL	3.9
3	N	1047	LYS	3.9
3	N	1456	LYS	3.9
3	D	224	ARG	3.9
5	P	138	SER	3.9
3	D	928	ALA	3.9
2	C	65	VAL	3.9
3	D	58	CYS	3.9
4	E	32	ARG	3.9
3	D	771	SER	3.9
2	C	59	LYS	3.9
2	C	879	ARG	3.9
5	F	284	ARG	3.9
2	M	1114	GLY	3.9
3	N	206	ARG	3.9
2	M	162	ILE	3.9
2	C	757	GLY	3.9
2	M	524	VAL	3.9
2	C	162	ILE	3.8
2	C	604	ALA	3.8
3	N	1324	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
2	M	266	ARG	3.8
3	N	1137	ARG	3.8
2	M	544	THR	3.8
3	D	1358	ALA	3.8
2	C	178	PRO	3.8
5	F	339	PRO	3.8
3	N	63	TYR	3.8
2	M	562	SER	3.8
3	D	78	VAL	3.8
2	C	102	HIS	3.8
2	C	217	LEU	3.8
3	N	707	THR	3.8
1	B	140	MET	3.8
1	K	1	MET	3.8
2	M	521	PRO	3.8
3	N	1131	SER	3.8
3	D	862	ASP	3.8
3	D	1294	VAL	3.8
2	C	457	ALA	3.8
3	D	22	SER	3.8
3	D	715	ALA	3.8
1	L	77	GLU	3.8
2	C	990	GLY	3.8
3	N	92	HIS	3.8
2	C	254	VAL	3.8
1	L	89	PHE	3.8
2	C	368	THR	3.8
2	M	444	PRO	3.8
2	M	465	GLY	3.8
2	M	875	GLY	3.8
3	D	797	LYS	3.8
1	A	186	LEU	3.8
3	D	1292	VAL	3.8
2	M	25	SER	3.8
3	N	1478	SER	3.8
2	M	1035	MET	3.7
3	N	1272	ALA	3.7
5	P	87	GLU	3.7
3	N	242	LEU	3.7
3	N	591	VAL	3.7
5	P	323	ASP	3.7
5	P	358	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	L	146	ARG	3.7
2	M	454	SER	3.7
3	D	718	PRO	3.7
5	F	213	ILE	3.7
5	F	376	ILE	3.7
5	F	143	HIS	3.7
1	A	185	ARG	3.7
1	A	87	VAL	3.7
3	D	1443	THR	3.7
2	C	909	ALA	3.7
3	D	559	ALA	3.7
2	M	722	ILE	3.7
3	D	555	LYS	3.7
3	N	215	TYR	3.7
4	O	32	ARG	3.7
2	M	774	LEU	3.7
3	N	554	LEU	3.7
4	O	73	LEU	3.7
2	C	35	PRO	3.7
2	C	859	PRO	3.7
3	N	866	VAL	3.7
5	P	362	SER	3.7
3	N	411	THR	3.7
5	F	388	ALA	3.7
1	K	87	VAL	3.7
2	C	1114	GLY	3.7
2	M	873	PRO	3.7
2	C	1059	ASP	3.7
5	P	176	ILE	3.7
1	B	207	PRO	3.7
3	N	1312	LEU	3.7
1	A	7	LYS	3.7
2	C	794	PRO	3.7
3	N	1430	SER	3.7
1	K	153	ALA	3.7
5	F	301	ALA	3.7
1	B	58	ILE	3.6
2	C	710	ILE	3.6
3	N	801	GLY	3.6
2	M	859	PRO	3.6
2	C	816	LYS	3.6
2	M	102	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
3	N	1294	VAL	3.6
3	N	589	ALA	3.6
3	N	798	GLU	3.6
5	F	333	ILE	3.6
3	D	872	ARG	3.6
1	K	193	ASP	3.6
2	C	174	LEU	3.6
3	D	107	ASP	3.6
3	N	519	VAL	3.6
1	L	23	PHE	3.6
5	P	146	GLY	3.6
2	C	367	LEU	3.6
5	F	166	LEU	3.6
2	M	936	VAL	3.6
1	L	140	MET	3.6
3	N	796	ARG	3.6
1	A	227	ASN	3.6
5	F	118	GLU	3.6
2	C	443	THR	3.6
2	M	82	GLU	3.6
3	N	560	GLN	3.6
5	F	340	SER	3.6
4	E	68	LEU	3.6
2	C	785	VAL	3.6
2	M	65	VAL	3.6
2	C	562	SER	3.6
2	C	591	SER	3.6
2	M	879	ARG	3.6
1	B	138	LEU	3.6
3	D	122	GLU	3.6
3	D	1303	TYR	3.6
1	B	217	ILE	3.5
2	C	141	HIS	3.5
5	P	321	ILE	3.5
2	C	601	GLY	3.5
2	C	646	GLY	3.5
2	C	1062	GLY	3.5
3	N	604	THR	3.5
2	C	95	TYR	3.5
1	L	21	GLY	3.5
3	N	24	GLY	3.5
2	C	1119	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
5	P	84	TYR	3.5
5	P	357	ALA	3.5
1	B	56	VAL	3.5
2	C	1026	GLN	3.5
2	M	201	GLY	3.5
5	P	361	LEU	3.5
1	A	20	TYR	3.5
3	D	205	TYR	3.5
2	C	980	GLY	3.5
5	P	88	ILE	3.5
2	M	457	ALA	3.5
3	D	866	VAL	3.5
3	N	453	ASP	3.5
3	N	1400	VAL	3.5
2	C	1112	PHE	3.5
1	L	197	LEU	3.5
3	N	1004	THR	3.5
5	P	139	ALA	3.5
2	M	45	GLN	3.5
5	P	137	GLY	3.5
3	N	234	GLU	3.4
3	N	692	GLU	3.4
5	P	351	SER	3.4
1	A	187	GLY	3.4
3	N	35	ARG	3.4
2	M	272	ALA	3.4
3	D	604	THR	3.4
3	N	472	ALA	3.4
2	C	7	GLY	3.4
5	P	118	GLU	3.4
2	M	422	ARG	3.4
2	M	66	LEU	3.4
4	E	31	LEU	3.4
2	C	501	THR	3.4
2	M	954	THR	3.4
3	D	203	ALA	3.4
3	N	1016	PRO	3.4
1	L	148	VAL	3.4
2	C	176	VAL	3.4
5	F	195	VAL	3.4
2	M	1043	TYR	3.4
2	M	416	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
3	D	865	THR	3.4
3	N	1077	ALA	3.4
4	O	42	PRO	3.4
3	N	925	GLU	3.4
3	D	582	LEU	3.4
3	D	608	SER	3.4
3	N	169	TYR	3.4
1	B	219	ARG	3.4
2	C	741	GLY	3.4
2	M	951	GLY	3.4
2	C	262	ALA	3.4
2	C	459	ALA	3.4
2	M	955	PRO	3.4
2	C	585	GLU	3.4
2	M	697	ARG	3.4
1	B	147	GLY	3.3
3	N	27	GLU	3.3
5	P	282	LEU	3.3
3	N	1338	ALA	3.3
2	M	573	ARG	3.3
2	C	743	VAL	3.3
3	N	1040	GLY	3.3
5	P	422	LEU	3.3
3	N	136	ASP	3.3
2	C	783	ARG	3.3
3	D	767	HIS	3.3
4	E	59	ASN	3.3
1	L	122	ILE	3.3
2	M	592	LEU	3.3
3	N	1041	LEU	3.3
3	D	1061	PHE	3.3
3	N	708	LEU	3.3
3	N	843	PHE	3.3
3	N	1035	ILE	3.3
1	K	147	GLY	3.3
3	N	164	GLY	3.3
5	F	84	TYR	3.3
3	D	1273	VAL	3.3
1	B	199	ILE	3.3
3	D	166	GLN	3.3
3	N	97	THR	3.3
3	D	632	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
3	D	809	PRO	3.3
3	D	1068	LEU	3.3
3	N	1429	LEU	3.3
2	C	54	ILE	3.3
2	M	1045	ALA	3.3
2	C	63	GLY	3.3
2	C	145	GLY	3.3
3	N	214	GLU	3.3
2	M	345	ARG	3.3
2	M	440	PRO	3.2
1	K	84	GLU	3.2
3	D	184	GLU	3.2
3	D	950	GLY	3.2
3	D	1274	ILE	3.2
1	K	191	ASP	3.2
2	C	268	ASP	3.2
5	P	244	ARG	3.2
3	N	1303	TYR	3.2
2	M	613	VAL	3.2
3	N	402	PRO	3.2
3	N	1333	HIS	3.2
5	F	402	ASN	3.2
3	D	949	ILE	3.2
3	D	226	PRO	3.2
3	D	846	PRO	3.2
3	N	1224	VAL	3.2
2	C	203	ASP	3.2
2	C	503	LEU	3.2
3	D	1420	LEU	3.2
3	N	764	LEU	3.2
3	N	1386	ASP	3.2
5	F	343	ASP	3.2
3	D	21	TRP	3.2
5	P	177	ALA	3.2
5	P	203	THR	3.2
3	D	1227	GLN	3.2
1	L	182	GLU	3.2
1	K	149	GLY	3.2
2	M	156	GLY	3.2
1	A	131	THR	3.2
1	L	98	THR	3.2
1	A	220	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
3	N	808	THR	3.2
2	C	777	ILE	3.2
3	D	947	ILE	3.2
5	P	213	ILE	3.2
1	K	142	VAL	3.2
2	M	275	TYR	3.2
2	M	742	VAL	3.2
5	F	132	ARG	3.2
2	M	68	PHE	3.2
5	F	328	PHE	3.2
2	C	58	ASP	3.2
2	M	784	ASP	3.2
4	E	47	LYS	3.2
1	B	170	VAL	3.2
4	E	64	ALA	3.1
2	M	1021	LEU	3.1
3	D	1006	ALA	3.1
2	M	54	ILE	3.1
5	P	143	HIS	3.1
1	A	219	ARG	3.1
2	C	278	GLU	3.1
2	C	1047	HIS	3.1
3	D	1130	ARG	3.1
3	N	1419	PRO	3.1
1	A	115	LEU	3.1
1	L	142	VAL	3.1
5	P	204	GLY	3.1
1	L	152	PRO	3.1
5	F	279	GLN	3.1
1	K	184	THR	3.1
3	D	95	LEU	3.1
3	D	1440	PHE	3.1
3	N	366	LYS	3.1
1	L	101	LEU	3.1
2	M	883	GLY	3.1
2	M	974	LEU	3.1
3	D	1000	THR	3.1
3	N	1000	THR	3.1
3	N	1481	VAL	3.1
5	F	400	ILE	3.1
2	M	408	ARG	3.1
5	P	405	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	117	HIS	3.1
2	C	70	GLU	3.0
2	M	885	ILE	3.0
1	B	211	LEU	3.0
3	N	1436	SER	3.0
4	O	68	LEU	3.0
3	D	231	VAL	3.0
3	D	1324	PRO	3.0
3	N	877	PRO	3.0
5	F	176	ILE	3.0
3	N	1328	GLY	3.0
2	C	647	GLN	3.0
2	M	372	LEU	3.0
3	D	1184	GLN	3.0
5	F	138	SER	3.0
3	N	1486	VAL	3.0
4	O	39	VAL	3.0
2	C	9	ILE	3.0
2	C	602	GLU	3.0
2	M	596	TYR	3.0
2	C	422	ARG	3.0
3	D	961	LYS	3.0
2	M	1046	ALA	3.0
3	N	972	LEU	3.0
1	B	53	VAL	3.0
2	M	959	PRO	3.0
3	D	1099	VAL	3.0
3	N	417	PRO	3.0
2	M	652	GLY	3.0
2	C	642	ARG	3.0
3	N	709	HIS	3.0
1	K	220	GLU	3.0
2	C	36	PRO	3.0
4	O	44	GLU	3.0
2	M	609	ASN	3.0
3	D	716	PHE	3.0
3	D	557	LEU	3.0
3	D	896	ALA	3.0
5	F	404	ALA	3.0
3	N	1418	LYS	3.0
2	M	534	VAL	3.0
3	N	1100	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
5	F	173	TYR	3.0
3	N	59	ALA	3.0
5	P	388	ALA	3.0
2	M	150	PRO	3.0
2	M	41	ASN	3.0
3	N	77	GLY	3.0
3	N	126	VAL	2.9
4	O	43	GLU	2.9
3	D	1445	HIS	2.9
3	D	796	ARG	2.9
3	N	166	GLN	2.9
5	P	210	LEU	2.9
5	P	412	GLU	2.9
3	N	155	ASP	2.9
5	F	342	VAL	2.9
5	P	376	ILE	2.9
3	N	212	ARG	2.9
3	N	699	VAL	2.9
2	C	13	ILE	2.9
3	N	1454	GLY	2.9
2	C	737	LEU	2.9
2	M	367	LEU	2.9
2	M	456	ALA	2.9
5	P	96	LEU	2.9
2	C	108	ILE	2.9
2	M	646	GLY	2.9
3	N	772	PRO	2.9
1	K	6	LEU	2.9
2	M	368	THR	2.9
3	N	1226	ALA	2.9
4	O	54	LEU	2.9
2	C	218	VAL	2.9
3	D	631	ILE	2.9
3	N	1330	ILE	2.9
5	P	109	GLY	2.9
1	A	112	ARG	2.9
2	C	888	THR	2.9
2	M	418	LEU	2.9
3	N	1483	PHE	2.9
2	C	383	ARG	2.9
2	M	318	PRO	2.9
3	N	178	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	N	759	ALA	2.9
2	M	1047	HIS	2.9
5	P	192	LEU	2.9
2	C	822	VAL	2.8
2	M	649	VAL	2.8
5	F	253	ASP	2.8
5	F	378	GLY	2.8
2	C	237	ARG	2.8
1	L	114	PHE	2.8
3	D	754	PHE	2.8
3	D	1330	ILE	2.8
2	C	850	ALA	2.8
5	F	337	HIS	2.8
2	M	520	GLU	2.8
5	P	201	LYS	2.8
3	N	146	PRO	2.8
2	C	712	ALA	2.8
2	M	85	GLU	2.8
3	N	1407	LEU	2.8
2	M	63	GLY	2.8
5	P	222	ARG	2.8
2	M	998	TYR	2.8
1	B	96	THR	2.8
2	M	673	LEU	2.8
2	M	737	LEU	2.8
1	A	47	SER	2.8
3	D	774	SER	2.8
3	D	886	VAL	2.8
2	C	93	PRO	2.8
2	C	135	VAL	2.8
2	C	209	ARG	2.8
3	N	741	ASP	2.8
3	N	1006	ALA	2.8
3	N	1329	ALA	2.8
5	F	133	ALA	2.8
1	B	94	LEU	2.8
1	L	25	LEU	2.8
2	C	779	GLY	2.8
3	D	94	GLU	2.8
3	N	1421	LEU	2.8
2	M	765	SER	2.8
1	A	144	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
4	O	7	ASP	2.8
2	C	563	ASN	2.8
2	M	611	ILE	2.8
4	O	53	GLY	2.8
5	P	300	ASP	2.8
3	D	189	GLN	2.7
3	N	904	VAL	2.7
2	C	797	GLY	2.7
2	C	78	PHE	2.7
2	C	1045	ALA	2.7
3	D	726	ILE	2.7
2	C	619	ARG	2.7
3	N	743	ASP	2.7
1	L	151	VAL	2.7
2	C	38	LYS	2.7
3	N	1292	VAL	2.7
2	C	230	ARG	2.7
2	C	344	PHE	2.7
2	C	648	ARG	2.7
2	M	934	PHE	2.7
3	D	1008	PHE	2.7
3	N	956	ILE	2.7
3	N	1450	ALA	2.7
5	F	246	ALA	2.7
3	N	115	LEU	2.7
2	M	563	ASN	2.7
1	K	76	VAL	2.7
2	M	741	GLY	2.7
2	C	353	ARG	2.7
2	C	895	TYR	2.7
3	D	650	LEU	2.7
5	F	369	LEU	2.7
3	N	66	GLN	2.7
3	N	73	CYS	2.7
2	C	904	PRO	2.7
1	B	91	ASN	2.7
2	M	278	GLU	2.7
3	N	467	GLU	2.7
3	N	965	GLU	2.7
1	L	11	PHE	2.7
2	M	871	LEU	2.7
2	M	895	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	M	723	THR	2.7
3	D	943	THR	2.7
1	B	171	PHE	2.7
2	C	871	LEU	2.7
2	M	963	LEU	2.7
3	D	899	LEU	2.7
2	M	802	ARG	2.7
5	F	412	GLU	2.7
1	B	135	GLY	2.7
2	M	532	MET	2.7
2	C	534	VAL	2.7
2	M	515	ALA	2.7
2	M	568	ALA	2.7
2	M	906	PHE	2.7
5	F	170	HIS	2.7
2	M	1012	PRO	2.7
2	M	606	VAL	2.6
3	D	1486	VAL	2.6
2	M	1039	ALA	2.6
3	D	1346	ARG	2.6
3	N	1225	ALA	2.6
1	L	58	ILE	2.6
2	M	952	LEU	2.6
4	E	73	LEU	2.6
2	M	1044	GLY	2.6
1	L	9	PRO	2.6
2	C	959	PRO	2.6
2	M	202	TYR	2.6
2	C	976	ASP	2.6
3	N	1269	LYS	2.6
1	A	142	VAL	2.6
2	M	552	HIS	2.6
4	O	38	THR	2.6
2	M	668	LEU	2.6
3	D	1454	GLY	2.6
1	A	212	ASN	2.6
2	C	355	VAL	2.6
2	M	1040	LEU	2.6
3	N	652	LEU	2.6
5	P	108	GLU	2.6
3	D	162	ARG	2.6
3	D	63	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	878	SER	2.6
3	N	608	SER	2.6
1	L	103	ALA	2.6
2	C	908	GLY	2.6
2	C	107	LEU	2.6
3	N	1447	LEU	2.6
2	C	521	PRO	2.6
2	M	6	PHE	2.6
2	M	76	PRO	2.6
3	N	710	ARG	2.6
3	D	564	GLU	2.6
1	B	38	ASN	2.6
3	D	391	ALA	2.6
3	N	72	VAL	2.6
3	N	1309	ALA	2.6
1	L	132	LEU	2.6
2	C	668	LEU	2.6
3	N	1048	PRO	2.6
4	E	69	LEU	2.6
3	D	467	GLU	2.6
4	E	43	GLU	2.6
2	C	256	TYR	2.6
2	M	286	SER	2.6
3	D	59	ALA	2.6
3	D	96	ALA	2.6
3	N	15	PRO	2.6
5	F	174	LEU	2.6
2	C	127	PHE	2.6
2	M	249	LYS	2.6
3	D	1071	PHE	2.6
3	N	754	PHE	2.6
2	C	903	SER	2.6
2	M	757	GLY	2.6
2	C	471	TYR	2.6
2	C	83	CYS	2.5
5	F	81	VAL	2.5
1	A	113	ASP	2.5
2	C	787	ASP	2.5
3	D	584	ASN	2.5
2	M	525	SER	2.5
2	M	880	MET	2.5
5	F	109	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
5	P	298	GLY	2.5
3	D	1326	THR	2.5
1	K	144	VAL	2.5
1	L	80	LEU	2.5
2	C	867	VAL	2.5
2	M	587	VAL	2.5
4	E	42	PRO	2.5
5	P	314	PRO	2.5
5	F	178	ARG	2.5
2	C	684	PHE	2.5
3	D	1277	ILE	2.5
3	N	1011	PHE	2.5
4	E	57	ASP	2.5
3	N	28	LYS	2.5
1	B	201	THR	2.5
2	M	570	PRO	2.5
2	C	418	LEU	2.5
3	D	895	VAL	2.5
3	D	972	LEU	2.5
3	N	26	VAL	2.5
1	A	149	GLY	2.5
3	D	1039	CYS	2.5
1	K	46	SER	2.5
3	D	1439	SER	2.5
3	N	1311	LEU	2.5
5	P	195	VAL	2.5
2	M	43	GLY	2.5
3	D	876	SER	2.5
4	E	11	GLY	2.5
3	D	14	SER	2.5
3	N	1359	GLN	2.5
5	P	78	SER	2.5
1	K	116	PRO	2.5
3	N	52	PRO	2.5
1	L	109	VAL	2.5
1	K	93	SER	2.5
2	M	619	ARG	2.5
1	L	211	LEU	2.4
2	M	217	LEU	2.4
3	N	760	ARG	2.4
5	F	140	ARG	2.4
3	D	378	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
4	E	67	GLU	2.4
1	B	101	LEU	2.4
3	D	115	LEU	2.4
3	D	1041	LEU	2.4
5	P	224	VAL	2.4
3	D	868	TYR	2.4
1	L	145	ASP	2.4
3	D	666	ILE	2.4
3	N	53	ILE	2.4
2	M	898	GLY	2.4
3	D	768	ASN	2.4
3	D	1328	GLY	2.4
3	D	1384	PRO	2.4
2	M	1115	LEU	2.4
3	N	623	VAL	2.4
4	E	83	ASP	2.4
3	D	187	LYS	2.4
1	B	21	GLY	2.4
2	C	875	GLY	2.4
3	D	563	PRO	2.4
2	M	1116	ALA	2.4
1	L	220	GLU	2.4
3	D	1308	GLU	2.4
3	N	25	GLU	2.4
3	D	1479	ASP	2.4
3	N	1275	SER	2.4
1	A	53	VAL	2.4
1	B	23	PHE	2.4
2	C	156	GLY	2.4
2	M	7	GLY	2.4
3	D	68	PHE	2.4
1	B	206	THR	2.4
3	N	583	ASP	2.4
2	M	569	VAL	2.4
3	D	1224	VAL	2.4
1	K	140	MET	2.4
3	N	766	ALA	2.4
1	K	99	LEU	2.4
3	N	1132	LEU	2.4
5	F	210	LEU	2.4
1	A	147	GLY	2.4
5	P	156	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	759	ALA	2.4
3	N	162	ARG	2.4
3	N	1479	ASP	2.4
5	F	199	ALA	2.4
1	A	223	THR	2.4
3	D	1275	SER	2.4
5	F	401	GLU	2.4
2	M	62	GLY	2.3
2	M	823	VAL	2.3
2	M	869	VAL	2.3
3	N	1200	VAL	2.3
5	F	156	VAL	2.3
2	M	108	ILE	2.3
3	N	957	PRO	2.3
2	M	471	TYR	2.3
2	M	699	PHE	2.3
3	D	887	ALA	2.3
3	N	228	ALA	2.3
3	D	652	LEU	2.3
4	O	40	LEU	2.3
5	F	354	LEU	2.3
2	M	843	HIS	2.3
1	A	15	THR	2.3
1	L	201	THR	2.3
2	C	62	GLY	2.3
1	L	143	ARG	2.3
2	C	1006	HIS	2.3
5	F	305	GLU	2.3
2	M	647	GLN	2.3
3	N	202	VAL	2.3
3	N	633	VAL	2.3
3	N	1487	VAL	2.3
3	D	1329	ALA	2.3
2	C	985	GLY	2.3
3	D	999	THR	2.3
2	C	831	ARG	2.3
2	M	602	GLU	2.3
5	P	107	GLU	2.3
2	M	926	PHE	2.3
2	C	296	GLY	2.3
2	M	601	GLY	2.3
3	D	61	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	626	SER	2.3
3	D	1138	ALA	2.3
3	N	1428	ALA	2.3
2	M	925	TYR	2.3
2	M	462	ASP	2.3
2	M	882	LEU	2.3
2	C	612	VAL	2.3
1	L	200	TRP	2.3
2	M	69	LEU	2.3
3	D	178	LEU	2.3
3	N	781	PRO	2.3
3	D	28	LYS	2.3
5	P	296	GLY	2.3
2	M	733	ALA	2.3
2	C	773	LEU	2.3
3	D	691	LEU	2.3
3	N	650	LEU	2.3
2	C	8	ARG	2.2
2	C	805	ARG	2.2
1	K	53	VAL	2.2
2	C	588	VAL	2.2
3	D	498	VAL	2.2
2	M	868	ASP	2.2
3	D	469	ASP	2.2
3	N	968	ASP	2.2
3	D	1225	ALA	2.2
2	C	1090	LYS	2.2
3	D	169	TYR	2.2
2	C	531	PHE	2.2
2	C	660	ALA	2.2
3	D	535	PHE	2.2
2	M	383	ARG	2.2
2	M	420	ARG	2.2
5	P	297	PRO	2.2
2	C	677	MET	2.2
2	M	743	VAL	2.2
3	D	409	VAL	2.2
2	M	516	ARG	2.2
3	N	715	ALA	2.2
2	M	922	PHE	2.2
1	L	207	PRO	2.2
3	D	728	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	1489	GLN	2.2
3	N	1435	LEU	2.2
5	F	116	LEU	2.2
3	N	1410	GLU	2.2
3	D	77	GLY	2.2
4	O	5	GLY	2.2
2	M	651	LYS	2.2
3	D	1158	VAL	2.2
3	N	41	ARG	2.2
2	C	704	HIS	2.2
1	B	210	ALA	2.2
2	M	128	ILE	2.2
3	N	422	ALA	2.2
3	N	726	ILE	2.2
2	M	70	GLU	2.2
2	M	764	GLU	2.2
3	D	1297	GLU	2.2
4	O	55	PHE	2.2
5	F	97	GLU	2.2
3	D	222	GLY	2.2
3	D	681	ARG	2.2
3	N	1036	ARG	2.2
1	A	226	SER	2.2
2	C	143	SER	2.2
2	C	392	SER	2.2
1	A	86	VAL	2.2
1	A	140	MET	2.2
2	C	941	VAL	2.2
1	L	29	GLU	2.2
2	C	1042	ALA	2.2
3	D	757	ALA	2.2
5	P	345	ALA	2.2
1	K	129	ILE	2.2
1	K	158	ILE	2.2
3	D	64	LYS	2.2
1	A	99	LEU	2.2
2	C	626	ARG	2.2
5	F	104	ARG	2.2
2	M	392	SER	2.2
3	N	753	SER	2.2
3	D	560	GLN	2.2
3	D	1339	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	1490	LYS	2.2
2	C	124	ASP	2.2
2	M	111	ASP	2.2
2	C	106	GLY	2.2
5	F	216	GLY	2.2
3	D	52	PRO	2.2
3	N	421	LEU	2.2
5	P	189	GLU	2.2
3	D	1005	GLN	2.1
4	O	13	VAL	2.1
2	M	660	ALA	2.1
2	M	939	ARG	2.1
1	L	195	LEU	2.1
3	D	976	GLN	2.1
2	C	5	ARG	2.1
3	N	569	ASN	2.1
2	C	951	GLY	2.1
2	M	132	ALA	2.1
5	P	196	VAL	2.1
2	M	239	PHE	2.1
2	C	241	LEU	2.1
3	D	204	LEU	2.1
3	N	621	LYS	2.1
3	N	878	GLY	2.1
2	C	825	VAL	2.1
2	M	850	ALA	2.1
1	K	225	PHE	2.1
5	F	194	LEU	2.1
3	N	197	SER	2.1
5	F	175	HIS	2.1
3	D	1040	GLY	2.1
5	P	367	MET	2.1
2	C	975	TYR	2.1
2	M	645	VAL	2.1
3	D	578	VAL	2.1
1	A	58	ILE	2.1
1	K	65	PHE	2.1
3	D	658	LEU	2.1
3	N	1130	ARG	2.1
3	N	1305	LEU	2.1
5	F	418	LEU	2.1
2	M	909	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	M	1036	GLU	2.1
3	D	414	ARG	2.1
3	N	158	TYR	2.1
3	N	963	TYR	2.1
1	K	74	ASP	2.1
1	L	72	LYS	2.1
3	D	596	SER	2.1
3	D	1293	PHE	2.1
5	F	160	ASP	2.1
4	E	54	LEU	2.1
5	F	209	PHE	2.1
1	B	200	TRP	2.1
5	P	347	GLN	2.1
2	C	913	GLU	2.1
1	B	39	PRO	2.1
2	C	29	ALA	2.1
2	M	188	LYS	2.1
3	D	807	ALA	2.1
4	O	64	ALA	2.1
1	K	98	THR	2.1
2	M	135	VAL	2.1
2	M	989	VAL	2.1
2	C	129	ILE	2.1
2	M	37	GLU	2.1
3	D	476	GLU	2.1
3	D	413	ASP	2.0
3	N	243	ALA	2.0
3	N	590	PRO	2.0
3	D	707	THR	2.0
3	N	205	TYR	2.0
3	D	925	GLU	2.0
3	D	992	ILE	2.0
1	L	82	LEU	2.0
2	C	952	LEU	2.0
3	N	1209	LEU	2.0
5	F	157	GLU	2.0
1	B	194	LYS	2.0
3	N	996	TRP	2.0
2	C	698	ASP	2.0
1	L	8	ALA	2.0
2	C	570	PRO	2.0
2	C	399	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	102	ILE	2.0
3	N	1008	PHE	2.0
1	A	215	VAL	2.0
2	M	756	VAL	2.0
2	M	250	ARG	2.0
4	E	53	GLY	2.0
4	E	40	LEU	2.0
2	M	533	ASP	2.0
2	M	1041	GLU	2.0
4	O	96	GLU	2.0
1	A	123	MET	2.0
2	C	444	PRO	2.0
3	D	648	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

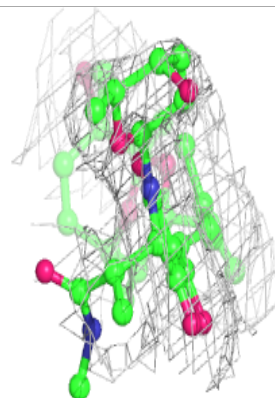
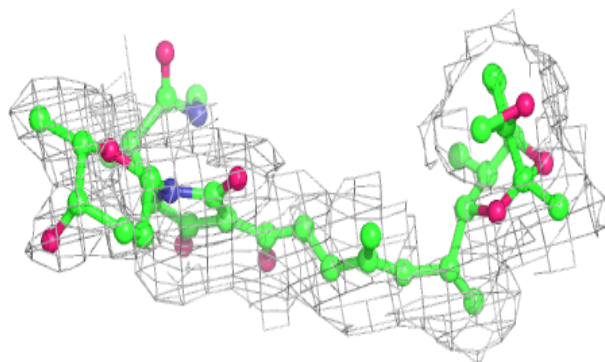
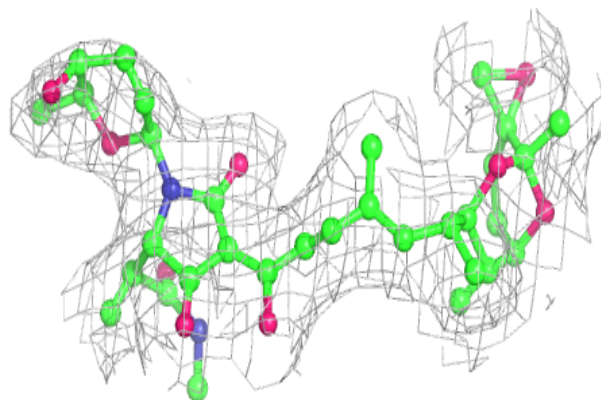
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	STD	N	8002	43/43	0.76	0.15	27,35,41,48	0
6	STD	D	8001	43/43	0.86	0.13	25,35,40,43	0
8	MG	N	9002	1/1	0.88	0.51	53,53,53,53	0
8	MG	D	9001	1/1	0.94	0.19	29,29,29,29	0
7	ZN	N	7459	1/1	0.95	0.10	64,64,64,64	0
7	ZN	N	7413	1/1	0.99	0.11	65,65,65,65	0
7	ZN	D	7458	1/1	0.99	0.09	64,64,64,64	0
7	ZN	D	7412	1/1	0.99	0.06	58,58,58,58	0

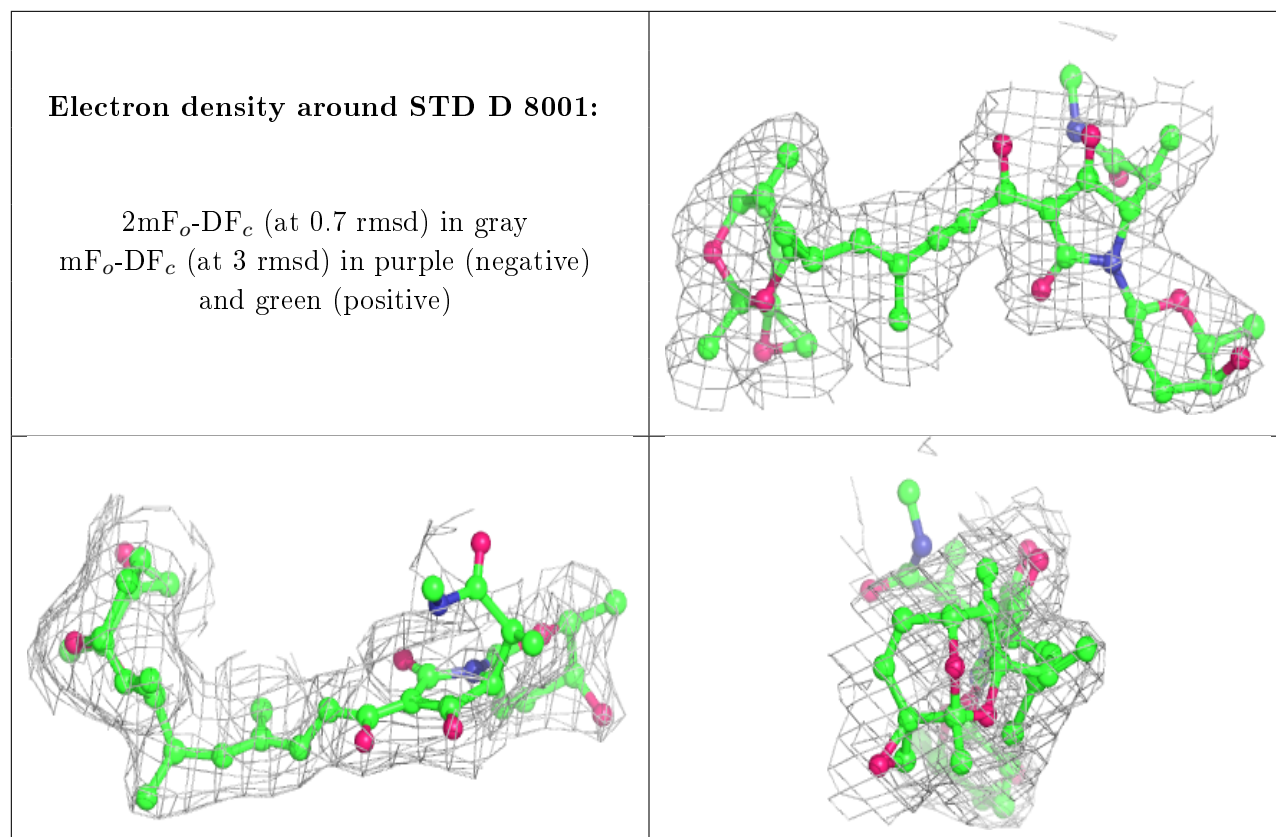
The following is a graphical depiction of the model fit to experimental electron density of all

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 STD N 8002:

$2mF_o-DF_c$ (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.