Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 10:49 PM EDT

PDB ID	:	3EQL
Title	:	Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with antibiotic myxopyronin
Authors	:	Vassylyev, D.G.; Vassylyeva, M.N.; Artsimovitch, I.
Deposited on	:	2008-09-30
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

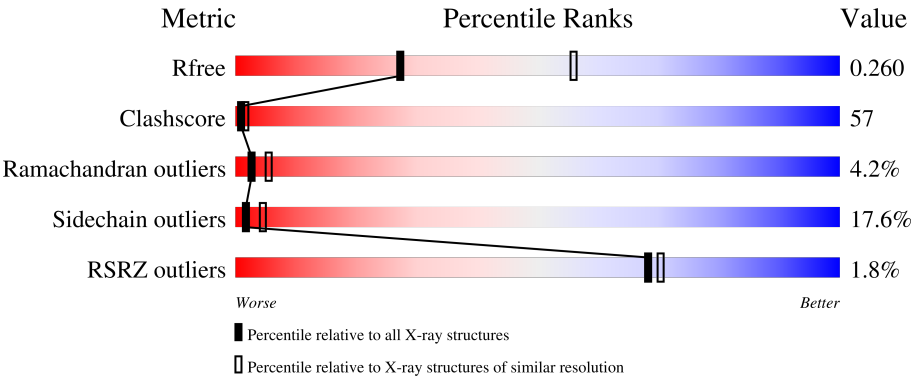
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	18% 44% 10% • 27%
1	B	315	3% 19% 44% 9% 27%
1	K	315	20% 42% 10% • 27%
1	L	315	17% 46% 9% • 27%
2	C	1119	25% 58% 16% •

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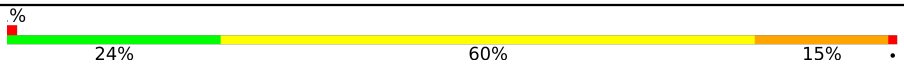
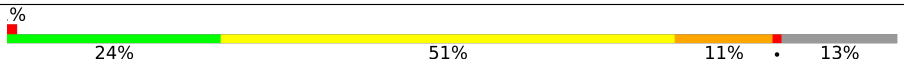
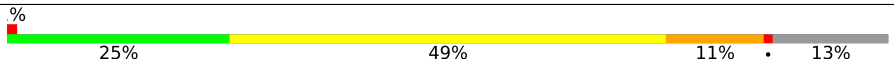
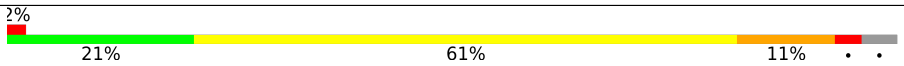
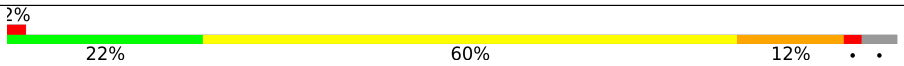
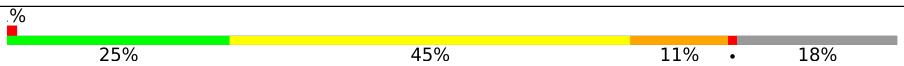
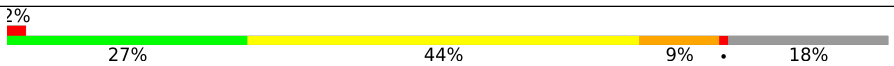
Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 57340 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 subunit alpha.

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 subunit beta.

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 subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1321	Total	C	N	O	S	0	0	0
			10407	6585	1845	1944	33			
3	N	1321	Total	C	N	O	S	0	0	0
			10407	6585	1845	1944	33			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			
4	O	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			

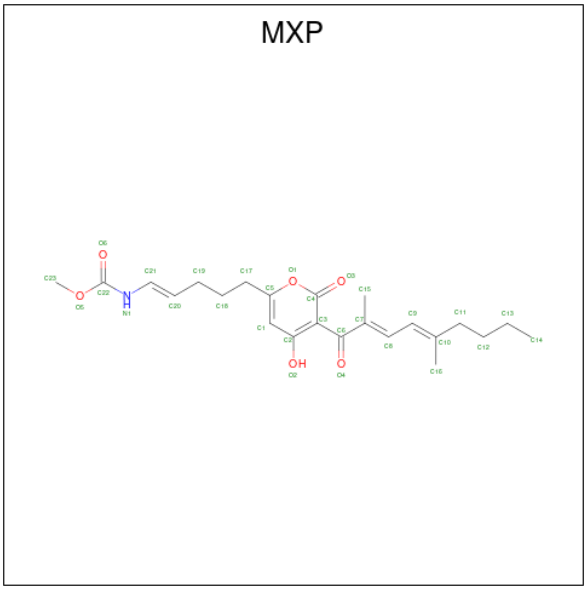
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is Myxopyronin B (three-letter code: MXP) (formula: $C_{23}H_{31}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			30	23	1	6		
7	N	1	Total	C	N	O	0	0
			30	23	1	6		

- 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.

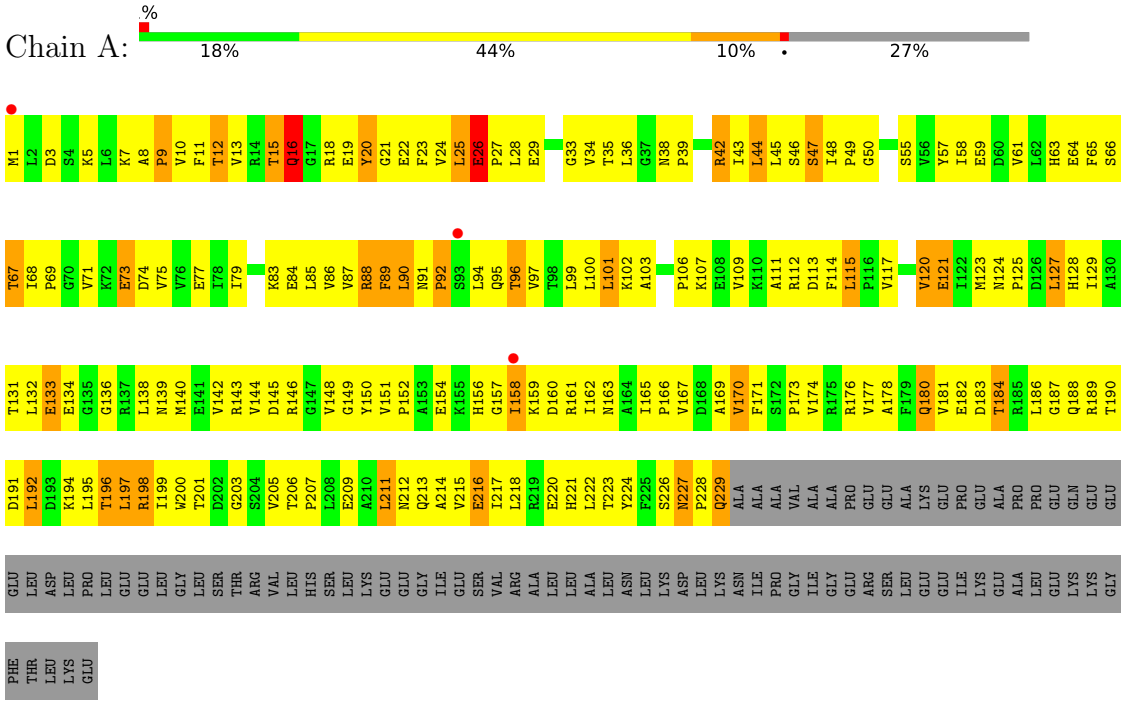
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	141	Total O 141 141	0	0
9	B	149	Total O 149 149	0	0
9	C	704	Total O 704 704	0	0
9	D	927	Total O 927 927	0	0
9	E	82	Total O 82 82	0	0
9	F	305	Total O 305 305	0	0
9	K	152	Total O 152 152	0	0
9	L	148	Total O 148 148	0	0
9	M	680	Total O 680 680	0	0
9	N	864	Total O 864 864	0	0
9	O	84	Total O 84 84	0	0
9	P	260	Total O 260 260	0	0

3 Residue-property plots (i)

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

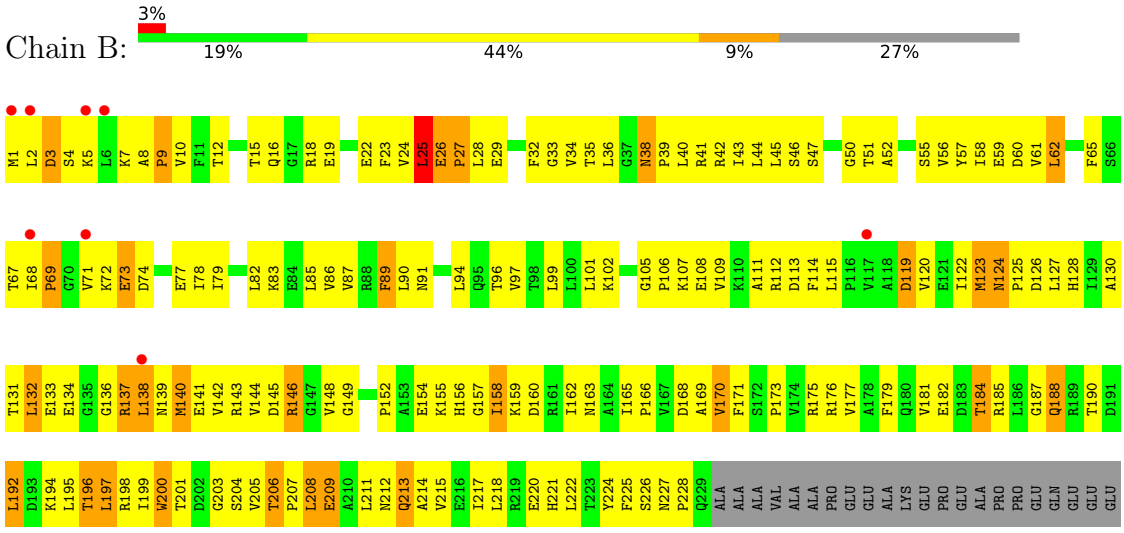
• Molecule 1: DNA-directed RNA polymerase subunit alpha

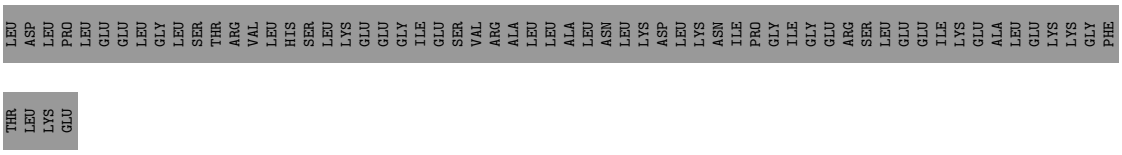
Chain A:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

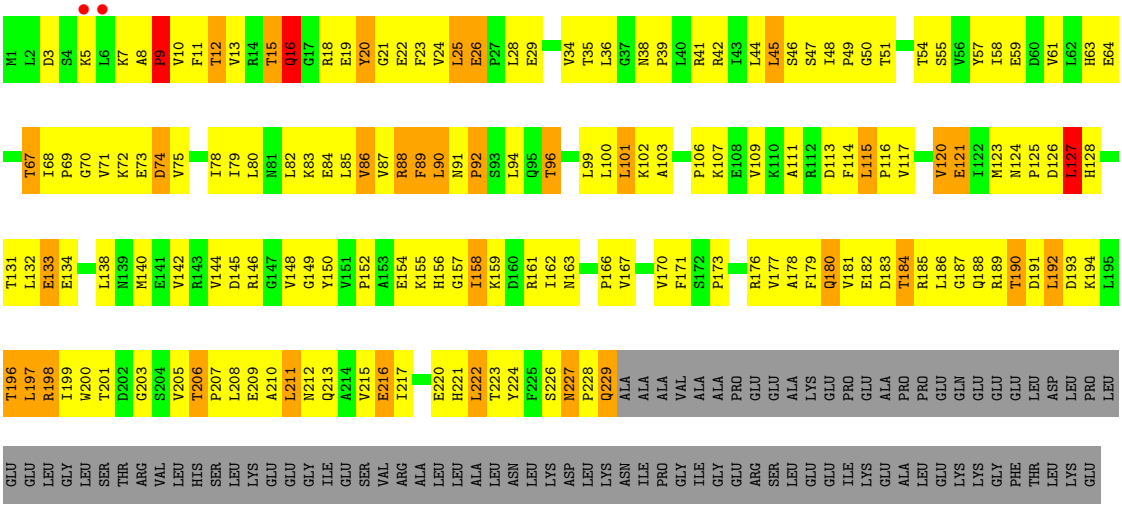
Chain B:





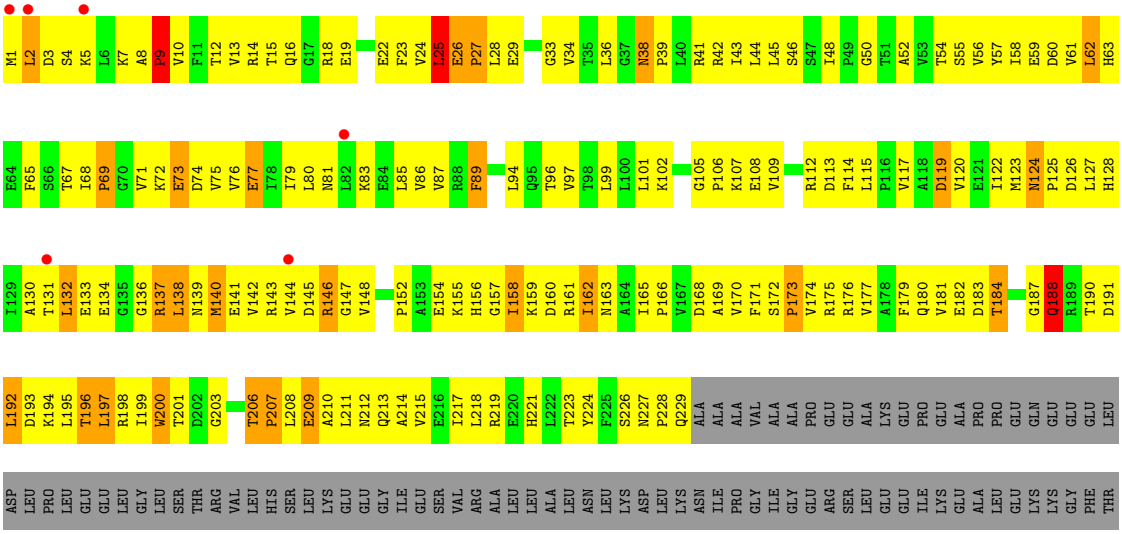
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain K:



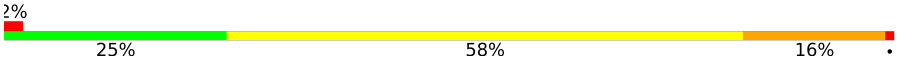
• Molecule 1: DNA-directed RNA polymerase subunit alpha

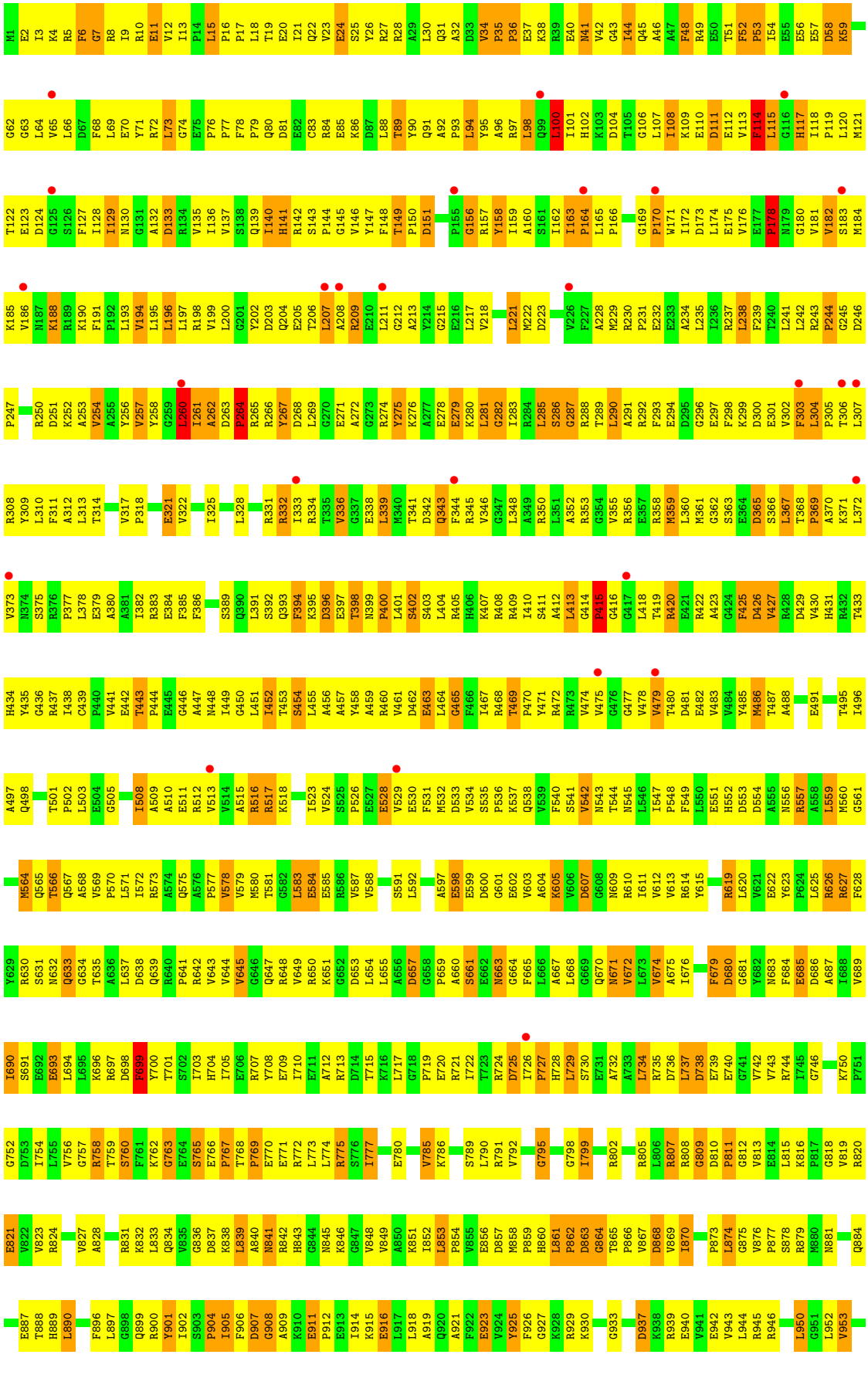
Chain L:

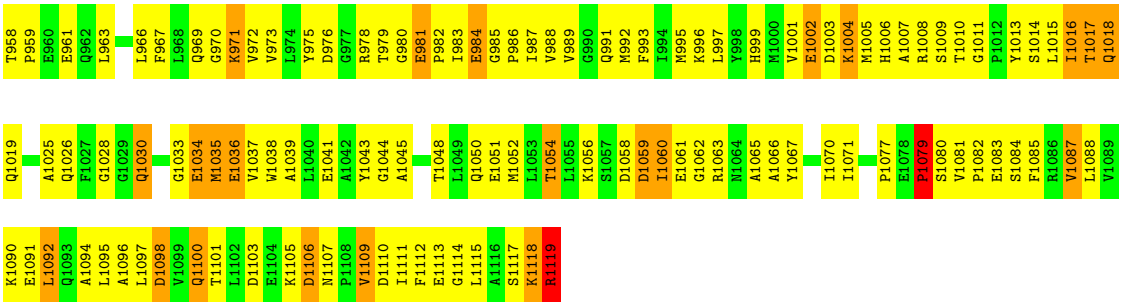


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:

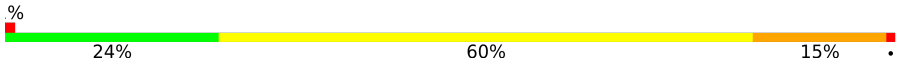


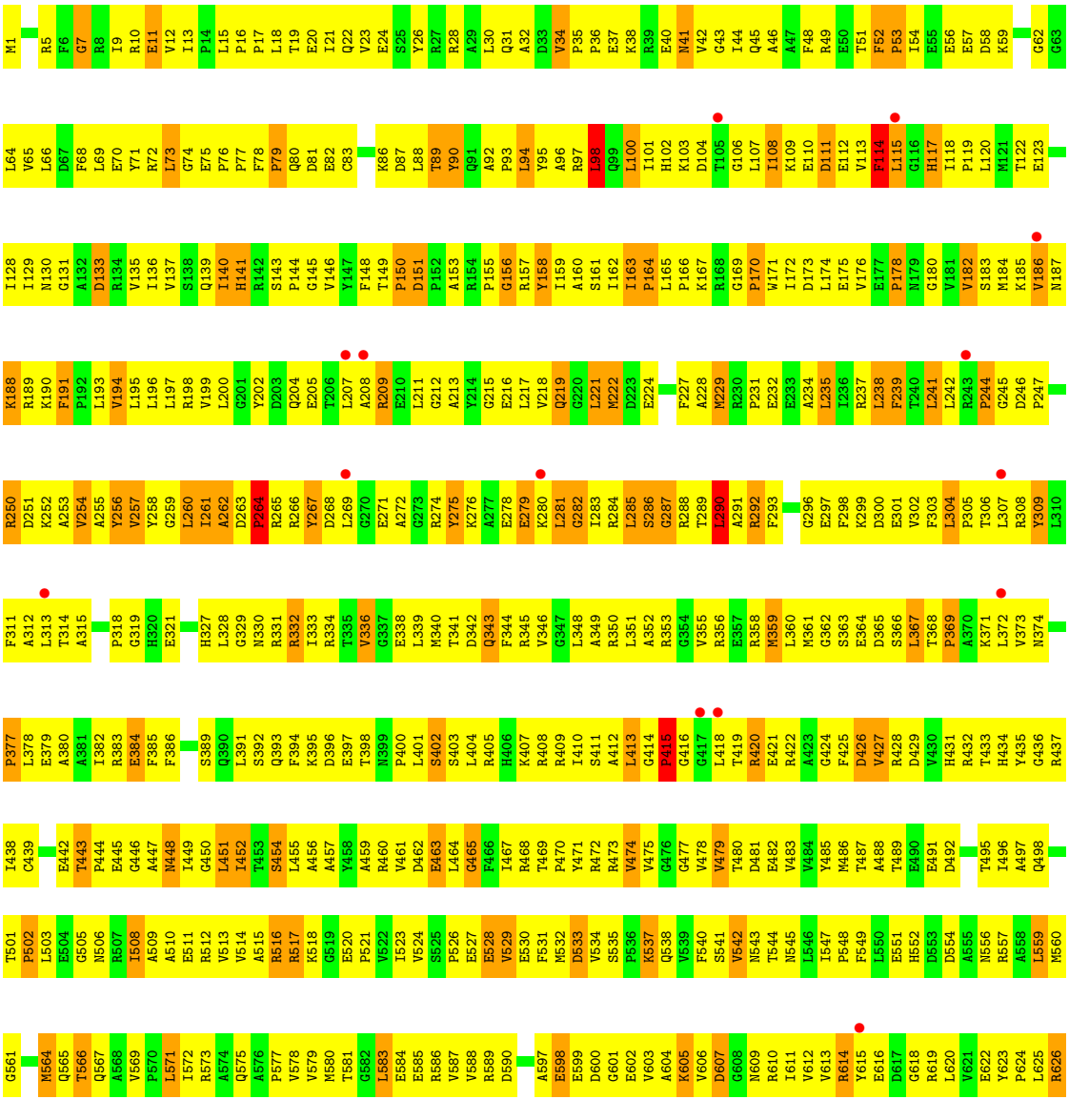


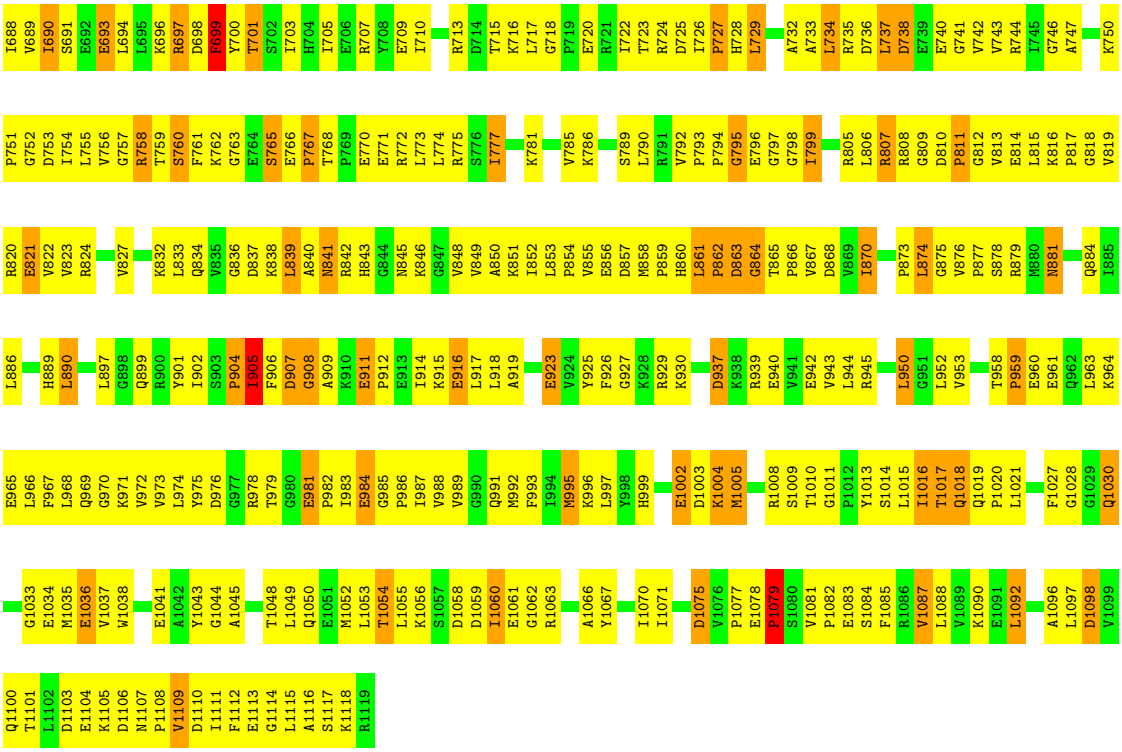


• Molecule 2: DNA-directed RNA polymerase subunit beta

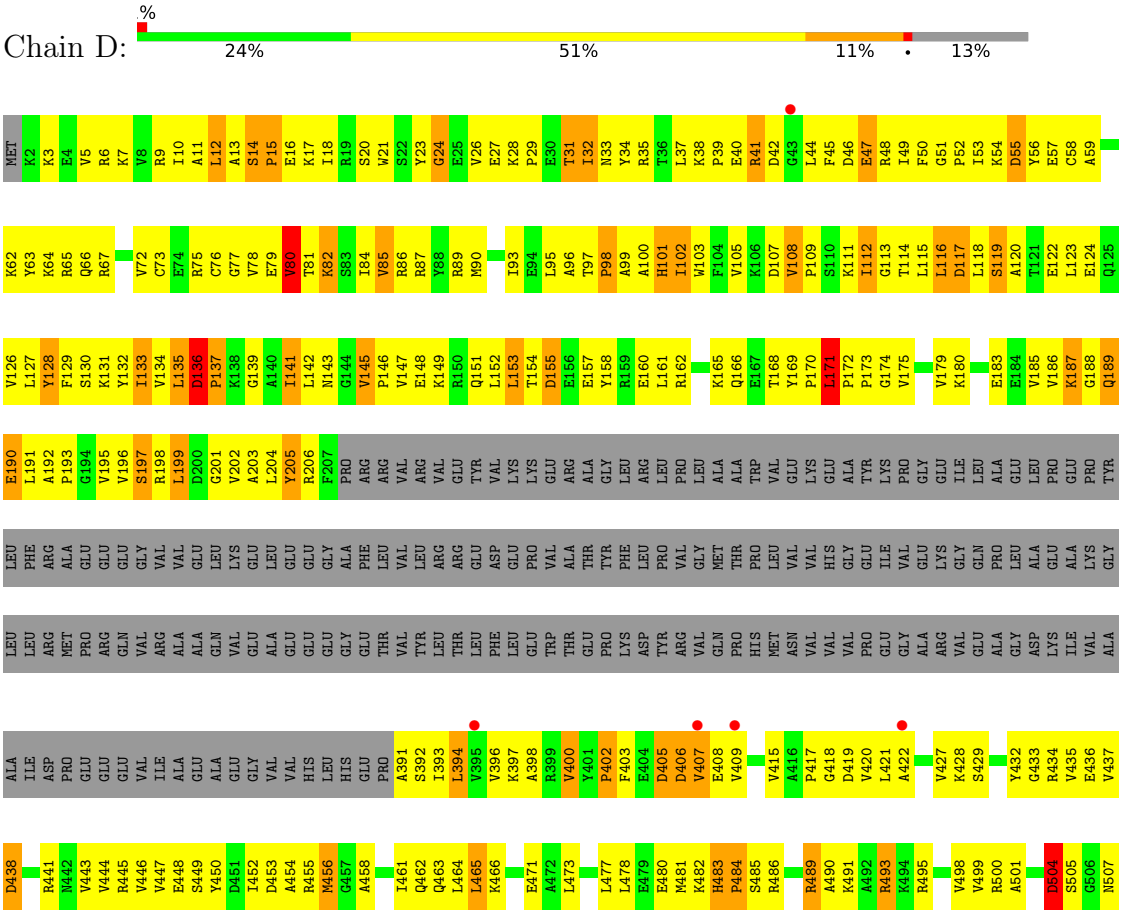
Chain M:

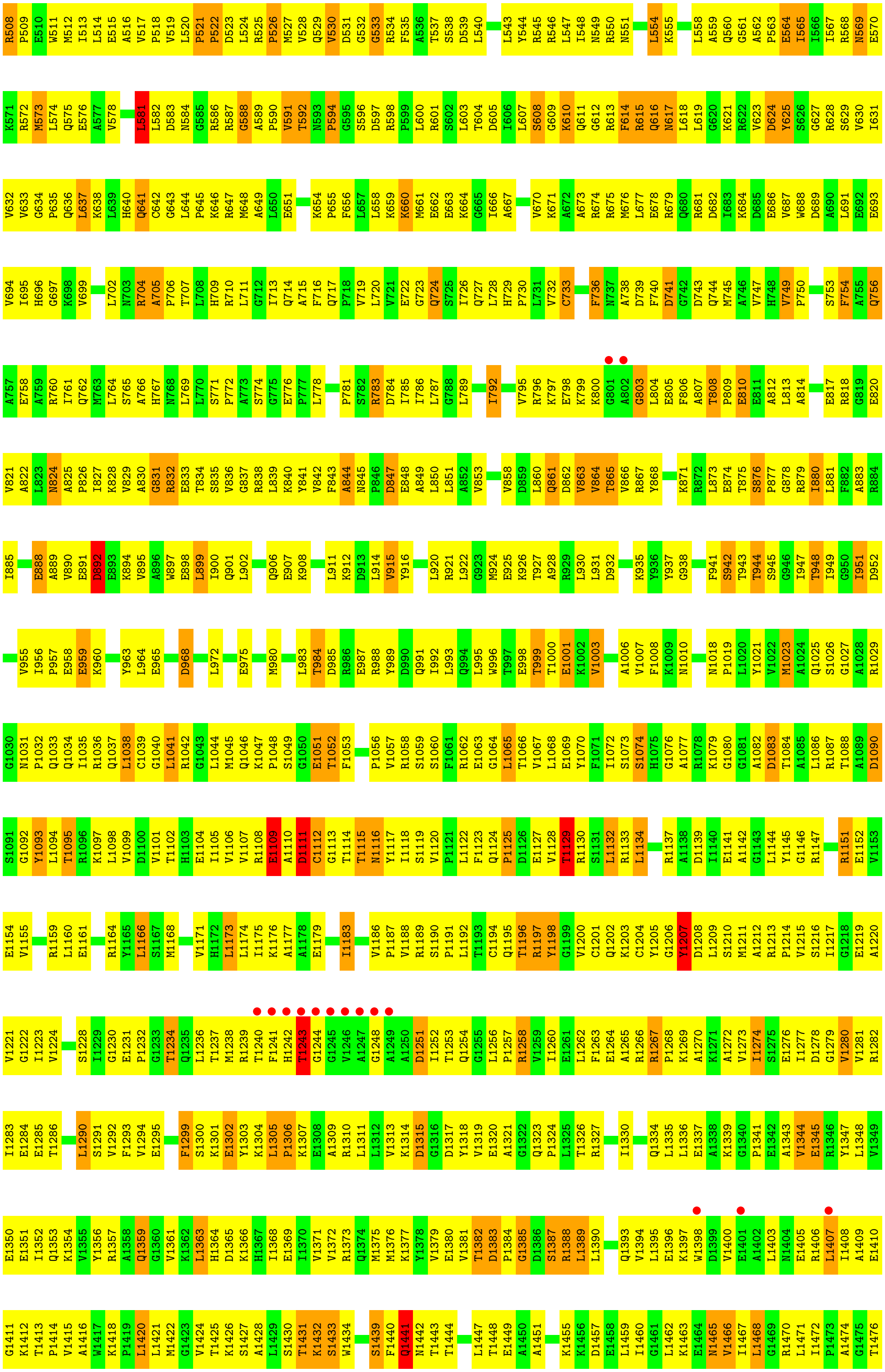




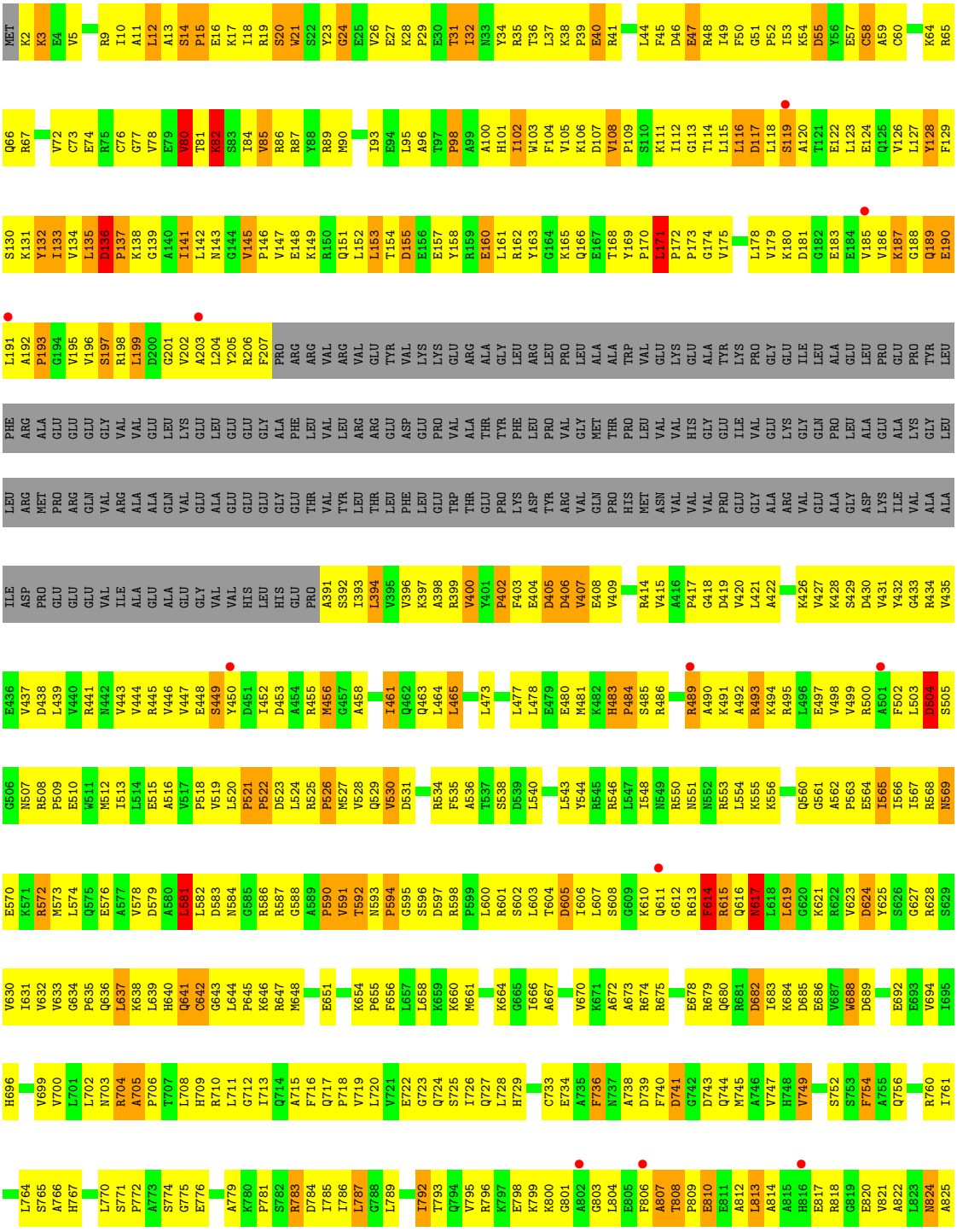


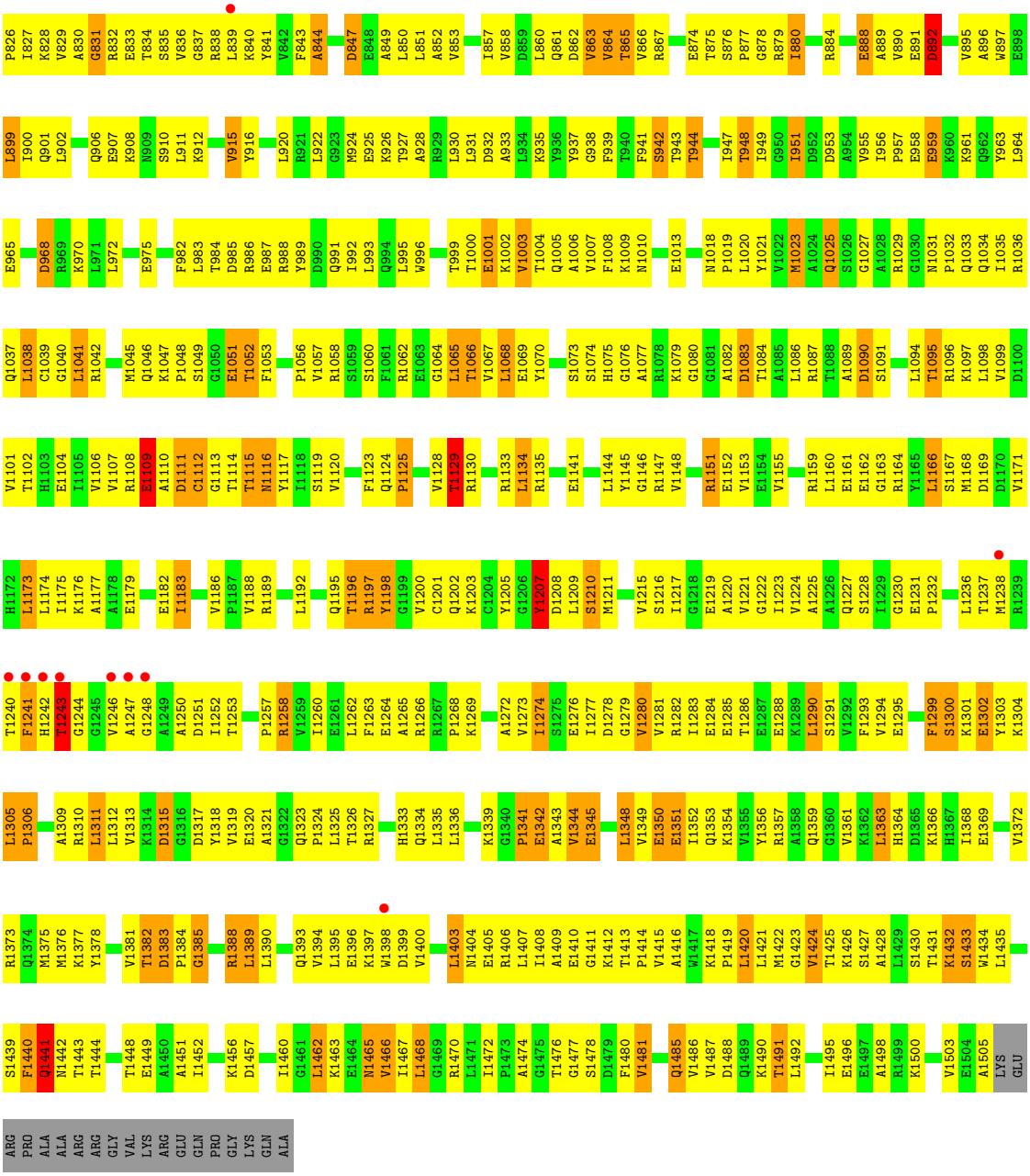
• Molecule 3: DNA-directed RNA polymerase subunit beta'



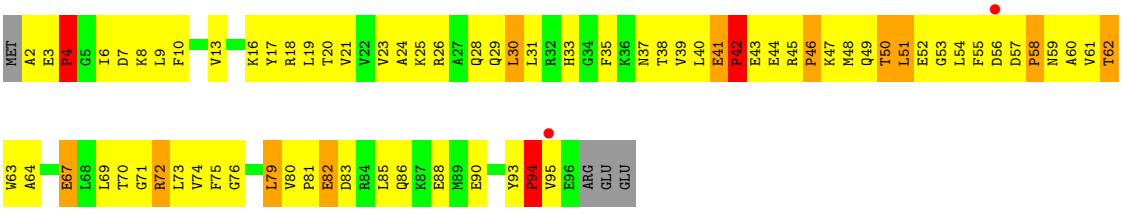


• Molecule 3: DNA-directed RNA polymerase subunit beta'



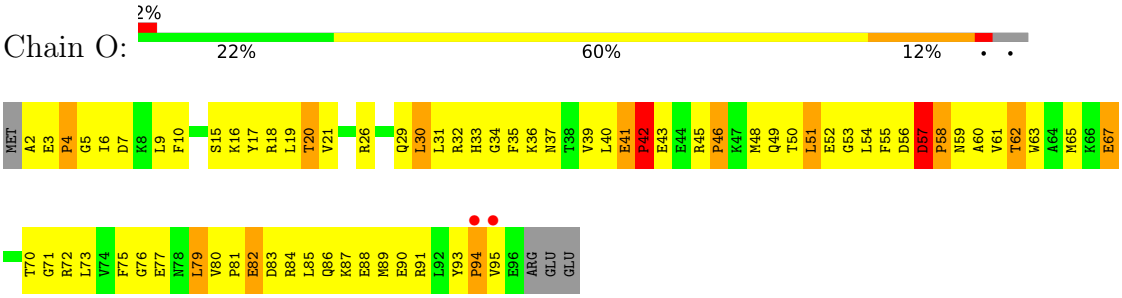


• Molecule 4: DNA-directed RNA polymerase subunit omega



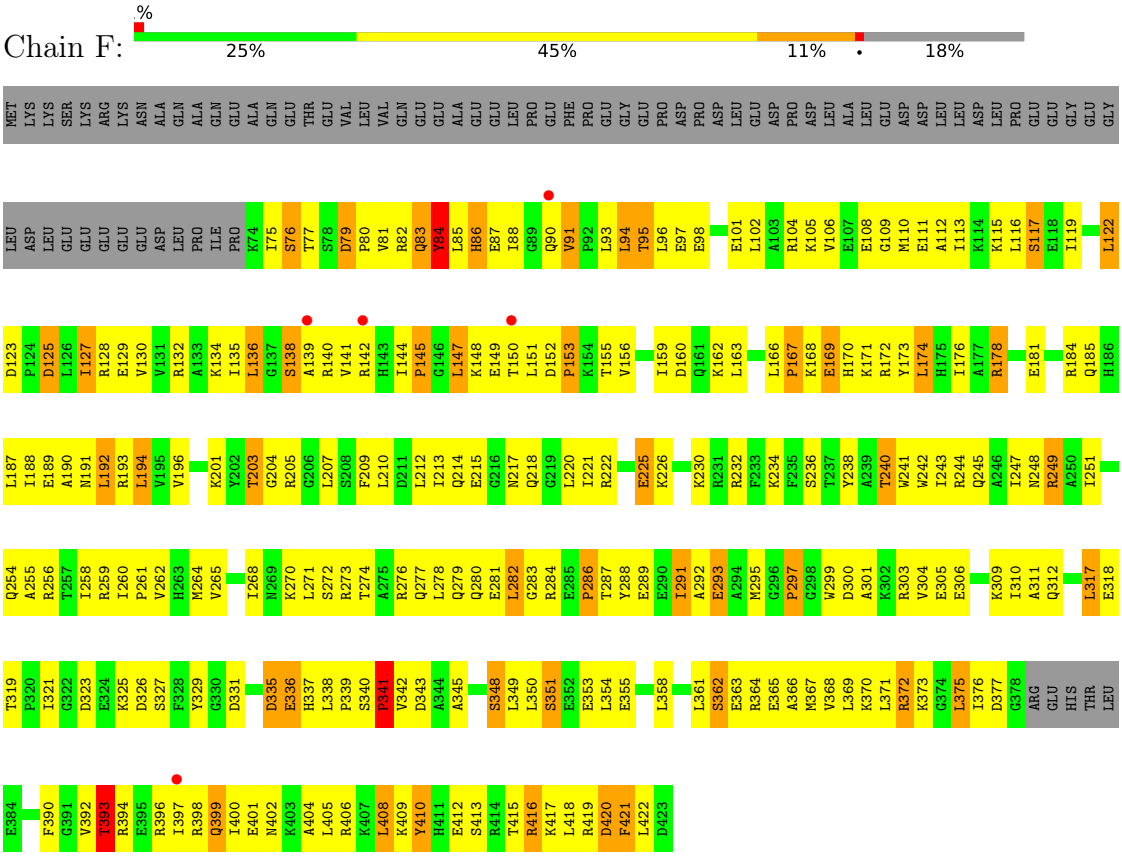
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain O:



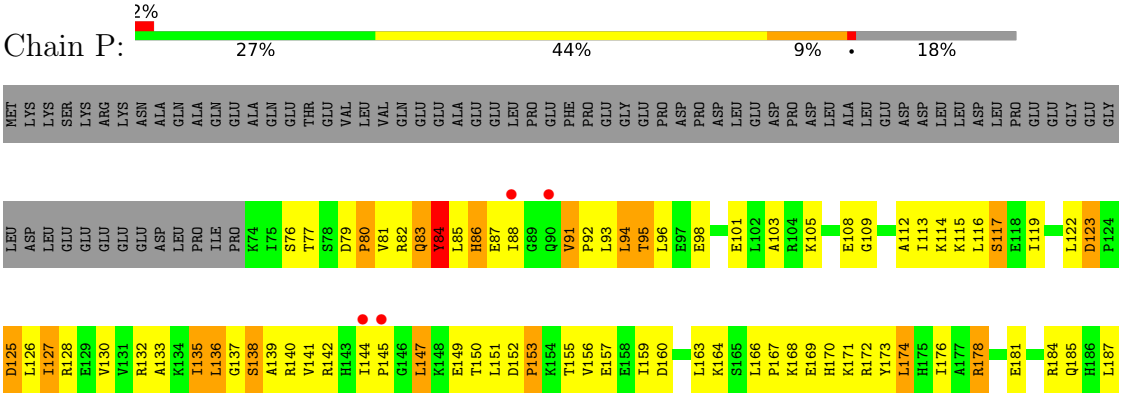
• Molecule 5: RNA polymerase sigma factor rpoD

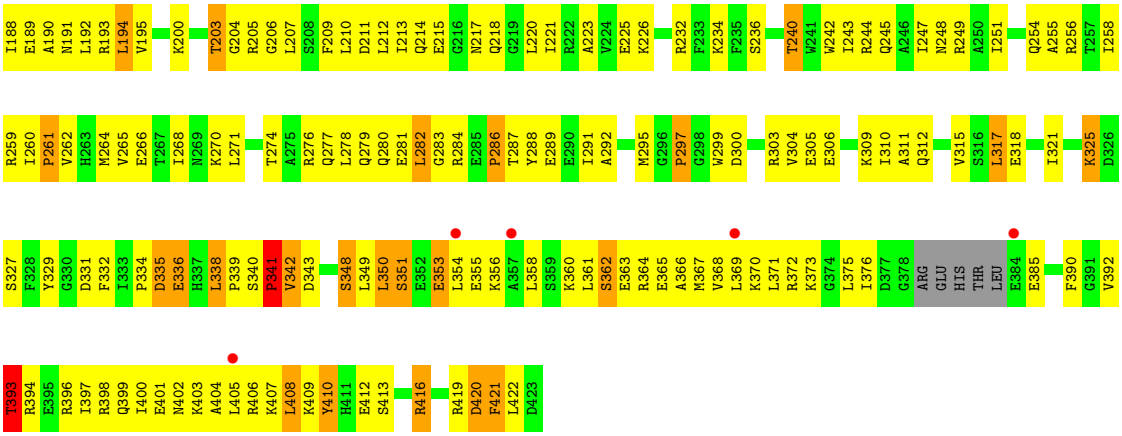
Chain F:



• Molecule 5: RNA polymerase sigma factor rpoD

Chain P:




I188 E189 A190 N191 L192 R193 L194 V195 K200 T203 G204 R205 G206 L207 S208 F209 L210 D211 L212 I213 Q214 E215 G216 N217 Q218 G219 L220 I221 R222 A223 V224 E225 K226 R232 F233 K234 F235 S236 T240 W241 W242 I243 R244 Q245 A246 I247 N248 R249 A250 I251 Q254 A255 R256 T257 I258
R259 I260 P261 V262 H263 M264 V265 E266 T267 I268 N269 K270 L271 T274 A275 R276 Q277 L278 Q279 Q280 E281 L282 G283 R284 E285 P286 T287 Y288 E289 E290 I291 A292 M295 G296 P297 G298 W299 D300 R303 V304 E305 E306 K309 I310 A311 Q312 V315 S316 L317 E318 I321 K325 D326
S327 F328 Y329 G330 D331 F332 I333 P334 D335 E336 H337 L338 P339 S340 P341 V342 D343 S348 L349 L350 S351 E352 E353 L354 E355 K356 A357 L358 S359 K360 L361 S362 E363 R364 E365 A366 M367 V368 L369 K370 L371 R372 K373 G374 L375 I376 D377 G378 ARG GLU HIS THR LEU E384 E385 F390 G391 V392
T393 R394 E395 R396 I397 R398 Q399 I400 E401 N402 K403 A404 L405 R406 K407 L408 K409 Y410 H411 E412 S413 R416 R419 D420 F421 L422 D423

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	235.00Å 235.00Å 254.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 39.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.00-2.70) 90.4 (39.96-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.270 0.238 , 0.260	Depositor DCC
R_{free} test set	18510 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 71.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.166 for -h,-k,l 0.048 for h,-h-k,-l 0.047 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	57340	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, MXP

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	0.84	2/1838 (0.1%)	1.04	9/2498 (0.4%)
1	B	0.74	1/1838 (0.1%)	0.95	9/2498 (0.4%)
1	K	0.81	2/1838 (0.1%)	1.00	8/2498 (0.3%)
1	L	0.75	1/1838 (0.1%)	0.96	10/2498 (0.4%)
2	C	0.73	0/8997	0.94	14/12164 (0.1%)
2	M	0.73	0/8997	0.94	14/12164 (0.1%)
3	D	0.75	2/10582 (0.0%)	0.97	15/14294 (0.1%)
3	N	0.75	1/10582 (0.0%)	0.97	18/14294 (0.1%)
4	E	0.73	0/784	1.23	5/1057 (0.5%)
4	O	0.71	0/784	1.08	3/1057 (0.3%)
5	F	0.65	0/2812	0.85	3/3781 (0.1%)
5	P	0.65	0/2812	0.86	2/3781 (0.1%)
All	All	0.74	9/53702 (0.0%)	0.96	110/72584 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	N	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	GLU	C-O	-11.04	1.02	1.23
1	K	26	GLU	C-O	-10.57	1.03	1.23
1	B	26	GLU	C-O	-10.23	1.03	1.23
1	L	26	GLU	C-O	-9.82	1.04	1.23
1	A	16	GLN	CB-CG	5.82	1.68	1.52
1	K	16	GLN	CB-CG	5.80	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	407	VAL	CB-CG2	-5.45	1.41	1.52
3	D	733	CYS	CB-SG	-5.41	1.73	1.81
3	D	407	VAL	CB-CG2	-5.33	1.41	1.52

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	94	PRO	CA-N-CD	-18.30	85.89	111.50
1	B	138	LEU	CA-CB-CG	12.41	143.84	115.30
1	L	138	LEU	CA-CB-CG	12.19	143.33	115.30
4	O	94	PRO	CA-N-CD	-9.89	97.65	111.50
1	K	26	GLU	CA-C-N	9.51	143.72	117.10
1	A	26	GLU	CA-C-N	9.00	142.30	117.10
3	N	1411	GLY	N-CA-C	-8.94	90.74	113.10
4	E	94	PRO	N-CA-C	8.91	135.26	112.10
3	D	1411	GLY	N-CA-C	-8.89	90.88	113.10
1	K	26	GLU	CA-C-O	-8.69	101.84	120.10
1	A	26	GLU	CA-C-O	-8.19	102.90	120.10
1	A	158	ILE	CG1-CB-CG2	-8.17	93.42	111.40
1	K	158	ILE	CG1-CB-CG2	-8.08	93.63	111.40
1	K	192	LEU	CA-CB-CG	7.83	133.31	115.30
1	A	42	ARG	NE-CZ-NH1	-7.74	116.43	120.30
3	D	614	PHE	CA-CB-CG	7.52	131.96	113.90
1	B	25	LEU	CA-CB-CG	7.34	132.17	115.30
3	N	581	LEU	CA-CB-CG	7.24	131.94	115.30
4	O	94	PRO	N-CA-C	7.03	130.37	112.10
1	L	26	GLU	CA-C-N	6.96	136.58	117.10
1	A	192	LEU	CA-CB-CG	6.92	131.22	115.30
5	F	136	LEU	CA-CB-CG	6.77	130.88	115.30
1	L	138	LEU	CB-CG-CD1	-6.65	99.70	111.00
3	D	637	LEU	CA-CB-CG	6.64	130.57	115.30
1	B	158	ILE	CB-CA-C	-6.64	98.33	111.60
1	L	25	LEU	CA-CB-CG	6.62	130.53	115.30
1	L	158	ILE	CB-CA-C	-6.57	98.47	111.60
1	A	197	LEU	CA-CB-CG	6.46	130.16	115.30
4	E	94	PRO	CA-CB-CG	-6.45	91.75	104.00
3	D	1207	TYR	CA-CB-CG	6.38	125.53	113.40
3	D	581	LEU	CA-CB-CG	6.38	129.98	115.30
5	P	84	TYR	CA-CB-CG	6.32	125.41	113.40
3	D	1109	GLU	CA-C-N	-6.30	103.34	117.20
3	N	813	LEU	CA-CB-CG	6.28	129.74	115.30
1	L	26	GLU	CA-C-O	-6.26	106.95	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	1109	GLU	C-N-CA	6.26	137.34	121.70
3	N	1389	LEU	CA-CB-CG	6.24	129.65	115.30
1	B	26	GLU	CA-C-N	6.23	134.55	117.10
3	D	171	LEU	CA-CB-CG	6.19	129.53	115.30
3	N	1207	TYR	CA-CB-CG	6.18	125.14	113.40
2	C	1119	ARG	CB-CA-C	6.17	122.75	110.40
3	N	80	VAL	CA-C-N	-6.13	103.70	117.20
2	C	114	PHE	CB-CG-CD1	6.13	125.09	120.80
3	N	1109	GLU	CA-C-N	-6.12	103.73	117.20
3	N	80	VAL	C-N-CA	6.05	136.82	121.70
3	D	1109	GLU	C-N-CA	6.04	136.79	121.70
1	B	138	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	K	188	GLN	CA-CB-CG	-6.01	100.19	113.40
2	M	114	PHE	CB-CG-CD1	5.93	124.95	120.80
2	C	58	ASP	C-N-CA	5.91	136.48	121.70
2	C	100	LEU	CA-CB-CG	5.87	128.79	115.30
2	M	114	PHE	CB-CG-CD2	-5.83	116.72	120.80
2	M	503	LEU	CA-CB-CG	5.82	128.69	115.30
3	N	637	LEU	CA-CB-CG	5.82	128.68	115.30
3	N	572	ARG	NE-CZ-NH1	-5.81	117.40	120.30
4	E	94	PRO	N-CD-CG	5.78	111.87	103.20
3	D	80	VAL	CA-C-N	-5.77	104.50	117.20
2	M	58	ASP	C-N-CA	5.77	136.12	121.70
1	A	90	LEU	CA-CB-CG	-5.71	102.18	115.30
3	D	1389	LEU	CA-CB-CG	5.70	128.42	115.30
3	N	58	CYS	CA-CB-SG	5.69	124.25	114.00
2	C	728	HIS	CA-C-N	5.69	129.72	117.20
2	M	287	GLY	N-CA-C	-5.68	98.89	113.10
2	C	114	PHE	CB-CG-CD2	-5.68	116.83	120.80
2	M	571	LEU	CB-CG-CD2	-5.66	101.39	111.00
3	D	831	GLY	N-CA-C	-5.65	98.97	113.10
3	N	831	GLY	N-CA-C	-5.65	98.98	113.10
3	N	171	LEU	CA-CB-CG	5.63	128.25	115.30
1	L	188	GLN	CA-CB-CG	5.62	125.78	113.40
1	B	26	GLU	CA-C-O	-5.60	108.33	120.10
2	C	287	GLY	N-CA-C	-5.60	99.10	113.10
4	E	50	THR	C-N-CA	5.59	135.68	121.70
1	L	146	ARG	CA-CB-CG	5.58	125.69	113.40
5	P	136	LEU	CA-CB-CG	5.58	128.14	115.30
2	M	728	HIS	CA-C-N	5.58	129.48	117.20
4	O	50	THR	C-N-CA	5.53	135.51	121.70
1	K	90	LEU	CA-CB-CG	-5.50	102.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	198	ARG	C-N-CA	5.48	135.40	121.70
2	C	98	LEU	CA-CB-CG	5.48	127.90	115.30
3	N	198	ARG	C-N-CA	5.47	135.39	121.70
1	K	25	LEU	C-N-CA	-5.46	108.06	121.70
3	D	564	GLU	CA-CB-CG	-5.43	101.45	113.40
2	C	264	PRO	C-N-CA	-5.43	108.13	121.70
1	B	188	GLN	CA-CB-CG	5.41	125.31	113.40
5	F	84	TYR	CA-CB-CG	5.41	123.68	113.40
2	C	795	GLY	N-CA-C	-5.41	99.58	113.10
2	M	264	PRO	C-N-CA	-5.40	108.20	121.70
2	M	795	GLY	N-CA-C	-5.37	99.67	113.10
2	M	98	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	188	GLN	CA-CB-CG	-5.35	101.63	113.40
3	N	21	TRP	CA-CB-CG	5.29	123.76	113.70
2	M	974	LEU	CA-CB-CG	5.26	127.39	115.30
1	B	146	ARG	CA-CB-CG	5.26	124.97	113.40
2	C	58	ASP	CA-C-N	-5.22	105.72	117.20
1	L	132	LEU	CA-CB-CG	5.21	127.29	115.30
2	M	58	ASP	CA-C-N	-5.20	105.77	117.20
1	L	2	LEU	CA-CB-CG	5.20	127.25	115.30
1	K	127	LEU	CA-CB-CG	5.17	127.20	115.30
5	F	377	ASP	CB-CG-OD2	5.17	122.96	118.30
3	D	41	ARG	NE-CZ-NH2	-5.17	117.72	120.30
3	D	80	VAL	C-N-CA	5.16	134.60	121.70
3	N	1351	GLU	CA-CB-CG	-5.16	102.05	113.40
2	C	260	LEU	CA-CB-CG	5.10	127.03	115.30
3	N	614	PHE	CB-CG-CD1	5.09	124.37	120.80
2	C	207	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	25	LEU	C-N-CA	-5.07	109.03	121.70
2	M	728	HIS	C-N-CA	-5.05	109.07	121.70
1	B	132	LEU	CA-CB-CG	5.02	126.85	115.30
2	M	1027	PHE	CA-C-N	5.02	126.25	116.20
2	C	763	GLY	C-N-CA	-5.02	109.16	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	132	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	184	0
1	B	1806	0	1861	197	0
1	K	1806	0	1861	212	0
1	L	1806	0	1861	198	0
2	C	8829	0	8933	1145	0
2	M	8829	0	8933	1073	0
3	D	10407	0	10633	1296	0
3	N	10407	0	10633	1283	0
4	E	770	0	784	121	0
4	O	770	0	784	113	0
5	F	2771	0	2844	316	0
5	P	2771	0	2844	312	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	30	0	31	18	0
7	N	30	0	31	18	0
8	D	1	0	0	0	0
8	N	1	0	0	0	0
9	A	141	0	0	28	0
9	B	149	0	0	30	0
9	C	704	0	0	215	0
9	D	927	0	0	239	0
9	E	82	0	0	29	0
9	F	305	0	0	77	0
9	K	152	0	0	41	0
9	L	148	0	0	34	0
9	M	680	0	0	180	0
9	N	864	0	0	235	0
9	O	84	0	0	26	0
9	P	260	0	0	71	0
All	All	57340	0	53894	6054	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 57.

All (6054) 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:D:610:LYS:HD3	7:D:1527:MXP:C15	1.49	1.41
3:N:610:LYS:HD3	7:N:1527:MXP:C15	1.55	1.37
3:N:136:ASP:HB3	3:N:137:PRO:HD3	1.27	1.15
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.27	1.13
3:D:610:LYS:HD3	7:D:1527:MXP:H15B	1.19	1.10
1:L:109:VAL:HG21	1:L:138:LEU:HD11	1.33	1.08
3:N:610:LYS:HD3	7:N:1527:MXP:H15	1.08	1.06
1:A:42:ARG:HH12	1:B:34:VAL:HB	1.00	1.06
1:B:109:VAL:HG21	1:B:138:LEU:HD11	1.35	1.06
2:M:877:PRO:HG2	3:N:1023:MET:HE2	1.27	1.06
3:D:611:GLN:HE22	3:D:1463:LYS:HE2	1.20	1.05
3:N:613:ARG:HG3	3:N:1441:GLN:HB2	1.39	1.04
3:N:101:HIS:HD1	3:N:103:TRP:HB2	1.21	1.04
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.34	1.04
3:N:180:LYS:HG2	3:N:183:GLU:HB2	1.35	1.04
3:D:180:LYS:HG2	3:D:183:GLU:HB2	1.37	1.03
2:C:795:GLY:HA3	2:C:1004:LYS:HE2	1.41	1.02
3:D:187:LYS:HE2	3:D:199:LEU:HB3	1.42	1.02
3:D:1335:LEU:HD23	3:D:1344:VAL:HA	1.41	1.02
3:N:610:LYS:CD	7:N:1527:MXP:C15	2.37	1.02
1:K:67:THR:HG21	2:M:609:ASN:HD21	1.24	1.02
2:M:150:PRO:HA	2:M:158:TYR:HB3	1.40	1.01
3:N:100:ALA:HB2	3:N:513:ILE:HD13	1.41	1.01
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.42	1.01
3:D:610:LYS:CD	7:D:1527:MXP:C15	2.38	1.01
1:A:7:LYS:HE2	1:A:186:LEU:HD11	1.42	1.01
4:E:94:PRO:HD3	9:E:180:HOH:O	1.60	1.00
1:K:7:LYS:HE2	1:K:186:LEU:HD11	1.40	1.00
3:N:1209:LEU:HD21	4:O:16:LYS:HD2	1.38	1.00
3:N:1160:LEU:HD11	3:N:1174:LEU:HD21	1.45	0.98
2:C:150:PRO:HA	2:C:158:TYR:HB3	1.42	0.98
3:D:907:GLU:HA	9:D:2416:HOH:O	1.65	0.97
3:N:148:GLU:HB3	3:N:151:GLN:HB2	1.43	0.97
2:C:2:GLU:HG3	2:C:899:GLN:HB3	1.46	0.97
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.44	0.96
1:A:152:PRO:HA	9:A:351:HOH:O	1.66	0.95
3:N:957:PRO:HG2	3:N:1007:VAL:HA	1.49	0.95
2:M:169:GLY:HA2	2:M:263:ASP:HB3	1.45	0.95
3:N:610:LYS:CD	7:N:1527:MXP:H15	1.96	0.95
1:K:42:ARG:HH12	1:L:34:VAL:HB	1.31	0.95
3:N:1405:GLU:O	3:N:1410:GLU:HA	1.67	0.95
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1465:ASN:HD21	3:N:1470:ARG:HD3	1.33	0.94
3:D:1393:GLN:HB2	3:D:1398:TRP:HE1	1.32	0.94
1:A:42:ARG:NH1	1:B:34:VAL:HB	1.82	0.94
3:D:581:LEU:HD12	3:D:603:LEU:HD11	1.50	0.94
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.48	0.94
5:P:268:ILE:HA	5:P:271:LEU:HD12	1.49	0.94
1:A:42:ARG:HH12	1:B:34:VAL:CB	1.80	0.93
1:L:152:PRO:HD2	1:L:155:LYS:HD3	1.46	0.93
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.50	0.93
2:C:862:PRO:HA	2:C:975:TYR:HE1	1.32	0.93
2:C:890:LEU:HA	2:C:914:ILE:HD11	1.50	0.93
5:P:361:LEU:HD22	5:P:366:ALA:HB2	1.48	0.93
2:C:66:LEU:HD22	2:C:372:LEU:HD23	1.52	0.92
3:D:957:PRO:HG2	3:D:1007:VAL:HA	1.52	0.92
2:M:757:GLY:HA2	2:M:789:SER:HB3	1.52	0.92
3:D:1194:CYS:HB2	9:D:1762:HOH:O	1.70	0.92
2:M:890:LEU:HA	2:M:914:ILE:HD11	1.52	0.92
3:D:610:LYS:HD3	7:D:1527:MXP:H15	1.52	0.92
2:M:1054:THR:HG23	2:M:1082:PRO:HG3	1.48	0.92
5:F:268:ILE:HA	5:F:271:LEU:HD12	1.51	0.91
3:N:581:LEU:HD12	3:N:603:LEU:HD11	1.51	0.91
3:D:611:GLN:HE22	3:D:1463:LYS:CE	1.84	0.91
2:M:437:ARG:CZ	2:M:488:ALA:HA	2.01	0.91
3:D:508:ARG:HG2	3:D:509:PRO:HD2	1.52	0.91
2:M:66:LEU:HD22	2:M:372:LEU:HD23	1.53	0.91
3:D:100:ALA:HB2	3:D:513:ILE:HD13	1.50	0.91
3:D:611:GLN:NE2	3:D:1463:LYS:HE2	1.84	0.91
3:N:675:ARG:HH12	5:P:421:PHE:HD2	1.15	0.91
2:M:409:ARG:HA	2:M:454:SER:HA	1.53	0.91
3:D:1405:GLU:O	3:D:1410:GLU:HA	1.71	0.90
2:C:41:ASN:HD22	2:C:41:ASN:H	1.16	0.90
2:M:862:PRO:HA	2:M:975:TYR:HE1	1.34	0.90
2:C:1114:GLY:H	2:C:1115:LEU:HD12	1.35	0.90
1:K:190:THR:HA	9:K:1309:HOH:O	1.70	0.90
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.53	0.90
3:D:406:ASP:HB3	5:F:168:LYS:HE2	1.54	0.89
3:D:87:ARG:HA	9:D:1713:HOH:O	1.71	0.89
1:B:152:PRO:HD2	1:B:155:LYS:HD3	1.54	0.89
3:N:18:ILE:HG23	3:N:518:PRO:HG3	1.54	0.89
1:A:24:VAL:HG22	1:A:196:THR:HB	1.54	0.88
3:D:204:LEU:HA	3:D:441:ARG:HH22	1.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:874:LEU:HD21	3:N:787:LEU:HD22	1.53	0.88
3:N:508:ARG:HG2	3:N:509:PRO:HD2	1.54	0.88
5:P:128:ARG:O	5:P:132:ARG:HG3	1.72	0.88
1:B:87:VAL:HG21	1:B:144:VAL:HG11	1.56	0.88
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	1.54	0.88
2:C:367:LEU:HA	2:C:371:LYS:HG3	1.53	0.88
2:C:1087:VAL:CG1	3:D:610:LYS:NZ	2.36	0.88
3:N:400:VAL:HG22	3:N:443:VAL:HG21	1.54	0.88
2:C:1054:THR:HG22	2:C:1059:ASP:HB2	1.52	0.88
5:P:205:ARG:HD2	5:P:251:ILE:HD13	1.56	0.88
2:C:191:PHE:HZ	2:C:196:LEU:HB2	1.37	0.88
3:N:165:LYS:HB2	3:N:397:LYS:HB3	1.56	0.88
2:C:431:HIS:HB3	2:C:434:HIS:HD2	1.39	0.88
2:C:952:LEU:HD12	2:C:969:GLN:HE22	1.35	0.88
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.39	0.88
5:F:128:ARG:O	5:F:132:ARG:HG3	1.74	0.88
1:L:184:THR:HG23	1:L:192:LEU:HB3	1.55	0.87
2:M:41:ASN:HD22	2:M:41:ASN:H	1.17	0.87
1:B:86:VAL:HG12	1:B:124:ASN:HD22	1.39	0.87
2:C:671:ASN:N	2:C:671:ASN:HD22	1.70	0.87
4:O:41:GLU:HA	4:O:45:ARG:HD3	1.57	0.87
3:N:131:LYS:HG2	3:N:568:ARG:HG2	1.56	0.87
1:L:194:LYS:HG2	9:L:1676:HOH:O	1.74	0.87
2:M:367:LEU:HA	2:M:371:LYS:HG3	1.57	0.87
3:N:1406:ARG:HA	3:N:1410:GLU:HG2	1.56	0.87
3:N:1393:GLN:HB2	3:N:1398:TRP:HE1	1.40	0.87
1:L:86:VAL:HG12	1:L:124:ASN:HD22	1.39	0.86
1:L:132:LEU:HG	1:L:136:GLY:HA3	1.57	0.86
3:N:59:ALA:HB3	3:N:76:CYS:SG	2.14	0.86
3:N:494:LYS:HA	9:N:1731:HOH:O	1.73	0.86
3:N:116:LEU:HD21	3:N:464:LEU:HB3	1.56	0.86
1:A:20:TYR:HD2	1:A:21:GLY:N	1.72	0.86
2:C:121:MET:HA	9:C:1509:HOH:O	1.73	0.86
2:M:140:ILE:HD11	2:M:412:ALA:HA	1.56	0.86
2:M:762:LYS:HB2	2:M:786:LYS:HD2	1.55	0.86
2:M:597:ALA:HB2	2:M:655:LEU:HD21	1.56	0.86
1:L:94:LEU:HD21	1:L:119:ASP:HB2	1.55	0.86
3:N:1383:ASP:HB2	3:N:1416:ALA:HB3	1.56	0.86
1:K:222:LEU:HD21	1:L:218:LEU:HD23	1.58	0.86
3:N:489:ARG:HH22	3:N:1389:LEU:HD21	1.40	0.85
3:N:1232:PRO:HB3	3:N:1361:VAL:HG21	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HD21	1:B:119:ASP:HB2	1.56	0.85
2:M:1054:THR:HG22	2:M:1059:ASP:HB2	1.58	0.85
3:N:187:LYS:HE2	3:N:199:LEU:HB3	1.56	0.85
3:N:201:GLY:HA2	3:N:396:VAL:O	1.74	0.85
5:P:291:ILE:HG21	5:P:304:VAL:HG11	1.57	0.85
2:C:1087:VAL:CG1	3:D:610:LYS:HZ1	1.87	0.85
3:D:201:GLY:HA2	3:D:396:VAL:O	1.76	0.85
3:D:400:VAL:HG22	3:D:443:VAL:HG21	1.57	0.85
5:F:205:ARG:HD2	5:F:251:ILE:HD13	1.56	0.85
3:N:204:LEU:HA	3:N:441:ARG:HH22	1.40	0.85
4:E:41:GLU:HA	4:E:45:ARG:HD3	1.56	0.85
2:M:302:VAL:HG12	9:M:1862:HOH:O	1.75	0.85
5:P:166:LEU:HB3	5:P:170:HIS:HB2	1.57	0.85
1:B:184:THR:HG23	1:B:192:LEU:HB3	1.57	0.85
2:C:1084:SER:HB2	7:D:1527:MXP:O4	1.76	0.85
3:D:561:GLY:HA3	5:F:184:ARG:HH12	1.42	0.85
3:D:1160:LEU:HD11	3:D:1174:LEU:HD21	1.57	0.85
2:M:710:ILE:HB	2:M:790:LEU:HD13	1.59	0.85
1:A:103:ALA:HB1	1:A:107:LYS:HE2	1.57	0.84
3:N:908:LYS:HB3	3:N:1027:GLY:HA3	1.58	0.84
1:B:58:ILE:HG22	1:B:137:ARG:HH21	1.41	0.84
3:D:59:ALA:HB3	3:D:76:CYS:SG	2.17	0.84
3:N:617:ASN:OD1	3:N:617:ASN:N	2.09	0.84
5:F:166:LEU:HB3	5:F:170:HIS:HB2	1.59	0.84
3:D:558:LEU:HD13	5:F:145:PRO:HB3	1.58	0.84
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.59	0.84
3:D:101:HIS:HD1	3:D:103:TRP:HB2	1.42	0.84
3:D:611:GLN:OE1	7:D:1527:MXP:H16B	1.78	0.84
4:O:95:VAL:HG13	9:O:1302:HOH:O	1.75	0.84
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.59	0.84
4:E:25:LYS:HE2	9:E:136:HOH:O	1.78	0.83
2:M:733:ALA:HB2	3:N:679:ARG:NH2	1.93	0.83
1:B:158:ILE:HD11	1:B:166:PRO:HA	1.59	0.83
1:L:158:ILE:HD11	1:L:166:PRO:HA	1.60	0.83
3:D:1465:ASN:HD21	3:D:1470:ARG:HD3	1.43	0.83
2:C:461:VAL:HG13	2:C:465:GLY:HA2	1.58	0.83
4:O:54:LEU:HG	4:O:58:PRO:HG2	1.61	0.83
1:A:35:THR:HG21	1:B:43:ILE:HD11	1.58	0.83
2:C:1009:SER:HB2	3:D:651:GLU:O	1.78	0.83
2:M:18:LEU:HD23	2:M:404:LEU:HD21	1.59	0.83
2:M:1114:GLY:H	2:M:1115:LEU:HD12	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:108:VAL:HB	3:N:109:PRO:HD3	1.60	0.83
1:K:42:ARG:HH21	2:M:857:ASP:HB3	1.44	0.83
3:D:1466:VAL:HG23	3:D:1472:ILE:HD11	1.60	0.83
2:M:952:LEU:HD12	2:M:969:GLN:HE22	1.41	0.83
2:M:1005:MET:HE1	3:N:648:MET:HB2	1.61	0.82
3:N:611:GLN:HG2	3:N:619:LEU:CD1	2.09	0.82
1:B:132:LEU:HD13	1:B:138:LEU:HD12	1.61	0.82
5:F:291:ILE:HG21	5:F:304:VAL:HG11	1.59	0.82
2:C:148:PHE:HZ	2:C:281:LEU:HD13	1.43	0.82
1:L:87:VAL:HG21	1:L:144:VAL:HG11	1.59	0.82
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.61	0.82
3:N:615:ARG:HH21	3:N:1089:ALA:HB2	1.44	0.82
2:C:409:ARG:HA	2:C:454:SER:HA	1.61	0.82
2:C:877:PRO:HG2	3:D:1023:MET:HE2	1.59	0.82
2:C:114:PHE:H	2:C:114:PHE:HD1	1.25	0.82
3:D:1406:ARG:HA	3:D:1410:GLU:HG2	1.61	0.82
3:N:32:ILE:HA	9:N:1836:HOH:O	1.79	0.82
2:C:1044:GLY:HA3	4:E:17:TYR:HE1	1.45	0.82
3:D:614:PHE:CD1	3:D:617:ASN:HA	2.14	0.82
3:N:465:LEU:HD21	9:N:1664:HOH:O	1.80	0.82
2:M:571:LEU:HD21	2:M:700:TYR:HA	1.60	0.82
3:N:152:LEU:HD23	3:N:152:LEU:H	1.43	0.82
3:N:1057:VAL:HG13	3:N:1069:GLU:HB3	1.60	0.82
2:C:750:LYS:HG3	3:D:681:ARG:HH21	1.45	0.82
2:M:603:VAL:HG21	2:M:643:VAL:HG11	1.60	0.82
2:M:643:VAL:HG23	9:M:1789:HOH:O	1.80	0.82
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.61	0.81
3:N:119:SER:HB2	3:N:123:LEU:HB2	1.58	0.81
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.62	0.81
3:N:1466:VAL:HG23	3:N:1472:ILE:HD11	1.60	0.81
3:D:798:GLU:HB2	3:D:828:LYS:HE3	1.62	0.81
2:M:114:PHE:HD1	2:M:114:PHE:H	1.23	0.81
3:N:1115:THR:HB	9:N:1624:HOH:O	1.80	0.81
3:D:136:ASP:HB3	3:D:137:PRO:CD	2.10	0.81
3:N:136:ASP:HB3	3:N:137:PRO:CD	2.10	0.81
2:M:513:VAL:HB	9:M:1622:HOH:O	1.80	0.81
4:O:10:PHE:HE2	4:O:16:LYS:HG3	1.45	0.81
3:N:795:VAL:HG11	3:N:863:VAL:HG13	1.61	0.81
5:P:117:SER:HA	9:P:595:HOH:O	1.81	0.81
1:B:132:LEU:HG	1:B:136:GLY:HA3	1.60	0.80
2:C:169:GLY:HA2	2:C:263:ASP:HB3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:860:HIS:HB2	9:C:1269:HOH:O	1.81	0.80
3:D:633:VAL:HG22	3:D:635:PRO:HD3	1.62	0.80
3:N:610:LYS:HD3	7:N:1527:MXP:H15B	1.58	0.80
3:N:843:PHE:HE1	3:N:864:VAL:HG11	1.44	0.80
2:C:436:GLY:O	2:C:459:ALA:HB2	1.81	0.80
3:D:592:THR:H	3:D:600:LEU:HD21	1.46	0.80
5:F:350:LEU:HD12	5:F:422:LEU:HD12	1.63	0.80
2:C:413:LEU:H	2:C:413:LEU:HD12	1.45	0.80
1:L:4:SER:HA	1:L:7:LYS:HE2	1.63	0.80
2:M:675:ALA:HA	2:M:989:VAL:HG12	1.63	0.80
3:N:699:VAL:H	3:N:756:GLN:NE2	1.80	0.80
3:D:1161:GLU:HG3	3:D:1164:ARG:HB2	1.64	0.80
2:M:599:GLU:HG3	2:M:600:ASP:H	1.46	0.80
2:M:786:LYS:HA	9:M:1657:HOH:O	1.80	0.80
3:N:1277:ILE:HD12	3:N:1301:LYS:HB2	1.63	0.80
3:N:135:LEU:HD11	9:N:2226:HOH:O	1.82	0.80
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.62	0.80
2:M:943:VAL:HG23	2:M:985:GLY:H	1.46	0.80
2:M:611:ILE:HD11	2:M:641:PRO:HG3	1.64	0.80
3:D:1220:ALA:HB1	3:D:1223:ILE:HD13	1.63	0.80
3:D:1223:ILE:H	3:D:1223:ILE:HD12	1.47	0.80
1:K:100:LEU:HB2	1:K:115:LEU:HD11	1.64	0.80
1:K:185:ARG:HA	9:K:1309:HOH:O	1.82	0.80
2:C:76:PRO:HB3	9:C:1229:HOH:O	1.83	0.79
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.64	0.79
3:D:1393:GLN:HB2	3:D:1398:TRP:NE1	1.96	0.79
1:K:87:VAL:HG21	1:K:144:VAL:HG11	1.64	0.79
1:L:55:SER:HB3	1:L:143:ARG:HB3	1.64	0.79
2:C:54:ILE:HD11	2:C:356:ARG:HG2	1.63	0.79
1:K:20:TYR:HD2	1:K:21:GLY:N	1.80	0.79
2:M:260:LEU:HB2	2:M:291:ALA:HB1	1.62	0.79
3:N:1095:THR:HG23	3:N:1230:GLY:HA3	1.62	0.79
5:P:132:ARG:HG2	5:P:181:GLU:OE1	1.81	0.79
3:N:613:ARG:NH2	3:N:1097:LYS:HE2	1.97	0.79
1:B:4:SER:HA	1:B:7:LYS:HE2	1.64	0.79
2:C:199:VAL:HG21	9:C:1705:HOH:O	1.82	0.79
2:M:1008:ARG:HH11	2:M:1028:GLY:HA2	1.47	0.79
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.63	0.79
4:E:94:PRO:CD	9:E:180:HOH:O	2.25	0.79
2:M:578:VAL:HG11	2:M:991:GLN:HB3	1.62	0.79
3:D:119:SER:H	3:D:123:LEU:HD22	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:1937:HOH:O	3:N:1068:LEU:HD11	1.82	0.79
3:N:783:ARG:NH1	3:N:1029:ARG:HG3	1.96	0.79
3:D:1095:THR:HG23	3:D:1230:GLY:HA3	1.64	0.79
2:M:774:LEU:HA	2:M:777:ILE:HD12	1.64	0.79
1:A:222:LEU:HD23	1:B:215:VAL:HB	1.64	0.79
2:C:512:ARG:HD3	2:C:523:ILE:HD11	1.65	0.79
3:D:162:ARG:HB3	9:D:2186:HOH:O	1.81	0.79
5:F:293:GLU:HB3	9:F:578:HOH:O	1.82	0.79
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.65	0.78
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.64	0.78
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.65	0.78
2:M:148:PHE:HZ	2:M:281:LEU:HD13	1.47	0.78
2:M:630:ARG:NH1	2:M:707:ARG:H	1.81	0.78
3:N:546:ARG:O	3:N:550:ARG:HG2	1.81	0.78
1:K:150:TYR:CE1	2:M:696:LYS:HA	2.19	0.78
1:K:206:THR:HG22	1:K:209:GLU:HG3	1.64	0.78
3:N:798:GLU:HB2	3:N:828:LYS:HE3	1.65	0.78
3:N:1273:VAL:HG22	3:N:1326:THR:OG1	1.84	0.78
2:C:256:TYR:CE1	2:C:293:PHE:HB2	2.18	0.78
2:C:474:VAL:HG11	2:C:529:VAL:HG12	1.64	0.78
2:M:571:LEU:HD21	2:M:700:TYR:HD2	1.47	0.78
3:N:493:ARG:HD2	3:N:1390:LEU:O	1.83	0.78
3:N:592:THR:H	3:N:600:LEU:HD21	1.47	0.78
4:O:46:PRO:HB3	4:O:54:LEU:HD22	1.64	0.78
2:M:413:LEU:H	2:M:413:LEU:HD12	1.48	0.78
3:N:630:VAL:HA	3:N:744:GLN:HG2	1.64	0.78
2:C:143:SER:HB2	2:C:276:LYS:HZ1	1.49	0.78
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.64	0.78
3:D:1277:ILE:HD12	3:D:1301:LYS:HB2	1.65	0.78
5:F:85:LEU:HA	5:F:88:ILE:HD12	1.66	0.78
1:L:58:ILE:HG22	1:L:137:ARG:HH21	1.48	0.78
3:N:55:ASP:HB3	9:N:1551:HOH:O	1.84	0.78
1:A:88:ARG:HA	9:A:344:HOH:O	1.82	0.78
2:C:578:VAL:HG23	2:C:579:VAL:HG12	1.64	0.78
2:C:1087:VAL:HG13	3:D:610:LYS:HZ1	1.48	0.78
3:D:1198:TYR:HA	9:D:2099:HOH:O	1.83	0.78
2:M:862:PRO:HA	2:M:975:TYR:CE1	2.19	0.78
2:C:100:LEU:HD23	2:C:368:THR:HA	1.66	0.78
4:E:31:LEU:HD21	4:E:60:ALA:HB2	1.65	0.78
5:P:130:VAL:HG21	5:P:159:ILE:HG21	1.65	0.78
1:B:41:ARG:HG3	1:B:177:VAL:HG21	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:HIS:HA	1:B:224:TYR:HD2	1.46	0.78
2:C:178:PRO:HA	9:C:1213:HOH:O	1.82	0.78
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.65	0.78
3:N:1312:LEU:HB2	9:N:2368:HOH:O	1.84	0.78
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.65	0.77
2:M:12:VAL:HG12	2:M:534:VAL:HG13	1.64	0.77
3:N:1291:SER:HB2	3:N:1293:PHE:HE1	1.48	0.77
1:B:32:PHE:HB2	9:B:398:HOH:O	1.84	0.77
3:D:610:LYS:CD	7:D:1527:MXP:H15B	2.06	0.77
3:N:116:LEU:HD22	3:N:118:LEU:HD11	1.67	0.77
2:C:1083:GLU:HG2	9:D:1751:HOH:O	1.82	0.77
2:M:797:GLY:HA2	9:M:1828:HOH:O	1.83	0.77
1:A:186:LEU:HB2	1:A:192:LEU:HD11	1.67	0.77
3:D:116:LEU:HD21	3:D:464:LEU:HB3	1.66	0.77
3:D:615:ARG:O	3:D:617:ASN:N	2.17	0.77
1:A:9:PRO:HB2	1:B:224:TYR:HB3	1.67	0.77
3:D:403:PHE:HD1	3:D:405:ASP:O	1.67	0.77
2:C:157:ARG:HD2	2:C:314:THR:HG22	1.67	0.77
2:C:163:ILE:HB	2:C:171:TRP:CH2	2.18	0.77
2:C:597:ALA:HB2	2:C:655:LEU:HD21	1.64	0.77
2:M:115:LEU:HD22	2:M:373:VAL:HG11	1.64	0.77
3:N:32:ILE:HG22	5:P:258:ILE:HD12	1.66	0.77
2:C:766:GLU:HG2	2:C:772:ARG:HH12	1.50	0.77
3:D:400:VAL:CG2	3:D:443:VAL:HG21	2.15	0.77
2:M:87:ASP:HA	9:M:1651:HOH:O	1.83	0.77
2:M:512:ARG:HD3	2:M:523:ILE:HD11	1.65	0.77
3:D:1495:ILE:HG12	4:E:80:VAL:HG11	1.66	0.77
5:F:132:ARG:HG2	5:F:181:GLU:OE1	1.85	0.77
2:M:1115:LEU:HD23	3:N:85:VAL:HG13	1.65	0.77
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.67	0.77
3:D:1389:LEU:HD12	3:D:1390:LEU:H	1.49	0.77
2:M:431:HIS:HB3	2:M:434:HIS:HD2	1.48	0.77
3:N:1223:ILE:H	3:N:1223:ILE:HD12	1.49	0.77
5:P:142:ARG:HD2	9:P:502:HOH:O	1.85	0.77
5:P:144:ILE:HB	5:P:145:PRO:HD3	1.67	0.77
2:C:760:SER:HA	9:C:1430:HOH:O	1.85	0.76
3:D:135:LEU:HD23	9:D:1592:HOH:O	1.86	0.76
2:M:1019:GLN:HE22	3:N:621:LYS:HA	1.49	0.76
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.66	0.76
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.65	0.76
3:D:1112:CYS:HB2	3:D:1195:GLN:HG2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.66	0.76
3:D:478:LEU:HD21	3:D:500:ARG:NH2	2.01	0.76
3:D:1191:PRO:HA	9:D:1762:HOH:O	1.86	0.76
2:C:468:ARG:HB2	2:C:486:MET:O	1.85	0.76
2:C:1103:ASP:OD1	3:D:3:LYS:HB2	1.85	0.76
3:D:1057:VAL:HG13	3:D:1069:GLU:HB3	1.65	0.76
1:L:60:ASP:HB2	1:L:137:ARG:CZ	2.16	0.76
3:N:611:GLN:HG2	3:N:619:LEU:HG	1.66	0.76
3:N:863:VAL:HG23	9:N:1635:HOH:O	1.85	0.76
3:D:152:LEU:HD23	3:D:152:LEU:H	1.50	0.76
3:D:1262:LEU:HD23	3:D:1352:ILE:HG13	1.66	0.76
5:F:260:ILE:HG23	5:F:264:MET:HB2	1.66	0.76
3:N:1040:GLY:O	3:N:1060:SER:HB3	1.85	0.76
2:M:914:ILE:HB	9:M:1825:HOH:O	1.85	0.76
2:C:862:PRO:HA	2:C:975:TYR:CE1	2.17	0.76
1:K:117:VAL:HB	1:K:120:VAL:HG12	1.66	0.76
3:N:489:ARG:NH2	3:N:1389:LEU:HD21	2.00	0.76
3:N:1041:LEU:HD12	3:N:1058:ARG:HA	1.68	0.76
3:D:544:TYR:O	3:D:548:ILE:HG12	1.85	0.76
5:F:144:ILE:HB	5:F:145:PRO:HD3	1.68	0.76
3:N:850:LEU:H	3:N:850:LEU:HD12	1.48	0.76
1:K:103:ALA:HB1	1:K:107:LYS:HE2	1.67	0.76
2:C:108:ILE:HB	2:C:368:THR:OG1	1.86	0.76
2:C:260:LEU:HB2	2:C:291:ALA:HB1	1.66	0.76
2:C:905:ILE:HD12	2:C:905:ILE:H	1.50	0.76
3:D:28:LYS:HG3	3:D:41:ARG:HH11	1.50	0.76
3:D:1205:TYR:CD2	3:D:1215:VAL:HG21	2.21	0.76
3:N:608:SER:HA	3:N:1443:THR:HG21	1.66	0.76
3:N:1094:LEU:O	3:N:1098:LEU:HD13	1.86	0.76
3:N:1495:ILE:HG12	4:O:80:VAL:HG11	1.66	0.76
4:O:31:LEU:HD21	4:O:60:ALA:HB2	1.67	0.76
5:F:155:THR:O	5:F:159:ILE:HG12	1.86	0.75
2:M:199:VAL:HG13	2:M:235:LEU:HG	1.66	0.75
3:N:400:VAL:CG2	3:N:443:VAL:HG21	2.17	0.75
3:N:637:LEU:HD21	3:N:642:CYS:HA	1.67	0.75
3:N:1062:ARG:HB2	9:N:1637:HOH:O	1.84	0.75
3:D:13:ALA:HA	9:D:1541:HOH:O	1.86	0.75
3:D:804:LEU:HB2	3:D:830:ALA:O	1.86	0.75
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.68	0.75
3:N:101:HIS:ND1	3:N:103:TRP:HB2	1.99	0.75
2:C:1081:VAL:HG21	2:C:1111:ILE:HG22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:232:GLU:HA	2:C:235:LEU:HD12	1.67	0.75
2:M:163:ILE:HB	2:M:171:TRP:CH2	2.22	0.75
2:C:54:ILE:HG21	9:C:1578:HOH:O	1.86	0.75
2:M:534:VAL:HB	9:M:1660:HOH:O	1.87	0.75
2:M:18:LEU:HB2	2:M:590:ASP:HB3	1.69	0.75
3:N:100:ALA:HB2	3:N:513:ILE:CD1	2.16	0.75
5:P:139:ALA:HA	5:P:152:ASP:CG	2.06	0.75
5:P:155:THR:O	5:P:159:ILE:HG12	1.86	0.75
1:A:224:TYR:HB3	1:B:9:PRO:HB2	1.66	0.75
2:C:197:LEU:HD22	2:C:202:TYR:HD2	1.51	0.75
3:D:1040:GLY:O	3:D:1060:SER:HB3	1.86	0.75
2:M:129:ILE:HG12	2:M:386:PHE:HB3	1.68	0.75
2:M:671:ASN:HD22	2:M:671:ASN:N	1.83	0.75
2:M:691:SER:HB2	2:M:858:MET:SD	2.26	0.75
1:B:55:SER:HB3	1:B:143:ARG:HB3	1.68	0.75
3:D:508:ARG:HB3	9:D:1761:HOH:O	1.86	0.75
3:D:850:LEU:HD12	3:D:850:LEU:H	1.49	0.75
5:F:87:GLU:O	5:F:91:VAL:HG23	1.85	0.75
1:K:18:ARG:HH11	1:K:123:MET:HE2	1.52	0.75
2:C:325:ILE:HG23	9:C:1315:HOH:O	1.86	0.75
3:N:611:GLN:HE22	7:N:1527:MXP:H16B	1.50	0.75
5:P:132:ARG:O	5:P:136:LEU:HG	1.87	0.75
1:B:34:VAL:HG22	1:B:181:VAL:HG21	1.68	0.74
4:E:45:ARG:HE	4:E:55:PHE:HD2	1.33	0.74
3:N:611:GLN:HG2	3:N:619:LEU:CG	2.17	0.74
3:D:458:ALA:HB1	3:D:513:ILE:HD12	1.67	0.74
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.68	0.74
3:N:171:LEU:HG	9:N:1934:HOH:O	1.86	0.74
3:N:1101:VAL:HG22	3:N:1428:ALA:HB2	1.70	0.74
3:N:1420:LEU:HD12	3:N:1421:LEU:H	1.51	0.74
2:C:979:THR:HG23	2:C:981:GLU:H	1.52	0.74
3:D:1045:MET:HB2	3:D:1072:ILE:HG22	1.70	0.74
2:C:101:ILE:HG23	2:C:107:LEU:HD22	1.69	0.74
3:N:890:VAL:HG11	3:N:922:LEU:HD13	1.70	0.74
2:C:1056:LYS:O	3:D:624:ASP:HB2	1.87	0.74
3:D:586:ARG:NH1	3:D:1444:THR:HG21	2.02	0.74
5:F:274:THR:O	5:F:278:LEU:HG	1.88	0.74
1:K:221:HIS:HA	1:K:224:TYR:CD2	2.22	0.74
3:N:1264:GLU:HG3	3:N:1424:VAL:HG12	1.69	0.74
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.69	0.74
1:K:226:SER:O	1:K:228:PRO:HD3	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1147:ARG:HB3	3:N:1188:VAL:HG21	1.68	0.74
3:D:1273:VAL:HG22	3:D:1326:THR:OG1	1.88	0.74
1:L:221:HIS:HA	1:L:224:TYR:HD2	1.51	0.74
2:M:139:GLN:OE1	2:M:415:PRO:HD2	1.88	0.74
3:N:458:ALA:HB1	3:N:513:ILE:HD12	1.68	0.74
3:N:1324:PRO:HA	9:N:1761:HOH:O	1.87	0.74
3:D:171:LEU:HB2	3:D:391:ALA:O	1.86	0.74
9:M:2128:HOH:O	3:N:1047:LYS:HE2	1.86	0.74
5:P:101:GLU:HB3	5:P:105:LYS:HE3	1.69	0.74
2:M:431:HIS:HB3	2:M:434:HIS:CD2	2.23	0.74
3:N:489:ARG:HG3	3:N:1388:ARG:HH22	1.53	0.74
1:B:201:THR:HG22	1:B:203:GLY:H	1.53	0.73
2:C:683:ASN:HA	2:C:687:ALA:HB3	1.70	0.73
9:C:1263:HOH:O	5:F:331:ASP:HA	1.88	0.73
3:N:206:ARG:HH12	5:P:98:GLU:HA	1.50	0.73
1:K:42:ARG:HH21	2:M:857:ASP:CB	2.00	0.73
2:M:256:TYR:CE1	2:M:293:PHE:HB2	2.23	0.73
3:N:1209:LEU:HD23	3:N:1211:MET:SD	2.28	0.73
1:B:176:ARG:HH21	3:D:850:LEU:HD13	1.53	0.73
2:C:222:MET:HB3	9:C:1633:HOH:O	1.88	0.73
2:C:1014:SER:HB3	2:C:1017:THR:O	1.88	0.73
3:N:37:LEU:HB3	9:N:1894:HOH:O	1.88	0.73
2:C:191:PHE:CZ	2:C:196:LEU:HB2	2.22	0.73
3:D:569:ASN:HB3	5:F:214:GLN:NE2	2.03	0.73
5:F:400:ILE:HG22	9:F:568:HOH:O	1.88	0.73
3:D:677:LEU:HD11	9:D:2185:HOH:O	1.88	0.73
4:E:46:PRO:HB3	4:E:54:LEU:HD22	1.71	0.73
1:K:22:GLU:HB3	9:K:1055:HOH:O	1.88	0.73
3:N:171:LEU:HB2	3:N:391:ALA:O	1.87	0.73
3:N:804:LEU:HB2	3:N:830:ALA:O	1.87	0.73
2:C:1008:ARG:HD2	2:C:1028:GLY:H	1.53	0.73
5:F:394:ARG:CZ	5:F:398:ARG:HB2	2.19	0.73
2:M:169:GLY:HA2	2:M:263:ASP:CB	2.19	0.73
2:C:654:LEU:HD11	2:C:663:ASN:ND2	2.03	0.73
3:D:477:LEU:HD11	3:D:495:ARG:HD3	1.69	0.73
1:L:213:GLN:O	1:L:217:ILE:HD12	1.88	0.73
1:B:60:ASP:HB2	1:B:137:ARG:CZ	2.19	0.73
2:C:109:LYS:HE2	2:C:111:ASP:OD1	1.88	0.73
5:P:112:ALA:HA	5:P:173:TYR:HD2	1.54	0.73
1:A:226:SER:O	1:A:228:PRO:HD3	1.89	0.73
2:C:431:HIS:HB3	2:C:434:HIS:CD2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:603:VAL:HG21	2:C:643:VAL:HG11	1.69	0.73
2:M:431:HIS:CD2	2:M:433:THR:H	2.07	0.73
1:A:49:PRO:HB3	1:A:148:VAL:HG22	1.71	0.73
1:B:58:ILE:HG22	1:B:137:ARG:NH2	2.03	0.73
1:B:138:LEU:HD23	1:B:140:MET:SD	2.28	0.73
3:D:453:ASP:HB2	9:D:1592:HOH:O	1.87	0.73
2:M:232:GLU:HA	2:M:235:LEU:HD12	1.70	0.73
3:N:536:ALA:HA	5:P:315:VAL:O	1.88	0.73
2:C:42:VAL:HG12	2:C:43:GLY:H	1.54	0.72
2:C:943:VAL:HG23	2:C:985:GLY:H	1.54	0.72
2:C:1010:THR:HG21	5:F:341:PRO:HB2	1.69	0.72
3:D:80:VAL:HG23	9:D:1536:HOH:O	1.87	0.72
2:M:140:ILE:HA	2:M:332:ARG:O	1.88	0.72
2:M:256:TYR:HE1	2:M:293:PHE:HB2	1.52	0.72
1:B:36:LEU:O	1:B:39:PRO:HD2	1.90	0.72
2:M:738:ASP:HB2	2:M:744:ARG:HB3	1.70	0.72
5:P:260:ILE:HG23	5:P:264:MET:HB2	1.69	0.72
2:C:140:ILE:HD11	2:C:412:ALA:HA	1.71	0.72
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.70	0.72
5:F:394:ARG:HA	5:F:397:ILE:HD12	1.69	0.72
1:K:67:THR:CG2	2:M:609:ASN:HD21	1.98	0.72
1:L:80:LEU:HD12	9:L:3794:HOH:O	1.88	0.72
2:C:115:LEU:HD22	2:C:373:VAL:HG11	1.70	0.72
2:C:276:LYS:HB3	9:C:1337:HOH:O	1.87	0.72
2:M:139:GLN:NE2	2:M:418:LEU:HD22	2.04	0.72
2:M:437:ARG:NH2	2:M:488:ALA:HA	2.05	0.72
2:M:549:PHE:HB3	2:M:552:HIS:HD2	1.54	0.72
5:P:260:ILE:HD11	5:P:310:ILE:HG22	1.71	0.72
1:A:150:TYR:HE2	1:A:152:PRO:HG3	1.54	0.72
2:C:147:TYR:HE2	2:C:280:LYS:HZ3	1.36	0.72
2:C:274:ARG:HD2	2:C:285:LEU:O	1.90	0.72
2:C:768:THR:HB	2:C:771:GLU:HB3	1.71	0.72
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.72	0.72
3:D:400:VAL:HG12	9:D:2306:HOH:O	1.87	0.72
3:D:806:PHE:CE1	3:D:813:LEU:HB3	2.25	0.72
2:M:191:PHE:HZ	2:M:196:LEU:HB2	1.53	0.72
2:M:958:THR:HA	9:M:1887:HOH:O	1.89	0.72
3:N:570:GLU:N	5:P:214:GLN:HE22	1.88	0.72
3:N:808:THR:HB	3:N:809:PRO:HD3	1.70	0.72
2:C:352:ALA:O	2:C:356:ARG:HG3	1.89	0.72
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1115:LEU:HB3	3:N:85:VAL:HG13	1.71	0.72
3:N:572:ARG:HH12	5:P:79:ASP:CG	1.92	0.72
3:N:1393:GLN:HB2	3:N:1398:TRP:NE1	2.04	0.72
5:P:92:PRO:HB3	9:P:672:HOH:O	1.88	0.72
2:C:305:PRO:HA	2:C:308:ARG:HB2	1.70	0.72
1:A:10:VAL:HG12	1:A:12:THR:HG22	1.70	0.72
2:C:952:LEU:HD12	2:C:969:GLN:NE2	2.04	0.72
3:D:810:GLU:O	3:D:813:LEU:HG	1.88	0.72
2:C:603:VAL:HG12	9:C:1531:HOH:O	1.90	0.72
3:D:546:ARG:O	3:D:550:ARG:HG2	1.90	0.72
2:M:683:ASN:HA	2:M:687:ALA:HB3	1.71	0.72
1:B:97:VAL:HG11	1:B:120:VAL:HG21	1.72	0.71
3:D:206:ARG:HH12	5:F:98:GLU:CA	2.03	0.71
3:D:1377:LYS:HA	9:D:2039:HOH:O	1.89	0.71
5:F:218:GLN:HA	5:F:221:ILE:HD12	1.69	0.71
2:M:305:PRO:HA	2:M:308:ARG:HB2	1.70	0.71
2:M:535:SER:HB2	2:M:537:LYS:HE3	1.72	0.71
5:P:132:ARG:HD2	9:P:505:HOH:O	1.89	0.71
2:C:630:ARG:HA	9:C:1414:HOH:O	1.90	0.71
2:C:654:LEU:HD11	2:C:663:ASN:HD22	1.56	0.71
1:K:28:LEU:HD12	9:K:2517:HOH:O	1.88	0.71
2:M:31:GLN:HB3	2:M:71:TYR:OH	1.90	0.71
2:M:408:ARG:HH21	2:M:542:VAL:HG22	1.55	0.71
3:N:406:ASP:HB3	5:P:168:LYS:HE2	1.70	0.71
4:O:45:ARG:HG2	9:O:1147:HOH:O	1.90	0.71
3:D:1239:ARG:HG3	9:D:2068:HOH:O	1.91	0.71
5:F:139:ALA:HA	5:F:152:ASP:CG	2.11	0.71
3:N:705:ALA:HB3	3:N:706:PRO:HD3	1.73	0.71
5:P:204:GLY:HA3	9:P:572:HOH:O	1.89	0.71
1:K:150:TYR:HE1	2:M:696:LYS:HA	1.54	0.71
2:M:461:VAL:HG13	2:M:465:GLY:HA2	1.71	0.71
2:M:569:VAL:HG12	2:M:996:LYS:O	1.89	0.71
3:N:1210:SER:HA	9:N:1732:HOH:O	1.90	0.71
1:B:61:VAL:HG23	1:B:137:ARG:HH22	1.56	0.71
2:C:713:ARG:NH2	3:D:531:ASP:HB3	2.06	0.71
5:F:88:ILE:HG21	5:F:193:ARG:HD3	1.73	0.71
1:L:83:LYS:HE2	1:L:168:ASP:HB2	1.71	0.71
1:A:221:HIS:HA	1:A:224:TYR:HD2	1.55	0.71
2:C:685:GLU:N	9:C:1222:HOH:O	2.23	0.71
2:M:298:PHE:HA	9:M:2058:HOH:O	1.90	0.71
2:C:724:ARG:HG2	2:C:734:LEU:HD23	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:738:ASP:HB2	2:C:744:ARG:HB3	1.71	0.71
3:N:86:ARG:O	3:N:522:PRO:HD2	1.91	0.71
2:C:157:ARG:HA	9:C:1318:HOH:O	1.90	0.71
2:C:671:ASN:HD22	2:C:671:ASN:H	1.36	0.71
2:C:139:GLN:HE22	2:C:415:PRO:HD2	1.56	0.71
3:D:105:VAL:HG21	3:D:128:TYR:HE2	1.55	0.71
3:D:894:LYS:HA	9:D:1776:HOH:O	1.91	0.71
5:F:151:LEU:O	5:F:155:THR:HB	1.90	0.71
2:M:420:ARG:HB2	9:M:1926:HOH:O	1.90	0.71
2:M:1021:LEU:HD21	5:P:332:PHE:O	1.91	0.71
3:N:611:GLN:O	3:N:1439:SER:O	2.09	0.71
2:C:676:ILE:HG23	2:C:676:ILE:O	1.91	0.71
3:D:574:LEU:O	3:D:578:VAL:HG23	1.90	0.71
2:M:428:ARG:HE	2:M:451:LEU:HD21	1.54	0.71
2:M:551:GLU:HG3	2:M:552:HIS:CD2	2.25	0.71
3:N:15:PRO:HB3	9:N:1827:HOH:O	1.90	0.71
3:N:574:LEU:O	3:N:578:VAL:HG23	1.91	0.71
1:A:35:THR:HG21	1:B:43:ILE:CD1	2.21	0.70
2:C:83:CYS:HA	2:C:88:LEU:HB3	1.73	0.70
3:D:131:LYS:HG2	3:D:568:ARG:HG2	1.72	0.70
1:L:56:VAL:HG13	1:L:142:VAL:HG12	1.73	0.70
2:M:514:VAL:HB	9:M:2025:HOH:O	1.91	0.70
3:N:1472:ILE:HG22	3:N:1474:ALA:H	1.56	0.70
1:A:20:TYR:CE2	1:A:22:GLU:HG3	2.26	0.70
2:M:904:PRO:HD2	2:M:908:GLY:HA2	1.72	0.70
3:N:611:GLN:CD	3:N:619:LEU:HD21	2.12	0.70
2:C:76:PRO:HB2	9:C:1121:HOH:O	1.91	0.70
3:D:185:VAL:HG22	3:D:191:LEU:HD21	1.71	0.70
2:M:12:VAL:HG21	2:M:472:ARG:HD3	1.74	0.70
2:M:716:LYS:HB2	9:M:2121:HOH:O	1.91	0.70
3:N:1161:GLU:HG3	3:N:1164:ARG:HB2	1.73	0.70
1:B:55:SER:CB	1:B:158:ILE:HD13	2.21	0.70
2:C:163:ILE:HD13	9:C:1347:HOH:O	1.90	0.70
5:F:361:LEU:HD12	5:F:408:LEU:HD11	1.74	0.70
1:L:197:LEU:HD21	1:L:199:ILE:HD11	1.73	0.70
2:M:789:SER:HB2	9:M:1726:HOH:O	1.90	0.70
3:N:1215:VAL:HG13	9:N:1985:HOH:O	1.90	0.70
2:C:399:ASN:O	2:C:402:SER:HB2	1.92	0.70
5:F:358:LEU:HD21	5:F:370:LYS:HZ2	1.54	0.70
2:M:889:HIS:HE1	3:N:951:ILE:H	1.37	0.70
2:M:890:LEU:HD12	2:M:914:ILE:HD13	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1077:ALA:HA	9:N:1738:HOH:O	1.90	0.70
3:N:1481:VAL:HG11	4:O:18:ARG:HA	1.74	0.70
1:A:107:LYS:HG2	9:A:404:HOH:O	1.91	0.70
3:D:614:PHE:C	3:D:615:ARG:O	2.26	0.70
1:L:132:LEU:HD13	1:L:138:LEU:HD12	1.74	0.70
2:M:45:GLN:HA	9:M:1991:HOH:O	1.89	0.70
2:M:157:ARG:HD2	2:M:314:THR:HG22	1.72	0.70
3:N:785:ILE:HD13	3:N:935:LYS:HA	1.74	0.70
3:N:1205:TYR:CD2	3:N:1215:VAL:HG21	2.25	0.70
1:A:117:VAL:HB	1:A:120:VAL:HG12	1.72	0.70
1:B:85:LEU:HD12	1:B:124:ASN:HB3	1.72	0.70
2:C:156:GLY:HA3	9:C:1282:HOH:O	1.90	0.70
2:C:611:ILE:HD11	2:C:641:PRO:HG3	1.72	0.70
3:D:206:ARG:HH12	5:F:98:GLU:N	1.90	0.70
2:M:83:CYS:HA	2:M:88:LEU:HB3	1.73	0.70
3:N:433:GLY:HA3	3:N:447:VAL:O	1.90	0.70
2:C:3:ILE:HA	2:C:900:ARG:O	1.91	0.70
2:C:838:LYS:HE3	2:C:846:LYS:HE2	1.71	0.70
3:D:433:GLY:HA3	3:D:447:VAL:O	1.90	0.70
3:D:1101:VAL:HA	3:D:1428:ALA:HB2	1.72	0.70
1:K:186:LEU:HB2	1:K:192:LEU:HD11	1.73	0.70
2:M:163:ILE:HG13	2:M:163:ILE:O	1.91	0.70
2:M:855:VAL:HG12	9:M:1977:HOH:O	1.90	0.70
3:N:1147:ARG:HB3	3:N:1188:VAL:CG2	2.21	0.70
1:B:59:GLU:HG3	1:B:139:ASN:HD22	1.57	0.70
2:C:276:LYS:HD2	9:C:1736:HOH:O	1.90	0.70
3:D:105:VAL:HG21	3:D:128:TYR:CE2	2.27	0.70
3:D:1114:THR:H	3:D:1195:GLN:HE21	1.39	0.70
4:E:10:PHE:HE2	4:E:16:LYS:HG3	1.55	0.70
1:L:55:SER:CB	1:L:158:ILE:HD13	2.21	0.70
1:L:201:THR:HG22	1:L:203:GLY:H	1.55	0.70
2:M:191:PHE:HB2	2:M:241:LEU:HD13	1.74	0.70
2:M:1009:SER:HB2	3:N:651:GLU:O	1.91	0.70
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.27	0.70
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.74	0.70
3:D:1356:TYR:CD2	3:D:1363:LEU:HD23	2.27	0.70
1:L:148:VAL:HG22	9:L:3229:HOH:O	1.92	0.70
2:M:312:ALA:HB1	2:M:318:PRO:HG2	1.73	0.70
2:M:436:GLY:HA2	2:M:538:GLN:O	1.92	0.70
3:N:584:ASN:ND2	3:N:590:PRO:HD2	2.06	0.70
3:N:810:GLU:O	3:N:813:LEU:HG	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1498:ALA:HB2	4:O:88:GLU:OE1	1.92	0.70
5:P:394:ARG:CZ	5:P:398:ARG:HB2	2.21	0.70
1:B:158:ILE:HD11	1:B:166:PRO:CA	2.22	0.69
2:C:139:GLN:NE2	2:C:415:PRO:HD2	2.07	0.69
3:D:73:CYS:HB3	3:D:76:CYS:O	1.92	0.69
3:D:1279:GLY:O	3:D:1318:TYR:HA	1.91	0.69
2:M:511:GLU:O	2:M:526:PRO:HD3	1.92	0.69
3:N:481:MET:HG3	3:N:1388:ARG:CZ	2.22	0.69
4:O:45:ARG:HD2	9:O:1011:HOH:O	1.92	0.69
2:C:572:ILE:HG13	9:C:1310:HOH:O	1.92	0.69
2:M:219:GLN:HG3	9:M:1965:HOH:O	1.90	0.69
2:C:671:ASN:N	2:C:671:ASN:ND2	2.40	0.69
3:D:607:LEU:O	3:D:610:LYS:HB2	1.92	0.69
1:K:50:GLY:HA3	1:K:173:PRO:HG3	1.74	0.69
2:M:578:VAL:HG23	2:M:579:VAL:HG12	1.73	0.69
3:N:10:ILE:HG13	3:N:1434:TRP:CZ2	2.27	0.69
3:N:680:GLN:HB2	9:N:2087:HOH:O	1.92	0.69
9:N:2060:HOH:O	5:P:147:LEU:HD21	1.91	0.69
4:O:45:ARG:HB2	4:O:46:PRO:HD2	1.74	0.69
1:B:221:HIS:HA	1:B:224:TYR:CD2	2.26	0.69
2:C:307:LEU:HG	2:C:311:PHE:HE2	1.57	0.69
3:D:611:GLN:HB2	7:D:1527:MXP:H11A	1.73	0.69
3:D:1243:THR:OG1	3:D:1253:THR:HB	1.92	0.69
5:F:279:GLN:HA	9:F:487:HOH:O	1.91	0.69
1:K:24:VAL:HG22	1:K:196:THR:HB	1.74	0.69
1:K:184:THR:HG23	1:K:192:LEU:HB2	1.74	0.69
3:N:705:ALA:CB	3:N:706:PRO:HD3	2.22	0.69
5:P:367:MET:HB2	9:P:493:HOH:O	1.92	0.69
2:C:276:LYS:O	2:C:280:LYS:HB2	1.93	0.69
3:D:795:VAL:HG11	3:D:863:VAL:HG13	1.73	0.69
1:K:7:LYS:NZ	1:K:186:LEU:HD21	2.07	0.69
3:N:1274:ILE:HD11	3:N:1334:GLN:NE2	2.08	0.69
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.75	0.69
1:B:158:ILE:HG22	1:B:160:ASP:H	1.56	0.69
2:C:139:GLN:OE1	2:C:415:PRO:HD2	1.92	0.69
2:C:436:GLY:HA2	2:C:538:GLN:O	1.92	0.69
2:C:603:VAL:HG13	9:C:1654:HOH:O	1.93	0.69
2:C:732:ALA:HB3	9:C:1588:HOH:O	1.93	0.69
3:N:1086:LEU:HB2	9:N:2385:HOH:O	1.91	0.69
4:E:47:LYS:HA	9:E:150:HOH:O	1.93	0.69
5:F:171:LYS:HD3	9:F:640:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:183:ASP:HB3	9:K:3288:HOH:O	1.93	0.69
2:M:143:SER:HB2	2:M:276:LYS:NZ	2.07	0.69
2:M:838:LYS:HE3	2:M:846:LYS:HE2	1.72	0.69
3:N:1001:GLU:HG2	9:N:2222:HOH:O	1.93	0.69
5:P:160:ASP:HA	5:P:163:LEU:HD12	1.73	0.69
5:P:166:LEU:O	5:P:171:LYS:HB2	1.93	0.69
2:C:909:ALA:HB1	9:C:1225:HOH:O	1.92	0.69
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.73	0.69
5:F:392:VAL:HG12	9:F:496:HOH:O	1.92	0.69
1:K:9:PRO:HD2	1:L:224:TYR:CD1	2.27	0.69
2:M:141:HIS:HB3	2:M:418:LEU:HG	1.75	0.69
2:M:311:PHE:HB3	9:M:1792:HOH:O	1.92	0.69
2:M:352:ALA:O	2:M:356:ARG:HG3	1.93	0.69
2:M:468:ARG:HB2	2:M:486:MET:O	1.92	0.69
2:M:905:ILE:H	2:M:905:ILE:HD12	1.57	0.69
3:N:149:LYS:HG3	9:N:2241:HOH:O	1.91	0.69
3:N:675:ARG:NH1	5:P:421:PHE:HD2	1.90	0.69
3:N:877:PRO:O	3:N:880:ILE:HG22	1.93	0.69
3:N:1095:THR:O	3:N:1099:VAL:HG23	1.91	0.69
5:P:85:LEU:HA	5:P:88:ILE:HD12	1.74	0.69
1:A:58:ILE:HB	1:A:61:VAL:HB	1.75	0.69
2:C:86:LYS:HD3	2:C:813:VAL:HG12	1.74	0.69
2:C:218:VAL:HG22	2:C:221:LEU:HD23	1.75	0.69
2:C:541:SER:HB2	9:C:1523:HOH:O	1.93	0.69
3:D:799:LYS:H	3:D:826:PRO:HG2	1.58	0.69
4:E:33:HIS:HB2	4:E:37:ASN:HD21	1.58	0.69
2:M:139:GLN:HE22	2:M:415:PRO:HG2	1.56	0.69
2:M:343:GLN:HG2	2:M:385:PHE:HB2	1.75	0.69
2:M:521:PRO:HG3	3:N:1068:LEU:HD23	1.75	0.69
2:M:751:PRO:HG3	2:M:795:GLY:O	1.92	0.69
3:N:484:PRO:HB3	9:N:1630:HOH:O	1.91	0.69
5:P:132:ARG:HG2	5:P:181:GLU:CD	2.14	0.69
1:A:97:VAL:HG23	9:A:349:HOH:O	1.92	0.69
2:C:176:VAL:HG12	2:C:182:VAL:HG13	1.73	0.69
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.08	0.69
3:D:584:ASN:ND2	3:D:590:PRO:HD2	2.07	0.69
2:M:28:ARG:NH1	2:M:463:GLU:HG2	2.07	0.69
3:N:124:GLU:O	3:N:128:TYR:HB2	1.93	0.69
1:A:111:ALA:HB2	1:A:127:LEU:HG	1.75	0.68
2:C:634:GLY:HA3	9:C:1157:HOH:O	1.92	0.68
3:D:206:ARG:HH12	5:F:98:GLU:HA	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:69:PRO:HB3	9:M:1747:HOH:O	1.93	0.68
3:N:36:THR:HA	9:N:2104:HOH:O	1.93	0.68
3:N:1354:LYS:HA	9:N:1826:HOH:O	1.92	0.68
4:O:46:PRO:HD2	9:O:1011:HOH:O	1.92	0.68
1:B:58:ILE:HB	1:B:61:VAL:HB	1.73	0.68
2:C:399:ASN:HB3	2:C:568:ALA:O	1.93	0.68
3:D:29:PRO:HG2	3:D:549:ASN:ND2	2.07	0.68
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.75	0.68
4:E:17:TYR:O	4:E:21:VAL:HG23	1.92	0.68
2:M:575:GLN:OE1	2:M:670:GLN:HB3	1.93	0.68
2:M:838:LYS:HE3	2:M:997:LEU:HD12	1.75	0.68
3:N:428:LYS:HD3	9:N:2334:HOH:O	1.93	0.68
3:N:646:LYS:HE2	3:N:722:GLU:HG2	1.75	0.68
3:N:1146:GLY:HA3	3:N:1207:TYR:HB2	1.74	0.68
3:N:1162:GLU:HB3	9:N:1922:HOH:O	1.92	0.68
5:P:87:GLU:O	5:P:91:VAL:HG23	1.92	0.68
3:D:1472:ILE:HG22	3:D:1474:ALA:H	1.58	0.68
1:L:101:LEU:HG	9:L:2708:HOH:O	1.91	0.68
3:N:555:LYS:HB3	9:N:1956:HOH:O	1.93	0.68
3:N:1112:CYS:HB2	3:N:1195:GLN:HG2	1.75	0.68
3:N:1317:ASP:HB2	9:N:1639:HOH:O	1.93	0.68
4:O:45:ARG:HE	4:O:55:PHE:HD2	1.40	0.68
1:B:52:ALA:HB2	1:B:170:VAL:O	1.93	0.68
2:C:73:LEU:HD22	2:C:118:ILE:HD11	1.75	0.68
1:L:97:VAL:HG11	1:L:120:VAL:HG21	1.73	0.68
2:M:69:LEU:HB2	2:M:97:ARG:HB2	1.76	0.68
3:N:403:PHE:HD1	3:N:405:ASP:O	1.76	0.68
3:N:523:ASP:HB3	9:N:1572:HOH:O	1.93	0.68
2:C:256:TYR:HE1	2:C:293:PHE:HB2	1.57	0.68
2:C:811:PRO:HB2	2:C:813:VAL:HG13	1.74	0.68
5:F:88:ILE:HD13	5:F:193:ARG:HD2	1.75	0.68
2:M:750:LYS:HD3	9:N:2087:HOH:O	1.93	0.68
3:N:119:SER:H	3:N:123:LEU:HD22	1.56	0.68
1:B:109:VAL:HG21	1:B:138:LEU:CD1	2.19	0.68
2:C:619:ARG:HG2	9:C:1584:HOH:O	1.94	0.68
2:C:1107:ASN:HB3	9:C:1226:HOH:O	1.94	0.68
3:D:565:ILE:HD12	5:F:192:LEU:HD13	1.75	0.68
5:P:248:ASN:HA	5:P:251:ILE:HD12	1.74	0.68
1:B:213:GLN:O	1:B:217:ILE:HD12	1.94	0.68
2:C:299:LYS:HB3	9:C:1267:HOH:O	1.94	0.68
3:D:704:ARG:HG2	3:D:705:ALA:H	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:147:LEU:HB2	9:F:2238:HOH:O	1.94	0.68
3:N:46:ASP:OD2	3:N:48:ARG:HG2	1.94	0.68
3:N:607:LEU:O	3:N:610:LYS:HB2	1.93	0.68
3:N:610:LYS:HB3	9:N:1557:HOH:O	1.94	0.68
5:P:77:THR:O	5:P:81:VAL:HG23	1.93	0.68
2:C:554:ASP:OD2	2:C:556:ASN:HB3	1.91	0.68
3:D:153:LEU:HD11	3:D:158:TYR:N	2.09	0.68
3:D:1239:ARG:HB2	9:D:2065:HOH:O	1.94	0.68
5:F:129:GLU:HG2	9:F:492:HOH:O	1.93	0.68
1:L:158:ILE:HG13	1:L:166:PRO:HB3	1.76	0.68
2:M:108:ILE:HB	2:M:368:THR:OG1	1.94	0.68
2:M:571:LEU:HD21	2:M:700:TYR:CD2	2.29	0.68
3:N:672:ALA:HB1	9:N:1656:HOH:O	1.93	0.68
1:A:100:LEU:HB2	1:A:115:LEU:HD11	1.76	0.68
1:A:136:GLY:HA3	9:A:320:HOH:O	1.93	0.68
2:C:145:GLY:O	2:C:163:ILE:HG23	1.93	0.68
3:D:162:ARG:HA	3:D:449:SER:CB	2.24	0.68
3:D:1141:GLU:HG2	3:D:1168:MET:HE1	1.75	0.68
1:K:133:GLU:HG2	1:K:134:GLU:N	2.07	0.68
1:L:128:HIS:HB2	9:L:3368:HOH:O	1.93	0.68
2:M:148:PHE:CZ	2:M:281:LEU:HD13	2.29	0.68
3:N:535:PHE:O	5:P:315:VAL:N	2.26	0.68
5:P:133:ALA:HA	9:P:567:HOH:O	1.92	0.68
5:P:218:GLN:HA	5:P:221:ILE:HD12	1.75	0.68
2:C:578:VAL:HG13	2:C:671:ASN:OD1	1.93	0.68
2:C:599:GLU:HG3	2:C:600:ASP:H	1.59	0.68
2:C:815:LEU:HD13	9:C:1286:HOH:O	1.94	0.68
2:C:874:LEU:HD12	3:D:784:ASP:OD2	1.94	0.68
2:C:915:LYS:HE3	9:C:1136:HOH:O	1.94	0.68
2:C:1096:ALA:O	3:D:13:ALA:HB2	1.94	0.68
3:D:723:GLY:HA3	9:D:1680:HOH:O	1.94	0.68
5:F:160:ASP:HA	5:F:163:LEU:HD12	1.75	0.68
2:M:492:ASP:HA	9:M:1901:HOH:O	1.92	0.68
3:N:108:VAL:HG21	9:N:2073:HOH:O	1.94	0.68
5:P:368:VAL:HG22	9:P:506:HOH:O	1.93	0.68
1:A:198:ARG:HB2	1:A:200:TRP:CZ3	2.29	0.67
1:B:158:ILE:HG13	1:B:166:PRO:HB3	1.76	0.67
2:C:333:ILE:HD13	2:C:467:ILE:HG13	1.76	0.67
3:D:586:ARG:HH12	3:D:1444:THR:HG21	1.58	0.67
2:M:145:GLY:O	2:M:163:ILE:HG23	1.94	0.67
3:N:1430:SER:HA	9:N:2035:HOH:O	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:339:LEU:HD11	9:C:1322:HOH:O	1.94	0.67
3:D:805:GLU:HG3	9:D:1779:HOH:O	1.93	0.67
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.76	0.67
2:M:93:PRO:HG3	2:M:117:HIS:CE1	2.29	0.67
2:M:292:ARG:HB3	9:M:2058:HOH:O	1.93	0.67
3:N:611:GLN:NE2	7:N:1527:MXP:H16B	2.09	0.67
3:N:1476:THR:HG23	4:O:21:VAL:HG22	1.75	0.67
4:O:9:LEU:HB3	4:O:19:LEU:HD21	1.76	0.67
4:O:88:GLU:HG3	9:O:2559:HOH:O	1.93	0.67
1:A:103:ALA:CB	1:A:107:LYS:HE2	2.24	0.67
2:C:914:ILE:HB	9:C:1225:HOH:O	1.93	0.67
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.75	0.67
1:L:180:GLN:HB3	9:L:1094:HOH:O	1.95	0.67
2:M:283:ILE:HD11	9:M:2124:HOH:O	1.95	0.67
2:M:445:GLU:HG2	9:M:1876:HOH:O	1.94	0.67
2:M:660:ALA:HB1	2:M:667:ALA:O	1.93	0.67
2:M:793:PRO:HD2	9:M:2061:HOH:O	1.93	0.67
2:M:966:LEU:HD11	2:M:986:PRO:HG2	1.74	0.67
3:N:130:SER:HB3	3:N:132:TYR:CE1	2.30	0.67
3:N:483:HIS:HB2	3:N:484:PRO:HD3	1.77	0.67
3:N:658:LEU:O	3:N:661:MET:HB2	1.94	0.67
3:N:1243:THR:OG1	3:N:1253:THR:HB	1.94	0.67
5:F:408:LEU:O	5:F:412:GLU:HG2	1.95	0.67
1:K:10:VAL:HG12	1:K:12:THR:HG22	1.77	0.67
2:M:979:THR:HG23	2:M:981:GLU:H	1.59	0.67
3:N:28:LYS:HG3	3:N:41:ARG:HH11	1.59	0.67
3:N:956:ILE:HG12	3:N:1039:CYS:O	1.95	0.67
2:M:318:PRO:HA	9:M:1903:HOH:O	1.94	0.67
3:N:544:TYR:O	3:N:548:ILE:HG12	1.93	0.67
3:N:1152:GLU:CD	3:N:1159:ARG:HH12	1.97	0.67
4:O:48:MET:O	4:O:52:GLU:HA	1.94	0.67
5:P:408:LEU:O	5:P:412:GLU:HG2	1.93	0.67
5:F:361:LEU:HD23	5:F:362:SER:H	1.58	0.67
2:M:724:ARG:HG2	2:M:734:LEU:HD23	1.77	0.67
3:N:141:ILE:CG2	3:N:450:TYR:H	2.08	0.67
5:P:268:ILE:HD13	5:P:311:ALA:HB2	1.77	0.67
2:C:551:GLU:HG3	2:C:552:HIS:CD2	2.30	0.67
2:C:944:LEU:HD21	2:C:963:LEU:HD23	1.77	0.67
3:D:809:PRO:HB2	3:D:812:ALA:HB2	1.76	0.67
3:D:906:GLN:HB3	3:D:911:LEU:CD1	2.24	0.67
3:D:1041:LEU:HD12	3:D:1058:ARG:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:VAL:HG23	1:L:137:ARG:HH22	1.59	0.67
3:N:764:LEU:HD23	3:N:767:HIS:ND1	2.10	0.67
3:N:1277:ILE:HA	9:N:1570:HOH:O	1.95	0.67
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.77	0.67
2:C:328:LEU:HD13	2:C:433:THR:HB	1.76	0.67
2:C:464:LEU:HG	9:C:1551:HOH:O	1.94	0.67
2:C:889:HIS:CD2	2:C:970:GLY:HA3	2.30	0.67
3:D:617:ASN:HB2	3:D:618:LEU:HD12	1.77	0.67
3:D:1432:LYS:HG2	9:D:1537:HOH:O	1.93	0.67
2:M:722:ILE:HG21	2:M:821:GLU:OE1	1.94	0.67
3:N:65:ARG:CG	3:N:66:GLN:H	2.07	0.67
3:N:508:ARG:HB3	9:N:1796:HOH:O	1.95	0.67
3:N:804:LEU:HD23	3:N:804:LEU:H	1.60	0.67
3:N:1220:ALA:HB1	3:N:1223:ILE:HD13	1.77	0.67
3:N:1279:GLY:O	3:N:1318:TYR:HA	1.94	0.67
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.75	0.67
1:B:60:ASP:H	1:B:137:ARG:NH2	1.92	0.67
2:C:244:PRO:HG2	2:C:246:ASP:OD2	1.95	0.67
3:D:637:LEU:HD21	3:D:642:CYS:HA	1.75	0.67
3:D:658:LEU:O	3:D:661:MET:HB2	1.95	0.67
5:F:191:ASN:HB3	5:F:220:LEU:HD11	1.76	0.67
1:K:123:MET:O	1:K:125:PRO:HD3	1.95	0.67
3:N:996:TRP:HA	3:N:999:THR:HG22	1.77	0.67
3:D:16:GLU:HA	9:D:2072:HOH:O	1.95	0.67
3:D:613:ARG:HB2	9:D:1834:HOH:O	1.95	0.67
3:D:785:ILE:HD13	3:D:935:LYS:HA	1.75	0.67
3:D:1481:VAL:HG11	4:E:18:ARG:HA	1.77	0.67
5:F:110:MET:HB2	9:F:483:HOH:O	1.94	0.67
1:K:46:SER:HB3	2:M:856:GLU:HG2	1.76	0.67
2:M:156:GLY:HA3	9:M:2199:HOH:O	1.95	0.67
2:M:770:GLU:HG2	9:M:2011:HOH:O	1.94	0.67
2:M:805:ARG:HG3	2:M:823:VAL:HG22	1.77	0.67
3:N:178:LEU:HD12	9:N:2234:HOH:O	1.94	0.67
3:N:556:LYS:HB3	5:P:218:GLN:HE22	1.59	0.67
5:P:295:MET:HG2	5:P:299:TRP:CD2	2.30	0.67
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.77	0.66
3:D:808:THR:HB	3:D:809:PRO:HD3	1.76	0.66
3:D:1094:LEU:O	3:D:1098:LEU:HD13	1.95	0.66
1:L:123:MET:C	1:L:125:PRO:HD3	2.15	0.66
2:M:204:GLN:NE2	2:M:222:MET:HA	2.10	0.66
2:M:1108:PRO:HD3	9:M:2055:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ALA:HB1	1:B:171:PHE:CD2	2.30	0.66
2:C:310:LEU:HD12	9:C:1562:HOH:O	1.94	0.66
2:C:397:GLU:HB2	9:C:1153:HOH:O	1.94	0.66
2:C:859:PRO:O	2:C:867:VAL:HG22	1.95	0.66
3:D:1410:GLU:OE2	3:D:1414:PRO:HG3	1.95	0.66
2:M:64:LEU:HD13	2:M:359:MET:HG3	1.76	0.66
2:M:1096:ALA:HB1	9:N:1592:HOH:O	1.94	0.66
3:N:188:GLY:N	3:N:199:LEU:HD23	2.11	0.66
3:N:1321:ALA:O	3:N:1339:LYS:HE3	1.96	0.66
3:D:609:GLY:O	3:D:617:ASN:ND2	2.28	0.66
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.25	0.66
3:D:965:GLU:HB2	9:D:1794:HOH:O	1.96	0.66
4:E:48:MET:O	4:E:52:GLU:HA	1.96	0.66
2:M:909:ALA:HB1	9:M:1825:HOH:O	1.94	0.66
2:M:952:LEU:HD12	2:M:969:GLN:NE2	2.08	0.66
2:M:1096:ALA:O	3:N:13:ALA:HB2	1.95	0.66
1:B:78:ILE:HA	9:B:438:HOH:O	1.95	0.66
3:D:116:LEU:HD22	3:D:118:LEU:HD11	1.76	0.66
3:D:805:GLU:HG2	9:D:1726:HOH:O	1.95	0.66
3:D:843:PHE:HE1	3:D:864:VAL:HG11	1.60	0.66
2:M:1:MET:HE2	9:M:2228:HOH:O	1.94	0.66
3:N:185:VAL:HG22	3:N:191:LEU:HD21	1.76	0.66
5:P:303:ARG:HB2	9:P:433:HOH:O	1.94	0.66
2:C:431:HIS:CD2	2:C:433:THR:H	2.13	0.66
2:C:693:GLU:HA	2:C:696:LYS:HG3	1.76	0.66
3:D:817:GLU:O	3:D:821:VAL:HG23	1.94	0.66
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.25	0.66
5:F:336:GLU:HA	9:F:469:HOH:O	1.94	0.66
3:N:82:LYS:HE2	9:N:1551:HOH:O	1.95	0.66
3:N:569:ASN:OD1	5:P:80:PRO:HB3	1.96	0.66
5:P:234:LYS:HG2	9:P:475:HOH:O	1.95	0.66
1:A:180:GLN:HB3	9:A:352:HOH:O	1.95	0.66
1:B:18:ARG:O	1:B:207:PRO:HD3	1.96	0.66
1:B:173:PRO:HG3	9:B:480:HOH:O	1.95	0.66
1:B:199:ILE:HD11	1:B:211:LEU:HD13	1.76	0.66
3:D:1166:LEU:HD12	3:D:1171:VAL:HG22	1.78	0.66
1:L:76:VAL:HG23	9:L:1317:HOH:O	1.95	0.66
2:M:21:ILE:H	2:M:21:ILE:HD12	1.60	0.66
2:M:1033:GLY:O	2:M:1036:GLU:HG2	1.96	0.66
2:M:1083:GLU:HG2	9:M:1724:HOH:O	1.96	0.66
3:N:126:VAL:HG21	9:N:2194:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:161:LEU:O	3:N:449:SER:HB3	1.95	0.66
5:P:335:ASP:OD1	5:P:338:LEU:HB2	1.95	0.66
2:C:15:LEU:CD2	2:C:583:LEU:HD11	2.26	0.66
2:C:498:GLN:O	2:C:501:THR:HG23	1.96	0.66
3:D:100:ALA:HB2	3:D:513:ILE:CD1	2.24	0.66
3:D:1498:ALA:HB2	4:E:88:GLU:OE1	1.96	0.66
4:E:6:ILE:HA	4:E:9:LEU:HD12	1.77	0.66
2:M:42:VAL:HG12	2:M:43:GLY:H	1.59	0.66
2:M:768:THR:HB	2:M:771:GLU:HB3	1.77	0.66
3:N:58:CYS:HA	3:N:78:VAL:HG11	1.77	0.66
3:N:133:ILE:HD11	3:N:155:ASP:OD1	1.96	0.66
3:N:924:MET:O	3:N:927:THR:HB	1.96	0.66
3:N:996:TRP:CD2	3:N:1056:PRO:HG2	2.31	0.66
3:N:1101:VAL:HG21	3:N:1424:VAL:HG22	1.77	0.66
2:C:141:HIS:HB3	2:C:418:LEU:HG	1.77	0.66
2:C:198:ARG:NE	2:C:228:ALA:HA	2.11	0.66
2:C:713:ARG:HH22	3:D:531:ASP:HB3	1.60	0.66
2:C:1018:GLN:OE1	2:C:1060:ILE:HD11	1.95	0.66
2:C:1019:GLN:HE22	3:D:621:LYS:HA	1.61	0.66
3:D:1310:ARG:HG3	3:D:1327:ARG:HB3	1.78	0.66
5:F:260:ILE:HD11	5:F:310:ILE:HG22	1.77	0.66
2:M:781:LYS:HG3	9:M:1700:HOH:O	1.95	0.66
3:N:633:VAL:HG22	3:N:635:PRO:HD3	1.76	0.66
3:N:704:ARG:HG2	3:N:705:ALA:H	1.59	0.66
3:N:1087:ARG:HB3	9:N:1678:HOH:O	1.95	0.66
2:C:864:GLY:O	2:C:866:PRO:HD3	1.96	0.66
2:M:350:ARG:HA	2:M:353:ARG:HD2	1.78	0.66
2:M:627:ARG:HA	9:M:1936:HOH:O	1.95	0.66
2:M:976:ASP:CB	2:M:979:THR:HG22	2.25	0.66
2:M:1014:SER:HB3	2:M:1017:THR:O	1.96	0.66
3:N:806:PHE:CE1	3:N:813:LEU:HB3	2.30	0.66
4:O:17:TYR:O	4:O:21:VAL:HG23	1.95	0.66
2:C:289:THR:HB	9:C:1392:HOH:O	1.96	0.66
3:D:679:ARG:HB2	3:D:682:ASP:OD2	1.95	0.66
3:D:1044:LEU:HD23	9:D:1976:HOH:O	1.95	0.66
5:F:321:ILE:HB	5:F:327:SER:OG	1.96	0.66
1:K:206:THR:HG22	1:K:209:GLU:H	1.61	0.66
3:N:1258:ARG:CZ	3:N:1262:LEU:HD11	2.26	0.66
5:P:292:ALA:HB1	5:P:299:TRP:O	1.96	0.66
2:C:439:CYS:HB3	9:C:1185:HOH:O	1.96	0.65
2:C:1015:LEU:HD11	9:F:451:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1141:GLU:CG	3:D:1168:MET:HE1	2.26	0.65
1:L:158:ILE:HG22	1:L:160:ASP:H	1.60	0.65
2:M:197:LEU:HD22	2:M:202:TYR:HD2	1.61	0.65
2:M:304:LEU:HD23	2:M:305:PRO:HD3	1.78	0.65
5:P:295:MET:HG2	5:P:299:TRP:CE2	2.31	0.65
5:P:407:LYS:HG2	9:P:600:HOH:O	1.95	0.65
3:D:403:PHE:CE1	3:D:407:VAL:HG23	2.31	0.65
5:F:273:ARG:HD3	9:F:735:HOH:O	1.96	0.65
2:M:312:ALA:HA	9:M:1882:HOH:O	1.96	0.65
3:N:139:GLY:HA3	9:N:2226:HOH:O	1.95	0.65
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.78	0.65
3:D:1102:THR:HG22	3:D:1222:GLY:HA2	1.78	0.65
5:F:415:THR:HG21	9:F:598:HOH:O	1.95	0.65
2:M:368:THR:HB	2:M:369:PRO:HD3	1.77	0.65
2:M:1081:VAL:HG21	2:M:1111:ILE:HG22	1.78	0.65
3:N:154:THR:HG23	3:N:157:GLU:H	1.60	0.65
3:N:493:ARG:HH11	3:N:1390:LEU:C	1.99	0.65
3:N:1035:ILE:HA	3:N:1038:LEU:CD1	2.26	0.65
5:P:151:LEU:O	5:P:155:THR:HB	1.96	0.65
5:P:261:PRO:HB3	9:P:570:HOH:O	1.94	0.65
3:D:128:TYR:HE1	3:D:461:ILE:HG13	1.61	0.65
3:D:611:GLN:NE2	3:D:1463:LYS:CE	2.53	0.65
3:D:1211:MET:HB3	9:D:2053:HOH:O	1.95	0.65
5:F:125:ASP:HA	9:F:652:HOH:O	1.97	0.65
1:L:58:ILE:HB	1:L:61:VAL:HB	1.77	0.65
1:L:206:THR:HG22	1:L:209:GLU:HB2	1.78	0.65
2:M:150:PRO:CA	2:M:158:TYR:HB3	2.22	0.65
2:M:528:GLU:HB3	9:M:1626:HOH:O	1.97	0.65
3:N:59:ALA:HB1	9:N:1806:HOH:O	1.96	0.65
3:N:65:ARG:HG3	3:N:66:GLN:H	1.62	0.65
3:N:644:LEU:HD12	3:N:645:PRO:HD2	1.78	0.65
2:C:237:ARG:HD2	9:C:1406:HOH:O	1.97	0.65
3:D:611:GLN:HE21	3:D:1439:SER:HB3	1.61	0.65
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.78	0.65
3:D:1502:ALA:HB1	9:D:2407:HOH:O	1.95	0.65
1:L:158:ILE:HD11	1:L:166:PRO:CA	2.25	0.65
1:L:176:ARG:HD3	3:N:884:ARG:NH2	2.11	0.65
2:M:571:LEU:CD2	2:M:700:TYR:HA	2.26	0.65
3:N:1301:LYS:HG2	9:N:2327:HOH:O	1.95	0.65
1:B:59:GLU:HG3	1:B:139:ASN:ND2	2.12	0.65
2:C:292:ARG:HD2	2:C:299:LYS:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:511:GLU:O	2:C:526:PRO:HD3	1.95	0.65
2:C:1030:GLN:NE2	3:D:628:ARG:HB3	2.11	0.65
2:C:1098:ASP:HB2	3:D:21:TRP:HZ2	1.60	0.65
3:D:583:ASP:OD2	3:D:604:THR:HG21	1.96	0.65
3:D:1109:GLU:OE1	3:D:1201:CYS:HB2	1.95	0.65
1:L:46:SER:O	1:L:148:VAL:HB	1.96	0.65
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.31	0.65
2:M:422:ARG:HA	9:M:1913:HOH:O	1.97	0.65
2:M:471:TYR:CE2	2:M:496:ILE:HG21	2.31	0.65
3:N:1109:GLU:OE1	3:N:1201:CYS:HB2	1.96	0.65
5:P:392:VAL:HG21	9:P:614:HOH:O	1.97	0.65
1:A:206:THR:CG2	1:A:209:GLU:H	2.10	0.65
2:C:1118:LYS:HG3	9:C:1317:HOH:O	1.95	0.65
3:D:1095:THR:O	3:D:1099:VAL:HG23	1.96	0.65
1:K:9:PRO:HB2	1:L:224:TYR:HB3	1.77	0.65
1:L:12:THR:HB	9:L:1867:HOH:O	1.96	0.65
1:L:109:VAL:HG12	9:L:1850:HOH:O	1.96	0.65
2:M:289:THR:HB	9:M:1685:HOH:O	1.97	0.65
2:M:724:ARG:O	2:M:734:LEU:HD21	1.97	0.65
3:N:105:VAL:HG21	3:N:128:TYR:CE2	2.30	0.65
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.79	0.65
1:B:179:PHE:HB2	1:B:195:LEU:HD11	1.77	0.65
2:C:442:GLU:HG2	2:C:454:SER:OG	1.96	0.65
2:C:1103:ASP:HB2	2:C:1107:ASN:O	1.96	0.65
3:D:493:ARG:NH1	3:D:1390:LEU:HB3	2.12	0.65
3:D:833:GLU:HG2	9:D:1935:HOH:O	1.97	0.65
1:K:16:GLN:HB3	9:K:1964:HOH:O	1.97	0.65
2:M:101:ILE:HG23	2:M:107:LEU:HD22	1.77	0.65
3:N:134:VAL:HG12	3:N:152:LEU:HB3	1.77	0.65
3:N:614:PHE:HD1	3:N:615:ARG:N	1.94	0.65
3:N:664:LYS:HE2	9:N:2324:HOH:O	1.96	0.65
2:C:610:ARG:HB2	9:C:1140:HOH:O	1.97	0.65
3:D:161:LEU:HD22	3:D:452:ILE:HG21	1.79	0.65
3:D:957:PRO:CG	3:D:1007:VAL:HA	2.25	0.65
3:D:1264:GLU:HG2	3:D:1425:THR:HG22	1.78	0.65
3:D:1422:MET:HE2	3:D:1427:SER:HA	1.79	0.65
1:L:221:HIS:HA	1:L:224:TYR:CD2	2.31	0.65
2:M:607:ASP:HB3	2:M:609:ASN:H	1.62	0.65
2:M:755:LEU:HB2	9:M:1781:HOH:O	1.97	0.65
3:N:508:ARG:CG	3:N:509:PRO:HD2	2.26	0.65
3:N:760:ARG:HH21	4:O:61:VAL:HG12	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:274:THR:O	5:P:278:LEU:HG	1.97	0.65
5:P:291:ILE:HG23	5:P:304:VAL:HG21	1.78	0.65
1:B:2:LEU:HD12	1:B:3:ASP:N	2.11	0.65
2:C:141:HIS:HB3	2:C:418:LEU:CG	2.27	0.65
2:C:627:ARG:HG3	2:C:628:PHE:H	1.61	0.65
3:D:1441:GLN:HB3	9:D:1557:HOH:O	1.97	0.65
5:F:166:LEU:O	5:F:171:LYS:HB2	1.96	0.65
2:M:916:GLU:HG2	9:M:2028:HOH:O	1.96	0.65
3:N:1166:LEU:HD12	3:N:1171:VAL:HG22	1.79	0.65
2:C:905:ILE:HB	9:C:1738:HOH:O	1.96	0.64
3:D:812:ALA:HB1	9:D:1779:HOH:O	1.98	0.64
3:D:906:GLN:HB3	3:D:911:LEU:HD11	1.78	0.64
5:F:187:LEU:HD23	5:F:187:LEU:O	1.97	0.64
1:K:38:ASN:HB3	1:K:39:PRO:HD3	1.77	0.64
1:L:54:THR:HG22	9:L:3428:HOH:O	1.96	0.64
1:L:61:VAL:N	1:L:137:ARG:HH22	1.95	0.64
2:M:838:LYS:HB2	2:M:848:VAL:HG22	1.78	0.64
3:N:611:GLN:HG2	3:N:619:LEU:HD11	1.77	0.64
3:D:1209:LEU:HD23	3:D:1211:MET:SD	2.37	0.64
2:M:54:ILE:HD11	2:M:356:ARG:HG2	1.79	0.64
2:M:73:LEU:HD22	2:M:118:ILE:HD11	1.79	0.64
2:M:429:ASP:HB3	9:M:2136:HOH:O	1.96	0.64
3:N:445:ARG:HB3	9:N:2112:HOH:O	1.98	0.64
3:N:817:GLU:O	3:N:821:VAL:HG23	1.96	0.64
1:A:13:VAL:HG12	1:A:15:THR:HG22	1.78	0.64
1:A:20:TYR:HB3	9:A:413:HOH:O	1.97	0.64
3:D:534:ARG:HG2	9:F:611:HOH:O	1.97	0.64
3:D:1237:THR:HG22	9:D:2068:HOH:O	1.98	0.64
5:F:401:GLU:O	5:F:405:LEU:HB2	1.97	0.64
1:K:13:VAL:HG12	1:K:15:THR:HG22	1.80	0.64
1:L:38:ASN:HB3	1:L:39:PRO:HD3	1.78	0.64
2:M:100:LEU:HD23	2:M:368:THR:HA	1.78	0.64
2:M:811:PRO:HB2	2:M:813:VAL:HG13	1.78	0.64
3:N:131:LYS:CG	3:N:568:ARG:HG2	2.26	0.64
3:N:141:ILE:HD12	9:N:2046:HOH:O	1.97	0.64
3:N:175:VAL:HG11	3:N:193:PRO:HB2	1.80	0.64
3:N:722:GLU:HA	9:N:1930:HOH:O	1.97	0.64
1:B:124:ASN:OD1	1:B:127:LEU:HB2	1.97	0.64
1:B:226:SER:O	1:B:228:PRO:HD3	1.97	0.64
2:C:645:VAL:HA	9:C:1531:HOH:O	1.96	0.64
2:C:976:ASP:CB	2:C:979:THR:HG22	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:55:ASP:HB3	3:D:82:LYS:HE2	1.79	0.64
3:D:149:LYS:HA	9:D:1632:HOH:O	1.98	0.64
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.80	0.64
5:F:349:LEU:HB2	9:F:433:HOH:O	1.98	0.64
2:M:263:ASP:HB2	2:M:264:PRO:HD3	1.78	0.64
3:N:1013:GLU:HB3	9:N:2351:HOH:O	1.97	0.64
2:C:691:SER:HB2	2:C:858:MET:SD	2.38	0.64
2:C:890:LEU:HD23	9:C:1640:HOH:O	1.97	0.64
3:D:124:GLU:O	3:D:128:TYR:HB2	1.97	0.64
1:K:41:ARG:HH22	2:M:866:PRO:HG3	1.63	0.64
1:L:9:PRO:HD3	9:L:1857:HOH:O	1.98	0.64
1:L:52:ALA:HB1	9:L:1023:HOH:O	1.98	0.64
1:L:109:VAL:HG21	1:L:138:LEU:CD1	2.18	0.64
2:M:170:PRO:HG2	2:M:258:TYR:CD2	2.32	0.64
2:M:176:VAL:HG12	2:M:182:VAL:HG13	1.78	0.64
2:M:549:PHE:CE2	2:M:886:LEU:HB3	2.32	0.64
3:N:565:ILE:HB	5:P:84:TYR:HD2	1.63	0.64
3:N:702:LEU:HD13	3:N:716:PHE:CD1	2.33	0.64
3:N:799:LYS:HB3	3:N:826:PRO:HG2	1.77	0.64
3:N:1209:LEU:HD12	3:N:1219:GLU:OE1	1.97	0.64
4:O:54:LEU:HG	4:O:58:PRO:CG	2.26	0.64
5:P:112:ALA:O	5:P:116:LEU:HG	1.98	0.64
5:P:315:VAL:HA	9:P:479:HOH:O	1.97	0.64
1:B:71:VAL:HG22	1:B:132:LEU:HD12	1.80	0.64
2:C:57:GLU:HB2	9:C:1254:HOH:O	1.97	0.64
2:C:79:PRO:HA	9:C:1251:HOH:O	1.97	0.64
2:C:84:ARG:HH21	2:C:128:ILE:HD11	1.63	0.64
2:C:140:ILE:CD1	2:C:412:ALA:HA	2.27	0.64
2:C:265:ARG:HG2	2:C:266:ARG:N	2.11	0.64
3:D:583:ASP:HB2	3:D:604:THR:OG1	1.97	0.64
3:D:1035:ILE:HA	3:D:1038:LEU:HD12	1.80	0.64
2:M:720:GLU:HA	2:M:759:THR:O	1.98	0.64
3:N:426:LYS:HD2	9:N:2209:HOH:O	1.96	0.64
4:O:67:GLU:OE1	4:O:73:LEU:HD11	1.97	0.64
2:C:218:VAL:HG22	2:C:221:LEU:CD2	2.28	0.64
2:C:549:PHE:HB3	2:C:552:HIS:HD2	1.63	0.64
2:C:573:ARG:HB2	9:C:1310:HOH:O	1.97	0.64
2:C:671:ASN:H	2:C:671:ASN:ND2	1.94	0.64
3:D:188:GLY:N	3:D:199:LEU:HD23	2.13	0.64
3:D:564:GLU:HA	3:D:567:ILE:HD13	1.80	0.64
3:D:614:PHE:CZ	5:F:326:ASP:HB3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:891:GLU:HG2	9:D:2400:HOH:O	1.96	0.64
5:F:327:SER:HA	9:F:456:HOH:O	1.96	0.64
2:M:545:ASN:OD1	2:M:905:ILE:HG12	1.96	0.64
2:M:603:VAL:HG22	2:M:613:VAL:HG12	1.79	0.64
4:O:88:GLU:HB3	9:O:2455:HOH:O	1.97	0.64
2:C:41:ASN:HD22	2:C:41:ASN:N	1.91	0.64
2:C:69:LEU:HB2	2:C:97:ARG:HB2	1.80	0.64
3:D:175:VAL:HG11	3:D:193:PRO:HB2	1.80	0.64
5:F:112:ALA:HA	5:F:173:TYR:HD2	1.63	0.64
2:M:118:ILE:HB	9:M:2032:HOH:O	1.98	0.64
2:M:331:ARG:CZ	2:M:427:VAL:HG12	2.28	0.64
3:N:148:GLU:HG2	3:N:151:GLN:NE2	2.11	0.64
3:N:546:ARG:HA	9:N:1614:HOH:O	1.98	0.64
3:N:679:ARG:HB2	3:N:682:ASP:OD2	1.98	0.64
3:N:1065:LEU:HG	3:N:1070:TYR:HD2	1.63	0.64
2:C:150:PRO:CA	2:C:158:TYR:HB3	2.23	0.64
2:C:314:THR:HG23	9:C:1562:HOH:O	1.98	0.64
2:C:773:LEU:HB2	9:C:1139:HOH:O	1.96	0.64
3:D:148:GLU:HG2	3:D:151:GLN:NE2	2.12	0.64
1:K:197:LEU:HD23	1:K:197:LEU:H	1.62	0.64
1:K:201:THR:HG22	1:K:203:GLY:H	1.63	0.64
3:N:153:LEU:HD11	3:N:158:TYR:N	2.13	0.64
3:N:595:GLY:HA2	9:N:2178:HOH:O	1.98	0.64
2:C:144:PRO:O	2:C:276:LYS:HD3	1.96	0.64
2:C:472:ARG:HB3	2:C:480:THR:O	1.97	0.64
3:D:154:THR:HG23	3:D:157:GLU:H	1.63	0.64
3:D:1434:TRP:CZ3	3:D:1457:ASP:HB2	2.33	0.64
1:K:117:VAL:HB	1:K:120:VAL:CG1	2.27	0.64
1:L:61:VAL:HG23	1:L:137:ARG:NH2	2.13	0.64
2:M:19:THR:O	2:M:23:VAL:HG23	1.97	0.64
3:N:615:ARG:HB3	9:N:2387:HOH:O	1.97	0.64
3:N:1023:MET:HB2	3:N:1029:ARG:O	1.98	0.64
4:O:59:ASN:HB3	4:O:62:THR:OG1	1.98	0.64
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.80	0.63
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.80	0.63
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.33	0.63
3:N:189:GLN:HG3	3:N:190:GLU:N	2.13	0.63
3:N:610:LYS:O	3:N:611:GLN:HG3	1.98	0.63
2:C:439:CYS:SG	2:C:441:VAL:HB	2.39	0.63
2:C:1014:SER:O	2:C:1018:GLN:HG3	1.97	0.63
3:D:52:PRO:HB2	3:D:80:VAL:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:558:LEU:HD13	5:F:145:PRO:CB	2.28	0.63
1:K:150:TYR:HE2	1:K:152:PRO:HG3	1.62	0.63
3:N:131:LYS:HE2	3:N:456:MET:HE1	1.80	0.63
3:N:569:ASN:HD21	5:P:210:LEU:HD22	1.62	0.63
1:B:61:VAL:N	1:B:137:ARG:HH22	1.96	0.63
2:C:200:LEU:HB2	9:C:1462:HOH:O	1.97	0.63
9:K:1622:HOH:O	2:M:640:ARG:HB2	1.98	0.63
5:P:166:LEU:HD11	9:P:491:HOH:O	1.98	0.63
3:D:764:LEU:HD23	3:D:767:HIS:CE1	2.33	0.63
1:K:120:VAL:HG13	9:K:2485:HOH:O	1.99	0.63
2:M:693:GLU:HA	2:M:696:LYS:HG3	1.80	0.63
2:M:1016:ILE:HG23	3:N:526:PRO:HG2	1.79	0.63
2:M:1098:ASP:HB2	3:N:21:TRP:HZ2	1.63	0.63
3:N:72:VAL:HG23	3:N:78:VAL:H	1.63	0.63
3:N:147:VAL:HA	9:N:1777:HOH:O	1.98	0.63
2:C:18:LEU:HD21	2:C:542:VAL:HG11	1.80	0.63
3:D:1397:LYS:HE3	9:D:2203:HOH:O	1.98	0.63
3:D:1439:SER:HB3	3:D:1463:LYS:HE2	1.79	0.63
1:K:177:VAL:HG12	9:K:1774:HOH:O	1.99	0.63
1:L:41:ARG:HG3	1:L:177:VAL:HG21	1.80	0.63
2:M:437:ARG:HG2	2:M:467:ILE:O	1.97	0.63
2:M:474:VAL:HG11	2:M:529:VAL:HG12	1.79	0.63
2:M:944:LEU:HD21	2:M:963:LEU:HD23	1.80	0.63
2:M:968:LEU:HB3	9:M:2164:HOH:O	1.98	0.63
3:N:169:TYR:CG	3:N:195:VAL:HG11	2.34	0.63
3:N:614:PHE:C	3:N:615:ARG:O	2.33	0.63
3:N:720:LEU:H	3:N:720:LEU:HD12	1.63	0.63
5:P:372:ARG:N	5:P:372:ARG:HD2	2.12	0.63
1:A:20:TYR:HE2	1:A:22:GLU:HG3	1.62	0.63
1:A:191:ASP:O	1:A:192:LEU:HD23	1.99	0.63
2:C:243:ARG:HG2	9:C:1218:HOH:O	1.99	0.63
2:C:358:ARG:HB3	2:C:371:LYS:O	1.98	0.63
3:D:562:ALA:HB1	3:D:567:ILE:HD11	1.80	0.63
3:D:614:PHE:HZ	5:F:326:ASP:HB3	1.63	0.63
3:D:785:ILE:HG22	3:D:789:LEU:HD12	1.80	0.63
3:D:1266:ARG:O	3:D:1268:PRO:HD3	1.98	0.63
5:F:115:LYS:HD2	5:F:173:TYR:CE2	2.33	0.63
5:F:132:ARG:O	5:F:136:LEU:HG	1.99	0.63
1:L:138:LEU:HD23	1:L:140:MET:SD	2.37	0.63
2:M:307:LEU:HG	2:M:311:PHE:HE2	1.62	0.63
3:N:890:VAL:HG13	3:N:926:LYS:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:34:GLY:HA2	9:O:3283:HOH:O	1.98	0.63
1:A:109:VAL:HG23	1:A:132:LEU:HD13	1.80	0.63
2:C:304:LEU:HD23	2:C:305:PRO:HD3	1.80	0.63
3:D:799:LYS:N	3:D:826:PRO:HG2	2.12	0.63
1:L:72:LYS:HD2	9:L:2772:HOH:O	1.98	0.63
2:M:397:GLU:HB2	9:M:1672:HOH:O	1.97	0.63
2:M:820:ARG:HG3	9:M:1785:HOH:O	1.99	0.63
3:N:161:LEU:HD22	3:N:452:ILE:HG21	1.79	0.63
3:N:478:LEU:HD21	3:N:500:ARG:NH2	2.13	0.63
3:N:925:GLU:HB3	4:O:2:ALA:HB3	1.79	0.63
4:O:60:ALA:O	4:O:63:TRP:HB2	1.97	0.63
2:C:185:LYS:HE2	2:C:190:LYS:HE2	1.80	0.63
2:C:660:ALA:HB1	2:C:667:ALA:O	1.98	0.63
3:D:65:ARG:HG3	3:D:66:GLN:H	1.64	0.63
3:D:1046:GLN:HG3	9:D:1606:HOH:O	1.98	0.63
3:D:1432:LYS:HG3	3:D:1433:SER:H	1.64	0.63
3:D:1465:ASN:ND2	3:D:1470:ARG:HD3	2.12	0.63
4:E:54:LEU:HG	4:E:58:PRO:CG	2.27	0.63
1:L:182:GLU:O	1:L:194:LYS:HB3	1.98	0.63
3:N:610:LYS:HG2	7:N:1527:MXP:H15A	1.80	0.63
5:P:401:GLU:O	5:P:405:LEU:HB2	1.99	0.63
1:B:61:VAL:HG23	1:B:137:ARG:NH2	2.13	0.63
2:C:599:GLU:HB2	9:C:1216:HOH:O	1.99	0.63
2:C:659:PRO:HD3	9:C:1639:HOH:O	1.98	0.63
5:F:88:ILE:HB	5:F:193:ARG:HH11	1.63	0.63
2:M:265:ARG:HG2	2:M:266:ARG:N	2.14	0.63
3:N:403:PHE:CE1	3:N:407:VAL:HG23	2.34	0.63
3:N:906:GLN:HB3	3:N:911:LEU:CD1	2.29	0.63
3:N:961:LYS:HA	9:N:2211:HOH:O	1.99	0.63
3:N:1272:ALA:HA	3:N:1326:THR:HB	1.81	0.63
3:N:1356:TYR:CD2	3:N:1363:LEU:HD23	2.33	0.63
1:A:91:ASN:OD1	1:A:92:PRO:HD2	1.98	0.62
2:C:142:ARG:HH21	2:C:325:ILE:CD1	2.12	0.62
3:D:1109:GLU:HG2	3:D:1201:CYS:HA	1.81	0.62
5:F:372:ARG:HD2	5:F:372:ARG:N	2.14	0.62
2:M:790:LEU:HG	9:M:1781:HOH:O	1.99	0.62
2:M:1103:ASP:HB2	2:M:1107:ASN:O	1.99	0.62
5:P:356:LYS:HB2	9:P:473:HOH:O	1.99	0.62
1:A:18:ARG:O	1:A:207:PRO:HD3	1.98	0.62
1:B:182:GLU:O	1:B:194:LYS:HB3	1.98	0.62
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:367:LEU:O	2:C:372:LEU:HD13	1.99	0.62
3:D:55:ASP:HB3	9:D:1577:HOH:O	1.99	0.62
3:D:179:VAL:HG13	3:D:183:GLU:HB3	1.81	0.62
3:D:996:TRP:CE2	3:D:1056:PRO:HG2	2.34	0.62
3:D:1037:GLN:HG2	3:D:1042:ARG:HB3	1.81	0.62
3:D:1488:ASP:HA	9:E:110:HOH:O	1.99	0.62
1:L:55:SER:OG	1:L:158:ILE:HD13	2.00	0.62
2:M:276:LYS:O	2:M:280:LYS:HB2	1.99	0.62
2:M:676:ILE:O	2:M:676:ILE:HG23	1.99	0.62
2:M:1067:TYR:HE1	3:N:655:PRO:HG3	1.62	0.62
3:N:188:GLY:HA2	9:N:1751:HOH:O	1.98	0.62
3:N:1109:GLU:HG2	3:N:1201:CYS:HA	1.81	0.62
4:O:37:ASN:HA	4:O:93:TYR:CE2	2.34	0.62
5:P:152:ASP:HA	9:P:502:HOH:O	1.98	0.62
2:C:162:ILE:O	2:C:164:PRO:HD3	1.99	0.62
2:C:1109:VAL:HG11	3:D:5:VAL:HG13	1.79	0.62
3:D:58:CYS:HA	3:D:78:VAL:HG11	1.80	0.62
4:E:45:ARG:HB2	4:E:46:PRO:HD2	1.80	0.62
4:E:95:VAL:O	4:E:95:VAL:HG12	1.99	0.62
2:M:166:PRO:HD3	2:M:265:ARG:HG3	1.79	0.62
2:M:709:GLU:HG3	2:M:824:ARG:HG2	1.82	0.62
3:N:538:SER:HB3	9:P:565:HOH:O	1.97	0.62
3:N:860:LEU:HD22	3:N:878:GLY:HA2	1.81	0.62
3:N:1262:LEU:HD23	3:N:1352:ILE:CG1	2.29	0.62
4:O:83:ASP:O	4:O:86:GLN:HG2	1.99	0.62
2:C:165:LEU:O	2:C:265:ARG:HD2	1.99	0.62
2:C:1005:MET:O	2:C:1005:MET:HG3	1.99	0.62
1:L:18:ARG:O	1:L:207:PRO:HD3	1.99	0.62
1:L:52:ALA:HB2	1:L:170:VAL:O	1.99	0.62
1:L:59:GLU:HG3	1:L:139:ASN:ND2	2.14	0.62
3:N:40:GLU:N	9:N:1836:HOH:O	2.31	0.62
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.80	0.62
3:N:1264:GLU:CD	3:N:1425:THR:HB	2.19	0.62
3:N:1290:LEU:CD2	3:N:1291:SER:H	2.12	0.62
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.81	0.62
2:C:395:LYS:HE2	2:C:403:SER:CB	2.20	0.62
2:C:838:LYS:CE	2:C:846:LYS:HE2	2.29	0.62
2:C:1001:VAL:HG13	9:C:1323:HOH:O	1.98	0.62
3:D:47:GLU:HG2	3:D:53:ILE:HG22	1.80	0.62
3:D:165:LYS:HB2	3:D:397:LYS:HB3	1.81	0.62
3:D:187:LYS:HG3	3:D:199:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:865:THR:HG22	9:D:1855:HOH:O	1.99	0.62
5:F:119:ILE:HD13	5:F:170:HIS:ND1	2.15	0.62
2:M:110:GLU:CB	2:M:369:PRO:HG3	2.30	0.62
2:M:741:GLY:HA3	9:M:1665:HOH:O	1.99	0.62
3:N:12:LEU:HD11	3:N:512:MET:HG2	1.80	0.62
3:N:52:PRO:HG3	3:N:78:VAL:HG13	1.81	0.62
3:N:185:VAL:HG23	3:N:202:VAL:C	2.18	0.62
3:N:510:GLU:HB3	9:N:2186:HOH:O	1.99	0.62
3:N:583:ASP:OD2	3:N:604:THR:HG21	1.99	0.62
5:P:375:LEU:HG	5:P:376:ILE:HG13	1.82	0.62
1:B:79:ILE:HD12	9:B:474:HOH:O	1.98	0.62
2:C:971:LYS:HA	2:C:988:VAL:HA	1.82	0.62
3:D:834:THR:HB	3:D:838:ARG:HB2	1.81	0.62
3:D:860:LEU:HA	3:D:877:PRO:HB2	1.82	0.62
2:M:333:ILE:HD13	2:M:467:ILE:HG13	1.81	0.62
2:M:472:ARG:HB3	2:M:480:THR:O	2.00	0.62
2:M:480:THR:HG22	2:M:481:ASP:H	1.64	0.62
3:N:775:GLY:HA2	9:N:2264:HOH:O	2.00	0.62
3:N:864:VAL:HG12	3:N:865:THR:H	1.65	0.62
3:N:1189:ARG:HH11	3:N:1203:LYS:HB2	1.64	0.62
5:P:172:ARG:O	5:P:176:ILE:HD13	1.99	0.62
2:C:877:PRO:HG2	3:D:1023:MET:CE	2.27	0.62
3:D:493:ARG:HH11	3:D:1390:LEU:HB3	1.63	0.62
3:D:877:PRO:O	3:D:880:ILE:HG22	1.99	0.62
3:D:1114:THR:CG2	3:D:1195:GLN:HB3	2.29	0.62
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.82	0.62
3:D:1356:TYR:HD2	3:D:1363:LEU:HD23	1.65	0.62
3:D:1467:ILE:HG23	7:D:1527:MXP:H16A	1.81	0.62
1:K:48:ILE:HG22	1:K:173:PRO:HD2	1.80	0.62
1:L:223:THR:HG22	9:L:4161:HOH:O	1.98	0.62
2:M:80:GLN:O	2:M:83:CYS:HB2	1.99	0.62
2:M:146:VAL:HG11	2:M:306:THR:HG22	1.81	0.62
2:M:431:HIS:HD2	2:M:433:THR:H	1.45	0.62
2:M:1002:GLU:HG2	2:M:1003:ASP:N	2.14	0.62
2:C:244:PRO:HG3	9:C:1642:HOH:O	1.98	0.62
3:D:491:LYS:HD3	9:D:1938:HOH:O	1.99	0.62
3:D:1321:ALA:O	3:D:1339:LYS:HE3	2.00	0.62
9:D:1795:HOH:O	4:E:50:THR:HB	2.00	0.62
3:N:723:GLY:HA3	9:N:1625:HOH:O	2.00	0.62
3:N:957:PRO:CG	3:N:1007:VAL:HA	2.27	0.62
4:O:30:LEU:O	4:O:35:PHE:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:THR:HG22	1:B:209:GLU:HB2	1.81	0.62
3:D:49:ILE:HG21	9:D:2241:HOH:O	2.00	0.62
3:D:1056:PRO:HD3	9:D:1650:HOH:O	1.99	0.62
3:D:1111:ASP:HB3	3:D:1203:LYS:HG3	1.82	0.62
5:F:396:ARG:HB2	9:F:496:HOH:O	1.98	0.62
2:M:86:LYS:CD	2:M:813:VAL:HG12	2.30	0.62
2:M:498:GLN:O	2:M:501:THR:HG23	2.00	0.62
2:M:557:ARG:NH1	2:M:879:ARG:HG2	2.15	0.62
2:M:559:LEU:HD23	2:M:560:MET:N	2.14	0.62
2:M:567:GLN:HB2	2:M:997:LEU:HD22	1.80	0.62
2:M:715:THR:HG22	2:M:717:LEU:HG	1.82	0.62
2:M:722:ILE:CD1	2:M:823:VAL:HG21	2.29	0.62
3:N:1192:LEU:HD13	3:N:1345:GLU:HG2	1.81	0.62
2:C:274:ARG:HG2	9:C:1142:HOH:O	1.99	0.62
2:C:307:LEU:HG	2:C:311:PHE:CE2	2.35	0.62
3:D:428:LYS:HE2	9:D:1881:HOH:O	2.00	0.62
3:N:394:LEU:HD21	9:N:2081:HOH:O	2.00	0.62
3:N:1013:GLU:HB2	9:N:1747:HOH:O	2.00	0.62
3:N:1258:ARG:NH2	3:N:1262:LEU:HD11	2.15	0.62
3:N:1293:PHE:CZ	3:N:1302:GLU:HB3	2.34	0.62
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.81	0.61
2:C:137:VAL:HG22	2:C:391:LEU:O	2.00	0.61
2:C:141:HIS:CB	2:C:418:LEU:HG	2.29	0.61
2:C:420:ARG:HA	9:C:1293:HOH:O	1.98	0.61
2:C:738:ASP:CB	2:C:744:ARG:HB3	2.29	0.61
2:C:902:ILE:O	2:C:904:PRO:HD3	2.00	0.61
3:D:107:ASP:O	3:D:108:VAL:C	2.37	0.61
3:D:1269:LYS:HD3	9:D:2029:HOH:O	1.99	0.61
3:D:1291:SER:HB2	3:D:1293:PHE:HE1	1.65	0.61
1:L:128:HIS:HE1	1:L:131:THR:HG23	1.64	0.61
1:L:169:ALA:HB1	1:L:171:PHE:CD2	2.35	0.61
3:N:80:VAL:HA	9:N:2248:HOH:O	1.99	0.61
3:N:683:ILE:HG22	9:N:1566:HOH:O	2.00	0.61
3:N:717:GLN:HG2	9:N:1629:HOH:O	2.00	0.61
3:N:1295:GLU:HB3	3:N:1300:SER:CB	2.30	0.61
2:C:31:GLN:HB3	2:C:71:TYR:OH	2.00	0.61
2:C:63:GLY:HA3	9:C:1168:HOH:O	1.98	0.61
2:C:528:GLU:HG2	9:C:1477:HOH:O	1.99	0.61
3:D:400:VAL:HG22	3:D:443:VAL:CG2	2.29	0.61
3:D:613:ARG:HG3	3:D:1441:GLN:HB2	1.82	0.61
3:D:955:VAL:HA	9:D:2261:HOH:O	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:30:LEU:O	4:E:35:PHE:HA	2.00	0.61
2:M:864:GLY:O	2:M:866:PRO:HD3	2.00	0.61
3:N:491:LYS:HD3	9:N:2284:HOH:O	1.98	0.61
3:N:611:GLN:CG	3:N:619:LEU:HG	2.29	0.61
3:N:1036:ARG:HH21	3:N:1042:ARG:HA	1.64	0.61
3:N:1274:ILE:HA	9:N:1761:HOH:O	2.00	0.61
3:N:1304:LYS:HA	9:N:1838:HOH:O	1.99	0.61
4:O:86:GLN:O	4:O:90:GLU:HG3	2.00	0.61
5:P:88:ILE:HG21	5:P:193:ARG:HD3	1.83	0.61
2:C:151:ASP:OD2	2:C:159:ILE:HG23	2.00	0.61
2:C:512:ARG:HB2	9:C:1201:HOH:O	2.00	0.61
3:D:50:PHE:CB	3:D:522:PRO:HG2	2.29	0.61
2:M:274:ARG:HD2	2:M:285:LEU:O	1.99	0.61
2:M:838:LYS:CE	2:M:846:LYS:HE2	2.29	0.61
2:M:926:PHE:CE1	2:M:929:ARG:HD3	2.35	0.61
5:P:284:ARG:HD2	9:P:504:HOH:O	1.99	0.61
2:C:305:PRO:HA	2:C:308:ARG:HD2	1.82	0.61
3:D:1097:LYS:HE3	9:D:2031:HOH:O	2.01	0.61
3:D:1430:SER:HA	9:D:1920:HOH:O	1.99	0.61
1:K:67:THR:HG21	2:M:609:ASN:ND2	2.07	0.61
1:K:109:VAL:HG23	1:K:132:LEU:HD13	1.81	0.61
2:M:144:PRO:HA	2:M:163:ILE:HG13	1.82	0.61
2:M:239:PHE:HB3	9:M:1968:HOH:O	2.00	0.61
3:N:702:LEU:HD13	3:N:716:PHE:HD1	1.64	0.61
3:N:1042:ARG:O	3:N:1057:VAL:HB	2.00	0.61
9:N:1961:HOH:O	5:P:168:LYS:HG2	2.01	0.61
9:N:2314:HOH:O	5:P:376:ILE:HD11	1.99	0.61
1:A:125:PRO:HD2	9:A:394:HOH:O	2.00	0.61
1:A:184:THR:HG23	1:A:192:LEU:HB2	1.82	0.61
2:C:143:SER:HB2	2:C:276:LYS:NZ	2.14	0.61
2:C:399:ASN:ND2	2:C:568:ALA:HB3	2.15	0.61
2:C:625:LEU:HB3	2:C:639:GLN:HB2	1.82	0.61
2:C:1002:GLU:HG2	2:C:1003:ASP:N	2.14	0.61
2:C:1056:LYS:NZ	3:D:749:VAL:O	2.33	0.61
3:D:847:ASP:O	3:D:851:LEU:HG	2.01	0.61
9:D:1675:HOH:O	5:F:337:HIS:HB3	2.01	0.61
5:F:230:LYS:HD3	9:F:439:HOH:O	1.99	0.61
5:F:361:LEU:HD23	5:F:362:SER:N	2.15	0.61
2:M:267:TYR:HB2	2:M:272:ALA:HB1	1.82	0.61
2:M:358:ARG:HB3	2:M:371:LYS:O	1.99	0.61
2:M:367:LEU:O	2:M:372:LEU:HD13	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:996:TRP:CE3	3:N:999:THR:HG21	2.35	0.61
3:N:1102:THR:HG22	3:N:1222:GLY:HA2	1.82	0.61
3:N:1173:LEU:HD23	3:N:1174:LEU:HD23	1.83	0.61
3:N:1389:LEU:HD12	3:N:1390:LEU:H	1.65	0.61
1:B:108:GLU:HB2	9:B:409:HOH:O	2.00	0.61
2:C:6:PHE:CG	2:C:909:ALA:HA	2.35	0.61
2:C:123:GLU:HB2	9:C:1197:HOH:O	2.00	0.61
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.83	0.61
2:C:1007:ALA:HB2	3:D:648:MET:HG3	1.82	0.61
2:C:1066:ALA:O	2:C:1070:ILE:HG13	1.99	0.61
3:D:119:SER:HB2	3:D:123:LEU:HD13	1.81	0.61
2:M:15:LEU:H	2:M:15:LEU:HD12	1.66	0.61
2:M:57:GLU:HG3	9:M:1902:HOH:O	1.99	0.61
2:M:176:VAL:HG12	2:M:182:VAL:CG1	2.31	0.61
3:N:52:PRO:HG2	3:N:80:VAL:HG13	1.81	0.61
3:N:119:SER:HB2	3:N:123:LEU:HD13	1.81	0.61
3:N:400:VAL:HG13	3:N:402:PRO:HD3	1.83	0.61
3:N:1377:LYS:HG3	3:N:1394:VAL:HG13	1.81	0.61
2:C:64:LEU:HD13	2:C:359:MET:HG3	1.82	0.61
2:C:108:ILE:HB	2:C:368:THR:HG1	1.65	0.61
2:C:333:ILE:CD1	2:C:467:ILE:HG13	2.30	0.61
3:D:204:LEU:HG	3:D:441:ARG:HH12	1.66	0.61
3:D:637:LEU:HD11	3:D:642:CYS:N	2.15	0.61
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.82	0.61
5:F:335:ASP:OD1	5:F:338:LEU:HB2	2.01	0.61
3:N:128:TYR:HE1	3:N:461:ILE:HG13	1.65	0.61
3:N:187:LYS:HG3	3:N:199:LEU:HD22	1.83	0.61
3:N:674:ARG:HD3	9:N:1957:HOH:O	2.01	0.61
5:P:203:THR:HG22	5:P:204:GLY:N	2.16	0.61
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.35	0.61
2:C:455:LEU:HD12	2:C:456:ALA:O	2.00	0.61
3:D:65:ARG:CG	3:D:66:GLN:H	2.13	0.61
3:D:1384:PRO:HG3	3:D:1389:LEU:HA	1.83	0.61
1:K:20:TYR:HD2	1:K:21:GLY:H	1.49	0.61
1:L:83:LYS:HA	9:L:2646:HOH:O	2.00	0.61
1:L:143:ARG:HD2	1:L:160:ASP:OD2	2.00	0.61
2:M:479:VAL:HG11	2:M:532:MET:HE2	1.81	0.61
3:N:500:ARG:HD2	9:N:2131:HOH:O	2.00	0.61
3:N:799:LYS:H	3:N:826:PRO:HG2	1.66	0.61
1:A:20:TYR:CD2	1:A:21:GLY:N	2.63	0.61
2:C:775:ARG:HG3	9:C:1214:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:919:ALA:HA	9:C:1166:HOH:O	2.00	0.61
3:D:169:TYR:CG	3:D:195:VAL:HG11	2.36	0.61
3:D:206:ARG:HH11	5:F:97:GLU:HB3	1.65	0.61
3:D:486:ARG:HD3	3:D:489:ARG:HD3	1.81	0.61
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.65	0.61
1:L:176:ARG:HH21	3:N:850:LEU:HD13	1.65	0.61
2:M:307:LEU:HG	2:M:311:PHE:CE2	2.36	0.61
3:N:31:THR:HG23	3:N:45:PHE:CE2	2.35	0.61
3:N:824:ASN:HB2	9:N:1978:HOH:O	2.01	0.61
3:N:1420:LEU:HD12	3:N:1421:LEU:N	2.14	0.61
2:C:73:LEU:HD23	2:C:94:LEU:HB2	1.83	0.61
2:C:325:ILE:HG12	9:C:1558:HOH:O	2.00	0.61
2:C:1065:ALA:HB1	2:C:1077:PRO:HG2	1.83	0.61
2:C:1067:TYR:O	2:C:1071:ILE:HG12	2.01	0.61
3:D:400:VAL:HG13	3:D:402:PRO:HD3	1.83	0.61
3:D:633:VAL:HG22	3:D:635:PRO:CD	2.30	0.61
3:D:850:LEU:HD12	3:D:850:LEU:N	2.15	0.61
3:D:1127:GLU:HB2	9:D:1604:HOH:O	2.00	0.61
3:D:1394:VAL:HG11	9:D:2203:HOH:O	2.00	0.61
2:M:41:ASN:H	2:M:41:ASN:ND2	1.94	0.61
3:N:860:LEU:HA	3:N:877:PRO:HB2	1.82	0.61
1:B:90:LEU:HD23	9:B:496:HOH:O	1.99	0.60
2:C:926:PHE:CE1	2:C:929:ARG:HD3	2.36	0.60
2:C:969:GLN:HA	9:D:1915:HOH:O	2.00	0.60
3:D:10:ILE:HG13	3:D:1434:TRP:CZ2	2.35	0.60
3:D:130:SER:HB3	3:D:132:TYR:CE1	2.36	0.60
3:D:471:GLU:HG3	9:D:1589:HOH:O	2.01	0.60
3:D:631:ILE:HG12	3:D:743:ASP:O	2.00	0.60
3:D:1393:GLN:CB	3:D:1398:TRP:HE1	2.10	0.60
3:D:1462:LEU:HD22	3:D:1472:ILE:HG23	1.83	0.60
1:K:206:THR:CG2	1:K:209:GLU:H	2.14	0.60
1:K:221:HIS:HA	1:K:224:TYR:HD2	1.64	0.60
3:N:204:LEU:HD21	3:N:445:ARG:HH12	1.65	0.60
2:C:331:ARG:HB2	9:C:1737:HOH:O	1.99	0.60
2:C:1067:TYR:HE1	3:D:655:PRO:HG3	1.65	0.60
2:C:1118:LYS:HG2	3:D:23:TYR:CE1	2.36	0.60
1:L:2:LEU:HD12	1:L:3:ASP:N	2.16	0.60
3:N:131:LYS:HE3	3:N:568:ARG:CB	2.31	0.60
3:N:809:PRO:HB2	3:N:812:ALA:HB2	1.82	0.60
3:N:1291:SER:HB2	3:N:1293:PHE:CE1	2.35	0.60
5:P:95:THR:HG21	9:P:531:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:247:ILE:HG22	5:P:251:ILE:HD11	1.82	0.60
1:B:106:PRO:HG3	1:B:134:GLU:HG2	1.82	0.60
1:B:206:THR:HG22	1:B:209:GLU:H	1.66	0.60
2:C:193:LEU:HD21	9:C:1526:HOH:O	2.02	0.60
3:D:507:ASN:HA	9:D:2352:HOH:O	2.01	0.60
3:D:728:LEU:HD22	3:D:745:MET:SD	2.42	0.60
1:K:42:ARG:NH2	2:M:857:ASP:HB3	2.15	0.60
1:K:157:GLY:HA3	9:K:2579:HOH:O	2.01	0.60
2:M:341:THR:O	2:M:345:ARG:HG3	2.00	0.60
3:N:27:GLU:HB2	9:N:2072:HOH:O	2.00	0.60
3:N:509:PRO:HB2	9:N:1664:HOH:O	2.00	0.60
3:N:1434:TRP:CZ3	3:N:1457:ASP:HB2	2.36	0.60
3:D:86:ARG:O	3:D:522:PRO:HD2	2.01	0.60
3:D:559:ALA:HA	9:F:646:HOH:O	2.01	0.60
3:D:829:VAL:H	3:D:835:SER:HB2	1.66	0.60
3:D:860:LEU:HD22	3:D:878:GLY:HA2	1.84	0.60
3:D:1299:PHE:HB2	9:D:2455:HOH:O	2.00	0.60
1:K:213:GLN:O	1:K:217:ILE:HG13	2.02	0.60
2:M:811:PRO:HG2	9:M:1891:HOH:O	2.00	0.60
3:N:52:PRO:CG	3:N:78:VAL:HG13	2.31	0.60
3:N:95:LEU:HA	3:N:551:ASN:ND2	2.16	0.60
3:N:107:ASP:O	3:N:108:VAL:C	2.39	0.60
3:N:566:ILE:HG23	5:P:217:ASN:HD22	1.66	0.60
2:C:720:GLU:HA	2:C:759:THR:O	2.02	0.60
2:C:1101:THR:HB	3:D:5:VAL:HG13	1.83	0.60
3:D:29:PRO:HB3	3:D:545:ARG:HG2	1.84	0.60
3:D:517:VAL:HG11	3:D:581:LEU:HD21	1.83	0.60
3:D:569:ASN:HB3	5:F:214:GLN:HE21	1.65	0.60
2:M:554:ASP:OD2	2:M:556:ASN:HB3	2.01	0.60
2:M:747:ALA:O	2:M:799:ILE:HA	2.01	0.60
2:M:971:LYS:HA	2:M:988:VAL:HA	1.84	0.60
3:N:80:VAL:HG12	3:N:81:THR:O	2.02	0.60
3:N:799:LYS:N	3:N:826:PRO:HG2	2.16	0.60
5:P:209:PHE:CE2	5:P:213:ILE:HD11	2.37	0.60
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.83	0.60
2:C:93:PRO:HG3	2:C:117:HIS:CE1	2.37	0.60
2:C:132:ALA:HB1	2:C:632:ASN:ND2	2.16	0.60
2:C:571:LEU:HD21	2:C:700:TYR:HA	1.82	0.60
5:F:369:LEU:HB2	9:F:426:HOH:O	2.02	0.60
9:K:3509:HOH:O	1:L:155:LYS:HE2	2.00	0.60
2:M:265:ARG:HB3	2:M:267:TYR:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:518:LYS:HA	9:M:1901:HOH:O	2.02	0.60
2:M:890:LEU:CA	2:M:914:ILE:HD11	2.31	0.60
3:N:1109:GLU:HG2	3:N:1202:GLN:H	1.66	0.60
4:O:54:LEU:CD2	4:O:63:TRP:HE1	2.14	0.60
5:P:325:LYS:HB2	9:P:652:HOH:O	2.01	0.60
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.37	0.60
2:C:169:GLY:HA3	9:C:1253:HOH:O	2.01	0.60
2:C:559:LEU:HD23	2:C:560:MET:N	2.17	0.60
3:D:519:VAL:HG13	3:D:544:TYR:CZ	2.36	0.60
3:D:984:THR:HG22	3:D:987:GLU:H	1.66	0.60
5:F:132:ARG:HD2	9:F:492:HOH:O	2.02	0.60
5:F:375:LEU:HG	5:F:376:ILE:HG13	1.83	0.60
1:K:18:ARG:HD2	1:K:123:MET:HE1	1.84	0.60
1:L:5:LYS:O	1:L:8:ALA:HB2	2.01	0.60
2:M:218:VAL:HA	2:M:221:LEU:HD23	1.84	0.60
2:M:218:VAL:HG22	2:M:221:LEU:HD23	1.84	0.60
2:M:1104:GLU:HG3	9:M:1982:HOH:O	2.01	0.60
3:N:142:LEU:HD11	9:N:2326:HOH:O	2.01	0.60
3:N:439:LEU:HB3	9:N:2015:HOH:O	1.99	0.60
3:N:583:ASP:OD1	3:N:586:ARG:HG3	2.01	0.60
3:N:647:ARG:HB3	9:N:2056:HOH:O	1.99	0.60
5:P:88:ILE:HD13	5:P:193:ARG:HB2	1.82	0.60
1:B:175:ARG:O	1:B:176:ARG:HG3	2.01	0.60
2:C:712:ALA:O	2:C:820:ARG:CB	2.50	0.60
2:C:818:GLY:N	5:F:309:LYS:HE2	2.17	0.60
3:D:1123:PHE:HA	3:D:1133:ARG:O	2.01	0.60
5:F:151:LEU:HB3	9:F:614:HOH:O	2.00	0.60
1:L:7:LYS:HG3	1:L:7:LYS:O	2.02	0.60
2:M:565:GLN:HA	2:M:995:MET:HE1	1.84	0.60
3:N:477:LEU:HD11	3:N:495:ARG:HD3	1.84	0.60
3:N:961:LYS:HB3	9:N:2007:HOH:O	2.00	0.60
1:B:132:LEU:HD21	1:B:136:GLY:O	2.01	0.60
2:C:260:LEU:HA	2:C:291:ALA:CB	2.31	0.60
2:C:591:SER:HA	9:C:1421:HOH:O	2.02	0.60
2:C:816:LYS:HB2	2:C:819:VAL:HG21	1.84	0.60
2:C:1017:THR:HG23	9:C:1263:HOH:O	2.00	0.60
3:D:408:GLU:HA	5:F:171:LYS:NZ	2.16	0.60
1:K:7:LYS:HZ1	1:K:186:LEU:HD21	1.67	0.60
1:K:18:ARG:NH1	1:K:88:ARG:HD3	2.16	0.60
2:M:9:ILE:O	2:M:9:ILE:HG13	2.02	0.60
3:N:73:CYS:HB3	3:N:76:CYS:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:141:ILE:HG22	3:N:450:TYR:H	1.66	0.60
3:N:161:LEU:O	3:N:161:LEU:HD23	2.02	0.60
3:N:1114:THR:CG2	3:N:1195:GLN:HB3	2.31	0.60
2:C:137:VAL:HG23	2:C:391:LEU:HG	1.83	0.60
2:C:1008:ARG:HD2	2:C:1028:GLY:N	2.17	0.60
3:D:776:GLU:HB3	3:D:912:LYS:HE2	1.84	0.60
3:D:1125:PRO:HB2	9:D:2360:HOH:O	2.01	0.60
3:D:1295:GLU:HB3	3:D:1300:SER:CB	2.32	0.60
3:D:1326:THR:HG23	9:D:2026:HOH:O	2.01	0.60
1:L:217:ILE:O	1:L:221:HIS:ND1	2.33	0.60
2:M:710:ILE:HD11	2:M:758:ARG:HD3	1.84	0.60
2:M:833:LEU:HD12	2:M:834:GLN:H	1.67	0.60
2:M:874:LEU:HD12	3:N:784:ASP:OD2	2.02	0.60
3:N:10:ILE:HG13	3:N:1434:TRP:CE2	2.37	0.60
3:N:130:SER:O	3:N:568:ARG:NH2	2.35	0.60
3:N:1114:THR:H	3:N:1195:GLN:HE21	1.50	0.60
4:O:9:LEU:HD22	4:O:19:LEU:HD11	1.83	0.60
4:O:61:VAL:O	4:O:65:MET:HG3	2.02	0.60
1:A:123:MET:C	1:A:125:PRO:HD3	2.22	0.59
1:B:123:MET:C	1:B:125:PRO:HD3	2.22	0.59
2:C:244:PRO:HD2	2:C:245:GLY:H	1.65	0.59
2:C:431:HIS:H	2:C:434:HIS:CD2	2.20	0.59
3:D:438:ASP:HB3	9:D:1574:HOH:O	2.02	0.59
3:D:519:VAL:HG13	3:D:544:TYR:CE1	2.37	0.59
3:D:1117:TYR:HB3	9:D:2262:HOH:O	2.02	0.59
1:K:191:ASP:O	1:K:192:LEU:HD23	2.01	0.59
2:M:139:GLN:NE2	2:M:415:PRO:HD2	2.17	0.59
2:M:1018:GLN:OE1	2:M:1060:ILE:HD11	2.02	0.59
2:M:1066:ALA:O	2:M:1070:ILE:HG13	2.02	0.59
3:N:204:LEU:HB2	3:N:394:LEU:HG	1.83	0.59
5:P:93:LEU:HG	5:P:190:ALA:CB	2.32	0.59
2:C:139:GLN:HE22	2:C:415:PRO:CD	2.15	0.59
2:C:712:ALA:O	2:C:820:ARG:HB2	2.02	0.59
2:C:933:GLY:HA2	9:C:1525:HOH:O	2.02	0.59
3:D:37:LEU:HD13	3:D:535:PHE:HZ	1.68	0.59
3:D:133:ILE:HG21	9:D:1764:HOH:O	2.02	0.59
3:D:409:VAL:CG1	3:D:435:VAL:HG11	2.31	0.59
3:D:786:ILE:HD13	3:D:1027:GLY:HA3	1.83	0.59
5:F:372:ARG:HG3	9:F:595:HOH:O	2.01	0.59
1:K:198:ARG:HG2	9:K:1904:HOH:O	2.01	0.59
1:L:59:GLU:HG3	1:L:139:ASN:HD22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:169:TYR:O	3:N:392:SER:HB2	2.01	0.59
3:N:550:ARG:HH11	3:N:573:MET:HB3	1.67	0.59
3:N:675:ARG:HG2	3:N:678:GLU:OE2	2.02	0.59
3:N:865:THR:HG22	9:N:1713:HOH:O	2.03	0.59
1:A:117:VAL:HB	1:A:120:VAL:CG1	2.31	0.59
1:B:89:PHE:HB3	1:B:94:LEU:HD22	1.84	0.59
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.36	0.59
3:D:47:GLU:HG2	9:D:1900:HOH:O	2.02	0.59
3:D:133:ILE:HG22	3:D:455:ARG:N	2.17	0.59
3:D:617:ASN:N	3:D:617:ASN:OD1	2.36	0.59
3:D:704:ARG:HD2	3:D:738:ALA:HB2	1.84	0.59
4:E:47:LYS:HE2	9:E:154:HOH:O	2.03	0.59
2:M:833:LEU:HD12	2:M:834:GLN:N	2.17	0.59
2:M:1085:PHE:CD2	3:N:1468:LEU:HA	2.36	0.59
3:N:50:PHE:HB3	3:N:522:PRO:HG2	1.83	0.59
3:N:95:LEU:HA	3:N:551:ASN:HD21	1.66	0.59
3:N:565:ILE:HD12	5:P:192:LEU:HD13	1.84	0.59
3:N:704:ARG:HD2	3:N:738:ALA:HB2	1.83	0.59
3:N:770:LEU:HB3	9:N:1689:HOH:O	2.01	0.59
3:N:1087:ARG:HG2	3:N:1238:MET:HB3	1.83	0.59
3:N:1264:GLU:O	3:N:1266:ARG:HG3	2.02	0.59
1:B:169:ALA:HB1	1:B:171:PHE:CE2	2.37	0.59
3:D:486:ARG:HD2	9:D:1689:HOH:O	2.03	0.59
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.83	0.59
3:D:804:LEU:HD23	3:D:804:LEU:H	1.68	0.59
3:D:980:MET:HG3	9:D:1653:HOH:O	2.01	0.59
3:D:1023:MET:HB2	3:D:1029:ARG:O	2.03	0.59
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.83	0.59
5:F:295:MET:HG2	5:F:299:TRP:CE2	2.37	0.59
1:K:50:GLY:O	1:K:146:ARG:HA	2.02	0.59
1:K:88:ARG:HG2	1:K:121:GLU:HG2	1.84	0.59
1:L:226:SER:O	1:L:228:PRO:HD3	2.02	0.59
2:M:328:LEU:HD22	2:M:437:ARG:HB3	1.83	0.59
2:M:468:ARG:HD3	9:M:2184:HOH:O	2.01	0.59
2:M:1038:TRP:HA	2:M:1041:GLU:HB2	1.84	0.59
3:N:165:LYS:HG3	3:N:397:LYS:HD3	1.84	0.59
3:N:734:GLU:HB2	9:N:1648:HOH:O	2.01	0.59
4:O:33:HIS:HB2	4:O:37:ASN:HD21	1.66	0.59
2:C:510:ALA:HB3	2:C:513:VAL:CG2	2.32	0.59
2:C:966:LEU:HD21	2:C:986:PRO:HG3	1.85	0.59
3:D:192:ALA:HB1	9:D:2083:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1088:THR:HG21	9:D:1813:HOH:O	2.02	0.59
1:K:89:PHE:HB3	1:K:94:LEU:HD22	1.84	0.59
2:M:208:ALA:O	2:M:218:VAL:HG21	2.02	0.59
2:M:305:PRO:HA	2:M:308:ARG:HD2	1.84	0.59
3:N:570:GLU:HB2	5:P:214:GLN:OE1	2.02	0.59
3:N:1342:GLU:HG3	9:N:1945:HOH:O	2.03	0.59
3:N:1357:ARG:HB2	9:N:1826:HOH:O	2.01	0.59
1:A:123:MET:O	1:A:125:PRO:HD3	2.03	0.59
1:B:40:LEU:HD21	1:B:215:VAL:HG12	1.84	0.59
2:C:984:GLU:HG3	3:D:944:THR:O	2.02	0.59
3:D:169:TYR:O	3:D:392:SER:HB2	2.02	0.59
3:D:408:GLU:HA	5:F:171:LYS:HZ1	1.67	0.59
3:D:926:LYS:HE2	9:D:1617:HOH:O	2.01	0.59
4:E:9:LEU:HB3	4:E:19:LEU:HD21	1.85	0.59
5:F:220:LEU:HD12	5:F:243:ILE:HD11	1.83	0.59
5:F:256:ARG:HD3	9:F:585:HOH:O	2.03	0.59
5:F:268:ILE:HD13	5:F:311:ALA:HB2	1.83	0.59
2:M:200:LEU:HD13	2:M:300:ASP:CG	2.23	0.59
2:M:404:LEU:HA	2:M:407:LYS:HD2	1.84	0.59
2:M:750:LYS:HB3	9:N:2087:HOH:O	2.02	0.59
3:N:133:ILE:HG22	3:N:455:ARG:N	2.18	0.59
3:N:434:ARG:HG2	9:N:2229:HOH:O	2.03	0.59
3:N:560:GLN:OE1	5:P:218:GLN:HG3	2.01	0.59
3:N:562:ALA:HB1	3:N:567:ILE:HD11	1.85	0.59
3:N:1117:TYR:HB3	9:N:1591:HOH:O	2.03	0.59
3:N:1403:LEU:HD23	9:N:1794:HOH:O	2.02	0.59
5:P:361:LEU:CD2	5:P:366:ALA:HB2	2.27	0.59
2:C:230:ARG:HG3	9:C:1406:HOH:O	2.01	0.59
2:C:260:LEU:HD21	9:C:1182:HOH:O	2.02	0.59
2:C:346:VAL:O	2:C:350:ARG:HG3	2.03	0.59
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.84	0.59
3:D:31:THR:HG23	3:D:45:PHE:CE2	2.37	0.59
3:D:490:ALA:HA	9:D:1529:HOH:O	2.03	0.59
4:E:41:GLU:N	4:E:42:PRO:HD2	2.17	0.59
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.83	0.59
2:M:208:ALA:HB1	2:M:218:VAL:HG13	1.84	0.59
2:M:482:GLU:HB3	9:M:2150:HOH:O	2.02	0.59
2:M:627:ARG:HG3	2:M:628:PHE:H	1.68	0.59
2:M:738:ASP:CB	2:M:744:ARG:HB3	2.31	0.59
2:M:816:LYS:HB2	2:M:819:VAL:HG21	1.84	0.59
2:M:1034:GLU:HA	2:M:1037:VAL:HG23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:113:ILE:HG23	5:P:127:ILE:HB	1.85	0.59
5:P:400:ILE:HD11	9:P:513:HOH:O	2.02	0.59
1:A:26:GLU:HG3	1:A:27:PRO:HD3	1.85	0.59
2:C:19:THR:O	2:C:23:VAL:HG23	2.02	0.59
2:C:69:LEU:HD12	2:C:97:ARG:HB3	1.85	0.59
2:C:773:LEU:O	2:C:777:ILE:HG13	2.03	0.59
3:D:47:GLU:HA	3:D:51:GLY:O	2.03	0.59
3:D:824:ASN:HB3	9:D:2122:HOH:O	2.01	0.59
4:E:7:ASP:HB2	9:E:100:HOH:O	2.03	0.59
5:F:369:LEU:O	5:F:373:LYS:HB2	2.02	0.59
5:F:400:ILE:HD11	9:F:643:HOH:O	2.03	0.59
2:M:191:PHE:CZ	2:M:196:LEU:HB2	2.35	0.59
2:M:579:VAL:HB	2:M:890:LEU:CD2	2.33	0.59
3:N:404:GLU:HB2	9:N:1640:HOH:O	2.03	0.59
2:C:185:LYS:HE2	2:C:190:LYS:HG2	1.84	0.59
2:C:200:LEU:HD13	2:C:300:ASP:CG	2.23	0.59
2:C:408:ARG:HH21	2:C:542:VAL:HG22	1.66	0.59
2:C:564:MET:HG3	2:C:997:LEU:HD11	1.84	0.59
2:C:841:ASN:HD21	2:C:845:ASN:H	1.50	0.59
2:C:1115:LEU:HB3	3:D:85:VAL:HG13	1.85	0.59
3:D:646:LYS:HE2	3:D:722:GLU:HG2	1.84	0.59
3:D:1102:THR:HG22	3:D:1222:GLY:CA	2.32	0.59
1:L:182:GLU:HB2	9:L:2617:HOH:O	2.01	0.59
2:M:585:GLU:HB3	9:M:1636:HOH:O	2.01	0.59
2:M:1053:LEU:HB3	9:N:2033:HOH:O	2.03	0.59
3:N:847:ASP:O	3:N:851:LEU:HG	2.02	0.59
3:N:897:TRP:CH2	3:N:902:LEU:HD21	2.38	0.59
3:N:1108:ARG:NH2	3:N:1198:TYR:HB2	2.16	0.59
3:N:1299:PHE:HB2	9:N:1861:HOH:O	2.02	0.59
3:N:1351:GLU:HG2	9:N:1724:HOH:O	2.02	0.59
5:P:130:VAL:HA	5:P:142:ARG:NH2	2.17	0.59
2:C:36:PRO:HG3	2:C:71:TYR:CE2	2.38	0.59
2:C:163:ILE:O	2:C:163:ILE:HG13	2.01	0.59
2:C:362:GLY:HA3	2:C:367:LEU:CD2	2.33	0.59
2:C:410:ILE:HD11	2:C:455:LEU:HB3	1.84	0.59
2:C:705:ILE:HG12	2:C:828:ALA:HB2	1.85	0.59
3:D:187:LYS:CE	3:D:199:LEU:HB3	2.27	0.59
3:D:448:GLU:HG2	3:D:448:GLU:O	2.02	0.59
5:F:361:LEU:HD22	5:F:366:ALA:HB2	1.85	0.59
1:K:158:ILE:H	1:K:166:PRO:HG3	1.68	0.59
1:L:101:LEU:HD11	9:L:1850:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:489:ARG:HH21	3:N:1389:LEU:HD11	1.67	0.59
5:P:406:ARG:O	5:P:409:LYS:HG2	2.02	0.59
1:A:161:ARG:NH1	1:A:161:ARG:HB2	2.18	0.58
2:C:294:GLU:HB3	9:C:1227:HOH:O	2.03	0.58
2:C:402:SER:OG	2:C:566:THR:HG22	2.02	0.58
2:C:437:ARG:CZ	2:C:488:ALA:HA	2.33	0.58
2:C:1087:VAL:HG13	3:D:610:LYS:NZ	2.13	0.58
3:D:153:LEU:CD1	3:D:157:GLU:HB2	2.33	0.58
3:D:481:MET:HG3	3:D:1388:ARG:CZ	2.32	0.58
3:D:498:VAL:HG23	3:D:499:VAL:N	2.18	0.58
3:D:592:THR:N	3:D:600:LEU:HD21	2.15	0.58
3:D:1243:THR:HB	3:D:1253:THR:HG22	1.85	0.58
3:D:1311:LEU:HD22	9:D:1836:HOH:O	2.03	0.58
4:E:83:ASP:O	4:E:86:GLN:HG2	2.03	0.58
2:M:185:LYS:HE2	2:M:190:LYS:HE2	1.84	0.58
2:M:218:VAL:HG22	2:M:221:LEU:CD2	2.32	0.58
2:M:292:ARG:HG2	9:M:1952:HOH:O	2.01	0.58
2:M:1056:LYS:NZ	3:N:749:VAL:O	2.35	0.58
3:N:84:ILE:HG13	3:N:85:VAL:N	2.18	0.58
3:N:117:ASP:HB2	3:N:495:ARG:NH2	2.17	0.58
3:N:715:ALA:HB3	3:N:764:LEU:HA	1.84	0.58
5:P:140:ARG:HG3	5:P:141:VAL:H	1.68	0.58
5:P:361:LEU:HD13	5:P:366:ALA:CB	2.33	0.58
1:A:36:LEU:O	1:A:39:PRO:HD2	2.02	0.58
3:D:702:LEU:HD23	3:D:745:MET:HE2	1.85	0.58
3:D:799:LYS:HB3	3:D:826:PRO:HG2	1.84	0.58
3:D:1109:GLU:HG2	3:D:1202:GLN:H	1.66	0.58
3:D:1177:ALA:HB3	3:D:1183:ILE:HD11	1.85	0.58
5:F:270:LYS:HG3	9:F:511:HOH:O	2.02	0.58
2:M:140:ILE:CD1	2:M:412:ALA:HA	2.32	0.58
2:M:194:VAL:HG21	2:M:221:LEU:O	2.02	0.58
2:M:300:ASP:HA	9:M:2239:HOH:O	2.03	0.58
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.85	0.58
3:N:206:ARG:HH12	5:P:98:GLU:CA	2.15	0.58
3:N:634:GLY:O	3:N:637:LEU:HB3	2.03	0.58
3:N:640:HIS:HE1	4:O:3:GLU:HG2	1.68	0.58
3:N:767:HIS:CD2	4:O:6:ILE:HG12	2.37	0.58
3:N:957:PRO:HG2	3:N:1007:VAL:CA	2.29	0.58
3:N:1114:THR:H	3:N:1195:GLN:NE2	2.01	0.58
1:A:39:PRO:CG	1:B:39:PRO:HG3	2.33	0.58
2:C:80:GLN:O	2:C:83:CYS:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:ALA:O	2:C:218:VAL:HG21	2.02	0.58
2:C:838:LYS:HE3	2:C:997:LEU:HD12	1.86	0.58
3:D:481:MET:HG2	3:D:482:LYS:N	2.18	0.58
3:D:992:ILE:O	3:D:995:LEU:HB3	2.03	0.58
4:E:69:LEU:HB3	9:E:140:HOH:O	2.02	0.58
5:F:132:ARG:HG2	5:F:181:GLU:CD	2.22	0.58
5:F:207:LEU:HB3	5:F:212:LEU:HG	1.84	0.58
1:L:99:LEU:HG	9:L:1066:HOH:O	2.03	0.58
2:M:212:GLY:HA3	2:M:218:VAL:HG23	1.85	0.58
2:M:654:LEU:HD11	2:M:663:ASN:ND2	2.18	0.58
2:M:694:LEU:HD11	2:M:868:ASP:HB3	1.85	0.58
2:M:838:LYS:NZ	2:M:846:LYS:HE2	2.18	0.58
2:M:859:PRO:O	2:M:867:VAL:HG22	2.03	0.58
3:N:169:TYR:CB	3:N:195:VAL:HG11	2.33	0.58
3:N:610:LYS:O	3:N:611:GLN:CG	2.50	0.58
1:B:46:SER:O	1:B:148:VAL:HB	2.03	0.58
2:C:110:GLU:CB	2:C:369:PRO:HG3	2.33	0.58
2:C:641:PRO:O	2:C:642:ARG:HD2	2.02	0.58
2:C:730:SER:HB2	9:C:1128:HOH:O	2.02	0.58
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.85	0.58
3:D:527:MET:CE	5:F:258:ILE:HD11	2.33	0.58
3:D:560:GLN:HB2	9:D:1923:HOH:O	2.03	0.58
2:M:137:VAL:HG23	2:M:391:LEU:HG	1.85	0.58
5:P:282:LEU:HD22	9:P:504:HOH:O	2.03	0.58
2:C:150:PRO:HD3	9:C:1150:HOH:O	2.04	0.58
2:C:328:LEU:HB2	2:C:433:THR:HG21	1.84	0.58
3:D:523:ASP:N	9:D:1713:HOH:O	2.30	0.58
3:D:957:PRO:HG2	3:D:1007:VAL:CA	2.30	0.58
3:D:1145:TYR:HE2	3:D:1168:MET:HB2	1.69	0.58
3:D:1152:GLU:CD	3:D:1159:ARG:HH12	2.06	0.58
4:E:59:ASN:HB3	4:E:62:THR:OG1	2.03	0.58
1:L:188:GLN:HG3	3:N:685:ASP:OD2	2.03	0.58
2:M:15:LEU:HD22	2:M:583:LEU:HD21	1.85	0.58
2:M:742:VAL:HG12	2:M:743:VAL:N	2.19	0.58
3:N:783:ARG:CZ	3:N:1029:ARG:HG3	2.32	0.58
3:N:813:LEU:O	3:N:817:GLU:HB2	2.03	0.58
1:A:218:LEU:O	1:A:222:LEU:HD12	2.04	0.58
2:C:429:ASP:HB3	9:C:1177:HOH:O	2.04	0.58
2:C:911:GLU:O	2:C:914:ILE:HG22	2.03	0.58
2:C:980:GLY:HA2	9:C:1431:HOH:O	2.03	0.58
5:F:323:ASP:HA	9:F:481:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:257:VAL:HG12	2:M:263:ASP:OD1	2.04	0.58
2:M:723:THR:HG21	9:M:1850:HOH:O	2.03	0.58
3:N:481:MET:SD	3:N:1388:ARG:HD2	2.44	0.58
3:N:829:VAL:H	3:N:835:SER:HB2	1.69	0.58
3:N:965:GLU:HA	3:N:968:ASP:HB2	1.84	0.58
3:N:1018:ASN:HB3	3:N:1021:TYR:HB3	1.85	0.58
2:C:265:ARG:HG2	2:C:267:TYR:H	1.68	0.58
2:C:1034:GLU:HA	2:C:1037:VAL:HG23	1.84	0.58
3:D:586:ARG:CZ	3:D:1444:THR:HG21	2.34	0.58
3:D:710:ARG:HH21	3:D:1210:SER:HB2	1.69	0.58
3:D:792:ILE:O	3:D:878:GLY:HA3	2.04	0.58
3:D:1026:SER:HA	9:D:2416:HOH:O	2.02	0.58
3:D:1063:GLU:HB3	9:D:1948:HOH:O	2.03	0.58
3:D:1422:MET:CE	3:D:1427:SER:HA	2.34	0.58
5:F:292:ALA:HB1	5:F:299:TRP:O	2.03	0.58
2:M:139:GLN:CD	2:M:415:PRO:HD2	2.24	0.58
2:M:151:ASP:OD2	2:M:159:ILE:HG23	2.03	0.58
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.86	0.58
3:N:116:LEU:HD21	3:N:464:LEU:CB	2.31	0.58
3:N:699:VAL:HG21	3:N:760:ARG:HB3	1.86	0.58
3:N:787:LEU:HD21	3:N:947:ILE:CD1	2.33	0.58
3:N:984:THR:HG22	3:N:987:GLU:H	1.68	0.58
3:N:1035:ILE:HA	3:N:1038:LEU:HD12	1.84	0.58
3:N:1145:TYR:HE2	3:N:1168:MET:HB2	1.67	0.58
1:B:108:GLU:HB3	9:B:522:HOH:O	2.02	0.58
2:C:56:GLU:OE1	2:C:64:LEU:HD22	2.03	0.58
2:C:86:LYS:CD	2:C:813:VAL:HG12	2.33	0.58
2:C:137:VAL:O	2:C:391:LEU:HD21	2.04	0.58
2:C:139:GLN:CD	2:C:415:PRO:HD2	2.24	0.58
2:C:208:ALA:HB1	2:C:218:VAL:HG13	1.85	0.58
2:C:267:TYR:HB2	2:C:272:ALA:HB1	1.84	0.58
5:F:77:THR:O	5:F:81:VAL:HG23	2.03	0.58
5:F:406:ARG:HA	5:F:409:LYS:HG2	1.85	0.58
1:K:96:THR:HG21	9:K:4199:HOH:O	2.03	0.58
2:M:101:ILE:HD11	9:M:1739:HOH:O	2.04	0.58
2:M:583:LEU:O	2:M:587:VAL:HG23	2.04	0.58
3:N:631:ILE:HG21	3:N:745:MET:SD	2.43	0.58
3:N:1102:THR:HG22	3:N:1222:GLY:CA	2.34	0.58
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.69	0.58
1:B:105:GLY:O	1:B:132:LEU:HB3	2.04	0.58
2:C:9:ILE:HG13	2:C:9:ILE:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:185:VAL:HG23	3:D:202:VAL:C	2.24	0.58
3:D:686:GLU:HA	3:D:689:ASP:OD2	2.04	0.58
3:D:1114:THR:H	3:D:1195:GLN:NE2	2.01	0.58
3:D:1206:GLY:HA3	3:D:1366:LYS:HZ1	1.68	0.58
3:D:1357:ARG:HG2	9:D:2067:HOH:O	2.04	0.58
5:F:95:THR:HG23	9:F:465:HOH:O	2.02	0.58
1:K:182:GLU:O	1:K:194:LYS:HB3	2.04	0.58
2:M:260:LEU:HA	2:M:291:ALA:CB	2.34	0.58
2:M:902:ILE:O	2:M:904:PRO:HD3	2.03	0.58
2:M:1056:LYS:O	3:N:624:ASP:HB2	2.04	0.58
2:M:1111:ILE:HG13	2:M:1112:PHE:H	1.69	0.58
1:A:133:GLU:HB3	9:C:1680:HOH:O	2.02	0.58
2:C:72:ARG:HB2	9:C:1804:HOH:O	2.04	0.58
2:C:182:VAL:HB	2:C:193:LEU:HD13	1.85	0.58
3:D:171:LEU:HD21	9:D:2083:HOH:O	2.03	0.58
3:D:633:VAL:HB	3:D:740:PHE:CE1	2.39	0.58
5:F:79:ASP:OD2	5:F:80:PRO:HD3	2.04	0.58
2:M:77:PRO:HD3	2:M:93:PRO:HD3	1.85	0.58
3:N:1286:THR:HG22	9:N:1537:HOH:O	2.02	0.58
4:O:31:LEU:HD23	4:O:35:PHE:HE1	1.68	0.58
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.39	0.57
2:C:102:HIS:HB2	2:C:106:GLY:O	2.04	0.57
2:C:184:MET:SD	2:C:303:PHE:HE2	2.27	0.57
2:C:242:LEU:HD23	9:C:1218:HOH:O	2.03	0.57
2:C:404:LEU:O	2:C:407:LYS:HB2	2.04	0.57
2:C:705:ILE:HA	2:C:827:VAL:O	2.04	0.57
3:D:81:THR:HB	3:D:85:VAL:CG2	2.34	0.57
3:D:561:GLY:HA3	5:F:184:ARG:NH1	2.17	0.57
3:D:813:LEU:O	3:D:817:GLU:HB2	2.04	0.57
3:D:1290:LEU:CD2	3:D:1291:SER:H	2.17	0.57
2:M:420:ARG:NH1	2:M:422:ARG:HH21	2.02	0.57
2:M:768:THR:HG21	9:P:562:HOH:O	2.04	0.57
2:M:1005:MET:CE	3:N:648:MET:HB2	2.33	0.57
3:N:572:ARG:HH21	5:P:83:GLN:HE21	1.50	0.57
2:C:165:LEU:HD12	2:C:166:PRO:HA	1.84	0.57
3:D:15:PRO:HG3	9:D:1709:HOH:O	2.04	0.57
3:D:204:LEU:HB2	3:D:394:LEU:HG	1.84	0.57
3:D:1045:MET:HG3	3:D:1073:SER:HA	1.86	0.57
3:D:1141:GLU:CD	3:D:1168:MET:HE1	2.25	0.57
2:M:671:ASN:N	2:M:671:ASN:ND2	2.48	0.57
2:M:697:ARG:HD2	2:M:699:PHE:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:733:ALA:HB2	3:N:679:ARG:HH21	1.69	0.57
3:N:415:VAL:HG13	3:N:419:ASP:HB2	1.86	0.57
3:N:525:ARG:N	3:N:526:PRO:HD3	2.18	0.57
3:N:1209:LEU:HD23	3:N:1211:MET:CG	2.34	0.57
5:P:365:GLU:OE1	5:P:400:ILE:HD12	2.04	0.57
1:A:224:TYR:CD1	1:B:9:PRO:HD2	2.39	0.57
1:B:206:THR:CG2	1:B:209:GLU:H	2.17	0.57
2:C:676:ILE:CG2	2:C:988:VAL:HG22	2.33	0.57
2:C:715:THR:HG22	2:C:717:LEU:HG	1.86	0.57
3:D:582:LEU:HA	3:D:603:LEU:HD12	1.87	0.57
3:D:996:TRP:CE3	3:D:999:THR:HG21	2.39	0.57
3:D:1112:CYS:HB2	3:D:1195:GLN:CG	2.33	0.57
3:D:1232:PRO:HB3	3:D:1361:VAL:CG2	2.34	0.57
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	2.03	0.57
1:K:58:ILE:HB	1:K:61:VAL:HB	1.85	0.57
1:L:62:LEU:HD12	1:L:62:LEU:H	1.69	0.57
1:L:99:LEU:HD21	1:L:122:ILE:HD11	1.86	0.57
1:L:101:LEU:HD12	1:L:114:PHE:N	2.18	0.57
2:M:144:PRO:O	2:M:276:LYS:HD3	2.04	0.57
3:N:152:LEU:HD23	3:N:152:LEU:N	2.18	0.57
3:N:493:ARG:HB2	3:N:1388:ARG:CZ	2.34	0.57
3:N:1293:PHE:CE2	3:N:1302:GLU:HB3	2.39	0.57
5:P:130:VAL:HG11	5:P:159:ILE:HB	1.86	0.57
1:A:186:LEU:CB	1:A:192:LEU:HD11	2.34	0.57
1:B:55:SER:OG	1:B:158:ILE:HD13	2.05	0.57
1:B:209:GLU:HB3	9:B:448:HOH:O	2.04	0.57
2:C:94:LEU:HD12	9:C:1545:HOH:O	2.04	0.57
1:K:9:PRO:HB3	1:K:25:LEU:HG	1.86	0.57
1:K:42:ARG:HH12	1:L:34:VAL:CB	2.13	0.57
2:M:136:ILE:HG22	2:M:336:VAL:HG22	1.86	0.57
2:M:139:GLN:O	2:M:333:ILE:HA	2.04	0.57
2:M:334:ARG:NH1	2:M:415:PRO:HG2	2.19	0.57
3:N:18:ILE:HD12	3:N:518:PRO:CG	2.34	0.57
3:N:1115:THR:HG22	9:N:1591:HOH:O	2.04	0.57
1:A:227:ASN:ND2	1:A:227:ASN:H	2.03	0.57
2:C:100:LEU:HD12	2:C:101:ILE:O	2.05	0.57
2:C:166:PRO:HD3	2:C:265:ARG:CG	2.34	0.57
2:C:611:ILE:HG22	2:C:613:VAL:HG13	1.86	0.57
9:C:1139:HOH:O	5:F:373:LYS:HB3	2.03	0.57
3:D:81:THR:O	3:D:82:LYS:O	2.21	0.57
3:D:189:GLN:HG3	3:D:190:GLU:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:195:VAL:HG13	9:D:2268:HOH:O	2.04	0.57
3:D:434:ARG:HB2	3:D:447:VAL:CG2	2.35	0.57
4:E:63:TRP:O	4:E:67:GLU:HG3	2.05	0.57
1:K:16:GLN:HG2	1:K:16:GLN:O	2.05	0.57
1:K:18:ARG:O	1:K:207:PRO:HD3	2.05	0.57
1:L:132:LEU:HD21	1:L:136:GLY:O	2.04	0.57
2:M:56:GLU:OE1	2:M:64:LEU:HD22	2.05	0.57
2:M:480:THR:HB	9:M:2150:HOH:O	2.03	0.57
3:N:480:GLU:HG3	3:N:480:GLU:O	2.04	0.57
3:N:614:PHE:CD1	3:N:615:ARG:N	2.72	0.57
4:O:41:GLU:N	4:O:42:PRO:HD2	2.20	0.57
1:B:143:ARG:HD2	1:B:160:ASP:OD2	2.04	0.57
2:C:15:LEU:HD22	2:C:583:LEU:HD11	1.85	0.57
2:C:142:ARG:HD3	9:C:1347:HOH:O	2.04	0.57
2:C:480:THR:HG22	2:C:481:ASP:N	2.19	0.57
3:D:576:GLU:HB2	9:D:1696:HOH:O	2.03	0.57
3:D:610:LYS:CD	7:D:1527:MXP:H15A	2.34	0.57
3:D:1109:GLU:CD	3:D:1202:GLN:H	2.07	0.57
3:D:1179:GLU:HA	9:D:2069:HOH:O	2.05	0.57
5:F:278:LEU:HB2	5:F:286:PRO:HG2	1.85	0.57
2:M:41:ASN:HD22	2:M:41:ASN:N	1.89	0.57
2:M:420:ARG:HG3	2:M:422:ARG:HG2	1.87	0.57
2:M:959:PRO:HD3	9:M:1887:HOH:O	2.04	0.57
3:N:455:ARG:HD2	9:N:2063:HOH:O	2.05	0.57
3:N:827:ILE:HB	9:N:2048:HOH:O	2.04	0.57
3:N:850:LEU:HD12	3:N:850:LEU:N	2.15	0.57
5:P:147:LEU:HB3	9:P:604:HOH:O	2.04	0.57
5:P:394:ARG:HA	5:P:397:ILE:HD12	1.87	0.57
2:C:21:ILE:H	2:C:21:ILE:HD12	1.70	0.57
2:C:430:VAL:HG11	3:D:1074:SER:OG	2.04	0.57
2:C:705:ILE:HB	9:C:1287:HOH:O	2.04	0.57
2:C:897:LEU:HD23	2:C:899:GLN:NE2	2.19	0.57
3:D:82:LYS:HE2	9:D:1577:HOH:O	2.05	0.57
2:M:1002:GLU:HG3	3:N:744:GLN:NE2	2.20	0.57
3:N:1037:GLN:HG2	3:N:1042:ARG:HB3	1.85	0.57
3:N:1189:ARG:NH1	3:N:1203:LYS:HB2	2.20	0.57
2:C:238:LEU:HD12	9:C:1705:HOH:O	2.05	0.57
2:C:495:THR:H	2:C:530:GLU:CD	2.08	0.57
2:C:724:ARG:O	2:C:734:LEU:HD21	2.05	0.57
2:C:774:LEU:HA	2:C:777:ILE:HD12	1.87	0.57
2:C:1008:ARG:NH1	2:C:1028:GLY:HA2	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:113:ILE:HG23	5:F:127:ILE:HB	1.87	0.57
1:K:178:ALA:HB2	2:M:864:GLY:H	1.69	0.57
1:K:227:ASN:H	1:K:227:ASN:ND2	2.02	0.57
1:L:39:PRO:O	1:L:43:ILE:HG12	2.05	0.57
2:M:189:ARG:HD2	9:M:2270:HOH:O	2.04	0.57
3:N:992:ILE:O	3:N:995:LEU:HB3	2.05	0.57
1:B:7:LYS:O	1:B:7:LYS:HG3	2.05	0.57
2:C:206:THR:HG21	9:C:1559:HOH:O	2.04	0.57
2:C:322:VAL:HG21	9:C:1390:HOH:O	2.04	0.57
2:C:341:THR:HG21	9:C:1365:HOH:O	2.05	0.57
2:C:615:TYR:HB2	9:C:1584:HOH:O	2.05	0.57
3:D:546:ARG:HA	9:D:1595:HOH:O	2.05	0.57
3:D:820:GLU:HG3	3:D:836:VAL:CG1	2.34	0.57
3:D:820:GLU:HG3	3:D:836:VAL:HG11	1.86	0.57
3:D:956:ILE:HG12	3:D:1039:CYS:O	2.05	0.57
3:D:1376:MET:HG2	3:D:1421:LEU:HD12	1.86	0.57
2:M:395:LYS:HE2	2:M:403:SER:HB2	1.86	0.57
2:M:876:VAL:HA	9:M:1870:HOH:O	2.03	0.57
2:M:939:ARG:HD3	2:M:975:TYR:CE2	2.40	0.57
3:N:77:GLY:O	3:N:78:VAL:HG23	2.05	0.57
3:N:834:THR:HB	3:N:838:ARG:HB2	1.86	0.57
4:O:54:LEU:O	4:O:54:LEU:HD23	2.05	0.57
5:P:138:SER:O	5:P:141:VAL:HG12	2.03	0.57
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.87	0.57
2:C:477:GLY:O	2:C:508:ILE:HG12	2.05	0.57
2:C:838:LYS:NZ	2:C:846:LYS:HE2	2.20	0.57
3:D:1443:THR:HG22	9:D:1543:HOH:O	2.03	0.57
1:K:18:ARG:HD2	1:K:123:MET:CE	2.35	0.57
1:K:91:ASN:OD1	1:K:92:PRO:HD2	2.05	0.57
1:L:44:LEU:HD21	1:L:199:ILE:HD13	1.85	0.57
3:N:171:LEU:HD13	9:N:1797:HOH:O	2.05	0.57
3:N:409:VAL:CG1	3:N:435:VAL:HG11	2.33	0.57
3:N:1295:GLU:HB3	3:N:1300:SER:HB3	1.87	0.57
3:N:1390:LEU:HB2	9:N:1897:HOH:O	2.05	0.57
4:O:33:HIS:CE1	4:O:89:MET:HG2	2.39	0.57
5:P:361:LEU:HD13	5:P:366:ALA:HB2	1.86	0.57
5:P:393:THR:O	5:P:397:ILE:HG13	2.05	0.57
1:A:34:VAL:HB	1:B:42:ARG:HH21	1.69	0.56
1:A:178:ALA:HB1	9:C:1688:HOH:O	2.05	0.56
1:B:201:THR:HG21	1:B:205:VAL:O	2.05	0.56
2:C:207:LEU:HD22	2:C:221:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:457:ALA:N	2:C:540:PHE:O	2.36	0.56
2:C:857:ASP:HB2	2:C:978:ARG:HB3	1.85	0.56
2:C:1038:TRP:HA	2:C:1041:GLU:HB2	1.87	0.56
9:C:1255:HOH:O	5:F:354:LEU:HD11	2.04	0.56
3:D:32:ILE:HG22	5:F:258:ILE:HD12	1.87	0.56
3:D:101:HIS:ND1	3:D:103:TRP:HB2	2.16	0.56
3:D:1090:ASP:HA	3:D:1093:TYR:HB2	1.87	0.56
3:D:1258:ARG:CZ	3:D:1262:LEU:HD11	2.36	0.56
2:M:144:PRO:HA	2:M:163:ILE:CG1	2.35	0.56
2:M:404:LEU:O	2:M:407:LYS:HB2	2.05	0.56
2:M:665:PHE:HB2	9:M:1978:HOH:O	2.04	0.56
2:M:1105:LYS:HG3	9:M:1731:HOH:O	2.04	0.56
3:N:957:PRO:HG3	3:N:1010:ASN:HD22	1.70	0.56
3:N:1231:GLU:HB3	3:N:1232:PRO:HD3	1.87	0.56
3:N:1384:PRO:HG3	3:N:1389:LEU:HA	1.86	0.56
3:N:1462:LEU:HD22	3:N:1472:ILE:HG23	1.87	0.56
1:A:149:GLY:O	1:A:171:PHE:HB2	2.06	0.56
1:A:158:ILE:H	1:A:166:PRO:HG3	1.70	0.56
1:A:206:THR:HG22	1:A:209:GLU:H	1.69	0.56
2:C:252:LYS:HE2	9:C:1771:HOH:O	2.04	0.56
2:C:766:GLU:HG2	2:C:772:ARG:NH1	2.19	0.56
2:C:1115:LEU:HD23	3:D:85:VAL:HA	1.85	0.56
3:D:428:LYS:HD3	9:D:1840:HOH:O	2.05	0.56
3:D:894:LYS:HB3	9:D:2117:HOH:O	2.05	0.56
3:D:1410:GLU:HG3	9:D:1966:HOH:O	2.04	0.56
1:K:103:ALA:CB	1:K:107:LYS:HE2	2.35	0.56
1:K:224:TYR:HB3	1:L:9:PRO:HB2	1.87	0.56
1:L:57:TYR:O	1:L:140:MET:HA	2.05	0.56
1:L:123:MET:O	1:L:125:PRO:HD3	2.05	0.56
2:M:102:HIS:HB2	2:M:106:GLY:O	2.05	0.56
2:M:110:GLU:H	2:M:368:THR:HG21	1.69	0.56
2:M:141:HIS:HB3	2:M:418:LEU:CG	2.35	0.56
2:M:722:ILE:HG23	2:M:722:ILE:O	2.04	0.56
3:N:2:LYS:HD3	9:N:2388:HOH:O	2.04	0.56
3:N:106:LYS:HB3	9:N:2026:HOH:O	2.05	0.56
3:N:1087:ARG:HG2	3:N:1238:MET:CB	2.34	0.56
3:N:1288:GLU:HA	9:N:1542:HOH:O	2.04	0.56
4:O:45:ARG:NH2	4:O:55:PHE:HB3	2.20	0.56
1:A:88:ARG:NH2	1:A:90:LEU:HD21	2.20	0.56
1:A:198:ARG:HB2	1:A:200:TRP:CH2	2.41	0.56
2:C:8:ARG:HB3	9:C:1721:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1018:GLN:NE2	3:D:87:ARG:HH12	2.03	0.56
2:C:1097:LEU:HD12	2:C:1097:LEU:N	2.20	0.56
3:D:81:THR:HG22	3:D:82:LYS:N	2.21	0.56
3:D:165:LYS:HA	9:D:2176:HOH:O	2.05	0.56
3:D:169:TYR:CE1	3:D:197:SER:HB2	2.40	0.56
3:D:611:GLN:NE2	3:D:1439:SER:HB3	2.20	0.56
3:D:1007:VAL:HG23	3:D:1008:PHE:N	2.21	0.56
4:E:45:ARG:NH2	4:E:55:PHE:HB3	2.20	0.56
4:E:54:LEU:CD2	4:E:63:TRP:HE1	2.18	0.56
5:F:88:ILE:HG12	5:F:193:ARG:HB2	1.87	0.56
5:F:203:THR:HG22	5:F:204:GLY:N	2.20	0.56
5:F:271:LEU:HG	5:F:295:MET:HE1	1.87	0.56
1:K:5:LYS:O	1:K:8:ALA:HB2	2.05	0.56
1:K:161:ARG:NH1	1:K:161:ARG:HB2	2.19	0.56
1:L:34:VAL:HG22	1:L:181:VAL:HG21	1.85	0.56
1:L:36:LEU:O	1:L:39:PRO:HD2	2.04	0.56
1:L:71:VAL:HG22	1:L:132:LEU:HD12	1.87	0.56
1:L:169:ALA:HB1	1:L:171:PHE:CE2	2.40	0.56
2:M:52:PHE:CG	2:M:68:PHE:HB2	2.40	0.56
2:M:328:LEU:HD23	2:M:467:ILE:HB	1.87	0.56
2:M:378:LEU:HG	2:M:382:ILE:HD11	1.87	0.56
2:M:480:THR:HG22	2:M:481:ASP:N	2.19	0.56
2:M:631:SER:HB3	2:M:637:LEU:HD21	1.87	0.56
2:M:733:ALA:HB2	3:N:679:ARG:HH22	1.66	0.56
2:M:863:ASP:O	2:M:865:THR:N	2.37	0.56
2:M:1015:LEU:HD12	9:P:651:HOH:O	2.04	0.56
3:N:114:THR:O	3:N:495:ARG:HG3	2.06	0.56
3:N:799:LYS:HB3	3:N:826:PRO:CG	2.34	0.56
3:N:1169:ASP:HA	9:N:1842:HOH:O	2.04	0.56
3:N:1232:PRO:HB3	3:N:1361:VAL:CG2	2.33	0.56
3:N:1356:TYR:HD2	3:N:1363:LEU:HD23	1.69	0.56
3:N:1388:ARG:HG3	3:N:1389:LEU:N	2.19	0.56
1:B:132:LEU:CD1	1:B:138:LEU:HD12	2.35	0.56
2:C:176:VAL:C	2:C:178:PRO:HD3	2.25	0.56
2:C:770:GLU:CG	3:D:65:ARG:HH12	2.17	0.56
3:D:394:LEU:HD21	9:D:1995:HOH:O	2.06	0.56
3:D:640:HIS:HB2	9:E:156:HOH:O	2.05	0.56
2:M:292:ARG:HD2	2:M:299:LYS:HG2	1.86	0.56
2:M:565:GLN:OE1	2:M:842:ARG:HG2	2.05	0.56
2:M:662:GLU:HB3	9:M:1978:HOH:O	2.05	0.56
3:N:113:GLY:HA3	3:N:120:ALA:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:560:GLN:HG2	5:P:221:ILE:HG21	1.86	0.56
1:A:66:SER:O	1:A:75:VAL:HG23	2.05	0.56
2:C:350:ARG:HA	2:C:353:ARG:HD2	1.87	0.56
2:C:413:LEU:HB3	9:C:1518:HOH:O	2.05	0.56
2:C:838:LYS:HB2	2:C:848:VAL:HG22	1.86	0.56
2:C:979:THR:HG23	2:C:981:GLU:N	2.18	0.56
3:D:55:ASP:O	3:D:80:VAL:HG11	2.06	0.56
3:D:1092:GLY:HA3	9:D:2012:HOH:O	2.05	0.56
3:D:1389:LEU:HD12	3:D:1390:LEU:N	2.19	0.56
5:F:140:ARG:HG3	5:F:141:VAL:H	1.69	0.56
1:K:34:VAL:HG13	2:M:939:ARG:HH21	1.70	0.56
1:K:91:ASN:CG	1:K:92:PRO:HD2	2.26	0.56
1:L:58:ILE:HG22	1:L:137:ARG:NH2	2.17	0.56
2:M:69:LEU:HD12	2:M:97:ARG:HB3	1.86	0.56
2:M:114:PHE:CE2	5:P:283:GLY:HA3	2.40	0.56
2:M:418:LEU:N	2:M:418:LEU:HD12	2.20	0.56
2:M:464:LEU:HD12	2:M:465:GLY:H	1.70	0.56
2:M:611:ILE:HG22	2:M:613:VAL:HG13	1.88	0.56
3:N:45:PHE:HD1	3:N:86:ARG:HH22	1.52	0.56
3:N:102:ILE:HD12	3:N:579:ASP:HB3	1.86	0.56
3:N:119:SER:HB2	3:N:123:LEU:CB	2.34	0.56
3:N:143:ASN:HD21	3:N:145:VAL:HG12	1.70	0.56
3:N:592:THR:N	3:N:600:LEU:HD21	2.18	0.56
3:N:814:ALA:O	3:N:818:ARG:HG3	2.05	0.56
3:N:1243:THR:HG22	3:N:1244:GLY:H	1.71	0.56
1:B:2:LEU:HD12	1:B:3:ASP:HB2	1.86	0.56
1:B:15:THR:HB	9:B:419:HOH:O	2.05	0.56
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.41	0.56
2:C:785:VAL:HG21	9:C:1244:HOH:O	2.05	0.56
3:D:169:TYR:CB	3:D:195:VAL:HG11	2.34	0.56
3:D:842:VAL:HG23	9:D:1531:HOH:O	2.06	0.56
3:D:996:TRP:HE3	3:D:999:THR:HG21	1.70	0.56
3:D:1495:ILE:HG12	4:E:80:VAL:CG1	2.35	0.56
5:F:291:ILE:HG23	5:F:304:VAL:HG21	1.87	0.56
2:M:141:HIS:HB2	9:M:2163:HOH:O	2.06	0.56
2:M:369:PRO:HD2	9:M:1905:HOH:O	2.06	0.56
2:M:408:ARG:HH21	2:M:542:VAL:CG2	2.17	0.56
2:M:510:ALA:HB3	2:M:513:VAL:CG2	2.36	0.56
2:M:510:ALA:HB3	2:M:513:VAL:HG23	1.88	0.56
2:M:660:ALA:HB3	9:M:1638:HOH:O	2.06	0.56
3:N:72:VAL:HG13	9:N:1744:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:485:SER:O	3:N:489:ARG:HB3	2.05	0.56
3:N:564:GLU:HA	3:N:567:ILE:HD13	1.88	0.56
3:N:637:LEU:HD11	3:N:642:CYS:N	2.21	0.56
3:N:1113:GLY:N	3:N:1195:GLN:HE22	2.03	0.56
5:P:113:ILE:HA	5:P:116:LEU:HD12	1.88	0.56
1:A:133:GLU:HG2	1:A:134:GLU:N	2.20	0.56
1:B:115:LEU:HD23	9:B:435:HOH:O	2.04	0.56
2:C:28:ARG:NH1	2:C:463:GLU:HG2	2.21	0.56
2:C:80:GLN:HB2	9:C:1803:HOH:O	2.04	0.56
2:C:176:VAL:HG12	2:C:182:VAL:CG1	2.36	0.56
2:C:607:ASP:HB3	2:C:609:ASN:H	1.70	0.56
2:C:818:GLY:HA2	5:F:309:LYS:NZ	2.20	0.56
3:D:1336:LEU:HA	3:D:1344:VAL:HG22	1.87	0.56
2:M:15:LEU:HD21	2:M:583:LEU:HD11	1.88	0.56
2:M:34:VAL:HG21	2:M:38:LYS:HD3	1.87	0.56
2:M:97:ARG:HG3	9:M:2157:HOH:O	2.05	0.56
2:M:599:GLU:HG3	2:M:600:ASP:N	2.18	0.56
2:M:857:ASP:HB2	2:M:978:ARG:HB3	1.87	0.56
3:N:602:SER:O	3:N:606:ILE:HG13	2.06	0.56
3:N:800:LYS:HE2	3:N:804:LEU:HD13	1.88	0.56
3:N:1007:VAL:HG23	3:N:1008:PHE:N	2.21	0.56
3:N:1495:ILE:HG12	4:O:80:VAL:CG1	2.35	0.56
5:P:108:GLU:HG3	5:P:176:ILE:HG21	1.88	0.56
5:P:138:SER:HB2	5:P:140:ARG:HG2	1.88	0.56
9:A:318:HOH:O	2:C:627:ARG:HA	2.05	0.56
2:C:1101:THR:HB	3:D:5:VAL:CG1	2.35	0.56
3:D:485:SER:O	3:D:489:ARG:HB3	2.06	0.56
5:F:101:GLU:HB3	5:F:105:LYS:HE3	1.87	0.56
5:F:225:GLU:HB3	9:F:605:HOH:O	2.06	0.56
1:K:20:TYR:CE2	1:K:22:GLU:HG3	2.41	0.56
2:M:167:LYS:HB2	9:M:1774:HOH:O	2.06	0.56
3:N:443:VAL:HG22	3:N:444:VAL:N	2.20	0.56
3:N:1047:LYS:HA	3:N:1053:PHE:CE1	2.41	0.56
3:N:1091:SER:HA	9:N:1706:HOH:O	2.06	0.56
4:O:84:ARG:HG3	9:O:2468:HOH:O	2.06	0.56
2:C:165:LEU:HD13	9:C:1292:HOH:O	2.05	0.56
2:C:580:MET:SD	2:C:584:GLU:HG3	2.46	0.56
2:C:750:LYS:HD2	3:D:681:ARG:HE	1.70	0.56
3:D:403:PHE:CD1	3:D:405:ASP:O	2.53	0.56
3:D:696:HIS:HB2	4:E:48:MET:HE3	1.87	0.56
4:E:33:HIS:HB2	4:E:37:ASN:ND2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:LYS:HE2	9:M:2012:HOH:O	2.05	0.56
2:M:193:LEU:HD11	9:M:1951:HOH:O	2.04	0.56
2:M:625:LEU:HB3	2:M:639:GLN:HB2	1.86	0.56
2:M:1115:LEU:HB3	3:N:85:VAL:CG1	2.35	0.56
3:N:1492:LEU:HD23	9:N:2099:HOH:O	2.04	0.56
4:O:95:VAL:HG22	9:O:1302:HOH:O	2.06	0.56
5:P:193:ARG:HD2	9:P:514:HOH:O	2.05	0.56
5:P:375:LEU:HD23	9:P:476:HOH:O	2.05	0.56
1:A:138:LEU:HD21	9:A:355:HOH:O	2.05	0.56
2:C:365:ASP:HB3	9:C:1410:HOH:O	2.06	0.56
2:C:729:LEU:HD22	9:D:1907:HOH:O	2.06	0.56
3:D:126:VAL:O	3:D:132:TYR:HD1	1.89	0.56
3:D:925:GLU:HB3	4:E:2:ALA:HB3	1.88	0.56
3:D:1113:GLY:N	3:D:1195:GLN:NE2	2.53	0.56
3:D:1204:CYS:HB3	9:D:1762:HOH:O	2.06	0.56
1:K:88:ARG:HG3	1:K:88:ARG:O	2.06	0.56
2:M:158:TYR:CE1	2:M:313:LEU:HG	2.40	0.56
2:M:235:LEU:HD11	9:M:2260:HOH:O	2.06	0.56
2:M:328:LEU:CD2	2:M:437:ARG:HB3	2.36	0.56
2:M:626:ARG:HB2	2:M:639:GLN:HE21	1.70	0.56
2:M:670:GLN:HE22	2:M:699:PHE:CA	2.19	0.56
2:M:1109:VAL:HG11	3:N:5:VAL:HG22	1.87	0.56
3:N:118:LEU:O	3:N:120:ALA:N	2.39	0.56
3:N:486:ARG:HD3	3:N:489:ARG:HD3	1.87	0.56
3:N:1466:VAL:HG23	3:N:1472:ILE:CD1	2.35	0.56
1:B:99:LEU:HD13	9:B:416:HOH:O	2.06	0.55
1:B:158:ILE:HG22	1:B:159:LYS:N	2.20	0.55
2:C:630:ARG:HG3	9:C:1287:HOH:O	2.07	0.55
3:D:80:VAL:N	9:D:1536:HOH:O	2.40	0.55
3:D:806:PHE:HE1	3:D:813:LEU:HB3	1.70	0.55
3:D:1035:ILE:HA	3:D:1038:LEU:CD1	2.36	0.55
3:D:1087:ARG:HD3	3:D:1236:LEU:O	2.06	0.55
5:F:416:ARG:HD3	5:F:419:ARG:HD3	1.89	0.55
1:K:88:ARG:NH2	1:K:90:LEU:HD21	2.21	0.55
1:L:85:LEU:HD13	1:L:127:LEU:HD23	1.88	0.55
1:L:206:THR:HG22	1:L:209:GLU:H	1.71	0.55
2:M:12:VAL:CG1	2:M:534:VAL:HG13	2.35	0.55
2:M:100:LEU:HD12	2:M:101:ILE:O	2.06	0.55
2:M:172:ILE:HA	2:M:185:LYS:O	2.07	0.55
2:M:208:ALA:HB1	2:M:218:VAL:CG1	2.36	0.55
3:N:421:LEU:HG	3:N:429:SER:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:592:THR:HG23	9:N:1987:HOH:O	2.06	0.55
4:O:54:LEU:HA	4:O:58:PRO:HG2	1.88	0.55
5:P:95:THR:HB	9:P:638:HOH:O	2.05	0.55
5:P:271:LEU:HG	5:P:295:MET:HE1	1.88	0.55
2:C:34:VAL:HG21	2:C:38:LYS:HD3	1.88	0.55
2:C:416:GLY:HA3	9:C:1419:HOH:O	2.06	0.55
2:C:605:LYS:HG3	2:C:612:VAL:HB	1.88	0.55
2:C:657:ASP:OD1	2:C:661:SER:HB2	2.06	0.55
2:C:670:GLN:O	2:C:672:VAL:HG12	2.06	0.55
3:D:408:GLU:HB3	9:D:2146:HOH:O	2.05	0.55
3:D:1305:LEU:HD13	9:D:1836:HOH:O	2.06	0.55
3:D:1486:VAL:HG12	4:E:73:LEU:HD22	1.89	0.55
4:E:76:GLY:HA3	4:E:79:LEU:HD12	1.88	0.55
5:F:234:LYS:HG3	5:F:236:SER:H	1.71	0.55
2:M:473:ARG:HB3	9:M:2150:HOH:O	2.05	0.55
2:M:598:GLU:O	2:M:651:LYS:HG3	2.06	0.55
2:M:987:ILE:HG23	3:N:948:THR:HG21	1.87	0.55
2:M:1008:ARG:NH1	2:M:1028:GLY:HA2	2.17	0.55
3:N:561:GLY:HA3	5:P:184:ARG:HH12	1.71	0.55
3:N:1422:MET:CE	3:N:1427:SER:HA	2.36	0.55
5:P:261:PRO:O	5:P:265:VAL:HG23	2.07	0.55
1:B:111:ALA:HB2	9:B:460:HOH:O	2.05	0.55
2:C:22:GLN:HE22	2:C:135:VAL:HG12	1.71	0.55
2:C:144:PRO:HA	2:C:163:ILE:CG1	2.37	0.55
2:C:149:THR:HA	9:C:1150:HOH:O	2.05	0.55
2:C:172:ILE:HA	2:C:185:LYS:O	2.07	0.55
2:C:197:LEU:HD22	2:C:202:TYR:CD2	2.38	0.55
2:C:1105:LYS:O	2:C:1107:ASN:N	2.38	0.55
3:D:421:LEU:HG	3:D:429:SER:HB3	1.87	0.55
3:D:646:LYS:HD3	9:D:1609:HOH:O	2.06	0.55
9:D:1806:HOH:O	5:F:309:LYS:HB3	2.07	0.55
1:K:184:THR:HG23	1:K:192:LEU:HD12	1.87	0.55
1:L:58:ILE:HD13	1:L:140:MET:HB3	1.88	0.55
2:M:654:LEU:HD11	2:M:663:ASN:HD22	1.70	0.55
2:M:770:GLU:HG3	3:N:65:ARG:HH12	1.70	0.55
3:N:19:ARG:NH2	9:N:1827:HOH:O	2.40	0.55
3:N:1463:LYS:O	3:N:1467:ILE:HG13	2.06	0.55
1:B:59:GLU:HG2	9:B:405:HOH:O	2.05	0.55
1:B:212:ASN:O	1:B:215:VAL:HG22	2.05	0.55
2:C:139:GLN:HG2	2:C:140:ILE:H	1.71	0.55
2:C:208:ALA:HB1	2:C:218:VAL:CG1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:583:LEU:O	2:C:587:VAL:HG23	2.06	0.55
2:C:1019:GLN:NE2	3:D:621:LYS:HA	2.20	0.55
2:C:1094:ALA:HB1	3:D:603:LEU:HD22	1.88	0.55
3:D:82:LYS:HG2	9:D:1675:HOH:O	2.06	0.55
4:E:86:GLN:O	4:E:90:GLU:HG3	2.06	0.55
5:F:138:SER:O	5:F:141:VAL:HG12	2.07	0.55
1:L:199:ILE:HD11	1:L:211:LEU:HD13	1.89	0.55
2:M:80:GLN:HB2	9:M:1668:HOH:O	2.07	0.55
2:M:261:ILE:HG21	9:M:2030:HOH:O	2.05	0.55
2:M:410:ILE:HD12	2:M:410:ILE:N	2.22	0.55
2:M:578:VAL:HG11	2:M:991:GLN:CB	2.35	0.55
2:M:589:ARG:HD2	9:M:1929:HOH:O	2.05	0.55
2:M:641:PRO:O	2:M:642:ARG:HD2	2.07	0.55
2:M:726:ILE:HG22	2:M:726:ILE:O	2.06	0.55
3:N:111:LYS:HE3	3:N:1449:GLU:HG2	1.88	0.55
3:N:128:TYR:HB3	3:N:129:PHE:HD1	1.71	0.55
3:N:703:ASN:HB2	3:N:713:ILE:HG12	1.89	0.55
3:N:1243:THR:HB	3:N:1253:THR:HG22	1.87	0.55
3:N:1281:VAL:HG23	3:N:1317:ASP:O	2.07	0.55
5:P:317:LEU:O	5:P:329:TYR:HB3	2.07	0.55
1:B:65:PHE:HB2	9:B:397:HOH:O	2.05	0.55
2:C:36:PRO:HB3	9:C:1632:HOH:O	2.06	0.55
2:C:770:GLU:HG3	3:D:65:ARG:HH12	1.70	0.55
3:D:16:GLU:HG3	9:D:1656:HOH:O	2.06	0.55
3:D:1398:TRP:HB2	9:D:2042:HOH:O	2.07	0.55
1:K:16:GLN:O	1:K:16:GLN:CG	2.55	0.55
2:M:73:LEU:HD23	2:M:94:LEU:HB2	1.88	0.55
2:M:701:THR:HG23	2:M:832:LYS:HA	1.88	0.55
2:M:877:PRO:HG3	3:N:1020:LEU:HD12	1.89	0.55
3:N:741:ASP:OD2	3:N:741:ASP:N	2.33	0.55
3:N:829:VAL:HG11	9:N:1877:HOH:O	2.07	0.55
3:N:1066:THR:HG22	3:N:1069:GLU:HG3	1.86	0.55
2:C:199:VAL:HG13	2:C:235:LEU:HG	1.89	0.55
2:C:318:PRO:HD2	9:C:1596:HOH:O	2.07	0.55
3:D:187:LYS:HG3	3:D:199:LEU:HB3	1.89	0.55
3:D:1095:THR:CG2	3:D:1230:GLY:HA3	2.36	0.55
5:F:373:LYS:HG3	9:F:450:HOH:O	2.06	0.55
1:K:74:ASP:O	1:K:78:ILE:HG13	2.06	0.55
1:K:198:ARG:HB2	1:K:200:TRP:CZ3	2.42	0.55
2:M:53:PRO:HD3	9:M:1709:HOH:O	2.06	0.55
2:M:128:ILE:HG22	9:M:1824:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:139:GLN:HE22	2:M:415:PRO:CG	2.19	0.55
2:M:918:LEU:HD23	2:M:967:PHE:O	2.07	0.55
3:N:586:ARG:HB2	9:N:1869:HOH:O	2.06	0.55
2:C:9:ILE:HG12	2:C:907:ASP:OD2	2.07	0.55
2:C:172:ILE:H	2:C:172:ILE:HD12	1.72	0.55
2:C:362:GLY:HA3	2:C:367:LEU:HD23	1.89	0.55
2:C:889:HIS:HE1	3:D:951:ILE:H	1.54	0.55
3:D:924:MET:O	3:D:927:THR:HB	2.06	0.55
3:D:1277:ILE:HD11	3:D:1301:LYS:HD2	1.89	0.55
5:F:256:ARG:HB2	9:F:658:HOH:O	2.07	0.55
1:K:94:LEU:HD13	9:K:1900:HOH:O	2.06	0.55
1:K:176:ARG:O	1:K:200:TRP:HE3	1.88	0.55
2:M:114:PHE:CD1	2:M:114:PHE:N	2.73	0.55
2:M:195:LEU:HD12	2:M:234:ALA:HB1	1.89	0.55
2:M:346:VAL:O	2:M:350:ARG:HG3	2.07	0.55
2:M:557:ARG:HD2	2:M:879:ARG:HG2	1.89	0.55
2:M:580:MET:O	2:M:902:ILE:HA	2.07	0.55
2:M:937:ASP:OD2	2:M:939:ARG:HD2	2.06	0.55
2:M:1010:THR:HG21	5:P:341:PRO:HB2	1.89	0.55
3:N:906:GLN:HB3	3:N:911:LEU:HD11	1.87	0.55
3:N:1312:LEU:HD22	9:N:2126:HOH:O	2.06	0.55
3:N:1432:LYS:HG3	3:N:1433:SER:H	1.72	0.55
3:D:111:LYS:HE2	3:D:498:VAL:HG12	1.88	0.55
3:D:482:LYS:HD2	9:D:2211:HOH:O	2.07	0.55
3:D:634:GLY:O	3:D:637:LEU:HB3	2.05	0.55
3:D:760:ARG:HD2	4:E:3:GLU:OE2	2.06	0.55
3:D:1311:LEU:HD23	3:D:1311:LEU:H	1.71	0.55
3:D:1397:LYS:HG2	9:D:1681:HOH:O	2.06	0.55
2:M:49:ARG:HA	9:M:1709:HOH:O	2.07	0.55
2:M:86:LYS:HD3	2:M:813:VAL:HG12	1.89	0.55
2:M:368:THR:HG22	9:M:2230:HOH:O	2.05	0.55
2:M:966:LEU:HD21	2:M:986:PRO:HG3	1.88	0.55
3:N:126:VAL:O	3:N:132:TYR:HD1	1.90	0.55
3:N:126:VAL:HG11	3:N:152:LEU:HD12	1.88	0.55
3:N:646:LYS:HD3	9:N:2006:HOH:O	2.06	0.55
3:N:774:SER:C	3:N:776:GLU:H	2.10	0.55
3:N:843:PHE:CD2	3:N:849:ALA:HA	2.42	0.55
3:N:843:PHE:CE1	3:N:864:VAL:HG11	2.32	0.55
3:N:1177:ALA:HB3	3:N:1183:ILE:HD11	1.88	0.55
3:N:1220:ALA:O	3:N:1224:VAL:HG23	2.07	0.55
3:N:1281:VAL:HG21	3:N:1313:VAL:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1396:GLU:O	3:N:1400:VAL:HG23	2.07	0.55
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.41	0.55
2:C:2:GLU:HG3	2:C:899:GLN:CB	2.29	0.55
2:C:551:GLU:OE1	2:C:906:PHE:HA	2.07	0.55
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.89	0.55
2:C:575:GLN:OE1	2:C:670:GLN:HB3	2.07	0.55
2:C:737:LEU:HD12	2:C:754:ILE:HB	1.88	0.55
2:C:1054:THR:CG2	2:C:1079:PRO:HB3	2.28	0.55
3:D:714:GLN:OE1	3:D:765:SER:HB2	2.07	0.55
3:D:890:VAL:HA	9:D:1617:HOH:O	2.07	0.55
3:D:1147:ARG:O	3:D:1166:LEU:HD23	2.06	0.55
3:D:1293:PHE:CE2	3:D:1302:GLU:HB3	2.42	0.55
5:F:172:ARG:O	5:F:176:ILE:HD13	2.07	0.55
1:L:179:PHE:HB2	1:L:195:LEU:HD11	1.88	0.55
2:M:137:VAL:CG2	2:M:391:LEU:HG	2.36	0.55
3:N:481:MET:HG3	3:N:1388:ARG:NH1	2.22	0.55
3:N:561:GLY:HA3	5:P:184:ARG:NH2	2.22	0.55
3:N:561:GLY:HA3	5:P:184:ARG:HH22	1.71	0.55
3:N:576:GLU:HB2	9:N:1886:HOH:O	2.06	0.55
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.42	0.55
1:A:127:LEU:C	1:A:127:LEU:HD12	2.27	0.55
1:A:132:LEU:HD21	1:A:138:LEU:HB2	1.89	0.55
2:C:56:GLU:OE2	2:C:356:ARG:HG2	2.07	0.55
2:C:57:GLU:O	2:C:62:GLY:HA3	2.06	0.55
2:C:553:ASP:OD1	2:C:843:HIS:ND1	2.40	0.55
2:C:670:GLN:HE22	2:C:699:PHE:CA	2.20	0.55
3:D:1090:ASP:HA	3:D:1093:TYR:CB	2.36	0.55
3:D:1431:THR:HB	9:D:1537:HOH:O	2.06	0.55
4:E:39:VAL:CG2	4:E:72:ARG:HD2	2.36	0.55
5:F:393:THR:HG22	9:F:485:HOH:O	2.07	0.55
2:M:632:ASN:N	9:M:1672:HOH:O	2.39	0.55
2:M:770:GLU:HA	9:M:1880:HOH:O	2.06	0.55
2:M:1060:ILE:CG2	2:M:1061:GLU:N	2.69	0.55
3:N:561:GLY:HA3	5:P:184:ARG:NH1	2.22	0.55
3:N:1225:ALA:HB2	9:N:1769:HOH:O	2.06	0.55
5:P:292:ALA:HB2	9:P:522:HOH:O	2.05	0.55
1:B:33:GLY:O	1:B:195:LEU:HD22	2.06	0.54
2:C:54:ILE:HD11	2:C:356:ARG:CG	2.35	0.54
2:C:136:ILE:HG22	2:C:336:VAL:HG22	1.89	0.54
2:C:194:VAL:HG21	2:C:221:LEU:O	2.07	0.54
2:C:260:LEU:HG	2:C:261:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:80:VAL:HG12	3:D:81:THR:O	2.06	0.54
3:D:149:LYS:HD2	9:D:1914:HOH:O	2.07	0.54
3:D:583:ASP:OD1	3:D:586:ARG:HG3	2.07	0.54
3:D:1101:VAL:CG2	3:D:1424:VAL:HG22	2.29	0.54
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.89	0.54
3:D:1382:THR:HG23	9:D:1608:HOH:O	2.07	0.54
3:D:1413:THR:HG23	9:D:1816:HOH:O	2.07	0.54
5:F:152:ASP:HB3	5:F:153:PRO:HD3	1.87	0.54
1:K:24:VAL:HG23	9:K:1055:HOH:O	2.06	0.54
1:L:52:ALA:HB2	1:L:170:VAL:C	2.28	0.54
1:L:105:GLY:O	1:L:132:LEU:HB3	2.07	0.54
1:L:175:ARG:O	1:L:176:ARG:HG3	2.07	0.54
2:M:254:VAL:O	2:M:257:VAL:HG23	2.07	0.54
2:M:413:LEU:H	2:M:413:LEU:CD1	2.13	0.54
2:M:455:LEU:HD12	2:M:456:ALA:O	2.07	0.54
2:M:1075:ASP:HA	9:M:2290:HOH:O	2.06	0.54
2:M:1084:SER:HB2	7:N:1527:MXP:O4	2.07	0.54
3:N:527:MET:HE3	3:N:535:PHE:HB3	1.89	0.54
3:N:1083:ASP:O	3:N:1087:ARG:HG3	2.07	0.54
3:N:1147:ARG:O	3:N:1166:LEU:HD23	2.08	0.54
3:N:1467:ILE:HG23	7:N:1527:MXP:H16A	1.89	0.54
1:A:88:ARG:HG2	1:A:121:GLU:HG2	1.89	0.54
2:C:41:ASN:O	2:C:46:ALA:HB2	2.08	0.54
2:C:510:ALA:HB3	2:C:513:VAL:HG23	1.89	0.54
2:C:580:MET:HB3	2:C:584:GLU:CD	2.28	0.54
2:C:805:ARG:HD2	9:C:1160:HOH:O	2.07	0.54
2:C:1056:LYS:HB3	3:D:623:VAL:HG13	1.89	0.54
3:D:400:VAL:C	3:D:402:PRO:HD3	2.26	0.54
3:D:611:GLN:OE1	7:D:1527:MXP:C16	2.53	0.54
3:D:675:ARG:HH12	5:F:421:PHE:HD2	1.55	0.54
3:D:786:ILE:HD13	3:D:908:LYS:HB3	1.87	0.54
5:F:84:TYR:O	5:F:88:ILE:HD12	2.07	0.54
5:F:94:LEU:HD23	9:F:642:HOH:O	2.07	0.54
1:L:85:LEU:HD12	1:L:124:ASN:HB3	1.89	0.54
2:M:197:LEU:HD12	2:M:207:LEU:HD11	1.89	0.54
3:N:77:GLY:HA3	9:N:2213:HOH:O	2.07	0.54
3:N:679:ARG:HB3	9:N:2172:HOH:O	2.06	0.54
3:N:996:TRP:CE2	3:N:1056:PRO:HG2	2.42	0.54
3:N:1144:LEU:HB3	3:N:1166:LEU:HD11	1.89	0.54
4:O:17:TYR:CD2	4:O:17:TYR:N	2.74	0.54
5:P:278:LEU:HB2	5:P:286:PRO:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TYR:HD2	1:A:21:GLY:H	1.53	0.54
1:A:57:TYR:CE2	1:A:59:GLU:HA	2.42	0.54
1:A:213:GLN:O	1:A:217:ILE:HG13	2.07	0.54
1:B:56:VAL:HG13	1:B:142:VAL:HG12	1.89	0.54
1:B:107:LYS:HG3	1:B:108:GLU:N	2.22	0.54
2:C:272:ALA:HB1	9:C:1127:HOH:O	2.06	0.54
2:C:724:ARG:HE	2:C:734:LEU:HD23	1.72	0.54
2:C:816:LYS:HE2	2:C:819:VAL:HG21	1.89	0.54
3:D:165:LYS:HG3	3:D:397:LYS:HD3	1.90	0.54
3:D:533:GLY:HA3	9:D:1806:HOH:O	2.07	0.54
3:D:568:ARG:O	3:D:572:ARG:HG3	2.06	0.54
3:D:675:ARG:HG2	3:D:678:GLU:OE2	2.06	0.54
3:D:1286:THR:HG22	9:D:1533:HOH:O	2.07	0.54
5:F:254:GLN:HA	9:F:443:HOH:O	2.08	0.54
1:L:106:PRO:HG3	1:L:134:GLU:HG2	1.88	0.54
1:L:158:ILE:HG22	1:L:159:LYS:N	2.21	0.54
2:M:1084:SER:O	2:M:1087:VAL:HG12	2.08	0.54
3:N:98:PRO:HG3	3:N:515:GLU:HB3	1.89	0.54
3:N:583:ASP:HB2	3:N:604:THR:OG1	2.07	0.54
3:N:820:GLU:HG3	3:N:836:VAL:CG1	2.36	0.54
3:N:1087:ARG:HD3	3:N:1237:THR:HA	1.90	0.54
3:N:1351:GLU:HG3	3:N:1354:LYS:HD2	1.90	0.54
5:P:205:ARG:HD3	5:P:251:ILE:HG21	1.89	0.54
5:P:358:LEU:HG	5:P:358:LEU:O	2.06	0.54
1:A:132:LEU:N	1:A:132:LEU:HD12	2.23	0.54
1:B:175:ARG:HA	9:B:492:HOH:O	2.08	0.54
1:B:211:LEU:O	1:B:214:ALA:HB3	2.07	0.54
2:C:84:ARG:NH2	2:C:128:ILE:HD11	2.23	0.54
2:C:120:LEU:HD23	9:C:1499:HOH:O	2.06	0.54
2:C:577:PRO:HG3	2:C:993:PHE:CE2	2.43	0.54
2:C:710:ILE:HD11	2:C:758:ARG:HD3	1.88	0.54
2:C:1087:VAL:CG1	3:D:610:LYS:HZ3	2.17	0.54
3:D:49:ILE:HB	3:D:50:PHE:CD1	2.42	0.54
3:D:570:GLU:N	5:F:214:GLN:HE22	2.05	0.54
3:D:711:LEU:C	3:D:713:ILE:H	2.11	0.54
3:D:1042:ARG:O	3:D:1057:VAL:HB	2.08	0.54
3:D:1293:PHE:CZ	3:D:1302:GLU:HB3	2.43	0.54
3:D:1381:VAL:HB	3:D:1389:LEU:O	2.08	0.54
5:F:305:GLU:O	5:F:309:LYS:HG3	2.07	0.54
2:M:565:GLN:HG2	2:M:995:MET:CE	2.37	0.54
2:M:889:HIS:CD2	2:M:970:GLY:HA3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:32:ILE:HD11	9:N:1596:HOH:O	2.06	0.54
3:N:566:ILE:HG12	5:P:192:LEU:HD21	1.88	0.54
3:N:610:LYS:C	3:N:611:GLN:HG3	2.28	0.54
3:N:1009:LYS:HE2	9:N:1963:HOH:O	2.07	0.54
3:N:1041:LEU:CD1	3:N:1058:ARG:HA	2.36	0.54
3:N:1262:LEU:HD23	3:N:1352:ILE:HG13	1.90	0.54
3:N:1472:ILE:O	3:N:1477:GLY:HA3	2.08	0.54
5:P:88:ILE:HB	9:P:514:HOH:O	2.06	0.54
1:A:184:THR:HG23	1:A:192:LEU:HD12	1.89	0.54
2:C:17:PRO:HB2	9:C:1289:HOH:O	2.07	0.54
2:C:292:ARG:NH1	2:C:299:LYS:HD3	2.22	0.54
3:D:41:ARG:HD2	9:D:2449:HOH:O	2.07	0.54
3:D:72:VAL:HG23	3:D:78:VAL:H	1.71	0.54
3:D:118:LEU:O	3:D:120:ALA:N	2.41	0.54
3:D:957:PRO:CD	3:D:1007:VAL:HG12	2.37	0.54
3:D:1045:MET:HG3	3:D:1073:SER:OG	2.07	0.54
3:D:1112:CYS:HA	9:D:2179:HOH:O	2.08	0.54
3:D:1142:ALA:HB3	9:D:2234:HOH:O	2.06	0.54
5:F:88:ILE:CB	5:F:193:ARG:HH11	2.20	0.54
2:M:137:VAL:HG22	2:M:391:LEU:O	2.08	0.54
2:M:362:GLY:HA3	2:M:367:LEU:CD2	2.37	0.54
3:N:764:LEU:HD23	3:N:767:HIS:CE1	2.42	0.54
3:N:799:LYS:O	3:N:826:PRO:HD2	2.08	0.54
3:N:1080:GLY:O	3:N:1084:THR:HG23	2.07	0.54
1:B:122:ILE:HG23	9:B:527:HOH:O	2.08	0.54
1:B:123:MET:O	1:B:125:PRO:HD3	2.08	0.54
2:C:398:THR:O	2:C:570:PRO:HD3	2.08	0.54
2:C:420:ARG:CZ	2:C:422:ARG:HH21	2.20	0.54
2:C:481:ASP:O	2:C:483:VAL:HG23	2.06	0.54
2:C:725:ASP:HA	9:C:1479:HOH:O	2.08	0.54
3:D:478:LEU:HD21	3:D:500:ARG:HH21	1.71	0.54
3:D:534:ARG:HE	5:F:312:GLN:HE22	1.56	0.54
1:K:86:VAL:HG13	1:K:124:ASN:HB2	1.89	0.54
2:M:157:ARG:NH1	2:M:314:THR:HB	2.22	0.54
2:M:252:LYS:HD3	2:M:296:GLY:HA2	1.89	0.54
2:M:1049:LEU:O	2:M:1053:LEU:HG	2.07	0.54
3:N:172:PRO:HA	9:N:2177:HOH:O	2.06	0.54
3:N:493:ARG:HB2	3:N:1388:ARG:NE	2.23	0.54
3:N:584:ASN:CG	3:N:590:PRO:HD2	2.27	0.54
2:C:191:PHE:HD2	2:C:195:LEU:HD23	1.72	0.54
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:99:ALA:HB1	3:D:575:GLN:CD	2.28	0.54
3:D:117:ASP:HB2	3:D:495:ARG:NH2	2.23	0.54
3:D:1109:GLU:CG	3:D:1202:GLN:H	2.21	0.54
3:D:1466:VAL:HG23	3:D:1472:ILE:CD1	2.33	0.54
1:K:111:ALA:HB2	1:K:127:LEU:HG	1.90	0.54
1:K:193:ASP:HA	9:K:2597:HOH:O	2.07	0.54
1:L:206:THR:CG2	1:L:209:GLU:H	2.21	0.54
2:M:185:LYS:HB3	2:M:188:LYS:O	2.07	0.54
2:M:281:LEU:CD1	2:M:306:THR:HA	2.38	0.54
2:M:669:GLY:HA3	2:M:995:MET:HA	1.90	0.54
3:N:1005:GLN:HB2	9:N:1763:HOH:O	2.07	0.54
3:N:1104:GLU:O	3:N:1106:VAL:HG23	2.08	0.54
3:N:1290:LEU:HD22	3:N:1291:SER:H	1.73	0.54
1:A:101:LEU:HD12	1:A:114:PHE:CD1	2.43	0.54
2:C:334:ARG:NH2	2:C:418:LEU:HD11	2.23	0.54
2:C:740:GLU:HB3	9:C:1664:HOH:O	2.08	0.54
3:D:1195:GLN:HG3	3:D:1196:THR:N	2.22	0.54
1:K:173:PRO:O	1:K:201:THR:HG23	2.08	0.54
2:M:129:ILE:CG1	2:M:386:PHE:HB3	2.35	0.54
2:M:250:ARG:HG3	9:M:2168:HOH:O	2.06	0.54
2:M:338:GLU:HA	2:M:341:THR:HG22	1.89	0.54
2:M:420:ARG:CZ	2:M:422:ARG:HH21	2.20	0.54
2:M:841:ASN:HD21	2:M:845:ASN:H	1.56	0.54
2:M:1034:GLU:OE2	3:N:616:GLN:HG2	2.08	0.54
3:N:127:LEU:HD11	3:N:461:ILE:HD11	1.89	0.54
3:N:187:LYS:HG3	3:N:199:LEU:HB3	1.89	0.54
3:N:477:LEU:HD23	9:N:1890:HOH:O	2.07	0.54
4:O:46:PRO:CB	4:O:54:LEU:HD22	2.35	0.54
4:O:70:THR:HG21	4:O:72:ARG:NE	2.23	0.54
5:P:142:ARG:CZ	5:P:156:VAL:HG22	2.38	0.54
5:P:207:LEU:HB3	5:P:212:LEU:HG	1.90	0.54
1:B:185:ARG:HD2	9:D:1847:HOH:O	2.08	0.54
2:C:51:THR:HB	2:C:348:LEU:HD23	1.89	0.54
2:C:77:PRO:HD3	2:C:93:PRO:HD3	1.89	0.54
2:C:130:ASN:HA	9:C:1363:HOH:O	2.07	0.54
2:C:438:ILE:HD11	2:C:467:ILE:HD12	1.89	0.54
2:C:774:LEU:HB2	9:C:1255:HOH:O	2.07	0.54
2:C:1115:LEU:HD12	2:C:1115:LEU:N	2.22	0.54
3:D:24:GLY:HA2	9:D:2024:HOH:O	2.07	0.54
3:D:119:SER:H	3:D:123:LEU:CD2	2.17	0.54
3:D:148:GLU:HG2	3:D:151:GLN:HE21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1113:GLY:HA2	9:D:1697:HOH:O	2.07	0.54
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.08	0.54
4:E:35:PHE:HZ	4:E:60:ALA:HA	1.73	0.54
5:F:94:LEU:HB2	5:F:98:GLU:OE2	2.08	0.54
1:K:184:THR:HG23	1:K:192:LEU:CB	2.36	0.54
1:L:173:PRO:O	1:L:201:THR:HG23	2.07	0.54
2:M:229:MET:HG3	9:M:1707:HOH:O	2.07	0.54
2:M:1008:ARG:HH11	2:M:1028:GLY:CA	2.20	0.54
3:N:187:LYS:CE	3:N:199:LEU:HB3	2.34	0.54
3:N:800:LYS:HD3	9:N:1722:HOH:O	2.08	0.54
3:N:891:GLU:HB2	9:N:2068:HOH:O	2.07	0.54
3:N:1389:LEU:HD22	9:N:1771:HOH:O	2.08	0.54
4:O:6:ILE:HA	4:O:9:LEU:HD12	1.89	0.54
1:B:83:LYS:O	1:B:170:VAL:HG21	2.08	0.54
2:C:602:GLU:HA	2:C:647:GLN:O	2.07	0.54
2:C:650:ARG:HG3	9:C:1791:HOH:O	2.08	0.54
2:C:863:ASP:O	2:C:865:THR:N	2.41	0.54
3:D:52:PRO:HG2	3:D:79:GLU:O	2.08	0.54
3:D:169:TYR:HB3	3:D:195:VAL:HG11	1.89	0.54
3:D:1176:LYS:O	3:D:1179:GLU:HB2	2.08	0.54
3:D:1369:GLU:O	3:D:1372:VAL:HG12	2.08	0.54
5:F:301:ALA:HB2	9:F:602:HOH:O	2.08	0.54
1:K:23:PHE:HE1	1:K:208:LEU:HD13	1.73	0.54
2:M:137:VAL:O	2:M:391:LEU:HD21	2.08	0.54
2:M:182:VAL:HG11	9:M:2050:HOH:O	2.08	0.54
2:M:216:GLU:HB3	9:M:1627:HOH:O	2.08	0.54
2:M:481:ASP:O	2:M:483:VAL:HG23	2.07	0.54
3:N:400:VAL:C	3:N:402:PRO:HD3	2.28	0.54
3:N:1277:ILE:HD11	3:N:1301:LYS:HD2	1.89	0.54
2:C:860:HIS:HE1	9:C:1431:HOH:O	1.91	0.53
2:C:1111:ILE:HG13	2:C:1112:PHE:H	1.73	0.53
3:D:550:ARG:HH11	3:D:573:MET:HB3	1.73	0.53
3:D:699:VAL:HG12	3:D:717:GLN:HA	1.88	0.53
3:D:820:GLU:HG2	3:D:825:ALA:O	2.08	0.53
3:D:1213:ARG:HG3	9:D:2053:HOH:O	2.06	0.53
3:D:1485:GLN:O	4:E:75:PHE:HA	2.08	0.53
5:F:399:GLN:HG3	9:F:571:HOH:O	2.08	0.53
1:K:123:MET:C	1:K:125:PRO:HD3	2.29	0.53
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.43	0.53
2:M:191:PHE:HD2	2:M:195:LEU:HD23	1.72	0.53
2:M:315:ALA:HB3	9:M:1882:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:352:ALA:HA	2:M:355:VAL:HG12	1.89	0.53
2:M:689:VAL:HB	2:M:870:ILE:HG13	1.89	0.53
3:N:81:THR:O	3:N:82:LYS:O	2.26	0.53
1:B:106:PRO:HG2	9:B:483:HOH:O	2.07	0.53
3:D:131:LYS:HD2	5:F:83:GLN:NE2	2.23	0.53
3:D:139:GLY:O	3:D:147:VAL:HB	2.08	0.53
3:D:161:LEU:O	3:D:161:LEU:HD23	2.08	0.53
3:D:1476:THR:HG23	4:E:21:VAL:HG22	1.90	0.53
4:E:49:GLN:HG2	9:E:108:HOH:O	2.09	0.53
5:F:271:LEU:HG	5:F:295:MET:CE	2.37	0.53
1:L:14:ARG:HA	9:L:3344:HOH:O	2.07	0.53
1:L:68:ILE:HG23	1:L:137:ARG:NH1	2.24	0.53
1:L:212:ASN:O	1:L:215:VAL:HG22	2.07	0.53
2:M:41:ASN:O	2:M:46:ALA:HB2	2.09	0.53
2:M:89:THR:HA	2:M:129:ILE:O	2.08	0.53
2:M:411:SER:HA	2:M:452:ILE:HA	1.90	0.53
2:M:685:GLU:CG	3:N:783:ARG:HD2	2.38	0.53
2:M:911:GLU:O	2:M:914:ILE:HG22	2.08	0.53
3:N:610:LYS:CG	7:N:1527:MXP:C15	2.85	0.53
3:N:615:ARG:O	3:N:616:GLN:C	2.46	0.53
3:N:820:GLU:HB2	3:N:836:VAL:HG11	1.90	0.53
3:N:983:LEU:HD13	3:N:991:GLN:OE1	2.08	0.53
3:N:1049:SER:OG	3:N:1051:GLU:HG3	2.08	0.53
3:N:1381:VAL:HB	3:N:1389:LEU:O	2.07	0.53
5:P:234:LYS:HG3	5:P:236:SER:H	1.74	0.53
1:B:44:LEU:HD21	1:B:199:ILE:HD13	1.89	0.53
2:C:254:VAL:O	2:C:257:VAL:HG23	2.09	0.53
2:C:736:ASP:C	2:C:738:ASP:H	2.12	0.53
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.91	0.53
3:D:454:ALA:HB3	9:D:2225:HOH:O	2.08	0.53
3:D:764:LEU:HD23	3:D:767:HIS:ND1	2.24	0.53
3:D:787:LEU:HD21	3:D:947:ILE:HD13	1.90	0.53
3:D:959:GLU:O	3:D:963:TYR:HD1	1.91	0.53
3:D:1273:VAL:HG13	9:D:2190:HOH:O	2.08	0.53
4:E:19:LEU:HB3	9:E:116:HOH:O	2.08	0.53
5:F:95:THR:HG22	5:F:96:LEU:HD23	1.90	0.53
1:K:126:ASP:HB2	9:K:1975:HOH:O	2.06	0.53
1:L:83:LYS:O	1:L:170:VAL:HG21	2.07	0.53
1:L:86:VAL:HG12	1:L:124:ASN:ND2	2.16	0.53
2:M:673:LEU:HD22	2:M:867:VAL:HA	1.90	0.53
2:M:690:ILE:CG2	2:M:852:ILE:HG13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:766:GLU:HG2	2:M:772:ARG:HH12	1.73	0.53
2:M:1103:ASP:OD1	3:N:3:LYS:HB2	2.09	0.53
3:N:407:VAL:HG13	3:N:421:LEU:O	2.09	0.53
3:N:1209:LEU:HD23	3:N:1211:MET:HG3	1.90	0.53
3:N:1278:ASP:HA	3:N:1319:VAL:O	2.08	0.53
3:N:1395:LEU:HD21	9:N:1988:HOH:O	2.08	0.53
3:D:408:GLU:O	3:D:408:GLU:HG2	2.07	0.53
3:D:662:GLU:HB2	9:D:1987:HOH:O	2.09	0.53
3:D:1080:GLY:O	3:D:1084:THR:HG23	2.08	0.53
3:D:1258:ARG:HG3	3:D:1262:LEU:HD13	1.89	0.53
3:D:1264:GLU:O	3:D:1266:ARG:HG3	2.07	0.53
4:E:29:GLN:HB2	4:E:33:HIS:CD2	2.43	0.53
5:F:162:LYS:HE2	9:F:641:HOH:O	2.08	0.53
5:F:345:ALA:HB1	9:F:710:HOH:O	2.08	0.53
1:K:63:HIS:HB3	2:M:746:GLY:HA2	1.89	0.53
2:M:52:PHE:O	2:M:54:ILE:N	2.41	0.53
2:M:182:VAL:CG1	2:M:193:LEU:HD13	2.38	0.53
2:M:227:PHE:HA	2:M:237:ARG:NH1	2.23	0.53
2:M:571:LEU:HD23	2:M:699:PHE:O	2.09	0.53
2:M:584:GLU:CD	2:M:584:GLU:H	2.10	0.53
2:M:604:ALA:HB3	2:M:612:VAL:O	2.08	0.53
2:M:611:ILE:CD1	2:M:625:LEU:HD11	2.38	0.53
2:M:632:ASN:HB2	9:M:1672:HOH:O	2.09	0.53
3:N:17:LYS:HA	3:N:20:SER:HB3	1.91	0.53
3:N:527:MET:CE	5:P:258:ILE:HD11	2.39	0.53
3:N:612:GLY:HA2	3:N:1441:GLN:HA	1.90	0.53
3:N:1144:LEU:HA	3:N:1147:ARG:HG3	1.90	0.53
3:N:1466:VAL:HG11	7:N:1527:MXP:H20	1.90	0.53
5:P:130:VAL:HA	5:P:142:ARG:HH21	1.73	0.53
2:C:4:LYS:O	2:C:901:TYR:HB3	2.08	0.53
2:C:378:LEU:HG	2:C:382:ILE:HD11	1.90	0.53
2:C:385:PHE:O	2:C:389:SER:HB3	2.08	0.53
2:C:765:SER:O	2:C:767:PRO:HD3	2.09	0.53
2:C:897:LEU:HB3	2:C:899:GLN:HE21	1.73	0.53
3:D:800:LYS:CE	3:D:804:LEU:HD13	2.39	0.53
3:D:1105:ILE:HD13	9:D:2099:HOH:O	2.09	0.53
3:D:1175:ILE:O	3:D:1179:GLU:HG3	2.08	0.53
3:D:1390:LEU:HA	9:D:2323:HOH:O	2.08	0.53
5:F:108:GLU:HG3	5:F:176:ILE:HG21	1.91	0.53
5:F:130:VAL:HG11	5:F:159:ILE:HB	1.90	0.53
2:M:328:LEU:HD21	2:M:438:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:806:LEU:HD22	9:M:1891:HOH:O	2.07	0.53
2:M:877:PRO:HG2	3:N:1023:MET:CE	2.18	0.53
3:N:448:GLU:O	3:N:448:GLU:HG2	2.08	0.53
3:N:1047:LYS:HB3	3:N:1048:PRO:CD	2.38	0.53
3:N:1486:VAL:HG12	4:O:73:LEU:HD22	1.90	0.53
1:B:140:MET:HB2	9:B:514:HOH:O	2.08	0.53
2:C:185:LYS:HB3	2:C:188:LYS:O	2.07	0.53
2:C:267:TYR:CD1	2:C:272:ALA:HB1	2.43	0.53
2:C:496:ILE:O	2:C:515:ALA:HB1	2.09	0.53
2:C:1008:ARG:HH11	2:C:1028:GLY:CA	2.18	0.53
3:D:493:ARG:HA	3:D:1388:ARG:NH1	2.24	0.53
3:D:799:LYS:HB3	3:D:826:PRO:CG	2.37	0.53
3:D:1485:GLN:NE2	4:E:80:VAL:H	2.07	0.53
5:F:415:THR:HB	9:F:522:HOH:O	2.09	0.53
1:K:20:TYR:CD2	1:K:21:GLY:N	2.69	0.53
1:K:45:LEU:HD21	9:K:2558:HOH:O	2.08	0.53
3:N:55:ASP:O	3:N:80:VAL:HG11	2.08	0.53
3:N:138:LYS:HD3	9:N:1530:HOH:O	2.08	0.53
3:N:169:TYR:CE1	3:N:197:SER:HB2	2.44	0.53
3:N:792:ILE:O	3:N:878:GLY:HA3	2.09	0.53
3:N:860:LEU:HD23	3:N:877:PRO:HB2	1.91	0.53
3:N:1236:LEU:HA	3:N:1359:GLN:NE2	2.24	0.53
4:O:39:VAL:CG2	4:O:72:ARG:HD2	2.39	0.53
5:P:94:LEU:HD23	9:P:638:HOH:O	2.09	0.53
2:C:403:SER:O	2:C:407:LYS:HG3	2.09	0.53
2:C:1054:THR:HG22	2:C:1059:ASP:CB	2.33	0.53
9:C:1255:HOH:O	5:F:354:LEU:HD21	2.08	0.53
3:D:113:GLY:HA3	3:D:120:ALA:HA	1.91	0.53
3:D:493:ARG:HB2	3:D:1388:ARG:CZ	2.39	0.53
3:D:591:VAL:HB	9:D:1809:HOH:O	2.08	0.53
3:D:615:ARG:O	3:D:616:GLN:C	2.44	0.53
3:D:996:TRP:HA	3:D:999:THR:HG22	1.89	0.53
3:D:1113:GLY:N	3:D:1195:GLN:HE22	2.07	0.53
3:D:1274:ILE:HD12	9:D:1674:HOH:O	2.08	0.53
3:D:1274:ILE:HD11	3:D:1334:GLN:NE2	2.24	0.53
1:L:60:ASP:H	1:L:137:ARG:NH2	2.06	0.53
2:M:328:LEU:HD21	2:M:438:ILE:CD1	2.38	0.53
2:M:410:ILE:HD12	2:M:410:ILE:H	1.73	0.53
2:M:874:LEU:HD23	3:N:1023:MET:CE	2.37	0.53
2:M:915:LYS:HB3	9:M:2164:HOH:O	2.09	0.53
3:N:46:ASP:HB3	3:N:49:ILE:HG13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:55:ASP:HB3	3:N:82:LYS:HE2	1.90	0.53
3:N:160:GLU:HG2	9:N:2310:HOH:O	2.09	0.53
3:N:785:ILE:HG22	3:N:789:LEU:HD12	1.91	0.53
3:N:860:LEU:O	3:N:877:PRO:HD2	2.07	0.53
3:N:908:LYS:CB	3:N:1027:GLY:HA3	2.33	0.53
3:N:996:TRP:HE3	3:N:999:THR:HG21	1.73	0.53
3:N:1087:ARG:HD3	3:N:1238:MET:N	2.23	0.53
3:N:1141:GLU:CG	3:N:1168:MET:HE1	2.39	0.53
3:N:1323:GLN:HG3	3:N:1324:PRO:HD2	1.90	0.53
4:O:29:GLN:HB2	4:O:33:HIS:CD2	2.43	0.53
5:P:368:VAL:O	5:P:372:ARG:HB2	2.09	0.53
2:C:496:ILE:H	2:C:496:ILE:HD12	1.74	0.53
2:C:690:ILE:CG2	2:C:852:ILE:HG13	2.39	0.53
2:C:816:LYS:HB2	2:C:819:VAL:CG2	2.39	0.53
3:D:52:PRO:CB	3:D:80:VAL:HG13	2.39	0.53
3:D:631:ILE:HG21	3:D:745:MET:SD	2.49	0.53
4:E:31:LEU:HD23	4:E:35:PHE:HE1	1.73	0.53
2:M:54:ILE:O	2:M:54:ILE:HG23	2.09	0.53
3:N:503:LEU:HD22	9:N:2051:HOH:O	2.09	0.53
3:N:550:ARG:NH1	3:N:573:MET:HB3	2.24	0.53
3:N:692:GLU:HG3	3:N:720:LEU:HD13	1.91	0.53
3:N:786:ILE:HD13	3:N:908:LYS:HB3	1.89	0.53
3:N:1066:THR:HA	9:N:1984:HOH:O	2.09	0.53
3:N:1377:LYS:O	3:N:1395:LEU:N	2.37	0.53
3:N:1422:MET:HE3	3:N:1427:SER:HA	1.89	0.53
2:C:535:SER:HB2	2:C:537:LYS:HG3	1.91	0.53
2:C:984:GLU:OE1	3:D:945:SER:HA	2.09	0.53
3:D:53:ILE:HG22	9:D:1900:HOH:O	2.08	0.53
3:D:1220:ALA:HB1	3:D:1223:ILE:CD1	2.36	0.53
3:D:1492:LEU:HD12	9:D:2354:HOH:O	2.09	0.53
5:F:321:ILE:O	5:F:327:SER:HB3	2.08	0.53
1:K:133:GLU:HG2	1:K:134:GLU:H	1.72	0.53
1:L:65:PHE:HB2	9:L:1134:HOH:O	2.08	0.53
2:M:64:LEU:HD11	2:M:100:LEU:HD13	1.90	0.53
2:M:162:ILE:O	2:M:164:PRO:HD3	2.09	0.53
2:M:607:ASP:HB2	2:M:610:ARG:HG3	1.91	0.53
2:M:737:LEU:HD12	2:M:754:ILE:HB	1.91	0.53
2:M:753:ASP:O	2:M:792:VAL:HG23	2.09	0.53
3:N:407:VAL:HG13	3:N:422:ALA:HB2	1.91	0.53
3:N:591:VAL:HG11	3:N:597:ASP:HA	1.91	0.53
3:N:1109:GLU:CD	3:N:1202:GLN:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1114:THR:HG23	3:N:1114:THR:O	2.09	0.53
3:N:1462:LEU:N	3:N:1462:LEU:HD23	2.23	0.53
2:C:495:THR:HB	2:C:530:GLU:HG3	1.91	0.53
2:C:1101:THR:OG1	2:C:1109:VAL:HG12	2.09	0.53
3:D:760:ARG:NH2	4:E:62:THR:N	2.57	0.53
3:D:1310:ARG:NE	3:D:1327:ARG:HB3	2.24	0.53
3:D:1330:ILE:HB	3:D:1347:TYR:CZ	2.43	0.53
1:K:23:PHE:O	1:K:196:THR:HA	2.09	0.53
1:L:80:LEU:HG	3:N:844:ALA:HB2	1.91	0.53
2:M:109:LYS:HE2	2:M:111:ASP:OD1	2.09	0.53
2:M:143:SER:HB2	2:M:276:LYS:HZ3	1.74	0.53
2:M:290:LEU:HD11	9:M:1886:HOH:O	2.09	0.53
2:M:413:LEU:HD12	2:M:413:LEU:N	2.21	0.53
2:M:549:PHE:HB3	2:M:552:HIS:CD2	2.42	0.53
3:N:81:THR:HG23	9:N:1885:HOH:O	2.09	0.53
3:N:1175:ILE:O	3:N:1179:GLU:HG3	2.09	0.53
5:P:127:ILE:HD11	9:P:595:HOH:O	2.08	0.53
1:A:181:VAL:HG11	9:A:337:HOH:O	2.10	0.52
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.44	0.52
1:B:58:ILE:HD13	1:B:140:MET:HB3	1.91	0.52
1:B:218:LEU:O	1:B:222:LEU:HG	2.08	0.52
2:C:52:PHE:O	2:C:54:ILE:N	2.42	0.52
2:C:110:GLU:H	2:C:368:THR:HG21	1.74	0.52
2:C:162:ILE:HD11	2:C:306:THR:HG21	1.90	0.52
2:C:818:GLY:HA2	5:F:309:LYS:HZ3	1.74	0.52
3:D:407:VAL:HG13	3:D:421:LEU:O	2.09	0.52
3:D:570:GLU:HB2	5:F:214:GLN:OE1	2.08	0.52
4:E:8:LYS:HG3	9:E:100:HOH:O	2.09	0.52
5:F:282:LEU:HD13	9:F:621:HOH:O	2.08	0.52
2:M:197:LEU:HB3	2:M:202:TYR:HB2	1.90	0.52
2:M:1115:LEU:HD12	2:M:1115:LEU:N	2.23	0.52
3:N:49:ILE:HB	3:N:50:PHE:CD1	2.44	0.52
3:N:104:PHE:CD2	3:N:1448:THR:HG23	2.44	0.52
3:N:567:ILE:N	3:N:567:ILE:HD12	2.24	0.52
3:N:826:PRO:HB3	9:N:1811:HOH:O	2.08	0.52
3:N:984:THR:HG21	9:N:1536:HOH:O	2.09	0.52
3:N:1176:LYS:O	3:N:1179:GLU:HB2	2.09	0.52
3:N:1243:THR:HG1	3:N:1253:THR:HB	1.73	0.52
4:O:33:HIS:HB2	4:O:37:ASN:ND2	2.24	0.52
5:P:369:LEU:O	5:P:373:LYS:HB2	2.09	0.52
1:A:211:LEU:O	1:A:214:ALA:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:PHE:CE2	1:B:199:ILE:HD12	2.44	0.52
1:B:197:LEU:HD21	1:B:199:ILE:HD11	1.91	0.52
2:C:166:PRO:HD3	2:C:265:ARG:HB2	1.91	0.52
2:C:260:LEU:HA	2:C:291:ALA:HB2	1.90	0.52
2:C:603:VAL:HG22	2:C:613:VAL:HG12	1.90	0.52
2:C:739:GLU:HA	9:C:1304:HOH:O	2.09	0.52
2:C:772:ARG:HB3	9:F:459:HOH:O	2.09	0.52
3:D:62:LYS:HD2	9:D:1735:HOH:O	2.08	0.52
3:D:102:ILE:HG13	9:D:1613:HOH:O	2.09	0.52
5:F:102:LEU:O	5:F:106:VAL:HG23	2.09	0.52
2:M:176:VAL:C	2:M:178:PRO:HD3	2.29	0.52
2:M:577:PRO:HG3	2:M:993:PHE:CE2	2.43	0.52
2:M:602:GLU:HA	2:M:647:GLN:O	2.09	0.52
2:M:1005:MET:HG3	2:M:1005:MET:O	2.09	0.52
3:N:32:ILE:O	5:P:258:ILE:HG23	2.09	0.52
3:N:104:PHE:HE2	3:N:1448:THR:HA	1.73	0.52
3:N:141:ILE:HG13	3:N:142:LEU:N	2.24	0.52
3:N:611:GLN:OE1	3:N:619:LEU:HD21	2.09	0.52
3:N:892:ASP:OD2	3:N:895:VAL:HG21	2.09	0.52
5:P:220:LEU:HD12	5:P:243:ILE:HD11	1.92	0.52
2:C:6:PHE:CD1	2:C:6:PHE:N	2.77	0.52
2:C:129:ILE:HG22	2:C:130:ASN:ND2	2.24	0.52
2:C:368:THR:HB	2:C:369:PRO:HD3	1.90	0.52
2:C:404:LEU:HA	2:C:407:LYS:HD2	1.91	0.52
5:F:371:LEU:HB2	5:F:372:ARG:HH11	1.74	0.52
5:F:393:THR:O	5:F:397:ILE:HG13	2.09	0.52
1:K:149:GLY:O	1:K:171:PHE:HB2	2.10	0.52
1:K:189:ARG:HD2	1:K:191:ASP:OD1	2.09	0.52
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.90	0.52
2:M:626:ARG:H	2:M:639:GLN:NE2	2.06	0.52
3:N:153:LEU:CD1	3:N:157:GLU:HB2	2.39	0.52
3:N:163:TYR:HB3	9:N:2151:HOH:O	2.10	0.52
3:N:179:VAL:HG13	3:N:183:GLU:HB3	1.92	0.52
3:N:408:GLU:HA	5:P:171:LYS:NZ	2.23	0.52
3:N:498:VAL:HG23	3:N:499:VAL:N	2.24	0.52
3:N:584:ASN:HD21	3:N:590:PRO:HD2	1.72	0.52
3:N:1305:LEU:HD22	3:N:1309:ALA:HB1	1.91	0.52
5:P:392:VAL:HG11	5:P:396:ARG:HD2	1.91	0.52
2:C:265:ARG:HB3	2:C:267:TYR:CD2	2.45	0.52
2:C:442:GLU:HB3	9:C:1185:HOH:O	2.08	0.52
2:C:643:VAL:HB	9:C:1145:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:114:THR:O	3:D:495:ARG:HG3	2.09	0.52
3:D:591:VAL:HG11	3:D:597:ASP:HA	1.92	0.52
3:D:710:ARG:HH21	3:D:1210:SER:CB	2.22	0.52
3:D:892:ASP:OD2	3:D:895:VAL:HG21	2.09	0.52
3:D:965:GLU:HA	3:D:968:ASP:HB2	1.91	0.52
1:K:127:LEU:C	1:K:127:LEU:HD12	2.30	0.52
1:L:45:LEU:HD21	1:L:177:VAL:HG13	1.91	0.52
2:M:289:THR:HG22	2:M:290:LEU:HD23	1.92	0.52
2:M:605:LYS:HG3	2:M:612:VAL:HB	1.92	0.52
3:N:408:GLU:HB3	9:N:1846:HOH:O	2.09	0.52
3:N:534:ARG:HG3	5:P:312:GLN:NE2	2.24	0.52
3:N:661:MET:O	3:N:664:LYS:O	2.26	0.52
3:N:1076:GLY:O	3:N:1079:LYS:HG2	2.09	0.52
3:N:1182:GLU:HG3	9:N:1552:HOH:O	2.08	0.52
3:N:1205:TYR:HE1	3:N:1221:VAL:HG13	1.73	0.52
5:P:115:LYS:O	5:P:119:ILE:HG13	2.08	0.52
5:P:141:VAL:O	5:P:145:PRO:HD2	2.09	0.52
1:B:198:ARG:HD2	9:B:489:HOH:O	2.09	0.52
2:C:142:ARG:HH21	2:C:325:ILE:HD11	1.72	0.52
2:C:208:ALA:HA	2:C:218:VAL:HG22	1.91	0.52
2:C:212:GLY:HA3	2:C:218:VAL:HG23	1.90	0.52
2:C:252:LYS:HD3	2:C:296:GLY:HA2	1.91	0.52
2:C:302:VAL:O	2:C:306:THR:HG23	2.09	0.52
2:C:480:THR:HG22	2:C:482:GLU:H	1.74	0.52
3:D:403:PHE:CZ	3:D:407:VAL:HG23	2.44	0.52
3:D:720:LEU:H	3:D:720:LEU:HD12	1.73	0.52
3:D:853:VAL:HA	3:D:858:VAL:O	2.10	0.52
3:D:1189:ARG:NH1	3:D:1203:LYS:HB2	2.24	0.52
3:D:1284:GLU:HG3	9:D:1992:HOH:O	2.10	0.52
4:E:54:LEU:HD23	4:E:54:LEU:O	2.09	0.52
5:F:181:GLU:O	5:F:184:ARG:HB3	2.10	0.52
5:F:338:LEU:HD12	9:F:562:HOH:O	2.09	0.52
1:K:206:THR:HG22	1:K:209:GLU:CG	2.36	0.52
1:L:101:LEU:HD11	1:L:113:ASP:HB2	1.91	0.52
2:M:131:GLY:N	9:M:1824:HOH:O	2.43	0.52
2:M:139:GLN:HE22	2:M:415:PRO:HD2	1.74	0.52
2:M:765:SER:O	2:M:767:PRO:HD3	2.10	0.52
3:N:169:TYR:HB3	3:N:195:VAL:HG11	1.91	0.52
3:N:633:VAL:HG22	3:N:635:PRO:CD	2.39	0.52
3:N:1109:GLU:CG	3:N:1202:GLN:H	2.22	0.52
3:N:1277:ILE:CD1	3:N:1301:LYS:HB2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:63:TRP:O	4:O:67:GLU:HG3	2.09	0.52
5:P:152:ASP:HB3	5:P:153:PRO:HD3	1.92	0.52
5:P:306:GLU:HG3	9:P:674:HOH:O	2.10	0.52
5:P:363:GLU:HA	5:P:367:MET:HG3	1.91	0.52
1:B:62:LEU:H	1:B:62:LEU:HD12	1.74	0.52
1:B:71:VAL:HG22	1:B:132:LEU:CD1	2.39	0.52
1:B:156:HIS:CG	1:B:157:GLY:H	2.27	0.52
2:C:145:GLY:H	2:C:163:ILE:HG12	1.72	0.52
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.40	0.52
3:D:116:LEU:HD21	3:D:464:LEU:CB	2.38	0.52
3:D:447:VAL:HA	9:D:2047:HOH:O	2.09	0.52
3:D:567:ILE:HD12	3:D:567:ILE:N	2.24	0.52
3:D:715:ALA:O	3:D:764:LEU:HD12	2.08	0.52
3:D:774:SER:C	3:D:776:GLU:H	2.13	0.52
3:D:809:PRO:HB2	3:D:812:ALA:CB	2.40	0.52
3:D:1363:LEU:HD12	3:D:1364:HIS:O	2.10	0.52
3:D:1394:VAL:HG21	9:D:2203:HOH:O	2.08	0.52
3:D:1503:VAL:HG13	9:D:1882:HOH:O	2.09	0.52
4:E:94:PRO:HA	9:E:126:HOH:O	2.08	0.52
1:K:90:LEU:HD11	9:K:1139:HOH:O	2.09	0.52
2:M:670:GLN:O	2:M:672:VAL:HG12	2.10	0.52
3:N:52:PRO:HB2	3:N:80:VAL:HG13	1.92	0.52
3:N:400:VAL:HG22	3:N:443:VAL:CG2	2.31	0.52
3:N:473:LEU:HD21	3:N:495:ARG:CZ	2.40	0.52
3:N:504:ASP:HB3	9:N:2286:HOH:O	2.08	0.52
3:N:710:ARG:NH2	3:N:1210:SER:OG	2.43	0.52
3:N:875:THR:HG22	3:N:879:ARG:HB2	1.92	0.52
3:N:1041:LEU:HD12	3:N:1058:ARG:CA	2.38	0.52
3:N:1097:LYS:O	3:N:1101:VAL:HG23	2.09	0.52
5:P:393:THR:HG22	5:P:394:ARG:H	1.75	0.52
2:C:64:LEU:HD22	2:C:359:MET:HG3	1.91	0.52
2:C:195:LEU:HD12	2:C:234:ALA:HB1	1.91	0.52
2:C:408:ARG:HH21	2:C:542:VAL:CG2	2.23	0.52
2:C:697:ARG:HD2	2:C:699:PHE:CD1	2.45	0.52
2:C:1059:ASP:OD1	2:C:1080:SER:HB3	2.10	0.52
9:C:1344:HOH:O	3:D:603:LEU:HB3	2.09	0.52
3:D:916:TYR:CE2	3:D:920:LEU:HD13	2.45	0.52
2:M:926:PHE:O	2:M:930:LYS:HG3	2.10	0.52
3:N:637:LEU:CD1	3:N:641:GLN:HB2	2.40	0.52
3:N:1019:PRO:O	3:N:1023:MET:HG2	2.10	0.52
3:N:1272:ALA:CA	3:N:1326:THR:HB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:181:GLU:O	5:P:184:ARG:HB3	2.10	0.52
5:P:288:TYR:HA	5:P:291:ILE:HG22	1.91	0.52
1:B:5:LYS:O	1:B:8:ALA:HB2	2.09	0.52
2:C:196:LEU:O	2:C:199:VAL:HB	2.10	0.52
2:C:209:ARG:O	2:C:213:ALA:HB2	2.10	0.52
2:C:338:GLU:O	2:C:341:THR:HG22	2.10	0.52
2:C:367:LEU:HD13	9:C:1770:HOH:O	2.10	0.52
2:C:435:TYR:C	2:C:437:ARG:H	2.13	0.52
2:C:713:ARG:HH12	3:D:531:ASP:CG	2.14	0.52
2:C:722:ILE:HG13	2:C:757:GLY:O	2.10	0.52
2:C:878:SER:HB3	3:D:1029:ARG:HH11	1.74	0.52
2:C:966:LEU:HD11	2:C:986:PRO:HG2	1.91	0.52
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.45	0.52
3:D:1101:VAL:HG21	3:D:1424:VAL:CG2	2.31	0.52
3:D:1321:ALA:O	3:D:1339:LYS:HG3	2.10	0.52
4:E:54:LEU:HD23	4:E:58:PRO:HD2	1.91	0.52
5:F:151:LEU:HD21	9:F:675:HOH:O	2.08	0.52
2:M:79:PRO:HA	9:M:2242:HOH:O	2.09	0.52
2:M:165:LEU:O	2:M:265:ARG:HD2	2.10	0.52
2:M:166:PRO:HD3	2:M:265:ARG:CG	2.39	0.52
2:M:208:ALA:HA	2:M:218:VAL:HG22	1.91	0.52
2:M:402:SER:OG	2:M:566:THR:HG22	2.09	0.52
2:M:773:LEU:O	2:M:777:ILE:HG13	2.10	0.52
3:N:408:GLU:HG2	3:N:408:GLU:O	2.10	0.52
3:N:947:ILE:O	3:N:947:ILE:HD12	2.09	0.52
3:N:1283:ILE:HG22	3:N:1284:GLU:N	2.24	0.52
5:P:191:ASN:HB3	5:P:220:LEU:HD11	1.90	0.52
5:P:358:LEU:CD2	5:P:370:LYS:HZ2	2.23	0.52
1:A:55:SER:CB	1:A:158:ILE:HG21	2.40	0.52
1:A:107:LYS:HE3	1:A:113:ASP:OD2	2.10	0.52
1:B:19:GLU:O	1:B:200:TRP:HA	2.10	0.52
2:C:170:PRO:HD3	2:C:263:ASP:HB3	1.92	0.52
2:C:281:LEU:CD1	2:C:306:THR:HA	2.40	0.52
2:C:971:LYS:HE2	9:C:1494:HOH:O	2.09	0.52
3:D:77:GLY:O	3:D:78:VAL:HG23	2.10	0.52
3:D:551:ASN:O	3:D:555:LYS:HG3	2.09	0.52
3:D:697:GLY:C	9:D:1581:HOH:O	2.48	0.52
3:D:863:VAL:HG12	9:D:1596:HOH:O	2.10	0.52
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.91	0.52
3:D:1462:LEU:N	3:D:1462:LEU:HD23	2.24	0.52
5:F:88:ILE:CD1	5:F:193:ARG:HB2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:54:ILE:HG22	2:M:66:LEU:HB3	1.92	0.52
2:M:385:PHE:O	2:M:389:SER:HB3	2.10	0.52
2:M:770:GLU:CG	3:N:65:ARG:HH12	2.23	0.52
2:M:807:ARG:HD3	9:M:1889:HOH:O	2.09	0.52
2:M:911:GLU:O	2:M:915:LYS:HG2	2.10	0.52
2:M:926:PHE:CD1	2:M:929:ARG:HD3	2.44	0.52
3:N:50:PHE:CB	3:N:522:PRO:HG2	2.40	0.52
3:N:1487:VAL:HG13	3:N:1491:THR:HB	1.91	0.52
5:P:279:GLN:HA	9:P:477:HOH:O	2.10	0.52
1:A:44:LEU:HB3	1:A:177:VAL:HG21	1.91	0.52
1:A:128:HIS:CE1	1:A:131:THR:HG23	2.45	0.52
2:C:70:GLU:HB3	9:C:1236:HOH:O	2.09	0.52
2:C:207:LEU:HD22	2:C:221:LEU:CD2	2.39	0.52
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.91	0.52
3:D:162:ARG:HA	3:D:449:SER:HB3	1.91	0.52
3:D:567:ILE:HD12	3:D:567:ILE:H	1.75	0.52
3:D:675:ARG:O	3:D:678:GLU:HG2	2.10	0.52
3:D:864:VAL:HG12	3:D:865:THR:H	1.73	0.52
3:D:1481:VAL:CG1	4:E:18:ARG:HG3	2.40	0.52
4:E:54:LEU:HA	4:E:58:PRO:HG2	1.91	0.52
5:F:163:LEU:HB3	5:F:174:LEU:HD13	1.92	0.52
1:K:146:ARG:HD2	9:K:2782:HOH:O	2.10	0.52
2:M:42:VAL:HG12	2:M:43:GLY:N	2.25	0.52
2:M:197:LEU:HD22	2:M:202:TYR:CD2	2.43	0.52
2:M:676:ILE:O	3:N:948:THR:HB	2.09	0.52
2:M:816:LYS:HE2	2:M:819:VAL:HG21	1.92	0.52
3:N:631:ILE:HG12	3:N:743:ASP:O	2.10	0.52
3:N:711:LEU:C	3:N:713:ILE:H	2.12	0.52
3:N:988:ARG:O	3:N:992:ILE:HG13	2.10	0.52
1:A:5:LYS:O	1:A:8:ALA:HB2	2.08	0.51
2:C:59:LYS:HB2	9:C:1378:HOH:O	2.08	0.51
2:C:815:LEU:HG	2:C:819:VAL:CG1	2.40	0.51
2:C:918:LEU:HD23	2:C:967:PHE:O	2.09	0.51
2:C:976:ASP:HB3	2:C:979:THR:HG22	1.92	0.51
2:C:1060:ILE:CG2	2:C:1061:GLU:N	2.72	0.51
3:D:105:VAL:HG13	3:D:124:GLU:OE1	2.10	0.51
3:D:1059:SER:OG	3:D:1065:LEU:HA	2.11	0.51
3:D:1280:VAL:O	3:D:1294:VAL:HA	2.10	0.51
3:D:1494:ALA:HB1	9:E:137:HOH:O	2.10	0.51
5:F:88:ILE:CG1	5:F:193:ARG:HB2	2.41	0.51
5:F:226:LYS:HD2	5:F:242:TRP:CZ2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:57:TYR:O	1:K:140:MET:HA	2.10	0.51
1:L:9:PRO:HB3	1:L:25:LEU:HG	1.93	0.51
1:L:117:VAL:HA	9:L:1875:HOH:O	2.10	0.51
1:L:156:HIS:CG	1:L:157:GLY:H	2.28	0.51
2:M:816:LYS:HB2	2:M:819:VAL:CG2	2.39	0.51
3:N:534:ARG:HG3	5:P:312:GLN:HE22	1.74	0.51
3:N:551:ASN:O	3:N:555:LYS:HG3	2.10	0.51
3:N:957:PRO:HD2	3:N:1007:VAL:HG12	1.91	0.51
3:N:1485:GLN:NE2	4:O:80:VAL:H	2.08	0.51
4:O:51:LEU:HB2	9:O:1054:HOH:O	2.09	0.51
5:P:336:GLU:HG3	9:P:629:HOH:O	2.09	0.51
3:D:126:VAL:HG11	3:D:152:LEU:HD12	1.92	0.51
3:D:127:LEU:HD11	3:D:461:ILE:HD11	1.92	0.51
3:D:133:ILE:HG22	3:D:455:ARG:C	2.31	0.51
3:D:661:MET:HE2	3:D:673:ALA:HB1	1.92	0.51
3:D:840:LYS:HB3	3:D:841:TYR:CD2	2.46	0.51
3:D:1118:ILE:HG23	9:D:1773:HOH:O	2.09	0.51
3:D:1385:GLY:CA	3:D:1413:THR:HG21	2.39	0.51
9:D:2077:HOH:O	5:F:349:LEU:HD22	2.10	0.51
5:F:278:LEU:CB	5:F:286:PRO:HG2	2.40	0.51
1:K:69:PRO:C	1:K:71:VAL:H	2.13	0.51
9:K:1749:HOH:O	2:M:929:ARG:HG3	2.08	0.51
1:L:25:LEU:HD23	1:L:28:LEU:HD11	1.91	0.51
2:M:260:LEU:HD22	9:M:2052:HOH:O	2.10	0.51
2:M:464:LEU:HD12	2:M:465:GLY:N	2.25	0.51
2:M:498:GLN:HE21	2:M:498:GLN:HA	1.74	0.51
3:N:192:ALA:HB2	3:N:393:ILE:HD11	1.92	0.51
3:N:428:LYS:HE2	9:N:1658:HOH:O	2.11	0.51
3:N:833:GLU:HG2	9:N:2184:HOH:O	2.08	0.51
5:P:189:GLU:HA	5:P:192:LEU:HD12	1.90	0.51
1:A:42:ARG:HH21	2:C:857:ASP:HB3	1.75	0.51
2:C:2:GLU:CG	2:C:899:GLN:HB3	2.28	0.51
2:C:141:HIS:O	2:C:331:ARG:HA	2.10	0.51
2:C:631:SER:HB3	2:C:637:LEU:HD21	1.92	0.51
3:D:10:ILE:HD11	3:D:1434:TRP:NE1	2.24	0.51
3:D:187:LYS:HG3	3:D:199:LEU:CD2	2.40	0.51
3:D:1205:TYR:HE1	3:D:1221:VAL:HG13	1.75	0.51
5:F:130:VAL:HA	5:F:142:ARG:NH2	2.26	0.51
5:F:361:LEU:HD21	5:F:404:ALA:HB1	1.92	0.51
1:L:57:TYR:CZ	1:L:161:ARG:HD3	2.45	0.51
1:L:196:THR:HG22	9:L:1676:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:489:THR:HG21	9:M:2237:HOH:O	2.09	0.51
3:N:31:THR:HG23	3:N:45:PHE:HE2	1.75	0.51
3:N:39:PRO:HB3	3:N:45:PHE:C	2.31	0.51
3:N:398:ALA:HB1	3:N:446:VAL:O	2.10	0.51
3:N:861:GLN:HG2	9:N:2139:HOH:O	2.09	0.51
3:N:1342:GLU:HB3	9:N:2128:HOH:O	2.10	0.51
2:C:211:LEU:HD11	2:C:308:ARG:HA	1.93	0.51
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.92	0.51
2:C:633:GLN:HG3	9:C:1153:HOH:O	2.09	0.51
2:C:810:ASP:N	2:C:811:PRO:HD3	2.25	0.51
2:C:987:ILE:HG12	3:D:948:THR:HG21	1.91	0.51
3:D:10:ILE:HG13	3:D:1434:TRP:CE2	2.45	0.51
3:D:18:ILE:HD12	3:D:518:PRO:CG	2.40	0.51
3:D:398:ALA:HB1	3:D:446:VAL:O	2.10	0.51
3:D:879:ARG:HD3	3:D:902:LEU:O	2.10	0.51
3:D:1115:THR:HG21	9:D:2063:HOH:O	2.10	0.51
3:D:1306:PRO:HG3	9:D:1723:HOH:O	2.10	0.51
3:D:1341:PRO:O	3:D:1345:GLU:HB2	2.10	0.51
4:E:33:HIS:CB	4:E:37:ASN:HD21	2.21	0.51
4:E:60:ALA:O	4:E:63:TRP:HB2	2.10	0.51
2:M:141:HIS:CB	2:M:418:LEU:HG	2.40	0.51
2:M:191:PHE:CZ	2:M:238:LEU:HD11	2.45	0.51
2:M:218:VAL:HG12	9:M:1965:HOH:O	2.11	0.51
2:M:264:PRO:HB2	9:M:1685:HOH:O	2.11	0.51
2:M:561:GLY:HA3	2:M:842:ARG:O	2.11	0.51
2:M:897:LEU:HB3	2:M:899:GLN:HE21	1.76	0.51
3:N:111:LYS:HE2	3:N:498:VAL:HG12	1.92	0.51
3:N:1264:GLU:HG2	3:N:1425:THR:HG22	1.92	0.51
3:N:1485:GLN:O	4:O:75:PHE:HA	2.11	0.51
5:P:416:ARG:HD3	5:P:419:ARG:HD3	1.92	0.51
1:A:19:GLU:O	1:A:200:TRP:HA	2.10	0.51
1:A:182:GLU:HG2	9:A:412:HOH:O	2.11	0.51
1:A:198:ARG:C	1:A:199:ILE:HD12	2.29	0.51
2:C:114:PHE:CD1	2:C:114:PHE:N	2.77	0.51
2:C:257:VAL:HG21	9:C:1517:HOH:O	2.11	0.51
2:C:278:GLU:HB2	9:C:1544:HOH:O	2.10	0.51
2:C:420:ARG:NH1	2:C:422:ARG:HH21	2.08	0.51
2:C:874:LEU:HD23	3:D:1023:MET:CE	2.41	0.51
2:C:876:VAL:O	2:C:879:ARG:O	2.29	0.51
2:C:1105:LYS:O	2:C:1105:LYS:HG3	2.10	0.51
2:C:1109:VAL:HG21	3:D:3:LYS:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:26:VAL:HG23	9:D:2241:HOH:O	2.10	0.51
3:D:137:PRO:N	9:D:1592:HOH:O	2.43	0.51
3:D:436:GLU:HB2	9:D:2406:HOH:O	2.10	0.51
3:D:480:GLU:HG3	3:D:480:GLU:O	2.10	0.51
3:D:1258:ARG:NH2	3:D:1262:LEU:HD11	2.26	0.51
3:D:1277:ILE:CD1	3:D:1301:LYS:HB2	2.40	0.51
5:F:410:TYR:O	5:F:413:SER:HB2	2.11	0.51
1:L:133:GLU:O	1:L:134:GLU:HG2	2.10	0.51
2:M:313:LEU:HD12	2:M:313:LEU:O	2.10	0.51
2:M:349:ALA:HB3	9:M:1970:HOH:O	2.10	0.51
2:M:398:THR:N	2:M:633:GLN:OE1	2.43	0.51
2:M:606:VAL:CG2	2:M:645:VAL:HG22	2.40	0.51
2:M:685:GLU:HG3	3:N:783:ARG:HD2	1.92	0.51
3:N:65:ARG:CG	3:N:66:GLN:N	2.73	0.51
3:N:145:VAL:HG13	3:N:146:PRO:N	2.26	0.51
3:N:1145:TYR:CE2	3:N:1168:MET:HB2	2.44	0.51
4:O:33:HIS:CB	4:O:37:ASN:HD21	2.24	0.51
5:P:350:LEU:HD12	5:P:422:LEU:HD12	1.92	0.51
2:C:334:ARG:HB2	9:C:1322:HOH:O	2.09	0.51
2:C:551:GLU:HB3	2:C:906:PHE:CD2	2.46	0.51
2:C:911:GLU:O	2:C:915:LYS:HG2	2.11	0.51
3:D:97:THR:HB	9:D:1781:HOH:O	2.10	0.51
3:D:586:ARG:NH2	3:D:1444:THR:HG21	2.26	0.51
3:D:637:LEU:CD1	3:D:641:GLN:HB2	2.41	0.51
3:D:799:LYS:O	3:D:826:PRO:HD2	2.09	0.51
3:D:1372:VAL:HG13	3:D:1373:ARG:N	2.26	0.51
5:F:273:ARG:HG2	9:F:688:HOH:O	2.10	0.51
1:K:19:GLU:HB3	9:K:2538:HOH:O	2.09	0.51
1:K:49:PRO:HB3	1:K:148:VAL:HG22	1.92	0.51
1:L:23:PHE:O	1:L:196:THR:HA	2.10	0.51
2:M:244:PRO:HD2	2:M:245:GLY:H	1.75	0.51
2:M:264:PRO:HB3	2:M:289:THR:HG21	1.93	0.51
2:M:411:SER:OG	2:M:452:ILE:HG23	2.11	0.51
2:M:477:GLY:O	2:M:508:ILE:HG12	2.11	0.51
2:M:976:ASP:HB3	2:M:979:THR:HG22	1.92	0.51
3:N:34:TYR:OH	5:P:261:PRO:HD2	2.10	0.51
3:N:204:LEU:HD21	3:N:445:ARG:NH1	2.26	0.51
3:N:613:ARG:CZ	3:N:1097:LYS:HE2	2.40	0.51
3:N:1113:GLY:N	3:N:1195:GLN:NE2	2.58	0.51
5:P:370:LYS:HD3	5:P:371:LEU:HG	1.93	0.51
2:C:165:LEU:HA	2:C:166:PRO:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:264:PRO:HB3	2:C:289:THR:HG21	1.91	0.51
2:C:551:GLU:OE2	2:C:552:HIS:NE2	2.43	0.51
3:D:52:PRO:HD2	9:D:1552:HOH:O	2.10	0.51
3:D:443:VAL:HG22	3:D:444:VAL:N	2.26	0.51
3:D:820:GLU:HA	3:D:825:ALA:O	2.10	0.51
3:D:1382:THR:HG21	3:D:1418:LYS:NZ	2.25	0.51
3:D:1441:GLN:HG3	3:D:1442:ASN:N	2.25	0.51
5:F:153:PRO:HD2	9:F:614:HOH:O	2.09	0.51
1:K:11:PHE:HB2	9:K:1022:HOH:O	2.10	0.51
1:K:70:GLY:N	2:M:607:ASP:OD1	2.38	0.51
2:M:516:ARG:HD2	9:M:1937:HOH:O	2.10	0.51
2:M:676:ILE:CG2	2:M:988:VAL:HG22	2.40	0.51
2:M:881:ASN:HD22	2:M:881:ASN:H	1.59	0.51
2:M:1058:ASP:HB2	3:N:621:LYS:HE2	1.93	0.51
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.91	0.51
3:N:141:ILE:HG21	3:N:449:SER:HA	1.92	0.51
3:N:658:LEU:HD11	3:N:674:ARG:HH11	1.76	0.51
3:N:754:PHE:HE2	3:N:1476:THR:HG21	1.76	0.51
3:N:986:ARG:HG3	9:N:1540:HOH:O	2.11	0.51
3:N:996:TRP:O	3:N:999:THR:HG22	2.11	0.51
3:N:1382:THR:HG21	3:N:1418:LYS:HE3	1.92	0.51
1:A:1:MET:HB3	9:A:440:HOH:O	2.10	0.51
1:A:49:PRO:O	1:A:173:PRO:HG2	2.10	0.51
2:C:334:ARG:NH1	2:C:415:PRO:HG2	2.25	0.51
3:D:687:VAL:HG13	9:D:2185:HOH:O	2.11	0.51
3:D:1101:VAL:CA	3:D:1428:ALA:HB2	2.40	0.51
3:D:1120:VAL:HB	3:D:1144:LEU:HD21	1.92	0.51
3:D:1243:THR:HG22	3:D:1244:GLY:H	1.76	0.51
3:D:1305:LEU:HD22	3:D:1309:ALA:HB1	1.92	0.51
4:E:17:TYR:N	4:E:17:TYR:CD2	2.78	0.51
5:F:339:PRO:HB3	5:F:343:ASP:HB2	1.92	0.51
1:K:180:GLN:HE22	2:M:929:ARG:HH21	1.59	0.51
2:M:98:LEU:HG	9:M:1826:HOH:O	2.10	0.51
2:M:208:ALA:HA	2:M:221:LEU:HD21	1.93	0.51
2:M:244:PRO:HG2	2:M:246:ASP:OD2	2.09	0.51
2:M:260:LEU:HA	2:M:291:ALA:HB2	1.91	0.51
2:M:333:ILE:HB	9:M:1750:HOH:O	2.10	0.51
2:M:1105:LYS:O	2:M:1107:ASN:N	2.44	0.51
3:N:14:SER:O	3:N:17:LYS:N	2.44	0.51
3:N:434:ARG:HB2	3:N:447:VAL:CG2	2.41	0.51
3:N:563:PRO:HG2	3:N:566:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:866:VAL:HG12	3:N:867:ARG:N	2.25	0.51
3:N:957:PRO:CD	3:N:1007:VAL:HG12	2.40	0.51
3:N:1250:ALA:HB2	9:N:1888:HOH:O	2.09	0.51
7:N:1527:MXP:H11A	9:N:1557:HOH:O	2.11	0.51
4:O:41:GLU:N	4:O:42:PRO:CD	2.74	0.51
5:P:103:ALA:HB3	9:P:455:HOH:O	2.11	0.51
2:C:6:PHE:CB	2:C:909:ALA:HA	2.40	0.51
2:C:129:ILE:CG1	2:C:386:PHE:HB3	2.41	0.51
2:C:275:TYR:HB2	9:C:1736:HOH:O	2.10	0.51
2:C:305:PRO:CA	2:C:308:ARG:HB2	2.41	0.51
2:C:676:ILE:O	2:C:676:ILE:CG2	2.56	0.51
2:C:742:VAL:HG12	2:C:743:VAL:N	2.26	0.51
3:D:46:ASP:OD2	3:D:48:ARG:HG2	2.11	0.51
3:D:50:PHE:HB3	3:D:522:PRO:HG2	1.91	0.51
3:D:633:VAL:O	3:D:633:VAL:HG13	2.11	0.51
3:D:661:MET:O	3:D:664:LYS:O	2.28	0.51
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.11	0.51
4:E:41:GLU:N	4:E:42:PRO:CD	2.72	0.51
5:F:260:ILE:CG2	5:F:264:MET:HB2	2.40	0.51
1:K:25:LEU:HB2	9:K:1260:HOH:O	2.11	0.51
1:L:128:HIS:CE1	1:L:131:THR:HG23	2.46	0.51
2:M:267:TYR:HD1	9:M:2269:HOH:O	1.94	0.51
2:M:644:VAL:HG22	2:M:647:GLN:OE1	2.11	0.51
3:N:399:ARG:HD2	9:N:1669:HOH:O	2.09	0.51
3:N:569:ASN:HB3	5:P:214:GLN:NE2	2.25	0.51
5:P:163:LEU:HD22	5:P:174:LEU:HD12	1.91	0.51
1:A:9:PRO:HD2	1:B:224:TYR:CE1	2.46	0.51
1:B:68:ILE:HG23	1:B:137:ARG:NH1	2.25	0.51
2:C:18:LEU:HD21	2:C:542:VAL:CG1	2.41	0.51
2:C:498:GLN:HA	2:C:498:GLN:NE2	2.26	0.51
2:C:952:LEU:HD22	9:C:1205:HOH:O	2.10	0.51
3:D:134:VAL:HG12	3:D:152:LEU:HB3	1.93	0.51
3:D:141:ILE:CG2	3:D:450:TYR:H	2.24	0.51
3:D:162:ARG:HD2	3:D:434:ARG:CZ	2.41	0.51
3:D:407:VAL:HG13	3:D:422:ALA:HB2	1.92	0.51
3:D:537:THR:C	5:F:317:LEU:HB2	2.32	0.51
3:D:581:LEU:O	3:D:603:LEU:HG	2.11	0.51
3:D:761:ILE:HG21	9:E:116:HOH:O	2.11	0.51
3:D:1145:TYR:CE2	3:D:1168:MET:HB2	2.45	0.51
3:D:1393:GLN:HB2	3:D:1398:TRP:CE2	2.46	0.51
1:K:89:PHE:HB3	1:K:94:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:50:GLY:HA3	1:L:171:PHE:O	2.11	0.51
2:M:437:ARG:HH22	2:M:491:GLU:CB	2.24	0.51
2:M:603:VAL:HG21	2:M:643:VAL:CG1	2.35	0.51
2:M:979:THR:HG23	2:M:981:GLU:N	2.24	0.51
3:N:569:ASN:HD21	5:P:210:LEU:CD2	2.22	0.51
3:N:615:ARG:O	3:N:617:ASN:N	2.44	0.51
3:N:820:GLU:HA	3:N:825:ALA:O	2.11	0.51
3:N:1280:VAL:O	3:N:1294:VAL:HA	2.11	0.51
9:N:2109:HOH:O	5:P:164:LYS:HE3	2.10	0.51
1:A:16:GLN:HG2	1:A:16:GLN:O	2.10	0.50
1:A:57:TYR:O	1:A:140:MET:HA	2.11	0.50
1:A:216:GLU:HG2	9:A:422:HOH:O	2.10	0.50
2:C:42:VAL:HG23	9:C:1299:HOH:O	2.10	0.50
2:C:861:LEU:HD21	2:C:925:TYR:HE2	1.76	0.50
2:C:890:LEU:HD12	2:C:914:ILE:HD13	1.93	0.50
2:C:942:GLU:O	2:C:945:ARG:HB3	2.11	0.50
3:D:6:ARG:HD3	9:D:1692:HOH:O	2.11	0.50
3:D:448:GLU:HA	9:D:2218:HOH:O	2.11	0.50
3:D:1147:ARG:HD2	3:D:1188:VAL:HG21	1.92	0.50
5:F:209:PHE:CE2	5:F:213:ILE:HD11	2.45	0.50
2:M:68:PHE:HE1	2:M:96:ALA:HB1	1.76	0.50
2:M:139:GLN:HE21	2:M:334:ARG:HD2	1.77	0.50
2:M:157:ARG:NH2	2:M:314:THR:O	2.44	0.50
2:M:275:TYR:HD2	9:M:1681:HOH:O	1.94	0.50
2:M:289:THR:O	2:M:291:ALA:N	2.44	0.50
2:M:358:ARG:HD3	2:M:371:LYS:O	2.11	0.50
2:M:463:GLU:HB3	9:M:1990:HOH:O	2.09	0.50
2:M:502:PRO:HB2	2:M:509:ALA:HB3	1.93	0.50
2:M:736:ASP:C	2:M:738:ASP:H	2.13	0.50
2:M:755:LEU:HD12	9:M:1781:HOH:O	2.10	0.50
3:N:137:PRO:HD2	3:N:453:ASP:OD2	2.11	0.50
3:N:955:VAL:O	3:N:1039:CYS:HB3	2.11	0.50
5:P:372:ARG:HD3	9:P:506:HOH:O	2.11	0.50
2:C:290:LEU:HB3	2:C:302:VAL:CG1	2.41	0.50
3:D:421:LEU:CG	3:D:429:SER:HB3	2.42	0.50
3:D:627:GLY:O	3:D:747:VAL:HG12	2.12	0.50
3:D:1018:ASN:HB3	3:D:1021:TYR:HB3	1.92	0.50
4:E:45:ARG:HH21	4:E:55:PHE:HB3	1.75	0.50
5:F:88:ILE:HD13	5:F:193:ARG:HB2	1.93	0.50
5:F:287:THR:HG23	5:F:289:GLU:HB3	1.92	0.50
1:K:179:PHE:HZ	2:M:939:ARG:HH22	1.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:69:PRO:C	1:L:71:VAL:H	2.13	0.50
2:M:573:ARG:HH12	2:M:697:ARG:HB3	1.75	0.50
2:M:671:ASN:ND2	2:M:671:ASN:H	2.08	0.50
2:M:710:ILE:CD1	2:M:790:LEU:HB2	2.41	0.50
2:M:930:LYS:HA	9:M:1678:HOH:O	2.11	0.50
3:N:9:ARG:HE	3:N:11:ALA:HB2	1.75	0.50
1:A:50:GLY:O	1:A:146:ARG:HA	2.11	0.50
2:C:41:ASN:H	2:C:41:ASN:ND2	1.97	0.50
2:C:181:VAL:HG11	9:C:1754:HOH:O	2.10	0.50
2:C:185:LYS:CE	2:C:190:LYS:HE2	2.40	0.50
2:C:480:THR:HG22	2:C:481:ASP:H	1.76	0.50
2:C:756:VAL:HG21	2:C:823:VAL:HG11	1.92	0.50
2:C:877:PRO:CG	3:D:1023:MET:HE2	2.36	0.50
2:C:1051:GLU:HG2	2:C:1056:LYS:HD2	1.93	0.50
2:C:1115:LEU:HD23	3:D:85:VAL:HG13	1.94	0.50
3:D:800:LYS:NZ	3:D:804:LEU:HD13	2.26	0.50
5:F:361:LEU:HD13	5:F:366:ALA:CB	2.42	0.50
2:M:136:ILE:CG2	2:M:336:VAL:HG22	2.41	0.50
2:M:253:ALA:O	2:M:256:TYR:HB2	2.11	0.50
2:M:274:ARG:HG2	9:M:1662:HOH:O	2.10	0.50
2:M:334:ARG:NH2	2:M:418:LEU:HD11	2.26	0.50
2:M:470:PRO:HD3	2:M:485:TYR:CE2	2.46	0.50
3:N:52:PRO:CG	3:N:80:VAL:HG13	2.41	0.50
3:N:414:ARG:HB3	9:N:2299:HOH:O	2.11	0.50
3:N:1299:PHE:N	3:N:1299:PHE:CD2	2.79	0.50
3:N:1495:ILE:HA	4:O:88:GLU:OE2	2.11	0.50
4:O:49:GLN:HB3	9:O:1772:HOH:O	2.11	0.50
1:A:183:ASP:HB3	9:A:322:HOH:O	2.11	0.50
2:C:42:VAL:HG12	2:C:43:GLY:N	2.23	0.50
2:C:578:VAL:HG11	2:C:991:GLN:HB3	1.93	0.50
2:C:759:THR:HB	2:C:785:VAL:CG2	2.41	0.50
3:D:543:LEU:HB2	9:D:1714:HOH:O	2.10	0.50
3:D:1276:GLU:HG3	3:D:1303:TYR:OH	2.12	0.50
3:D:1466:VAL:CG2	3:D:1472:ILE:HD11	2.36	0.50
3:D:1495:ILE:HD12	4:E:88:GLU:OE2	2.11	0.50
5:F:85:LEU:HD11	9:F:543:HOH:O	2.11	0.50
5:F:141:VAL:O	5:F:145:PRO:HD2	2.12	0.50
5:F:363:GLU:HA	5:F:367:MET:HG3	1.93	0.50
1:K:9:PRO:HB3	1:K:25:LEU:CD2	2.41	0.50
2:M:274:ARG:HG2	2:M:274:ARG:O	2.10	0.50
2:M:837:ASP:O	2:M:848:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:877:PRO:HG3	3:N:1020:LEU:CD1	2.41	0.50
2:M:1019:GLN:NE2	3:N:621:LYS:HA	2.22	0.50
3:N:561:GLY:CA	5:P:184:ARG:HH12	2.23	0.50
3:N:1189:ARG:HD3	9:N:1595:HOH:O	2.10	0.50
2:C:73:LEU:HD23	2:C:94:LEU:HD13	1.93	0.50
2:C:93:PRO:HG3	2:C:117:HIS:HE1	1.76	0.50
2:C:604:ALA:HB3	2:C:612:VAL:O	2.12	0.50
2:C:1005:MET:HE2	3:D:648:MET:HB2	1.94	0.50
3:D:145:VAL:HG22	3:D:146:PRO:CD	2.41	0.50
3:D:610:LYS:CG	7:D:1527:MXP:C15	2.90	0.50
3:D:1192:LEU:HD13	3:D:1345:GLU:HG2	1.94	0.50
3:D:1223:ILE:H	3:D:1223:ILE:CD1	2.22	0.50
4:E:9:LEU:HD22	4:E:19:LEU:HD11	1.94	0.50
5:F:288:TYR:HA	5:F:291:ILE:HG22	1.92	0.50
2:M:78:PHE:CG	2:M:88:LEU:HD21	2.46	0.50
2:M:96:ALA:HB3	9:M:1826:HOH:O	2.10	0.50
2:M:186:VAL:HG23	2:M:187:ASN:H	1.75	0.50
2:M:227:PHE:HA	2:M:237:ARG:HH12	1.75	0.50
2:M:290:LEU:HD23	2:M:290:LEU:H	1.76	0.50
2:M:545:ASN:O	2:M:581:THR:HG21	2.11	0.50
2:M:565:GLN:HG2	2:M:995:MET:HE2	1.93	0.50
3:N:34:TYR:OH	5:P:264:MET:HG3	2.11	0.50
3:N:627:GLY:O	3:N:747:VAL:HG12	2.12	0.50
3:N:728:LEU:HD22	3:N:745:MET:SD	2.52	0.50
3:N:970:LYS:HD3	9:N:2041:HOH:O	2.12	0.50
3:N:1128:VAL:HG13	9:N:2137:HOH:O	2.12	0.50
3:N:1481:VAL:HG13	4:O:18:ARG:HG3	1.93	0.50
5:P:214:GLN:O	5:P:217:ASN:HB2	2.12	0.50
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.47	0.50
2:C:6:PHE:HB2	2:C:908:GLY:C	2.32	0.50
2:C:897:LEU:HB3	2:C:899:GLN:HG2	1.93	0.50
3:D:11:ALA:HB1	3:D:507:ASN:OD1	2.12	0.50
3:D:641:GLN:HG2	9:D:1610:HOH:O	2.10	0.50
4:E:64:ALA:HA	4:E:67:GLU:OE1	2.12	0.50
5:F:88:ILE:CG2	5:F:193:ARG:HH11	2.24	0.50
1:K:18:ARG:HH11	1:K:123:MET:CE	2.21	0.50
1:K:19:GLU:O	1:K:200:TRP:HA	2.12	0.50
2:M:110:GLU:HB3	9:M:2230:HOH:O	2.10	0.50
2:M:153:ALA:O	2:M:155:PRO:HD3	2.12	0.50
2:M:269:LEU:HB3	9:M:2007:HOH:O	2.11	0.50
2:M:496:ILE:H	2:M:496:ILE:HD12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:517:ARG:HB2	9:M:2072:HOH:O	2.12	0.50
2:M:762:LYS:HG2	2:M:763:GLY:H	1.76	0.50
2:M:795:GLY:HA3	2:M:1004:LYS:HE2	1.93	0.50
3:N:403:PHE:HE2	3:N:443:VAL:N	2.10	0.50
3:N:567:ILE:HD12	3:N:567:ILE:H	1.77	0.50
3:N:699:VAL:HG12	3:N:717:GLN:HA	1.93	0.50
3:N:1128:VAL:HG11	9:N:1633:HOH:O	2.10	0.50
3:N:1408:ILE:O	3:N:1409:ALA:C	2.47	0.50
5:P:392:VAL:HG11	5:P:396:ARG:CD	2.41	0.50
1:A:106:PRO:HG3	1:A:134:GLU:HG3	1.93	0.50
2:C:64:LEU:HD13	2:C:359:MET:CG	2.41	0.50
2:C:197:LEU:HB3	2:C:202:TYR:HB2	1.92	0.50
2:C:244:PRO:CD	2:C:245:GLY:H	2.24	0.50
2:C:689:VAL:HB	2:C:870:ILE:HG13	1.93	0.50
2:C:808:ARG:HA	2:C:815:LEU:HD22	1.92	0.50
2:C:811:PRO:HD2	2:C:813:VAL:HG22	1.93	0.50
2:C:1004:LYS:HA	9:C:1776:HOH:O	2.11	0.50
3:D:418:GLY:N	3:D:429:SER:O	2.35	0.50
3:D:630:VAL:CA	3:D:744:GLN:HG2	2.38	0.50
3:D:753:SER:HB3	9:E:134:HOH:O	2.11	0.50
3:D:800:LYS:HE2	3:D:804:LEU:HD13	1.94	0.50
3:D:862:ASP:O	3:D:876:SER:HB2	2.12	0.50
3:D:1216:SER:HB3	9:D:2106:HOH:O	2.11	0.50
4:E:38:THR:HG22	9:E:103:HOH:O	2.12	0.50
5:F:196:VAL:HG13	5:F:213:ILE:HD11	1.94	0.50
5:F:282:LEU:HD12	9:F:487:HOH:O	2.11	0.50
1:K:186:LEU:CB	1:K:192:LEU:HD11	2.40	0.50
1:L:4:SER:HA	1:L:7:LYS:HG2	1.93	0.50
1:L:19:GLU:O	1:L:200:TRP:HA	2.12	0.50
2:M:878:SER:HB3	3:N:1029:ARG:HH11	1.75	0.50
3:N:630:VAL:CA	3:N:744:GLN:HG2	2.39	0.50
3:N:716:PHE:CE2	3:N:765:SER:HB3	2.47	0.50
3:N:806:PHE:HE1	3:N:813:LEU:HB3	1.74	0.50
3:N:1310:ARG:HG3	3:N:1327:ARG:HB3	1.94	0.50
5:P:163:LEU:HB3	5:P:174:LEU:HD13	1.93	0.50
2:C:650:ARG:HB2	2:C:653:ASP:HB2	1.93	0.50
2:C:1096:ALA:O	3:D:13:ALA:CB	2.60	0.50
3:D:999:THR:O	3:D:1003:VAL:HG13	2.12	0.50
3:D:1281:VAL:HG21	3:D:1313:VAL:CG2	2.42	0.50
3:D:1295:GLU:HB3	3:D:1300:SER:OG	2.12	0.50
5:F:406:ARG:O	5:F:409:LYS:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:216:GLU:O	1:K:220:GLU:HG3	2.11	0.50
2:M:57:GLU:O	2:M:62:GLY:HA3	2.11	0.50
2:M:145:GLY:H	2:M:163:ILE:HG12	1.76	0.50
2:M:618:GLY:HA2	9:M:1827:HOH:O	2.10	0.50
2:M:876:VAL:O	2:M:879:ARG:O	2.29	0.50
4:O:89:MET:HA	9:O:1936:HOH:O	2.12	0.50
1:A:73:GLU:HG3	9:A:363:HOH:O	2.11	0.50
1:A:85:LEU:HB2	1:A:127:LEU:HD21	1.94	0.50
2:C:32:ALA:HB2	2:C:73:LEU:HD11	1.93	0.50
2:C:70:GLU:HA	9:C:1632:HOH:O	2.12	0.50
2:C:165:LEU:HD12	2:C:166:PRO:C	2.32	0.50
2:C:262:ALA:O	2:C:264:PRO:O	2.30	0.50
2:C:584:GLU:CD	2:C:584:GLU:H	2.14	0.50
2:C:605:LYS:HB2	9:C:1120:HOH:O	2.11	0.50
2:C:1034:GLU:CA	2:C:1037:VAL:HG23	2.42	0.50
3:D:520:LEU:O	3:D:525:ARG:NH1	2.45	0.50
3:D:614:PHE:HB3	3:D:617:ASN:HB3	1.94	0.50
3:D:1214:PRO:HB2	9:D:2327:HOH:O	2.11	0.50
4:E:40:LEU:HD22	9:E:124:HOH:O	2.11	0.50
4:E:45:ARG:HB2	4:E:46:PRO:CD	2.42	0.50
4:E:70:THR:HG22	4:E:71:GLY:N	2.27	0.50
5:F:167:PRO:HB2	5:F:169:GLU:OE1	2.12	0.50
1:K:34:VAL:HG22	2:M:939:ARG:NH2	2.27	0.50
1:K:211:LEU:HD12	1:K:211:LEU:O	2.11	0.50
2:M:580:MET:HB3	2:M:584:GLU:CD	2.32	0.50
2:M:713:ARG:NH2	3:N:531:ASP:HB3	2.27	0.50
2:M:729:LEU:HD13	3:N:675:ARG:CZ	2.42	0.50
2:M:1116:ALA:HA	9:M:2070:HOH:O	2.12	0.50
3:N:19:ARG:HG2	9:N:2118:HOH:O	2.11	0.50
3:N:129:PHE:O	3:N:572:ARG:HG2	2.11	0.50
3:N:131:LYS:HE3	3:N:568:ARG:HB2	1.94	0.50
3:N:394:LEU:HD11	9:N:1920:HOH:O	2.11	0.50
3:N:1209:LEU:HD13	9:N:1985:HOH:O	2.12	0.50
3:N:1310:ARG:NE	3:N:1327:ARG:HB3	2.27	0.50
5:P:278:LEU:CB	5:P:286:PRO:HG2	2.42	0.50
5:P:358:LEU:HD21	5:P:367:MET:CE	2.42	0.50
5:P:358:LEU:HD13	5:P:370:LYS:CG	2.42	0.50
2:C:461:VAL:HG12	2:C:462:ASP:O	2.12	0.49
3:D:696:HIS:HB2	4:E:48:MET:CE	2.42	0.49
3:D:1147:ARG:HB3	3:D:1188:VAL:HG23	1.93	0.49
3:D:1383:ASP:HB2	3:D:1416:ALA:CB	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:74:VAL:HA	9:E:163:HOH:O	2.12	0.49
5:F:113:ILE:HG23	5:F:127:ILE:CG2	2.42	0.49
5:F:189:GLU:HA	5:F:192:LEU:HD12	1.94	0.49
1:L:211:LEU:O	1:L:214:ALA:HB3	2.12	0.49
2:M:36:PRO:HG2	2:M:70:GLU:HB3	1.94	0.49
2:M:196:LEU:O	2:M:199:VAL:HB	2.12	0.49
2:M:498:GLN:HB2	9:M:2088:HOH:O	2.11	0.49
2:M:1034:GLU:CA	2:M:1037:VAL:HG23	2.42	0.49
3:N:148:GLU:HG2	3:N:151:GLN:HE21	1.77	0.49
3:N:409:VAL:HB	3:N:421:LEU:HA	1.93	0.49
3:N:516:ALA:O	3:N:518:PRO:HD3	2.12	0.49
3:N:675:ARG:O	3:N:678:GLU:HG2	2.12	0.49
3:N:1003:VAL:O	3:N:1006:ALA:HB3	2.12	0.49
3:N:1353:GLN:NE2	3:N:1363:LEU:O	2.43	0.49
3:N:1389:LEU:HD12	3:N:1390:LEU:HG	1.94	0.49
5:P:115:LYS:HD2	5:P:173:TYR:CE2	2.47	0.49
5:P:187:LEU:O	5:P:187:LEU:HD23	2.11	0.49
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.32	0.49
1:B:25:LEU:HD23	1:B:28:LEU:HD11	1.94	0.49
1:B:85:LEU:HG	9:B:527:HOH:O	2.10	0.49
2:C:252:LYS:HB3	2:C:298:PHE:HZ	1.77	0.49
2:C:358:ARG:HG3	9:C:1597:HOH:O	2.11	0.49
2:C:523:ILE:HG22	9:C:1356:HOH:O	2.12	0.49
2:C:626:ARG:HB2	2:C:639:GLN:HE21	1.77	0.49
2:C:684:PHE:HE2	3:D:733:CYS:SG	2.35	0.49
2:C:789:SER:O	2:C:791:ARG:HG3	2.12	0.49
2:C:1087:VAL:HG12	3:D:610:LYS:NZ	2.27	0.49
3:D:17:LYS:HB2	9:D:1656:HOH:O	2.12	0.49
3:D:39:PRO:HB3	3:D:45:PHE:C	2.33	0.49
3:D:99:ALA:HB1	3:D:575:GLN:OE1	2.11	0.49
3:D:119:SER:HB2	3:D:123:LEU:CB	2.36	0.49
5:F:151:LEU:HD22	9:F:737:HOH:O	2.12	0.49
1:K:57:TYR:CE2	1:K:59:GLU:HA	2.46	0.49
2:M:305:PRO:CA	2:M:308:ARG:HB2	2.42	0.49
2:M:403:SER:O	2:M:407:LYS:HG3	2.12	0.49
1:A:189:ARG:HG3	9:A:334:HOH:O	2.12	0.49
2:C:435:TYR:OH	2:C:498:GLN:NE2	2.44	0.49
2:C:607:ASP:HB2	2:C:610:ARG:HG3	1.95	0.49
2:C:722:ILE:HG21	2:C:821:GLU:OE1	2.12	0.49
2:C:926:PHE:CD1	2:C:929:ARG:HD3	2.46	0.49
3:D:27:GLU:HA	9:D:2102:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:65:ARG:HB2	5:F:375:LEU:O	2.11	0.49
3:D:465:LEU:HD22	3:D:509:PRO:O	2.12	0.49
3:D:540:LEU:HA	3:D:543:LEU:HD12	1.94	0.49
3:D:656:PHE:HB3	3:D:694:VAL:HG11	1.93	0.49
3:D:984:THR:CG2	3:D:987:GLU:H	2.25	0.49
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.12	0.49
3:D:1291:SER:HB2	3:D:1293:PHE:CE1	2.45	0.49
3:D:1307:LYS:HE3	9:D:2288:HOH:O	2.12	0.49
3:D:1388:ARG:HG3	3:D:1389:LEU:N	2.26	0.49
3:D:1420:LEU:HD12	3:D:1421:LEU:N	2.26	0.49
5:F:259:ARG:HA	9:F:658:HOH:O	2.12	0.49
1:K:134:GLU:HG2	9:K:1422:HOH:O	2.11	0.49
1:L:12:THR:OG1	1:L:24:VAL:HB	2.12	0.49
2:M:191:PHE:CD2	2:M:195:LEU:HD23	2.48	0.49
2:M:302:VAL:O	2:M:306:THR:HG23	2.11	0.49
2:M:338:GLU:O	2:M:341:THR:HG22	2.12	0.49
2:M:629:TYR:HB3	9:M:1712:HOH:O	2.11	0.49
2:M:679:PHE:C	3:N:943:THR:HG22	2.33	0.49
2:M:897:LEU:HB3	2:M:899:GLN:HG2	1.94	0.49
2:M:1115:LEU:CD2	3:N:85:VAL:HG13	2.40	0.49
3:N:862:ASP:O	3:N:877:PRO:HD3	2.13	0.49
3:N:928:ALA:O	3:N:931:LEU:HB2	2.12	0.49
4:O:72:ARG:HB2	9:O:4461:HOH:O	2.12	0.49
5:P:299:TRP:CE3	5:P:303:ARG:HD3	2.46	0.49
5:P:361:LEU:HD21	5:P:404:ALA:HB1	1.93	0.49
2:C:21:ILE:O	2:C:25:SER:HB2	2.13	0.49
2:C:163:ILE:HG21	9:C:1347:HOH:O	2.11	0.49
2:C:625:LEU:O	2:C:627:ARG:N	2.46	0.49
2:C:775:ARG:HG2	9:C:1674:HOH:O	2.12	0.49
2:C:810:ASP:N	2:C:811:PRO:CD	2.75	0.49
3:D:14:SER:O	3:D:17:LYS:N	2.46	0.49
3:D:145:VAL:HG13	3:D:146:PRO:N	2.28	0.49
3:D:787:LEU:HD21	3:D:947:ILE:CD1	2.43	0.49
3:D:957:PRO:HG3	3:D:1010:ASN:HD22	1.77	0.49
3:D:1209:LEU:HD21	4:E:16:LYS:HD2	1.94	0.49
3:D:1396:GLU:O	3:D:1400:VAL:HG23	2.12	0.49
2:M:443:THR:CG2	2:M:449:ILE:HG13	2.42	0.49
2:M:810:ASP:N	2:M:811:PRO:CD	2.75	0.49
2:M:1060:ILE:HB	9:M:1724:HOH:O	2.12	0.49
3:N:141:ILE:HG23	3:N:161:LEU:HD21	1.95	0.49
3:N:502:PHE:CE1	3:N:509:PRO:HB3	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:820:GLU:HG2	3:N:825:ALA:O	2.13	0.49
3:N:1066:THR:CG2	3:N:1069:GLU:HG3	2.42	0.49
3:N:1262:LEU:HD23	3:N:1352:ILE:HG12	1.93	0.49
3:N:1372:VAL:HA	3:N:1375:MET:SD	2.53	0.49
5:P:185:GLN:O	5:P:189:GLU:HG3	2.12	0.49
5:P:369:LEU:HD11	5:P:401:GLU:HB2	1.94	0.49
1:B:86:VAL:HG12	1:B:124:ASN:ND2	2.18	0.49
1:B:149:GLY:O	1:B:171:PHE:HB2	2.13	0.49
2:C:85:GLU:OE2	2:C:802:ARG:NH2	2.45	0.49
3:D:481:MET:HG3	3:D:1388:ARG:NH2	2.27	0.49
3:D:527:MET:HB3	9:D:1582:HOH:O	2.11	0.49
3:D:1159:ARG:HB3	3:D:1159:ARG:CZ	2.43	0.49
3:D:1463:LYS:HB2	7:D:1527:MXP:H23B	1.95	0.49
5:F:364:ARG:HD2	9:F:435:HOH:O	2.12	0.49
2:M:678:PRO:O	3:N:943:THR:HA	2.11	0.49
2:M:818:GLY:N	5:P:309:LYS:HE2	2.26	0.49
2:M:985:GLY:C	9:N:1555:HOH:O	2.49	0.49
3:N:149:LYS:HA	9:N:2241:HOH:O	2.12	0.49
3:N:207:PHE:HA	9:N:1567:HOH:O	2.12	0.49
3:N:827:ILE:O	3:N:837:GLY:HA3	2.13	0.49
3:N:895:VAL:O	3:N:899:LEU:HG	2.12	0.49
5:P:299:TRP:HE3	9:P:492:HOH:O	1.94	0.49
1:A:133:GLU:HG2	1:A:134:GLU:H	1.77	0.49
2:C:113:VAL:HB	2:C:115:LEU:HD23	1.95	0.49
2:C:1004:LYS:HG3	9:C:1776:HOH:O	2.12	0.49
3:D:409:VAL:HB	3:D:421:LEU:HA	1.94	0.49
3:D:674:ARG:HD3	9:D:1564:HOH:O	2.11	0.49
3:D:767:HIS:CD2	4:E:6:ILE:HG12	2.47	0.49
3:D:1283:ILE:HB	3:D:1315:ASP:OD2	2.13	0.49
1:L:158:ILE:HG12	9:L:3428:HOH:O	2.13	0.49
2:M:5:ARG:HB3	2:M:902:ILE:HB	1.93	0.49
2:M:101:ILE:HG23	2:M:107:LEU:CD2	2.41	0.49
2:M:139:GLN:CD	2:M:418:LEU:HD22	2.33	0.49
2:M:209:ARG:O	2:M:213:ALA:HB2	2.12	0.49
2:M:364:GLU:O	2:M:367:LEU:HD21	2.12	0.49
2:M:442:GLU:HG2	2:M:454:SER:OG	2.12	0.49
3:N:185:VAL:HG22	3:N:203:ALA:HB2	1.95	0.49
3:N:527:MET:HE2	5:P:258:ILE:HD11	1.94	0.49
3:N:736:PHE:O	3:N:738:ALA:N	2.46	0.49
3:N:1393:GLN:CB	3:N:1398:TRP:HE1	2.20	0.49
3:N:1435:LEU:HA	9:N:1677:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:209:PHE:O	5:P:213:ILE:HG13	2.12	0.49
5:P:358:LEU:HD22	5:P:370:LYS:HE3	1.94	0.49
1:A:176:ARG:O	1:A:200:TRP:HE3	1.96	0.49
2:C:44:ILE:HG23	2:C:344:PHE:CE1	2.48	0.49
2:C:191:PHE:CD2	2:C:195:LEU:HD23	2.47	0.49
2:C:622:GLU:HB3	9:C:1635:HOH:O	2.12	0.49
2:C:681:GLY:O	3:D:633:VAL:HG21	2.12	0.49
2:C:722:ILE:O	2:C:722:ILE:HG23	2.13	0.49
2:C:815:LEU:HD23	2:C:819:VAL:O	2.12	0.49
2:C:816:LYS:O	2:C:819:VAL:HB	2.12	0.49
3:D:53:ILE:HG23	3:D:54:LYS:H	1.78	0.49
3:D:521:PRO:O	3:D:525:ARG:HG2	2.13	0.49
3:D:530:VAL:HG13	9:D:2079:HOH:O	2.12	0.49
3:D:664:LYS:HA	9:D:1859:HOH:O	2.12	0.49
3:D:988:ARG:O	3:D:992:ILE:HG13	2.13	0.49
3:D:1114:THR:HG23	3:D:1116:ASN:HD21	1.78	0.49
3:D:1177:ALA:CB	3:D:1183:ILE:HD11	2.42	0.49
3:D:1189:ARG:HH11	3:D:1203:LYS:HB2	1.77	0.49
3:D:1272:ALA:CA	3:D:1326:THR:HB	2.41	0.49
5:F:295:MET:HG2	5:F:299:TRP:CD2	2.47	0.49
1:L:2:LEU:HD12	1:L:3:ASP:HB2	1.95	0.49
2:M:93:PRO:HG3	2:M:117:HIS:HE1	1.76	0.49
2:M:136:ILE:HG21	2:M:336:VAL:HG13	1.93	0.49
2:M:185:LYS:HE2	2:M:190:LYS:HG2	1.95	0.49
2:M:358:ARG:HA	2:M:361:MET:HB2	1.95	0.49
2:M:923:GLU:O	2:M:927:GLY:HA3	2.12	0.49
2:M:1109:VAL:HA	3:N:3:LYS:HE3	1.93	0.49
3:N:28:LYS:CG	3:N:41:ARG:HH11	2.25	0.49
3:N:443:VAL:HG22	3:N:444:VAL:H	1.77	0.49
3:N:1066:THR:HG22	3:N:1069:GLU:CG	2.42	0.49
3:N:1128:VAL:O	3:N:1129:THR:C	2.49	0.49
3:N:1246:VAL:HG13	3:N:1269:LYS:NZ	2.28	0.49
5:P:287:THR:HG23	5:P:289:GLU:HB3	1.93	0.49
1:B:73:GLU:CD	1:B:130:ALA:HA	2.32	0.49
2:C:332:ARG:CZ	2:C:464:LEU:HD11	2.43	0.49
2:C:420:ARG:HG3	2:C:422:ARG:HG2	1.95	0.49
9:C:1813:HOH:O	3:D:532:GLY:HA3	2.13	0.49
3:D:122:GLU:O	3:D:126:VAL:HG23	2.13	0.49
3:D:507:ASN:HB2	9:D:1793:HOH:O	2.12	0.49
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.33	0.49
3:D:937:TYR:O	3:D:941:PHE:HD1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.95	0.49
4:E:23:VAL:HG12	4:E:61:VAL:HG13	1.95	0.49
5:F:81:VAL:O	5:F:85:LEU:HB2	2.12	0.49
2:M:139:GLN:HE22	2:M:415:PRO:CD	2.26	0.49
2:M:331:ARG:NH1	2:M:427:VAL:HG12	2.27	0.49
2:M:352:ALA:HA	2:M:355:VAL:CG1	2.43	0.49
2:M:506:ASN:HB2	9:M:1906:HOH:O	2.12	0.49
2:M:967:PHE:CD1	2:M:972:VAL:HG12	2.47	0.49
3:N:128:TYR:CE1	3:N:461:ILE:HG13	2.47	0.49
3:N:1161:GLU:HG3	3:N:1164:ARG:CB	2.41	0.49
3:N:1363:LEU:HD12	3:N:1364:HIS:O	2.12	0.49
5:P:226:LYS:HD2	5:P:242:TRP:CZ2	2.48	0.49
2:C:341:THR:O	2:C:345:ARG:HG3	2.12	0.49
2:C:418:LEU:N	2:C:418:LEU:HD12	2.28	0.49
2:C:1098:ASP:HB2	3:D:21:TRP:CZ2	2.46	0.49
2:C:1115:LEU:HD23	3:D:85:VAL:CA	2.43	0.49
3:D:32:ILE:HD12	3:D:527:MET:HG2	1.94	0.49
3:D:527:MET:HE2	5:F:258:ILE:HD11	1.93	0.49
3:D:572:ARG:NH2	5:F:83:GLN:HE21	2.10	0.49
3:D:1051:GLU:HA	9:D:1601:HOH:O	2.12	0.49
3:D:1161:GLU:HG3	3:D:1164:ARG:CB	2.39	0.49
3:D:1379:VAL:HG11	3:D:1395:LEU:HD12	1.95	0.49
2:M:108:ILE:HB	2:M:368:THR:HG1	1.76	0.49
2:M:442:GLU:O	2:M:442:GLU:HG3	2.11	0.49
2:M:1096:ALA:O	3:N:13:ALA:CB	2.61	0.49
3:N:34:TYR:HE2	5:P:260:ILE:HA	1.77	0.49
3:N:141:ILE:HG21	3:N:450:TYR:H	1.78	0.49
3:N:418:GLY:N	3:N:429:SER:O	2.34	0.49
3:N:528:VAL:O	3:N:535:PHE:HA	2.13	0.49
3:N:964:LEU:HD22	9:N:2037:HOH:O	2.13	0.49
5:P:191:ASN:OD1	5:P:194:LEU:HD13	2.13	0.49
1:B:45:LEU:HB2	9:B:399:HOH:O	2.12	0.49
1:B:101:LEU:HD12	1:B:114:PHE:N	2.28	0.49
2:C:148:PHE:CZ	2:C:281:LEU:HD13	2.35	0.49
2:C:358:ARG:HA	2:C:361:MET:HB2	1.93	0.49
2:C:367:LEU:HA	2:C:371:LYS:CG	2.35	0.49
2:C:890:LEU:CA	2:C:914:ILE:HD11	2.33	0.49
9:C:1162:HOH:O	3:D:943:THR:HG21	2.13	0.49
3:D:99:ALA:HA	3:D:575:GLN:HE22	1.77	0.49
3:D:116:LEU:HB3	3:D:118:LEU:HG	1.94	0.49
3:D:127:LEU:HD12	3:D:128:TYR:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:897:TRP:CH2	3:D:902:LEU:HD21	2.47	0.49
3:D:1101:VAL:HG22	3:D:1428:ALA:HB2	1.94	0.49
3:D:1481:VAL:HG13	4:E:18:ARG:HG3	1.93	0.49
5:F:112:ALA:O	5:F:116:LEU:HG	2.13	0.49
2:M:254:VAL:HG13	2:M:258:TYR:HE1	1.77	0.49
2:M:564:MET:HG3	2:M:997:LEU:HD11	1.94	0.49
2:M:770:GLU:O	2:M:773:LEU:HB3	2.13	0.49
2:M:987:ILE:HA	3:N:948:THR:HG21	1.95	0.49
3:N:709:HIS:CD2	3:N:711:LEU:HB2	2.48	0.49
3:N:804:LEU:HB3	9:N:1996:HOH:O	2.11	0.49
3:N:1141:GLU:HG2	3:N:1168:MET:HE1	1.95	0.49
3:N:1242:HIS:HE1	3:N:1266:ARG:HB3	1.78	0.49
5:P:116:LEU:HB2	5:P:127:ILE:HD12	1.95	0.49
5:P:135:ILE:O	5:P:135:ILE:HD13	2.13	0.49
2:C:17:PRO:HG2	9:C:1758:HOH:O	2.12	0.48
2:C:121:MET:HG3	9:C:1509:HOH:O	2.11	0.48
2:C:208:ALA:HA	2:C:221:LEU:HD21	1.94	0.48
2:C:379:GLU:O	2:C:383:ARG:HB3	2.13	0.48
2:C:976:ASP:HB2	2:C:979:THR:HG22	1.94	0.48
2:C:1033:GLY:O	2:C:1036:GLU:HG2	2.13	0.48
3:D:186:VAL:HB	3:D:189:GLN:HB2	1.95	0.48
3:D:610:LYS:CG	7:D:1527:MXP:H15A	2.42	0.48
3:D:834:THR:HA	9:D:2405:HOH:O	2.13	0.48
3:D:1049:SER:OG	3:D:1051:GLU:HG3	2.13	0.48
3:D:1114:THR:HG23	3:D:1114:THR:O	2.13	0.48
3:D:1310:ARG:CZ	3:D:1327:ARG:HD3	2.43	0.48
4:E:28:GLN:HG3	9:E:134:HOH:O	2.12	0.48
1:K:7:LYS:HE2	1:K:186:LEU:CD1	2.29	0.48
2:M:64:LEU:HD13	2:M:359:MET:CG	2.42	0.48
2:M:242:LEU:HD22	9:M:1924:HOH:O	2.11	0.48
2:M:858:MET:HB2	2:M:859:PRO:CD	2.43	0.48
2:M:1101:THR:HB	3:N:5:VAL:HG13	1.94	0.48
3:N:39:PRO:HB3	3:N:45:PHE:O	2.13	0.48
3:N:984:THR:CG2	3:N:987:GLU:H	2.25	0.48
3:N:1116:ASN:N	3:N:1116:ASN:ND2	2.60	0.48
3:N:1128:VAL:HG12	9:N:1593:HOH:O	2.13	0.48
5:P:220:LEU:HB2	5:P:243:ILE:HD11	1.95	0.48
1:A:9:PRO:HB3	1:A:25:LEU:HG	1.94	0.48
1:A:189:ARG:HD2	1:A:191:ASP:OD1	2.12	0.48
2:C:18:LEU:HD23	2:C:404:LEU:HD21	1.95	0.48
2:C:139:GLN:NE2	2:C:418:LEU:HD22	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:367:LEU:O	2:C:371:LYS:HB2	2.13	0.48
3:D:14:SER:HB2	9:D:1656:HOH:O	2.13	0.48
3:D:128:TYR:CE1	3:D:461:ILE:HG13	2.45	0.48
3:D:614:PHE:O	3:D:615:ARG:C	2.51	0.48
3:D:741:ASP:OD2	3:D:741:ASP:N	2.41	0.48
9:D:1893:HOH:O	4:E:85:LEU:HG	2.13	0.48
5:F:277:GLN:O	5:F:280:GLN:HB3	2.13	0.48
1:K:55:SER:CB	1:K:158:ILE:HG21	2.43	0.48
1:K:150:TYR:CE2	1:K:152:PRO:HG3	2.44	0.48
2:M:200:LEU:HD13	2:M:300:ASP:OD2	2.12	0.48
2:M:439:CYS:SG	2:M:540:PHE:HB3	2.53	0.48
2:M:461:VAL:HG12	2:M:462:ASP:O	2.13	0.48
2:M:636:ALA:HB2	2:M:703:ILE:HG22	1.95	0.48
2:M:671:ASN:ND2	2:M:993:PHE:HD2	2.10	0.48
3:N:112:ILE:HD12	3:N:461:ILE:HG21	1.94	0.48
3:N:180:LYS:HG3	3:N:183:GLU:H	1.77	0.48
3:N:417:PRO:HD2	3:N:432:TYR:CE1	2.48	0.48
3:N:610:LYS:HG2	7:N:1527:MXP:C15	2.43	0.48
3:N:754:PHE:CE2	3:N:1476:THR:HG21	2.49	0.48
5:P:371:LEU:HD12	9:P:669:HOH:O	2.11	0.48
1:A:5:LYS:HB2	9:A:440:HOH:O	2.12	0.48
1:A:201:THR:HG22	1:A:203:GLY:H	1.78	0.48
2:C:15:LEU:HD21	2:C:583:LEU:HD11	1.93	0.48
2:C:198:ARG:HD2	2:C:228:ALA:CB	2.44	0.48
2:C:468:ARG:NE	2:C:485:TYR:HB3	2.27	0.48
2:C:644:VAL:HG22	2:C:647:GLN:OE1	2.14	0.48
2:C:888:THR:HG22	9:C:1474:HOH:O	2.13	0.48
2:C:1054:THR:HG23	2:C:1082:PRO:HG3	1.93	0.48
3:D:190:GLU:HB2	9:D:1738:HOH:O	2.14	0.48
3:D:760:ARG:HH22	4:E:62:THR:CA	2.26	0.48
3:D:881:LEU:O	3:D:885:ILE:HG13	2.13	0.48
5:F:109:GLY:O	5:F:113:ILE:HG13	2.13	0.48
5:F:247:ILE:HG22	5:F:251:ILE:HD11	1.95	0.48
5:F:312:GLN:HB2	9:F:706:HOH:O	2.12	0.48
1:K:34:VAL:HG22	2:M:939:ARG:HH21	1.79	0.48
2:M:139:GLN:HG2	2:M:140:ILE:H	1.77	0.48
2:M:601:GLY:HA2	2:M:616:GLU:HG3	1.95	0.48
2:M:615:TYR:HH	2:M:623:TYR:HH	1.60	0.48
3:N:161:LEU:O	3:N:449:SER:CB	2.59	0.48
3:N:524:LEU:C	3:N:526:PRO:HD3	2.33	0.48
3:N:1123:PHE:CE1	3:N:1134:LEU:HD12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:93:LEU:HG	5:P:190:ALA:HB1	1.96	0.48
5:P:306:GLU:O	5:P:310:ILE:HG13	2.13	0.48
1:B:12:THR:OG1	1:B:24:VAL:HB	2.14	0.48
1:B:58:ILE:HG21	1:B:68:ILE:HD13	1.96	0.48
2:C:183:SER:CB	2:C:190:LYS:HD3	2.43	0.48
2:C:290:LEU:HB3	2:C:302:VAL:HG11	1.94	0.48
2:C:472:ARG:O	2:C:531:PHE:HD2	1.96	0.48
2:C:627:ARG:O	2:C:638:ASP:HA	2.13	0.48
2:C:809:GLY:HA2	9:C:1126:HOH:O	2.12	0.48
3:D:491:LYS:HE2	9:D:1851:HOH:O	2.12	0.48
5:F:369:LEU:HD11	5:F:401:GLU:HB2	1.94	0.48
1:L:22:GLU:HG2	1:L:198:ARG:HG2	1.94	0.48
2:M:101:ILE:HG22	2:M:102:HIS:N	2.28	0.48
2:M:258:TYR:HB3	9:M:1886:HOH:O	2.13	0.48
2:M:412:ALA:HB1	2:M:419:THR:CG2	2.43	0.48
2:M:1014:SER:O	2:M:1018:GLN:HG3	2.14	0.48
3:N:9:ARG:HH22	3:N:507:ASN:HD21	1.61	0.48
3:N:534:ARG:HG2	9:P:456:HOH:O	2.13	0.48
3:N:553:ARG:HH12	5:P:211:ASP:HA	1.78	0.48
3:N:572:ARG:NH1	5:P:79:ASP:OD1	2.39	0.48
3:N:1312:LEU:HD12	9:N:2368:HOH:O	2.12	0.48
5:P:339:PRO:HB3	5:P:343:ASP:HB2	1.94	0.48
1:B:107:LYS:HG3	1:B:108:GLU:H	1.78	0.48
2:C:140:ILE:HA	2:C:332:ARG:O	2.14	0.48
2:C:281:LEU:HD12	2:C:305:PRO:O	2.13	0.48
2:C:405:ARG:HA	9:C:1409:HOH:O	2.12	0.48
2:C:462:ASP:HB3	2:C:468:ARG:HD3	1.96	0.48
2:C:831:ARG:HD2	9:C:1303:HOH:O	2.14	0.48
2:C:1115:LEU:CB	3:D:85:VAL:HG13	2.43	0.48
3:D:32:ILE:HG12	9:D:1967:HOH:O	2.13	0.48
3:D:760:ARG:HB2	4:E:3:GLU:OE2	2.14	0.48
3:D:805:GLU:OE1	3:D:809:PRO:HG2	2.14	0.48
3:D:829:VAL:H	3:D:835:SER:CB	2.26	0.48
3:D:840:LYS:HB3	3:D:841:TYR:CE2	2.48	0.48
3:D:938:GLY:O	3:D:942:SER:HB3	2.14	0.48
5:F:369:LEU:HA	9:F:450:HOH:O	2.13	0.48
2:M:165:LEU:HB2	9:M:2226:HOH:O	2.14	0.48
2:M:212:GLY:HA3	2:M:218:VAL:CG2	2.44	0.48
2:M:305:PRO:HA	2:M:308:ARG:CD	2.44	0.48
2:M:380:ALA:O	2:M:384:GLU:HB2	2.14	0.48
2:M:968:LEU:HD22	9:M:2164:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:57:GLU:HG3	3:N:64:LYS:HG2	1.95	0.48
3:N:1198:TYR:HE2	9:N:2318:HOH:O	1.96	0.48
3:N:1264:GLU:OE2	3:N:1425:THR:HB	2.14	0.48
5:P:80:PRO:HA	5:P:83:GLN:HB2	1.95	0.48
5:P:136:LEU:HD23	5:P:181:GLU:OE2	2.13	0.48
1:A:16:GLN:O	1:A:16:GLN:CG	2.62	0.48
1:A:64:GLU:HG3	1:A:165:ILE:HD12	1.96	0.48
1:A:112:ARG:HA	9:A:397:HOH:O	2.13	0.48
1:B:101:LEU:HB2	1:B:114:PHE:CD2	2.48	0.48
2:C:672:VAL:CG2	2:C:868:ASP:HB2	2.44	0.48
2:C:1065:ALA:CB	2:C:1077:PRO:HG2	2.43	0.48
3:D:12:LEU:HD13	3:D:511:TRP:HB2	1.94	0.48
3:D:34:TYR:O	3:D:35:ARG:C	2.51	0.48
3:D:126:VAL:HG12	3:D:132:TYR:HB2	1.96	0.48
3:D:162:ARG:HH11	3:D:434:ARG:HH22	1.62	0.48
3:D:670:VAL:O	3:D:674:ARG:HG3	2.14	0.48
3:D:760:ARG:HH22	4:E:62:THR:N	2.11	0.48
3:D:947:ILE:HD12	3:D:947:ILE:O	2.14	0.48
3:D:1104:GLU:O	3:D:1106:VAL:HG23	2.14	0.48
3:D:1209:LEU:HD12	3:D:1219:GLU:OE1	2.14	0.48
3:D:1258:ARG:NH2	3:D:1351:GLU:OE2	2.46	0.48
3:D:1290:LEU:HD22	3:D:1291:SER:H	1.79	0.48
4:E:4:PRO:HB2	9:E:109:HOH:O	2.13	0.48
5:F:80:PRO:HA	5:F:83:GLN:HB2	1.94	0.48
5:F:82:ARG:HD3	9:F:608:HOH:O	2.14	0.48
5:F:134:LYS:HB2	5:F:178:ARG:NH2	2.28	0.48
2:M:435:TYR:C	2:M:437:ARG:H	2.15	0.48
2:M:544:THR:O	2:M:547:ILE:HG13	2.14	0.48
2:M:958:THR:HG23	2:M:961:GLU:H	1.79	0.48
3:N:409:VAL:O	3:N:437:VAL:HG21	2.13	0.48
3:N:417:PRO:HD2	3:N:432:TYR:CD1	2.48	0.48
3:N:443:VAL:HG11	3:N:445:ARG:HE	1.79	0.48
3:N:853:VAL:HA	3:N:858:VAL:O	2.14	0.48
3:N:1110:ALA:O	3:N:1111:ASP:C	2.49	0.48
3:N:1147:ARG:HD2	3:N:1188:VAL:HG21	1.95	0.48
3:N:1282:ARG:HA	3:N:1315:ASP:OD1	2.14	0.48
3:N:1310:ARG:HE	3:N:1327:ARG:HB3	1.78	0.48
3:N:1351:GLU:HA	3:N:1354:LYS:HG3	1.95	0.48
1:A:23:PHE:O	1:A:196:THR:HA	2.13	0.48
1:A:222:LEU:HD11	1:B:218:LEU:HD23	1.95	0.48
1:B:156:HIS:CG	1:B:157:GLY:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:120:LEU:HA	9:C:1499:HOH:O	2.12	0.48
2:C:412:ALA:HB1	2:C:419:THR:CG2	2.44	0.48
3:D:409:VAL:HG12	3:D:435:VAL:HG11	1.94	0.48
3:D:486:ARG:HB2	9:D:2292:HOH:O	2.12	0.48
3:D:565:ILE:HD12	5:F:192:LEU:CD1	2.42	0.48
3:D:1041:LEU:CD1	3:D:1058:ARG:HA	2.42	0.48
1:K:197:LEU:HD23	1:K:197:LEU:N	2.29	0.48
1:K:206:THR:CG2	1:K:209:GLU:HG3	2.39	0.48
2:M:682:TYR:CE1	2:M:851:LYS:HD2	2.49	0.48
3:N:521:PRO:O	3:N:525:ARG:HG2	2.13	0.48
3:N:1197:ARG:N	9:N:1577:HOH:O	2.46	0.48
1:B:7:LYS:HG3	9:B:434:HOH:O	2.13	0.48
2:C:211:LEU:CD1	2:C:308:ARG:HA	2.44	0.48
2:C:305:PRO:HA	2:C:308:ARG:CD	2.42	0.48
2:C:719:PRO:HB3	2:C:820:ARG:CZ	2.43	0.48
2:C:724:ARG:HG2	2:C:734:LEU:CD2	2.43	0.48
3:D:45:PHE:HB3	3:D:86:ARG:NH2	2.29	0.48
3:D:204:LEU:O	3:D:393:ILE:HA	2.13	0.48
3:D:466:LYS:NZ	9:D:1668:HOH:O	2.47	0.48
3:D:705:ALA:HB3	3:D:706:PRO:CD	2.43	0.48
4:E:73:LEU:N	9:E:131:HOH:O	2.46	0.48
5:F:172:ARG:NH1	9:F:462:HOH:O	2.45	0.48
2:M:431:HIS:H	2:M:434:HIS:CD2	2.30	0.48
2:M:625:LEU:O	2:M:627:ARG:N	2.47	0.48
2:M:1056:LYS:HB3	3:N:623:VAL:HG13	1.94	0.48
2:M:1088:LEU:HG	2:M:1092:LEU:HD12	1.95	0.48
3:N:615:ARG:HH21	3:N:1089:ALA:CB	2.20	0.48
3:N:820:GLU:HG3	3:N:836:VAL:HG11	1.95	0.48
3:N:1047:LYS:HB3	3:N:1048:PRO:HD2	1.94	0.48
3:N:1110:ALA:O	3:N:1112:CYS:N	2.46	0.48
3:N:1240:THR:O	3:N:1257:PRO:HB3	2.14	0.48
1:A:7:LYS:NZ	1:A:186:LEU:HD21	2.29	0.48
1:A:206:THR:HG22	1:A:209:GLU:CG	2.40	0.48
2:C:11:GLU:HB2	9:C:1190:HOH:O	2.14	0.48
2:C:139:GLN:OE1	2:C:414:GLY:HA3	2.14	0.48
2:C:165:LEU:HD12	2:C:166:PRO:CA	2.43	0.48
2:C:611:ILE:CD1	2:C:625:LEU:HD11	2.44	0.48
2:C:676:ILE:HG22	2:C:988:VAL:HG22	1.96	0.48
2:C:851:LYS:HG3	9:C:1250:HOH:O	2.12	0.48
3:D:12:LEU:HD23	3:D:13:ALA:H	1.79	0.48
3:D:702:LEU:HD13	3:D:716:PHE:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:2077:HOH:O	5:F:349:LEU:HD13	2.13	0.48
5:F:358:LEU:HD13	5:F:370:LYS:HG3	1.96	0.48
1:K:9:PRO:HB3	1:K:25:LEU:HD21	1.96	0.48
1:K:101:LEU:HD12	1:K:114:PHE:CD1	2.49	0.48
1:L:50:GLY:O	1:L:146:ARG:HA	2.13	0.48
1:L:207:PRO:HD2	9:L:3232:HOH:O	2.13	0.48
3:N:73:CYS:SG	3:N:74:GLU:N	2.86	0.48
3:N:81:THR:HG22	3:N:82:LYS:N	2.29	0.48
3:N:421:LEU:CG	3:N:429:SER:HB3	2.43	0.48
3:N:1321:ALA:O	3:N:1339:LYS:HG3	2.13	0.48
4:O:54:LEU:HD23	4:O:58:PRO:HD2	1.96	0.48
5:P:292:ALA:O	5:P:299:TRP:HB2	2.14	0.48
1:B:39:PRO:O	1:B:43:ILE:HG12	2.14	0.48
2:C:19:THR:O	2:C:19:THR:HG22	2.14	0.48
2:C:143:SER:CB	2:C:276:LYS:HZ1	2.23	0.48
2:C:289:THR:O	2:C:291:ALA:N	2.46	0.48
2:C:410:ILE:H	2:C:410:ILE:HD12	1.78	0.48
2:C:410:ILE:HD12	2:C:410:ILE:N	2.29	0.48
2:C:762:LYS:HG3	2:C:786:LYS:HD2	1.95	0.48
2:C:879:ARG:HB3	9:C:1196:HOH:O	2.14	0.48
3:D:550:ARG:NH1	3:D:573:MET:HB3	2.29	0.48
3:D:561:GLY:CA	5:F:184:ARG:HH12	2.21	0.48
3:D:1238:MET:HG3	3:D:1257:PRO:HG3	1.95	0.48
5:F:128:ARG:HB2	9:F:652:HOH:O	2.14	0.48
2:M:369:PRO:HG2	9:M:2247:HOH:O	2.14	0.48
2:M:496:ILE:O	2:M:515:ALA:HB1	2.14	0.48
2:M:644:VAL:HG22	9:M:2151:HOH:O	2.13	0.48
2:M:1098:ASP:HB2	3:N:21:TRP:CZ2	2.47	0.48
3:N:47:GLU:HA	3:N:51:GLY:O	2.13	0.48
3:N:116:LEU:HB3	3:N:118:LEU:HG	1.96	0.48
3:N:126:VAL:O	3:N:132:TYR:CD1	2.67	0.48
3:N:127:LEU:HD12	3:N:128:TYR:N	2.29	0.48
3:N:407:VAL:HA	3:N:422:ALA:CB	2.44	0.48
3:N:465:LEU:HB3	9:N:2360:HOH:O	2.14	0.48
3:N:540:LEU:HD21	3:N:603:LEU:HD23	1.95	0.48
3:N:1177:ALA:CB	3:N:1183:ILE:HD11	2.44	0.48
3:N:1384:PRO:O	3:N:1413:THR:HG21	2.13	0.48
4:O:31:LEU:HD23	4:O:35:PHE:CE1	2.48	0.48
5:P:240:THR:O	5:P:244:ARG:HG3	2.13	0.48
1:A:162:ILE:HG13	1:A:163:ASN:N	2.28	0.47
1:B:50:GLY:O	1:B:146:ARG:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:GLY:HA2	2:C:341:THR:OG1	2.13	0.47
2:C:544:THR:O	2:C:547:ILE:HG13	2.13	0.47
2:C:556:ASN:HA	9:C:1448:HOH:O	2.12	0.47
2:C:571:LEU:CD2	2:C:700:TYR:HA	2.44	0.47
2:C:679:PHE:CE1	2:C:870:ILE:HD13	2.49	0.47
2:C:843:HIS:CD2	2:C:884:GLN:HA	2.49	0.47
2:C:896:PHE:CD2	2:C:925:TYR:HB2	2.49	0.47
2:C:926:PHE:O	2:C:930:LYS:HG3	2.12	0.47
2:C:930:LYS:HD3	9:C:1707:HOH:O	2.14	0.47
3:D:133:ILE:HG22	3:D:455:ARG:CA	2.43	0.47
3:D:666:ILE:H	3:D:666:ILE:HG13	1.55	0.47
3:D:693:GLU:O	4:E:48:MET:HE1	2.14	0.47
3:D:1128:VAL:O	3:D:1129:THR:C	2.51	0.47
3:D:1323:GLN:HG3	3:D:1324:PRO:HD2	1.95	0.47
1:K:155:LYS:HD3	9:K:3774:HOH:O	2.14	0.47
1:K:180:GLN:NE2	2:M:929:ARG:HH21	2.11	0.47
2:M:252:LYS:NZ	2:M:296:GLY:HA3	2.29	0.47
2:M:614:ARG:HD3	9:M:2272:HOH:O	2.14	0.47
2:M:650:ARG:HB2	2:M:653:ASP:HB2	1.94	0.47
2:M:879:ARG:HD2	2:M:879:ARG:H	1.79	0.47
3:N:87:ARG:HA	3:N:523:ASP:HB2	1.96	0.47
3:N:147:VAL:HG21	9:N:2101:HOH:O	2.13	0.47
3:N:916:TYR:CE2	3:N:920:LEU:HD13	2.49	0.47
3:N:1000:THR:HG23	3:N:1001:GLU:N	2.29	0.47
5:P:139:ALA:HB1	9:P:558:HOH:O	2.13	0.47
5:P:358:LEU:HD21	5:P:367:MET:HE1	1.96	0.47
1:A:49:PRO:CB	1:A:148:VAL:HG22	2.42	0.47
2:C:101:ILE:HG22	2:C:102:HIS:N	2.28	0.47
2:C:218:VAL:HA	2:C:221:LEU:HD23	1.95	0.47
2:C:333:ILE:N	2:C:333:ILE:HD12	2.28	0.47
2:C:378:LEU:HG	2:C:382:ILE:CD1	2.44	0.47
2:C:704:HIS:O	2:C:828:ALA:HA	2.14	0.47
3:D:62:LYS:HB2	9:D:1735:HOH:O	2.14	0.47
3:D:1262:LEU:HD23	3:D:1352:ILE:CG1	2.38	0.47
3:D:1337:GLU:HB2	9:D:1785:HOH:O	2.14	0.47
4:E:94:PRO:CG	9:E:180:HOH:O	2.56	0.47
5:F:138:SER:H	5:F:140:ARG:HE	1.62	0.47
5:F:187:LEU:HD23	5:F:187:LEU:C	2.34	0.47
2:M:72:ARG:HB2	9:M:1985:HOH:O	2.13	0.47
2:M:176:VAL:O	2:M:178:PRO:HD3	2.13	0.47
2:M:276:LYS:HG2	2:M:280:LYS:HZ2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1002:GLU:HG3	3:N:744:GLN:HE22	1.79	0.47
3:N:133:ILE:HG22	3:N:455:ARG:CA	2.44	0.47
3:N:603:LEU:HA	3:N:606:ILE:HD12	1.96	0.47
3:N:633:VAL:C	3:N:635:PRO:HD3	2.35	0.47
3:N:1467:ILE:HG12	7:N:1527:MXP:H16A	1.96	0.47
5:P:119:ILE:HD13	5:P:170:HIS:ND1	2.29	0.47
5:P:277:GLN:O	5:P:280:GLN:HB3	2.13	0.47
1:B:69:PRO:C	1:B:71:VAL:H	2.18	0.47
1:B:120:VAL:HG11	9:B:416:HOH:O	2.15	0.47
2:C:115:LEU:HD22	2:C:373:VAL:CG1	2.41	0.47
2:C:207:LEU:O	2:C:211:LEU:HB3	2.14	0.47
2:C:281:LEU:O	2:C:282:GLY:O	2.32	0.47
2:C:837:ASP:O	2:C:848:VAL:HG13	2.14	0.47
2:C:1006:HIS:O	3:D:648:MET:HE3	2.14	0.47
2:C:1106:ASP:OD1	3:D:7:LYS:HD2	2.14	0.47
3:D:403:PHE:HE2	3:D:443:VAL:N	2.12	0.47
3:D:528:VAL:HG12	3:D:529:GLN:N	2.29	0.47
3:D:1087:ARG:NH1	3:D:1234:THR:O	2.47	0.47
3:D:1408:ILE:O	3:D:1409:ALA:C	2.49	0.47
3:D:1463:LYS:O	3:D:1467:ILE:HG13	2.13	0.47
3:D:1476:THR:CG2	4:E:21:VAL:HG22	2.44	0.47
4:E:4:PRO:HG2	9:E:175:HOH:O	2.12	0.47
4:E:82:GLU:HG3	4:E:83:ASP:H	1.78	0.47
1:K:9:PRO:HB3	1:K:25:LEU:CG	2.44	0.47
2:M:262:ALA:O	2:M:264:PRO:O	2.32	0.47
2:M:631:SER:HG	2:M:635:THR:H	1.59	0.47
3:N:1090:ASP:OD1	3:N:1241:PHE:CZ	2.68	0.47
3:N:1129:THR:HG23	3:N:1130:ARG:H	1.78	0.47
3:N:1238:MET:HG3	3:N:1257:PRO:HG3	1.96	0.47
3:N:1481:VAL:CG1	4:O:18:ARG:HG3	2.44	0.47
4:O:87:LYS:HD3	9:O:2559:HOH:O	2.15	0.47
5:P:321:ILE:O	5:P:327:SER:HB3	2.13	0.47
1:B:87:VAL:CG2	1:B:144:VAL:HG11	2.36	0.47
2:C:772:ARG:HD3	9:F:459:HOH:O	2.15	0.47
2:C:923:GLU:O	2:C:927:GLY:HA3	2.15	0.47
3:D:87:ARG:HB2	3:D:523:ASP:HB2	1.96	0.47
3:D:432:TYR:O	3:D:448:GLU:HA	2.15	0.47
3:D:895:VAL:O	3:D:899:LEU:HG	2.14	0.47
3:D:1372:VAL:O	3:D:1375:MET:HB2	2.13	0.47
4:E:67:GLU:OE1	4:E:73:LEU:HD11	2.15	0.47
5:F:358:LEU:CD2	5:F:370:LYS:HZ2	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:410:ILE:HD11	2:M:455:LEU:HB3	1.96	0.47
2:M:668:LEU:O	2:M:993:PHE:CZ	2.67	0.47
2:M:670:GLN:HE22	2:M:699:PHE:C	2.18	0.47
2:M:975:TYR:HA	2:M:982:PRO:HA	1.95	0.47
9:M:1815:HOH:O	3:N:1456:LYS:HD3	2.13	0.47
3:N:81:THR:HB	3:N:85:VAL:CG2	2.43	0.47
3:N:87:ARG:HD2	9:N:1572:HOH:O	2.14	0.47
3:N:162:ARG:HA	3:N:449:SER:CB	2.44	0.47
3:N:787:LEU:HD21	3:N:947:ILE:HD11	1.96	0.47
3:N:807:ALA:HB2	9:N:1559:HOH:O	2.15	0.47
3:N:957:PRO:HB3	3:N:959:GLU:HG3	1.95	0.47
3:N:1440:PHE:CD2	3:N:1440:PHE:N	2.82	0.47
1:A:184:THR:HG23	1:A:192:LEU:CB	2.42	0.47
1:B:102:LYS:HA	1:B:138:LEU:O	2.15	0.47
2:C:21:ILE:HG12	2:C:455:LEU:HD21	1.96	0.47
2:C:157:ARG:N	9:C:1172:HOH:O	2.46	0.47
2:C:1058:ASP:OD1	2:C:1084:SER:HB3	2.14	0.47
3:D:109:PRO:HB2	9:D:2000:HOH:O	2.13	0.47
3:D:119:SER:CB	3:D:123:LEU:HD13	2.44	0.47
3:D:589:ALA:HA	9:D:1703:HOH:O	2.12	0.47
3:D:1500:LYS:HE3	9:D:2173:HOH:O	2.13	0.47
5:F:365:GLU:HG2	5:F:397:ILE:HA	1.96	0.47
2:M:160:ALA:O	2:M:173:ASP:HA	2.14	0.47
2:M:164:PRO:HB3	9:M:1703:HOH:O	2.14	0.47
2:M:378:LEU:HG	2:M:382:ILE:CD1	2.44	0.47
2:M:817:PRO:HG3	5:P:288:TYR:OH	2.14	0.47
2:M:965:GLU:HG3	9:M:2274:HOH:O	2.15	0.47
9:M:2079:HOH:O	3:N:606:ILE:HG21	2.15	0.47
3:N:100:ALA:CB	3:N:513:ILE:HD13	2.29	0.47
3:N:611:GLN:CG	3:N:619:LEU:HD11	2.42	0.47
3:N:752:SER:HB2	9:N:1905:HOH:O	2.14	0.47
3:N:795:VAL:HA	3:N:861:GLN:O	2.15	0.47
3:N:1236:LEU:HD11	3:N:1356:TYR:CE1	2.48	0.47
3:N:1448:THR:O	3:N:1451:ALA:HB3	2.14	0.47
5:P:353:GLU:HG2	9:P:485:HOH:O	2.13	0.47
1:A:5:LYS:HD2	9:A:440:HOH:O	2.14	0.47
1:A:59:GLU:HG3	1:A:139:ASN:CG	2.35	0.47
1:B:27:PRO:HB3	1:B:192:LEU:CD2	2.45	0.47
2:C:129:ILE:HG22	2:C:130:ASN:N	2.29	0.47
2:C:313:LEU:HA	9:C:1596:HOH:O	2.15	0.47
2:C:422:ARG:HG3	2:C:423:ALA:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:479:VAL:HG21	2:C:503:LEU:HD11	1.96	0.47
2:C:726:ILE:O	2:C:726:ILE:HG22	2.14	0.47
3:D:17:LYS:HA	3:D:20:SER:HB3	1.95	0.47
3:D:75:ARG:HB2	9:D:1539:HOH:O	2.15	0.47
3:D:80:VAL:HG12	3:D:81:THR:N	2.29	0.47
3:D:133:ILE:H	3:D:133:ILE:HG12	1.35	0.47
3:D:180:LYS:HG3	3:D:183:GLU:H	1.79	0.47
3:D:524:LEU:C	3:D:526:PRO:HD3	2.35	0.47
3:D:1109:GLU:HG2	3:D:1202:GLN:N	2.29	0.47
5:F:350:LEU:O	5:F:354:LEU:HB2	2.14	0.47
1:L:195:LEU:C	9:L:1676:HOH:O	2.53	0.47
2:M:328:LEU:HD22	2:M:437:ARG:CB	2.44	0.47
2:M:421:GLU:O	2:M:421:GLU:HG2	2.15	0.47
2:M:497:ALA:HA	2:M:515:ALA:HA	1.96	0.47
3:N:34:TYR:O	3:N:35:ARG:C	2.52	0.47
3:N:137:PRO:HD2	3:N:453:ASP:CB	2.45	0.47
3:N:486:ARG:HH12	3:N:1389:LEU:HD11	1.78	0.47
3:N:844:ALA:O	3:N:867:ARG:HB3	2.14	0.47
3:N:900:ILE:O	3:N:900:ILE:HG13	2.15	0.47
5:P:280:GLN:O	5:P:280:GLN:HG2	2.14	0.47
1:A:133:GLU:N	9:A:320:HOH:O	2.46	0.47
1:A:182:GLU:O	1:A:194:LYS:HB3	2.14	0.47
1:B:185:ARG:HB3	9:D:1701:HOH:O	2.14	0.47
2:C:5:ARG:HB3	2:C:902:ILE:HB	1.97	0.47
2:C:129:ILE:HG23	9:C:1478:HOH:O	2.14	0.47
2:C:165:LEU:HG	2:C:265:ARG:HH12	1.79	0.47
2:C:274:ARG:HG2	2:C:274:ARG:O	2.15	0.47
2:C:279:GLU:HG3	2:C:280:LYS:N	2.30	0.47
2:C:289:THR:HG22	2:C:290:LEU:HD23	1.97	0.47
2:C:726:ILE:HG22	9:C:1346:HOH:O	2.14	0.47
2:C:865:THR:C	9:C:1269:HOH:O	2.52	0.47
2:C:875:GLY:HA2	2:C:879:ARG:NH1	2.30	0.47
2:C:958:THR:HG23	2:C:961:GLU:H	1.78	0.47
3:D:18:ILE:HG21	3:D:516:ALA:O	2.14	0.47
3:D:397:LYS:CE	3:D:448:GLU:HB3	2.45	0.47
3:D:455:ARG:HH11	3:D:463:GLN:HG3	1.78	0.47
3:D:520:LEU:HD23	3:D:540:LEU:CD2	2.45	0.47
3:D:637:LEU:HD11	3:D:642:CYS:CA	2.45	0.47
3:D:1066:THR:HG22	3:D:1069:GLU:HG3	1.96	0.47
3:D:1236:LEU:HA	3:D:1359:GLN:NE2	2.30	0.47
3:D:1403:LEU:HD12	9:D:1814:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:140:ARG:HG3	5:F:141:VAL:N	2.29	0.47
1:K:209:GLU:O	1:K:213:GLN:HG3	2.15	0.47
2:M:165:LEU:HD12	2:M:166:PRO:HA	1.95	0.47
2:M:175:GLU:HB3	2:M:183:SER:OG	2.14	0.47
2:M:267:TYR:HB2	2:M:272:ALA:CB	2.44	0.47
2:M:332:ARG:HH21	2:M:338:GLU:CD	2.17	0.47
2:M:362:GLY:HA3	2:M:367:LEU:HD23	1.95	0.47
2:M:448:ASN:HB3	2:M:452:ILE:HD11	1.97	0.47
2:M:472:ARG:O	2:M:531:PHE:HD2	1.97	0.47
2:M:839:LEU:HD21	2:M:849:VAL:CG2	2.45	0.47
2:M:1015:LEU:N	9:M:1708:HOH:O	2.47	0.47
2:M:1050:GLN:NE2	9:M:2160:HOH:O	2.48	0.47
2:M:1067:TYR:O	2:M:1071:ILE:HG12	2.14	0.47
3:N:84:ILE:O	3:N:87:ARG:HB3	2.15	0.47
3:N:171:LEU:HD22	3:N:175:VAL:HB	1.96	0.47
3:N:540:LEU:HA	3:N:543:LEU:HD12	1.97	0.47
3:N:543:LEU:HA	3:N:546:ARG:HG3	1.96	0.47
3:N:685:ASP:HB3	9:N:1697:HOH:O	2.14	0.47
3:N:827:ILE:HG23	3:N:837:GLY:HA2	1.97	0.47
3:N:1045:MET:HG3	3:N:1073:SER:HA	1.97	0.47
3:N:1111:ASP:HB3	3:N:1203:LYS:HG3	1.96	0.47
3:N:1394:VAL:HG21	9:N:1598:HOH:O	2.14	0.47
3:N:1490:LYS:HB2	9:O:3444:HOH:O	2.14	0.47
4:O:39:VAL:HG21	4:O:72:ARG:HD2	1.97	0.47
5:P:81:VAL:O	5:P:85:LEU:HB2	2.14	0.47
5:P:109:GLY:O	5:P:113:ILE:HG13	2.15	0.47
5:P:160:ASP:OD1	5:P:178:ARG:NH2	2.48	0.47
5:P:361:LEU:HD23	5:P:362:SER:N	2.29	0.47
2:C:290:LEU:HD23	2:C:290:LEU:H	1.78	0.47
2:C:535:SER:CB	2:C:537:LYS:HG3	2.45	0.47
2:C:627:ARG:HG3	2:C:628:PHE:N	2.29	0.47
3:D:205:TYR:HB2	3:D:393:ILE:HG12	1.95	0.47
3:D:443:VAL:HG11	3:D:445:ARG:HE	1.80	0.47
3:D:525:ARG:N	3:D:526:PRO:HD3	2.29	0.47
3:D:827:ILE:O	3:D:837:GLY:HA3	2.15	0.47
3:D:907:GLU:O	3:D:911:LEU:HD13	2.15	0.47
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.15	0.47
3:D:1212:ALA:HB3	9:D:1618:HOH:O	2.15	0.47
5:F:261:PRO:O	5:F:265:VAL:HG23	2.14	0.47
1:L:15:THR:C	1:L:16:GLN:HG2	2.35	0.47
2:M:405:ARG:CZ	9:M:1857:HOH:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:648:ARG:HG3	2:M:648:ARG:O	2.14	0.47
2:M:798:GLY:H	2:M:827:VAL:CG1	2.27	0.47
2:M:1034:GLU:O	2:M:1037:VAL:N	2.48	0.47
3:N:582:LEU:HA	3:N:603:LEU:HD12	1.96	0.47
3:N:874:GLU:HG3	9:N:1713:HOH:O	2.14	0.47
3:N:933:ALA:O	3:N:937:TYR:HD1	1.98	0.47
3:N:1341:PRO:O	3:N:1343:ALA:N	2.48	0.47
5:P:234:LYS:HE2	9:P:430:HOH:O	2.14	0.47
5:P:358:LEU:HD22	5:P:370:LYS:CE	2.45	0.47
1:A:89:PHE:HB3	1:A:94:LEU:HD22	1.97	0.47
1:B:165:ILE:HG22	9:B:502:HOH:O	2.14	0.47
2:C:301:GLU:O	2:C:305:PRO:HG2	2.15	0.47
2:C:497:ALA:HA	2:C:515:ALA:HA	1.96	0.47
3:D:65:ARG:CG	3:D:66:GLN:N	2.77	0.47
3:D:421:LEU:HB2	3:D:427:VAL:HG12	1.95	0.47
3:D:844:ALA:O	3:D:867:ARG:HB3	2.15	0.47
3:D:983:LEU:HD13	3:D:991:GLN:OE1	2.15	0.47
5:F:309:LYS:O	5:F:312:GLN:HB2	2.15	0.47
2:M:113:VAL:O	2:M:115:LEU:HD23	2.15	0.47
2:M:551:GLU:O	3:N:1065:LEU:HB3	2.15	0.47
2:M:983:ILE:HG23	3:N:944:THR:O	2.15	0.47
3:N:18:ILE:HD12	3:N:518:PRO:HD3	1.97	0.47
3:N:85:VAL:HG12	3:N:89:ARG:NE	2.30	0.47
3:N:204:LEU:HG	3:N:441:ARG:HH12	1.80	0.47
3:N:593:ASN:HD21	5:P:206:GLY:HA2	1.80	0.47
5:P:95:THR:HG22	5:P:96:LEU:HD23	1.97	0.47
5:P:410:TYR:O	5:P:413:SER:HB2	2.15	0.47
1:B:15:THR:C	1:B:16:GLN:HG2	2.35	0.47
1:B:46:SER:HB2	9:B:503:HOH:O	2.14	0.47
1:B:141:GLU:HG3	9:B:405:HOH:O	2.14	0.47
2:C:176:VAL:O	2:C:178:PRO:HD3	2.15	0.47
2:C:732:ALA:O	2:C:735:ARG:HG3	2.15	0.47
2:C:1025:ALA:C	2:C:1026:GLN:HG3	2.35	0.47
2:C:1035:MET:HG2	3:D:707:THR:O	2.14	0.47
2:C:1071:ILE:O	3:D:659:LYS:HB2	2.15	0.47
3:D:407:VAL:HA	3:D:422:ALA:CB	2.45	0.47
3:D:699:VAL:HG21	3:D:760:ARG:HB3	1.97	0.47
3:D:810:GLU:HG2	9:D:2253:HOH:O	2.14	0.47
3:D:843:PHE:CD2	3:D:849:ALA:HA	2.49	0.47
3:D:1051:GLU:HG3	3:D:1051:GLU:H	1.46	0.47
3:D:1240:THR:O	3:D:1257:PRO:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1478:SER:HG	3:D:1481:VAL:HG23	1.80	0.47
1:K:45:LEU:HD23	9:K:1231:HOH:O	2.14	0.47
1:K:89:PHE:HD1	1:K:120:VAL:HG23	1.80	0.47
2:M:172:ILE:H	2:M:172:ILE:HD12	1.78	0.47
2:M:224:GLU:HG3	9:M:2180:HOH:O	2.14	0.47
2:M:1060:ILE:HG22	2:M:1061:GLU:H	1.78	0.47
5:P:371:LEU:HD22	5:P:375:LEU:HD22	1.95	0.47
5:P:372:ARG:HB3	9:P:615:HOH:O	2.14	0.47
2:C:36:PRO:HB2	2:C:70:GLU:HG2	1.97	0.46
2:C:54:ILE:HG22	2:C:66:LEU:HB3	1.96	0.46
2:C:122:THR:HG22	2:C:123:GLU:N	2.31	0.46
2:C:166:PRO:HD3	2:C:265:ARG:HG3	1.97	0.46
2:C:183:SER:HB3	2:C:190:LYS:HD3	1.97	0.46
2:C:1030:GLN:CD	3:D:628:ARG:HB3	2.35	0.46
2:C:1115:LEU:HB3	3:D:85:VAL:CG1	2.44	0.46
3:D:39:PRO:HD2	3:D:47:GLU:OE1	2.15	0.46
3:D:204:LEU:HG	3:D:441:ARG:NH1	2.30	0.46
3:D:481:MET:HB2	3:D:1388:ARG:NH1	2.30	0.46
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.30	0.46
4:E:42:PRO:HD3	9:E:101:HOH:O	2.16	0.46
5:F:292:ALA:O	5:F:299:TRP:HB2	2.15	0.46
1:K:106:PRO:HG3	1:K:134:GLU:CG	2.45	0.46
1:L:162:ILE:HA	9:L:1885:HOH:O	2.15	0.46
2:M:379:GLU:O	2:M:383:ARG:HB3	2.15	0.46
2:M:439:CYS:SG	2:M:541:SER:N	2.87	0.46
2:M:627:ARG:O	2:M:638:ASP:HA	2.15	0.46
2:M:751:PRO:HG3	2:M:796:GLU:HG2	1.98	0.46
2:M:815:LEU:HD23	2:M:819:VAL:O	2.15	0.46
2:M:851:LYS:NZ	9:M:2027:HOH:O	2.48	0.46
3:N:133:ILE:HG22	3:N:455:ARG:C	2.35	0.46
3:N:153:LEU:HD12	3:N:157:GLU:HB2	1.97	0.46
3:N:421:LEU:HB2	3:N:427:VAL:HG12	1.96	0.46
3:N:702:LEU:HD23	3:N:745:MET:HE1	1.97	0.46
3:N:1112:CYS:HB2	3:N:1195:GLN:CG	2.45	0.46
4:O:45:ARG:HB3	9:O:1014:HOH:O	2.14	0.46
4:O:70:THR:HG21	4:O:72:ARG:HE	1.80	0.46
5:P:288:TYR:HA	5:P:291:ILE:CG2	2.45	0.46
1:A:227:ASN:H	1:A:227:ASN:HD22	1.61	0.46
1:B:217:ILE:O	1:B:221:HIS:ND1	2.43	0.46
2:C:204:GLN:NE2	2:C:222:MET:HA	2.29	0.46
2:C:267:TYR:HB2	2:C:272:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:328:LEU:CD1	2:C:433:THR:HB	2.44	0.46
2:C:557:ARG:NE	2:C:560:MET:SD	2.88	0.46
2:C:672:VAL:HG23	2:C:868:ASP:HB2	1.96	0.46
2:C:1050:GLN:HG2	2:C:1079:PRO:HG2	1.97	0.46
3:D:39:PRO:HB3	3:D:45:PHE:O	2.15	0.46
3:D:204:LEU:HA	3:D:441:ARG:NH2	2.18	0.46
3:D:204:LEU:HD21	3:D:445:ARG:NH1	2.30	0.46
3:D:422:ALA:O	3:D:427:VAL:HB	2.16	0.46
3:D:543:LEU:HA	3:D:546:ARG:HG3	1.96	0.46
3:D:702:LEU:HD13	3:D:716:PHE:CD1	2.50	0.46
3:D:863:VAL:HA	9:D:1596:HOH:O	2.14	0.46
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.16	0.46
5:F:396:ARG:HA	5:F:399:GLN:HB2	1.97	0.46
2:M:18:LEU:HB2	2:M:590:ASP:CB	2.44	0.46
2:M:279:GLU:HG3	2:M:280:LYS:N	2.29	0.46
2:M:400:PRO:HG2	9:M:1638:HOH:O	2.15	0.46
3:N:850:LEU:O	3:N:853:VAL:HB	2.14	0.46
3:N:1108:ARG:NE	3:N:1198:TYR:O	2.47	0.46
4:O:59:ASN:N	9:O:4171:HOH:O	2.48	0.46
5:P:398:ARG:HG3	5:P:402:ASN:ND2	2.29	0.46
2:C:648:ARG:HG3	2:C:648:ARG:O	2.14	0.46
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.96	0.46
3:D:112:ILE:HD12	3:D:461:ILE:HG21	1.96	0.46
3:D:527:MET:HE1	5:F:258:ILE:HD11	1.97	0.46
3:D:537:THR:O	5:F:317:LEU:HB2	2.15	0.46
3:D:730:PRO:HA	3:D:733:CYS:SG	2.55	0.46
3:D:795:VAL:HG22	3:D:876:SER:HB3	1.96	0.46
3:D:1037:GLN:OE1	3:D:1042:ARG:HD3	2.15	0.46
5:F:319:THR:O	5:F:321:ILE:HG12	2.15	0.46
2:M:62:GLY:HA2	2:M:359:MET:CE	2.45	0.46
2:M:1078:GLU:HA	2:M:1079:PRO:HD3	1.86	0.46
3:N:187:LYS:HG3	3:N:199:LEU:CD2	2.44	0.46
3:N:1217:ILE:HD12	3:N:1480:PHE:CE2	2.51	0.46
4:O:33:HIS:CD2	4:O:89:MET:HG2	2.49	0.46
1:A:65:PHE:CE1	2:C:799:ILE:HD11	2.51	0.46
1:A:161:ARG:HB2	1:A:161:ARG:HH11	1.79	0.46
1:B:23:PHE:O	1:B:196:THR:HA	2.14	0.46
2:C:64:LEU:HB2	2:C:359:MET:CE	2.45	0.46
2:C:139:GLN:HA	2:C:411:SER:O	2.15	0.46
2:C:147:TYR:HE1	9:C:1347:HOH:O	1.98	0.46
2:C:160:ALA:O	2:C:173:ASP:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:271:GLU:HA	2:C:275:TYR:CD1	2.51	0.46
2:C:328:LEU:HB2	2:C:433:THR:CG2	2.46	0.46
3:D:677:LEU:HD21	9:D:2185:HOH:O	2.14	0.46
3:D:928:ALA:O	3:D:931:LEU:HB2	2.16	0.46
3:D:951:ILE:CD1	3:D:1062:ARG:HG3	2.45	0.46
3:D:1382:THR:OG1	3:D:1418:LYS:HE3	2.16	0.46
1:K:42:ARG:HE	2:M:857:ASP:HB3	1.79	0.46
1:L:102:LYS:HA	1:L:138:LEU:O	2.16	0.46
1:L:200:TRP:HZ3	9:N:2120:HOH:O	1.98	0.46
2:M:426:ASP:OD1	2:M:427:VAL:HG22	2.14	0.46
2:M:459:ALA:HB1	2:M:467:ILE:CG2	2.46	0.46
2:M:760:SER:O	2:M:786:LYS:N	2.40	0.46
3:N:562:ALA:HB1	3:N:567:ILE:CD1	2.45	0.46
3:N:705:ALA:HB3	3:N:706:PRO:CD	2.45	0.46
3:N:705:ALA:HB2	9:N:1965:HOH:O	2.16	0.46
3:N:1195:GLN:CG	3:N:1196:THR:N	2.78	0.46
3:N:1281:VAL:HG21	3:N:1313:VAL:HG21	1.96	0.46
3:N:1476:THR:CG2	4:O:21:VAL:HG22	2.42	0.46
5:P:123:ASP:HB2	5:P:126:LEU:HD13	1.96	0.46
5:P:420:ASP:O	5:P:422:LEU:HD23	2.16	0.46
1:B:85:LEU:HD13	1:B:127:LEU:HD23	1.98	0.46
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.81	0.46
2:C:31:GLN:NE2	2:C:71:TYR:OH	2.49	0.46
2:C:89:THR:HA	2:C:129:ILE:O	2.15	0.46
2:C:479:VAL:HG11	2:C:532:MET:HE2	1.97	0.46
2:C:588:VAL:HG21	9:C:1718:HOH:O	2.15	0.46
2:C:798:GLY:H	2:C:827:VAL:CG1	2.29	0.46
3:D:23:TYR:O	3:D:49:ILE:HG23	2.16	0.46
3:D:795:VAL:HG12	3:D:796:ARG:N	2.31	0.46
3:D:860:LEU:O	3:D:877:PRO:HD2	2.14	0.46
3:D:952:ASP:HA	3:D:1062:ARG:NH2	2.31	0.46
5:F:116:LEU:CB	5:F:127:ILE:HD12	2.46	0.46
5:F:151:LEU:HD11	9:F:626:HOH:O	2.14	0.46
5:F:171:LYS:HA	9:F:473:HOH:O	2.16	0.46
1:K:58:ILE:HG21	1:K:68:ILE:HD11	1.97	0.46
1:L:89:PHE:HB3	1:L:94:LEU:HD22	1.98	0.46
2:M:468:ARG:HB3	2:M:487:THR:HA	1.97	0.46
2:M:718:GLY:HA3	2:M:761:PHE:CE1	2.51	0.46
2:M:843:HIS:CD2	2:M:884:GLN:HA	2.50	0.46
2:M:1077:PRO:HG3	9:M:2203:HOH:O	2.15	0.46
3:N:18:ILE:HD12	3:N:518:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:403:PHE:CD1	3:N:405:ASP:O	2.62	0.46
4:O:82:GLU:HG3	4:O:83:ASP:H	1.80	0.46
5:P:209:PHE:HE2	5:P:213:ILE:HD11	1.79	0.46
1:B:57:TYR:O	1:B:140:MET:HA	2.15	0.46
1:B:60:ASP:HB2	1:B:137:ARG:NH1	2.31	0.46
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.50	0.46
2:C:575:GLN:O	2:C:667:ALA:HB1	2.15	0.46
2:C:762:LYS:C	2:C:763:GLY:O	2.52	0.46
2:C:939:ARG:HD3	2:C:975:TYR:CE2	2.51	0.46
2:C:975:TYR:HA	2:C:982:PRO:HA	1.97	0.46
3:D:191:LEU:HD13	3:D:393:ILE:HG21	1.97	0.46
3:D:421:LEU:HD11	3:D:446:VAL:CG2	2.45	0.46
3:D:455:ARG:NH1	3:D:463:GLN:HG3	2.31	0.46
3:D:1076:GLY:O	3:D:1079:LYS:HG2	2.16	0.46
4:E:13:VAL:HG23	9:E:151:HOH:O	2.14	0.46
1:K:35:THR:HG21	1:L:43:ILE:HD11	1.98	0.46
1:K:132:LEU:HD12	1:K:132:LEU:N	2.30	0.46
1:L:69:PRO:O	1:L:71:VAL:HG23	2.15	0.46
1:L:73:GLU:CD	1:L:130:ALA:HA	2.34	0.46
2:M:491:GLU:OE1	2:M:516:ARG:NH2	2.48	0.46
2:M:810:ASP:N	2:M:811:PRO:HD3	2.30	0.46
3:N:145:VAL:HG22	3:N:146:PRO:CD	2.46	0.46
3:N:1115:THR:HG21	3:N:1151:ARG:HH21	1.80	0.46
3:N:1266:ARG:O	3:N:1268:PRO:HD3	2.15	0.46
5:P:396:ARG:HA	5:P:399:GLN:HB2	1.98	0.46
1:B:176:ARG:NH2	3:D:847:ASP:HA	2.31	0.46
1:B:179:PHE:HZ	9:B:437:HOH:O	1.99	0.46
2:C:89:THR:HB	2:C:129:ILE:O	2.16	0.46
2:C:140:ILE:HD13	2:C:331:ARG:HH21	1.80	0.46
2:C:674:VAL:HB	2:C:869:VAL:HG13	1.98	0.46
2:C:875:GLY:HA2	2:C:879:ARG:HH11	1.80	0.46
2:C:929:ARG:HH12	2:C:940:GLU:CD	2.19	0.46
3:D:53:ILE:HG23	3:D:54:LYS:N	2.30	0.46
3:D:73:CYS:HB2	9:D:2023:HOH:O	2.14	0.46
3:D:421:LEU:HD11	3:D:446:VAL:HG21	1.97	0.46
3:D:443:VAL:HG22	3:D:444:VAL:H	1.81	0.46
3:D:1377:LYS:NZ	9:D:1537:HOH:O	2.45	0.46
3:D:1389:LEU:HD12	3:D:1390:LEU:HG	1.98	0.46
3:D:1472:ILE:O	3:D:1477:GLY:HA3	2.14	0.46
1:L:27:PRO:HB3	1:L:192:LEU:HD22	1.98	0.46
2:M:333:ILE:HD12	2:M:333:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:119:SER:HB3	9:N:1620:HOH:O	2.15	0.46
3:N:407:VAL:HG22	3:N:422:ALA:HB2	1.98	0.46
3:N:522:PRO:HA	3:N:525:ARG:NH1	2.31	0.46
3:N:644:LEU:HD23	3:N:718:PRO:HB3	1.98	0.46
3:N:937:TYR:O	3:N:941:PHE:HD1	1.99	0.46
3:N:1311:LEU:HD23	3:N:1311:LEU:H	1.81	0.46
3:N:1382:THR:HG21	3:N:1418:LYS:NZ	2.31	0.46
3:N:1410:GLU:OE2	3:N:1414:PRO:HG3	2.16	0.46
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.97	0.46
1:B:205:VAL:HB	9:B:448:HOH:O	2.15	0.46
2:C:101:ILE:HG23	2:C:107:LEU:CD2	2.43	0.46
2:C:799:ILE:HD13	2:C:799:ILE:N	2.30	0.46
3:D:131:LYS:HG3	3:D:572:ARG:HH21	1.81	0.46
3:D:409:VAL:O	3:D:437:VAL:HG21	2.16	0.46
3:D:498:VAL:CG2	3:D:499:VAL:N	2.79	0.46
3:D:562:ALA:HB1	3:D:567:ILE:CD1	2.45	0.46
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.46	0.46
3:D:693:GLU:HG3	4:E:48:MET:CE	2.46	0.46
3:D:783:ARG:NH1	3:D:1029:ARG:HG3	2.30	0.46
3:D:800:LYS:HE3	3:D:830:ALA:HB3	1.98	0.46
3:D:1335:LEU:CD2	3:D:1344:VAL:HA	2.29	0.46
4:E:26:ARG:HH11	4:E:29:GLN:CD	2.18	0.46
5:F:241:TRP:HB2	9:F:438:HOH:O	2.15	0.46
5:F:398:ARG:HG3	5:F:402:ASN:ND2	2.31	0.46
2:M:82:GLU:OE2	2:M:86:LYS:HE3	2.16	0.46
2:M:122:THR:HG22	2:M:123:GLU:N	2.30	0.46
2:M:352:ALA:C	2:M:355:VAL:HG12	2.36	0.46
2:M:518:LYS:HG3	9:M:1841:HOH:O	2.16	0.46
2:M:988:VAL:HG11	3:N:949:ILE:O	2.16	0.46
2:M:1097:LEU:HD21	3:N:103:TRP:HZ3	1.81	0.46
3:N:137:PRO:HD2	3:N:453:ASP:CG	2.36	0.46
3:N:795:VAL:HG22	3:N:876:SER:HB3	1.97	0.46
3:N:1344:VAL:HG12	3:N:1348:LEU:HD22	1.97	0.46
3:N:1385:GLY:CA	3:N:1413:THR:HG21	2.46	0.46
3:N:1426:LYS:HA	9:N:1705:HOH:O	2.15	0.46
1:A:9:PRO:HD2	1:B:224:TYR:CD1	2.51	0.46
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.31	0.46
2:C:1067:TYR:CE1	3:D:655:PRO:HG3	2.49	0.46
3:D:48:ARG:NH2	9:D:1710:HOH:O	2.48	0.46
3:D:525:ARG:HA	3:D:538:SER:OG	2.15	0.46
3:D:866:VAL:HG12	3:D:867:ARG:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1083:ASP:O	3:D:1087:ARG:HG3	2.15	0.46
5:F:214:GLN:O	5:F:217:ASN:HB2	2.16	0.46
1:K:36:LEU:O	1:K:39:PRO:HD2	2.16	0.46
2:M:9:ILE:HG12	2:M:907:ASP:OD2	2.15	0.46
2:M:103:LYS:HB3	9:M:2059:HOH:O	2.15	0.46
2:M:115:LEU:HD22	2:M:373:VAL:CG1	2.41	0.46
2:M:211:LEU:HD11	2:M:308:ARG:HA	1.98	0.46
2:M:540:PHE:HE1	2:M:906:PHE:HE1	1.64	0.46
2:M:612:VAL:HG22	2:M:622:GLU:HA	1.97	0.46
3:N:560:GLN:O	5:P:184:ARG:NH2	2.48	0.46
3:N:1197:ARG:HG3	3:N:1198:TYR:H	1.80	0.46
5:P:113:ILE:HG23	5:P:127:ILE:CG2	2.46	0.46
5:P:266:GLU:O	5:P:270:LYS:HG3	2.16	0.46
5:P:358:LEU:HD13	5:P:370:LYS:HG3	1.97	0.46
5:P:400:ILE:HA	9:P:540:HOH:O	2.15	0.46
5:P:406:ARG:HA	5:P:409:LYS:HG2	1.97	0.46
1:A:198:ARG:HD2	1:A:200:TRP:CH2	2.51	0.46
1:A:212:ASN:O	1:A:215:VAL:HG22	2.16	0.46
2:C:199:VAL:HG13	2:C:235:LEU:CD2	2.46	0.46
2:C:292:ARG:HH11	2:C:299:LYS:HD3	1.81	0.46
2:C:564:MET:SD	2:C:846:LYS:HE3	2.55	0.46
2:C:841:ASN:C	2:C:841:ASN:HD22	2.19	0.46
3:D:27:GLU:O	3:D:28:LYS:HG2	2.16	0.46
3:D:45:PHE:HD1	3:D:86:ARG:HH22	1.64	0.46
3:D:539:ASP:OD2	5:F:318:GLU:HB2	2.15	0.46
3:D:704:ARG:CG	3:D:705:ALA:H	2.24	0.46
3:D:911:LEU:O	3:D:915:VAL:HG23	2.15	0.46
3:D:1295:GLU:HB3	3:D:1300:SER:HB3	1.97	0.46
3:D:1326:THR:HG22	3:D:1327:ARG:N	2.31	0.46
3:D:1485:GLN:HE21	4:E:80:VAL:H	1.63	0.46
5:F:176:ILE:HA	9:F:463:HOH:O	2.16	0.46
5:F:368:VAL:O	5:F:372:ARG:HB2	2.16	0.46
1:K:46:SER:HB3	2:M:856:GLU:CG	2.45	0.46
1:K:51:THR:HA	1:K:145:ASP:O	2.16	0.46
2:M:110:GLU:HB2	2:M:369:PRO:HG3	1.97	0.46
2:M:143:SER:C	2:M:163:ILE:HD11	2.37	0.46
2:M:538:GLN:CD	9:M:1660:HOH:O	2.54	0.46
2:M:976:ASP:HB2	2:M:979:THR:HG22	1.96	0.46
2:M:1097:LEU:N	2:M:1097:LEU:HD12	2.30	0.46
2:M:1109:VAL:HG11	3:N:5:VAL:HG13	1.97	0.46
2:M:1115:LEU:CB	3:N:85:VAL:HG13	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:18:ILE:HG21	3:N:516:ALA:O	2.15	0.46
3:N:131:LYS:HD2	5:P:83:GLN:OE1	2.15	0.46
3:N:884:ARG:O	3:N:888:GLU:HB2	2.16	0.46
4:O:53:GLY:C	4:O:55:PHE:N	2.67	0.46
5:P:88:ILE:HD13	5:P:193:ARG:CB	2.46	0.46
5:P:138:SER:H	5:P:140:ARG:HE	1.64	0.46
1:A:69:PRO:C	1:A:71:VAL:H	2.18	0.45
1:B:9:PRO:HD3	9:B:452:HOH:O	2.17	0.45
2:C:6:PHE:HB2	2:C:908:GLY:O	2.16	0.45
2:C:86:LYS:HD2	9:C:1425:HOH:O	2.16	0.45
2:C:411:SER:OG	2:C:452:ILE:HG23	2.16	0.45
2:C:437:ARG:HG2	2:C:467:ILE:HG22	1.97	0.45
2:C:791:ARG:HD3	9:C:1572:HOH:O	2.15	0.45
2:C:1087:VAL:HG12	3:D:610:LYS:HZ3	1.81	0.45
3:D:803:GLY:CA	9:D:1726:HOH:O	2.64	0.45
3:D:1144:LEU:HB3	3:D:1166:LEU:HD11	1.97	0.45
3:D:1267:ARG:O	3:D:1267:ARG:HG2	2.16	0.45
3:D:1455:LYS:NZ	9:D:2342:HOH:O	2.48	0.45
5:F:148:LYS:HE3	9:F:489:HOH:O	2.16	0.45
1:L:124:ASN:OD1	1:L:127:LEU:HB2	2.17	0.45
2:M:9:ILE:HD11	2:M:537:LYS:CE	2.45	0.45
2:M:217:LEU:HB2	2:M:311:PHE:CE1	2.50	0.45
2:M:265:ARG:NH2	9:M:2236:HOH:O	2.48	0.45
2:M:612:VAL:HG22	2:M:622:GLU:HG3	1.99	0.45
2:M:675:ALA:CA	2:M:989:VAL:HG12	2.41	0.45
2:M:1114:GLY:HA2	9:M:1820:HOH:O	2.15	0.45
3:N:10:ILE:HD11	3:N:1434:TRP:NE1	2.31	0.45
3:N:102:ILE:HD12	3:N:579:ASP:CG	2.36	0.45
3:N:573:MET:SD	5:P:210:LEU:HB3	2.56	0.45
3:N:625:TYR:O	3:N:749:VAL:HG23	2.16	0.45
3:N:1258:ARG:NE	3:N:1262:LEU:HD11	2.31	0.45
3:N:1283:ILE:CG2	3:N:1290:LEU:HD21	2.46	0.45
4:O:45:ARG:HB2	4:O:46:PRO:CD	2.45	0.45
4:O:70:THR:HG22	4:O:71:GLY:N	2.31	0.45
4:O:87:LYS:HB3	9:O:2559:HOH:O	2.15	0.45
2:C:18:LEU:CD2	2:C:542:VAL:HG11	2.45	0.45
2:C:137:VAL:CG2	2:C:391:LEU:HG	2.46	0.45
2:C:146:VAL:HG22	2:C:162:ILE:HG23	1.97	0.45
2:C:425:PHE:O	2:C:429:ASP:OD2	2.35	0.45
2:C:536:PRO:HB2	9:C:1738:HOH:O	2.16	0.45
2:C:916:GLU:O	2:C:919:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1044:GLY:CA	4:E:17:TYR:HE1	2.21	0.45
3:D:66:GLN:O	3:D:67:ARG:C	2.53	0.45
3:D:195:VAL:HG12	3:D:196:VAL:N	2.31	0.45
3:D:736:PHE:O	3:D:738:ALA:N	2.50	0.45
3:D:907:GLU:HG2	3:D:908:LYS:H	1.81	0.45
3:D:1031:ASN:O	3:D:1034:GLN:HB2	2.16	0.45
5:F:80:PRO:O	5:F:83:GLN:HB2	2.16	0.45
5:F:94:LEU:HD12	5:F:98:GLU:OE2	2.16	0.45
5:F:288:TYR:HA	5:F:291:ILE:CG2	2.46	0.45
1:K:55:SER:HB2	1:K:158:ILE:HG21	1.98	0.45
1:K:158:ILE:HD12	1:K:158:ILE:HG23	1.88	0.45
1:K:162:ILE:HG13	1:K:163:ASN:N	2.32	0.45
2:M:49:ARG:HG2	2:M:266:ARG:HH12	1.82	0.45
2:M:165:LEU:HA	2:M:166:PRO:O	2.15	0.45
2:M:367:LEU:O	2:M:371:LYS:HB2	2.17	0.45
2:M:914:ILE:HD12	2:M:914:ILE:HA	1.75	0.45
3:N:23:TYR:O	3:N:24:GLY:O	2.35	0.45
3:N:204:LEU:O	3:N:393:ILE:HA	2.15	0.45
3:N:570:GLU:CA	5:P:214:GLN:HE22	2.29	0.45
3:N:1203:LYS:HG2	9:N:1955:HOH:O	2.15	0.45
3:N:1264:GLU:HG2	3:N:1425:THR:H	1.81	0.45
5:P:142:ARG:NH1	5:P:150:THR:OG1	2.49	0.45
5:P:157:GLU:HG2	9:P:498:HOH:O	2.16	0.45
1:A:158:ILE:HG22	1:A:160:ASP:H	1.81	0.45
2:C:271:GLU:HA	2:C:275:TYR:HD1	1.81	0.45
2:C:460:ARG:NE	2:C:485:TYR:CZ	2.84	0.45
2:C:551:GLU:HA	2:C:906:PHE:CE2	2.51	0.45
2:C:612:VAL:HG22	2:C:622:GLU:HA	1.99	0.45
2:C:905:ILE:H	2:C:905:ILE:CD1	2.13	0.45
2:C:1002:GLU:HA	9:C:1756:HOH:O	2.15	0.45
3:D:421:LEU:HB3	3:D:444:VAL:HG11	1.98	0.45
3:D:667:ALA:HB2	3:D:676:MET:SD	2.56	0.45
3:D:699:VAL:H	3:D:756:GLN:NE2	2.15	0.45
3:D:710:ARG:NH2	3:D:1210:SER:HB2	2.31	0.45
3:D:754:PHE:HA	4:E:24:ALA:HB1	1.98	0.45
3:D:814:ALA:O	3:D:818:ARG:HG3	2.17	0.45
3:D:1116:ASN:N	3:D:1116:ASN:ND2	2.63	0.45
3:D:1350:GLU:OE2	3:D:1357:ARG:NH1	2.48	0.45
5:F:82:ARG:O	5:F:86:HIS:HB2	2.15	0.45
2:M:19:THR:O	2:M:19:THR:HG22	2.16	0.45
2:M:51:THR:HB	2:M:348:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:838:LYS:HZ2	2:M:846:LYS:HE2	1.81	0.45
2:M:1044:GLY:HA3	4:O:17:TYR:HE1	1.80	0.45
3:N:102:ILE:HD12	3:N:579:ASP:CB	2.45	0.45
3:N:157:GLU:HA	3:N:160:GLU:OE1	2.16	0.45
3:N:455:ARG:NH2	9:N:2369:HOH:O	2.49	0.45
3:N:584:ASN:HD21	3:N:590:PRO:CD	2.29	0.45
3:N:684:LYS:HD2	9:N:2165:HOH:O	2.16	0.45
3:N:999:THR:O	3:N:1003:VAL:HG13	2.16	0.45
3:N:1378:TYR:HA	3:N:1394:VAL:HA	1.98	0.45
4:O:16:LYS:HB2	9:O:3818:HOH:O	2.14	0.45
5:P:300:ASP:HB3	9:P:433:HOH:O	2.16	0.45
5:P:419:ARG:O	5:P:421:PHE:N	2.49	0.45
1:B:169:ALA:HB1	1:B:171:PHE:HD2	1.80	0.45
2:C:64:LEU:HB2	2:C:359:MET:SD	2.56	0.45
2:C:110:GLU:HB2	2:C:369:PRO:HG3	1.98	0.45
2:C:114:PHE:CE2	5:F:283:GLY:HA3	2.51	0.45
2:C:212:GLY:HA3	2:C:218:VAL:CG2	2.45	0.45
2:C:352:ALA:HA	2:C:355:VAL:CG1	2.46	0.45
3:D:9:ARG:HA	3:D:1434:TRP:CH2	2.50	0.45
3:D:87:ARG:HA	3:D:523:ASP:HB2	1.98	0.45
3:D:473:LEU:HD21	3:D:495:ARG:CZ	2.46	0.45
3:D:684:LYS:HD3	3:D:686:GLU:OE1	2.17	0.45
3:D:1110:ALA:O	3:D:1111:ASP:C	2.52	0.45
3:D:1299:PHE:CD2	3:D:1299:PHE:N	2.84	0.45
3:D:1492:LEU:HA	9:D:2354:HOH:O	2.16	0.45
4:E:44:GLU:HG2	9:E:142:HOH:O	2.16	0.45
5:F:336:GLU:N	9:F:562:HOH:O	2.48	0.45
5:F:371:LEU:HB2	5:F:372:ARG:NH1	2.32	0.45
5:F:392:VAL:HG11	5:F:396:ARG:CD	2.46	0.45
1:L:156:HIS:CG	1:L:157:GLY:N	2.84	0.45
1:L:165:ILE:O	1:L:165:ILE:HG13	2.16	0.45
2:M:285:LEU:HD22	9:M:1655:HOH:O	2.15	0.45
2:M:329:GLY:HA3	2:M:489:THR:HG23	1.98	0.45
2:M:418:LEU:N	2:M:418:LEU:CD1	2.80	0.45
2:M:752:GLY:H	2:M:792:VAL:HB	1.82	0.45
3:N:93:ILE:HD13	3:N:548:ILE:HD11	1.98	0.45
3:N:104:PHE:CE2	3:N:1448:THR:HG23	2.51	0.45
3:N:1369:GLU:O	3:N:1372:VAL:HG12	2.17	0.45
3:N:1505:ALA:HB1	9:N:2193:HOH:O	2.17	0.45
4:O:75:PHE:HE1	9:O:3411:HOH:O	1.98	0.45
4:O:76:GLY:HA3	4:O:79:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:54:ILE:HG23	2:C:54:ILE:O	2.16	0.45
2:C:265:ARG:HD3	2:C:267:TYR:HB3	1.99	0.45
2:C:443:THR:HA	2:C:444:PRO:HD3	1.79	0.45
2:C:474:VAL:HA	2:C:478:VAL:O	2.17	0.45
2:C:565:GLN:OE1	2:C:842:ARG:HG2	2.17	0.45
2:C:1060:ILE:HG22	2:C:1061:GLU:H	1.81	0.45
3:D:72:VAL:CG2	3:D:78:VAL:H	2.29	0.45
3:D:540:LEU:HD21	3:D:603:LEU:HD23	1.98	0.45
3:D:563:PRO:HG2	5:F:188:ILE:HG21	1.99	0.45
3:D:760:ARG:HD2	4:E:3:GLU:OE1	2.17	0.45
3:D:1000:THR:HG23	3:D:1001:GLU:N	2.31	0.45
3:D:1047:LYS:HG2	3:D:1053:PHE:CE2	2.51	0.45
4:E:31:LEU:HD23	4:E:35:PHE:CE1	2.52	0.45
5:F:340:SER:O	5:F:342:VAL:N	2.50	0.45
5:F:394:ARG:NE	5:F:398:ARG:HB2	2.31	0.45
2:M:118:ILE:O	2:M:118:ILE:HD12	2.16	0.45
2:M:807:ARG:HA	2:M:821:GLU:HB2	1.99	0.45
3:N:45:PHE:HD1	3:N:86:ARG:NH2	2.15	0.45
3:N:126:VAL:CG1	3:N:132:TYR:HB2	2.47	0.45
3:N:675:ARG:HH22	5:P:421:PHE:HE2	1.63	0.45
3:N:700:VAL:HG22	3:N:718:PRO:HG3	1.98	0.45
3:N:779:ALA:HA	9:N:1773:HOH:O	2.16	0.45
3:N:796:ARG:NH1	3:N:861:GLN:HE21	2.14	0.45
3:N:939:PHE:O	3:N:943:THR:HG23	2.17	0.45
3:N:1299:PHE:N	3:N:1299:PHE:HD2	2.15	0.45
3:N:1420:LEU:HD23	9:N:1853:HOH:O	2.15	0.45
5:P:91:VAL:HG21	9:P:550:HOH:O	2.17	0.45
5:P:360:LYS:HG2	9:P:511:HOH:O	2.17	0.45
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.75	0.45
1:A:151:VAL:H	1:A:169:ALA:HB3	1.81	0.45
2:C:68:PHE:HE1	2:C:96:ALA:HB1	1.82	0.45
2:C:418:LEU:N	2:C:418:LEU:CD1	2.79	0.45
2:C:598:GLU:HG3	2:C:623:TYR:OH	2.17	0.45
3:D:95:LEU:HD23	3:D:574:LEU:HD11	1.98	0.45
3:D:892:ASP:O	3:D:895:VAL:N	2.49	0.45
2:M:455:LEU:HD12	2:M:456:ALA:N	2.32	0.45
3:N:28:LYS:HG3	3:N:41:ARG:CD	2.47	0.45
3:N:403:PHE:CE2	3:N:443:VAL:N	2.85	0.45
3:N:409:VAL:HG12	3:N:435:VAL:HG11	1.98	0.45
3:N:560:GLN:NE2	5:P:221:ILE:HB	2.31	0.45
3:N:704:ARG:CG	3:N:705:ALA:H	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:728:LEU:HD12	9:N:1892:HOH:O	2.17	0.45
3:N:861:GLN:HG2	3:N:861:GLN:H	1.55	0.45
3:N:1084:THR:HG21	9:N:2214:HOH:O	2.16	0.45
5:P:351:SER:O	5:P:355:GLU:HB2	2.15	0.45
5:P:361:LEU:HD21	5:P:404:ALA:CB	2.46	0.45
1:A:58:ILE:HG21	1:A:68:ILE:CD1	2.45	0.45
1:B:61:VAL:H	1:B:137:ARG:HH22	1.65	0.45
2:C:342:ASP:O	2:C:346:VAL:HG23	2.16	0.45
2:C:469:THR:OG1	2:C:470:PRO:HD2	2.16	0.45
2:C:739:GLU:CD	2:C:742:VAL:HB	2.37	0.45
2:C:837:ASP:OD1	2:C:999:HIS:NE2	2.49	0.45
2:C:876:VAL:HB	2:C:877:PRO:HD3	1.98	0.45
2:C:1009:SER:CB	3:D:651:GLU:HG2	2.47	0.45
3:D:584:ASN:HD21	3:D:590:PRO:HB2	1.82	0.45
3:D:617:ASN:C	3:D:618:LEU:HD12	2.37	0.45
3:D:640:HIS:HE1	4:E:3:GLU:HG2	1.80	0.45
3:D:1108:ARG:HB2	9:D:2164:HOH:O	2.15	0.45
3:D:1173:LEU:HD23	3:D:1174:LEU:HD23	1.98	0.45
3:D:1242:HIS:NE2	3:D:1266:ARG:HD3	2.31	0.45
3:D:1285:GLU:O	3:D:1285:GLU:HG2	2.17	0.45
3:D:1487:VAL:HG13	3:D:1491:THR:HB	1.97	0.45
5:F:284:ARG:HB2	9:F:621:HOH:O	2.17	0.45
5:F:393:THR:HG22	5:F:394:ARG:H	1.82	0.45
2:M:92:ALA:HB2	2:M:120:LEU:CD1	2.45	0.45
2:M:551:GLU:HB3	2:M:906:PHE:CD2	2.51	0.45
2:M:1059:ASP:CG	2:M:1062:GLY:HA3	2.37	0.45
3:N:16:GLU:HG3	9:N:1701:HOH:O	2.16	0.45
3:N:105:VAL:HG21	3:N:128:TYR:HE2	1.75	0.45
3:N:486:ARG:HG2	9:N:1964:HOH:O	2.15	0.45
3:N:569:ASN:ND2	5:P:210:LEU:HD22	2.29	0.45
3:N:586:ARG:HG2	9:N:2201:HOH:O	2.16	0.45
3:N:770:LEU:HB2	3:N:1210:SER:O	2.17	0.45
3:N:838:ARG:HB3	9:N:2366:HOH:O	2.17	0.45
3:N:1335:LEU:O	3:N:1335:LEU:HG	2.16	0.45
3:N:1350:GLU:O	3:N:1350:GLU:HG3	2.16	0.45
9:N:1980:HOH:O	5:P:210:LEU:HD12	2.17	0.45
5:P:125:ASP:HA	9:P:579:HOH:O	2.16	0.45
2:C:266:ARG:HA	2:C:288:ARG:HD3	1.97	0.45
2:C:471:TYR:CD2	2:C:496:ILE:HG21	2.51	0.45
2:C:475:VAL:O	2:C:475:VAL:HG12	2.17	0.45
2:C:810:ASP:H	2:C:811:PRO:HD3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:971:LYS:HG2	9:C:1494:HOH:O	2.17	0.45
3:D:137:PRO:HD2	3:D:453:ASP:CB	2.46	0.45
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.46	0.45
4:E:37:ASN:HA	4:E:93:TYR:CE2	2.52	0.45
5:F:361:LEU:HD13	5:F:366:ALA:HB2	1.98	0.45
2:M:18:LEU:HD13	2:M:590:ASP:OD2	2.16	0.45
2:M:694:LEU:CD1	2:M:868:ASP:HB3	2.47	0.45
2:M:715:THR:CG2	2:M:717:LEU:HG	2.45	0.45
2:M:1048:THR:O	2:M:1052:MET:HG2	2.17	0.45
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.82	0.45
3:N:119:SER:CB	3:N:123:LEU:HD13	2.46	0.45
3:N:809:PRO:HB2	3:N:812:ALA:CB	2.45	0.45
3:N:896:ALA:O	3:N:900:ILE:HG23	2.17	0.45
3:N:1107:VAL:HA	3:N:1200:VAL:O	2.17	0.45
3:N:1372:VAL:HG13	3:N:1373:ARG:N	2.32	0.45
1:A:64:GLU:O	1:A:64:GLU:HG2	2.14	0.45
1:A:158:ILE:HG22	1:A:159:LYS:N	2.32	0.45
2:C:13:ILE:HG12	2:C:534:VAL:HG13	1.98	0.45
2:C:36:PRO:HG2	2:C:70:GLU:HB3	1.97	0.45
2:C:185:LYS:NZ	2:C:190:LYS:HE2	2.32	0.45
2:C:670:GLN:HE22	2:C:699:PHE:C	2.21	0.45
2:C:841:ASN:HD21	2:C:845:ASN:N	2.15	0.45
2:C:926:PHE:HE1	2:C:929:ARG:NH1	2.15	0.45
3:D:72:VAL:HG23	3:D:78:VAL:N	2.32	0.45
3:D:141:ILE:HG13	3:D:142:LEU:N	2.31	0.45
3:D:850:LEU:O	3:D:853:VAL:HB	2.16	0.45
3:D:1124:GLN:HA	3:D:1125:PRO:HD3	1.79	0.45
4:E:46:PRO:CB	4:E:54:LEU:HD22	2.46	0.45
5:F:248:ASN:HA	5:F:251:ILE:HD12	1.98	0.45
2:M:9:ILE:HD11	2:M:537:LYS:HE2	1.98	0.45
2:M:537:LYS:H	2:M:537:LYS:HG2	1.44	0.45
2:M:854:PRO:C	2:M:856:GLU:N	2.70	0.45
2:M:987:ILE:HG22	2:M:988:VAL:O	2.17	0.45
3:N:28:LYS:HA	3:N:29:PRO:HD3	1.72	0.45
3:N:863:VAL:HG11	9:N:2345:HOH:O	2.17	0.45
3:N:1045:MET:HG3	3:N:1073:SER:OG	2.17	0.45
3:N:1120:VAL:HB	3:N:1144:LEU:HD21	1.99	0.45
5:P:132:ARG:HB3	5:P:136:LEU:HD21	1.99	0.45
1:B:55:SER:HB2	1:B:158:ILE:HD13	1.96	0.45
2:C:9:ILE:HG12	2:C:907:ASP:CG	2.38	0.45
2:C:338:GLU:HA	2:C:341:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:358:ARG:HD3	2:C:371:LYS:O	2.17	0.45
2:C:889:HIS:HD2	2:C:970:GLY:HA3	1.81	0.45
2:C:939:ARG:HB3	2:C:982:PRO:HG3	1.98	0.45
2:C:1109:VAL:CG1	3:D:5:VAL:HG13	2.46	0.45
3:D:31:THR:HG23	3:D:45:PHE:HE2	1.80	0.45
3:D:76:CYS:N	9:D:1539:HOH:O	2.49	0.45
3:D:637:LEU:HD12	3:D:641:GLN:HB2	1.99	0.45
3:D:1087:ARG:CD	3:D:1236:LEU:O	2.65	0.45
3:D:1254:GLN:HB2	9:D:1984:HOH:O	2.17	0.45
3:D:1368:ILE:H	3:D:1368:ILE:HG13	1.57	0.45
3:D:1448:THR:O	3:D:1451:ALA:HB3	2.16	0.45
1:K:198:ARG:C	1:K:199:ILE:HD12	2.37	0.45
2:M:90:TYR:HE1	9:M:2242:HOH:O	2.00	0.45
2:M:165:LEU:O	2:M:265:ARG:HB2	2.17	0.45
2:M:572:ILE:HD11	2:M:701:THR:HB	1.99	0.45
2:M:673:LEU:CD2	2:M:867:VAL:HG12	2.46	0.45
3:N:50:PHE:HB3	3:N:522:PRO:CG	2.46	0.45
3:N:54:LYS:O	3:N:55:ASP:O	2.34	0.45
3:N:103:TRP:NE1	3:N:1444:THR:HG23	2.31	0.45
3:N:477:LEU:HD22	3:N:492:ALA:HB1	1.99	0.45
3:N:500:ARG:HH11	3:N:500:ARG:HG3	1.82	0.45
3:N:656:PHE:HB3	3:N:694:VAL:HG11	1.98	0.45
3:N:1376:MET:HG2	3:N:1421:LEU:HD12	1.98	0.45
2:C:102:HIS:CE1	2:C:365:ASP:HA	2.52	0.44
2:C:221:LEU:HD11	9:C:1633:HOH:O	2.17	0.44
2:C:410:ILE:CD1	2:C:455:LEU:HB3	2.46	0.44
2:C:750:LYS:HG3	3:D:681:ARG:NH2	2.24	0.44
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.82	0.44
3:D:514:LEU:HA	9:D:1709:HOH:O	2.15	0.44
3:D:609:GLY:O	3:D:610:LYS:O	2.35	0.44
3:D:820:GLU:HB2	3:D:836:VAL:HG11	1.99	0.44
3:D:1465:ASN:HD22	3:D:1465:ASN:HA	1.50	0.44
5:F:420:ASP:O	5:F:422:LEU:HD23	2.16	0.44
2:M:281:LEU:O	2:M:282:GLY:O	2.35	0.44
2:M:690:ILE:HG12	2:M:694:LEU:HD12	1.99	0.44
2:M:863:ASP:OD1	2:M:865:THR:HG22	2.16	0.44
2:M:988:VAL:HG13	3:N:948:THR:OG1	2.17	0.44
2:M:1058:ASP:OD1	2:M:1084:SER:HB3	2.16	0.44
2:M:1115:LEU:HD12	2:M:1115:LEU:H	1.81	0.44
3:N:486:ARG:N	9:N:1964:HOH:O	2.49	0.44
3:N:644:LEU:HD12	3:N:645:PRO:CD	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:860:LEU:HB2	9:N:2139:HOH:O	2.17	0.44
4:O:32:ARG:HD2	9:O:4200:HOH:O	2.16	0.44
5:P:195:VAL:HG11	5:P:217:ASN:OD1	2.17	0.44
5:P:340:SER:OG	5:P:342:VAL:HG23	2.17	0.44
2:C:158:TYR:CE1	2:C:313:LEU:HG	2.52	0.44
2:C:598:GLU:O	2:C:651:LYS:HG3	2.16	0.44
3:D:625:TYR:O	3:D:749:VAL:HG23	2.16	0.44
3:D:810:GLU:HA	3:D:813:LEU:HD23	1.98	0.44
3:D:960:LYS:HG2	3:D:964:LEU:HD12	1.99	0.44
3:D:1161:GLU:CG	3:D:1164:ARG:HD2	2.46	0.44
5:F:191:ASN:OD1	5:F:194:LEU:HD13	2.17	0.44
5:F:256:ARG:HH12	5:F:311:ALA:HA	1.82	0.44
1:L:228:PRO:O	1:L:229:GLN:HG3	2.17	0.44
2:M:355:VAL:CG2	2:M:372:LEU:HG	2.48	0.44
2:M:861:LEU:HD21	2:M:925:TYR:HE2	1.81	0.44
3:N:72:VAL:HG23	3:N:78:VAL:N	2.30	0.44
3:N:169:TYR:HA	3:N:170:PRO:HD3	1.83	0.44
3:N:455:ARG:HA	9:N:2093:HOH:O	2.17	0.44
3:N:611:GLN:OE1	3:N:619:LEU:HD11	2.17	0.44
3:N:708:LEU:HD23	3:N:708:LEU:HA	1.80	0.44
3:N:1010:ASN:HA	9:N:1747:HOH:O	2.17	0.44
3:N:1109:GLU:HG2	3:N:1202:GLN:N	2.30	0.44
3:N:1263:PHE:O	3:N:1375:MET:HE2	2.18	0.44
5:P:226:LYS:HD2	5:P:242:TRP:HZ2	1.82	0.44
1:A:86:VAL:CG1	1:A:124:ASN:HB2	2.48	0.44
2:C:208:ALA:CA	2:C:221:LEU:HD21	2.48	0.44
2:C:258:TYR:HB3	9:C:1773:HOH:O	2.17	0.44
2:C:265:ARG:CG	2:C:266:ARG:N	2.80	0.44
2:C:380:ALA:O	2:C:384:GLU:HB2	2.18	0.44
2:C:402:SER:OG	2:C:566:THR:O	2.36	0.44
2:C:601:GLY:O	2:C:649:VAL:HG22	2.18	0.44
2:C:684:PHE:HD2	3:D:740:PHE:HE1	1.65	0.44
2:C:690:ILE:HG12	2:C:694:LEU:HD12	1.99	0.44
2:C:1058:ASP:HB2	3:D:621:LYS:HE2	1.99	0.44
3:D:28:LYS:CG	3:D:41:ARG:HH11	2.24	0.44
3:D:136:ASP:CB	3:D:137:PRO:HD3	2.20	0.44
3:D:560:GLN:OE1	5:F:218:GLN:HG3	2.18	0.44
3:D:814:ALA:HB2	9:D:1889:HOH:O	2.18	0.44
3:D:1310:ARG:HE	3:D:1327:ARG:HB3	1.80	0.44
5:F:94:LEU:HB2	5:F:98:GLU:CD	2.37	0.44
1:L:152:PRO:HG2	3:N:857:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:12:VAL:HG13	2:M:13:ILE:HG23	1.98	0.44
2:M:36:PRO:HG3	2:M:71:TYR:CE2	2.53	0.44
2:M:78:PHE:HB3	2:M:79:PRO:HD2	1.99	0.44
2:M:729:LEU:HD13	3:N:675:ARG:NH2	2.33	0.44
2:M:762:LYS:C	2:M:763:GLY:O	2.53	0.44
2:M:850:ALA:HA	3:N:632:VAL:CG1	2.47	0.44
2:M:926:PHE:CE2	2:M:960:GLU:HG3	2.52	0.44
2:M:1021:LEU:HD13	5:P:331:ASP:O	2.18	0.44
3:N:666:ILE:H	3:N:666:ILE:HG13	1.61	0.44
3:N:826:PRO:HD2	3:N:829:VAL:HG22	1.99	0.44
3:N:1159:ARG:CZ	3:N:1159:ARG:HB3	2.47	0.44
3:N:1207:TYR:H	3:N:1366:LYS:HZ1	1.65	0.44
3:N:1326:THR:HG22	3:N:1327:ARG:N	2.33	0.44
5:P:318:GLU:HG2	9:P:448:HOH:O	2.16	0.44
1:B:10:VAL:HG12	1:B:12:THR:HG23	1.98	0.44
2:C:113:VAL:O	2:C:115:LEU:HD23	2.17	0.44
2:C:529:VAL:HG21	9:C:1134:HOH:O	2.18	0.44
2:C:598:GLU:HG2	9:C:1352:HOH:O	2.18	0.44
2:C:674:VAL:HB	2:C:869:VAL:CG1	2.47	0.44
2:C:759:THR:HB	2:C:785:VAL:HG21	1.99	0.44
2:C:863:ASP:OD1	2:C:865:THR:HG22	2.16	0.44
3:D:63:TYR:HB2	9:D:2023:HOH:O	2.17	0.44
3:D:85:VAL:HG11	3:D:89:ARG:CZ	2.48	0.44
3:D:614:PHE:CB	3:D:617:ASN:HB3	2.47	0.44
3:D:624:ASP:HB3	3:D:625:TYR:CD1	2.53	0.44
3:D:1376:MET:HA	9:D:2082:HOH:O	2.17	0.44
3:D:1380:GLU:HB2	3:D:1420:LEU:CD2	2.47	0.44
4:E:40:LEU:C	4:E:42:PRO:HD2	2.37	0.44
1:K:227:ASN:H	1:K:227:ASN:HD22	1.65	0.44
1:K:229:GLN:HE21	1:K:229:GLN:HB2	1.56	0.44
1:L:45:LEU:HD21	1:L:177:VAL:HG22	1.99	0.44
1:L:45:LEU:HD11	1:L:177:VAL:CG2	2.48	0.44
2:M:114:PHE:CD2	5:P:283:GLY:HA3	2.52	0.44
2:M:211:LEU:CD1	2:M:308:ARG:HA	2.47	0.44
2:M:810:ASP:H	2:M:811:PRO:HD3	1.82	0.44
2:M:862:PRO:HD3	2:M:973:VAL:O	2.18	0.44
2:M:968:LEU:CB	9:M:2164:HOH:O	2.58	0.44
2:M:1030:GLN:NE2	3:N:628:ARG:HB3	2.32	0.44
3:N:165:LYS:HE2	9:N:2305:HOH:O	2.17	0.44
3:N:420:VAL:HG13	9:N:2303:HOH:O	2.17	0.44
3:N:1182:GLU:HB3	9:N:2331:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:45:ARG:HH21	4:O:55:PHE:HB3	1.80	0.44
5:P:276:ARG:HA	9:P:451:HOH:O	2.17	0.44
1:A:88:ARG:HG3	1:A:88:ARG:O	2.16	0.44
1:A:127:LEU:HD11	1:A:129:ILE:CD1	2.47	0.44
1:B:23:PHE:HE2	1:B:199:ILE:HD12	1.81	0.44
1:B:27:PRO:HB3	1:B:192:LEU:HD22	1.99	0.44
2:C:139:GLN:HG2	2:C:140:ILE:N	2.33	0.44
2:C:278:GLU:HG3	2:C:283:ILE:HG23	2.00	0.44
2:C:443:THR:CG2	2:C:449:ILE:HG13	2.48	0.44
2:C:474:VAL:HG13	2:C:529:VAL:O	2.17	0.44
2:C:1043:TYR:HE1	3:D:710:ARG:O	2.00	0.44
3:D:28:LYS:HA	3:D:29:PRO:HD3	1.69	0.44
3:D:880:ILE:O	3:D:883:ALA:HB3	2.17	0.44
5:F:351:SER:O	5:F:355:GLU:HB2	2.17	0.44
1:K:132:LEU:HD21	1:K:138:LEU:HB2	2.00	0.44
1:K:212:ASN:O	1:K:215:VAL:HG22	2.18	0.44
1:L:191:ASP:O	1:L:192:LEU:HG	2.18	0.44
2:M:227:PHE:HD2	2:M:237:ARG:CZ	2.30	0.44
2:M:247:PRO:HB2	9:M:2082:HOH:O	2.16	0.44
2:M:474:VAL:HA	2:M:478:VAL:O	2.17	0.44
3:N:66:GLN:O	3:N:67:ARG:C	2.55	0.44
3:N:204:LEU:HA	3:N:441:ARG:NH2	2.20	0.44
3:N:204:LEU:O	3:N:393:ILE:HG23	2.17	0.44
3:N:421:LEU:HD11	3:N:446:VAL:CG2	2.48	0.44
3:N:953:ASP:O	3:N:955:VAL:HG23	2.17	0.44
3:N:1002:LYS:HA	9:N:1776:HOH:O	2.17	0.44
3:N:1217:ILE:H	3:N:1217:ILE:HG13	1.68	0.44
3:N:1326:THR:HG22	3:N:1327:ARG:H	1.81	0.44
3:N:1426:LYS:HG2	9:N:1735:HOH:O	2.18	0.44
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.44	0.44
1:A:229:GLN:HE21	1:A:229:GLN:HB2	1.57	0.44
1:B:59:GLU:HG3	1:B:139:ASN:HB3	2.00	0.44
2:C:48:PHE:CE1	2:C:348:LEU:HD11	2.53	0.44
2:C:217:LEU:HB2	2:C:311:PHE:CE1	2.53	0.44
2:C:873:PRO:HB3	3:D:949:ILE:HG12	2.00	0.44
3:D:631:ILE:O	3:D:632:VAL:HG23	2.18	0.44
3:D:660:LYS:HE3	3:D:663:GLU:CD	2.38	0.44
3:D:1155:VAL:CG1	3:D:1177:ALA:HB1	2.47	0.44
4:E:85:LEU:HD23	4:E:86:GLN:N	2.32	0.44
4:E:88:GLU:HB3	9:E:137:HOH:O	2.18	0.44
5:F:240:THR:O	5:F:244:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:299:TRP:CE3	5:F:303:ARG:HD3	2.52	0.44
5:F:300:ASP:CG	5:F:301:ALA:N	2.71	0.44
5:F:419:ARG:O	5:F:421:PHE:N	2.50	0.44
1:K:92:PRO:HB3	9:K:3732:HOH:O	2.17	0.44
2:M:118:ILE:HA	2:M:119:PRO:HD3	1.88	0.44
2:M:264:PRO:HA	9:M:1703:HOH:O	2.17	0.44
2:M:281:LEU:HD12	2:M:305:PRO:O	2.17	0.44
2:M:319:GLY:HA2	9:M:1910:HOH:O	2.18	0.44
2:M:405:ARG:NH1	2:M:566:THR:HG21	2.32	0.44
2:M:1010:THR:HG22	2:M:1011:GLY:N	2.32	0.44
2:M:1105:LYS:HB3	9:M:1845:HOH:O	2.16	0.44
3:N:122:GLU:O	3:N:126:VAL:HG23	2.18	0.44
3:N:1167:SER:O	3:N:1171:VAL:HG23	2.18	0.44
3:N:1247:ALA:HB3	9:N:1888:HOH:O	2.16	0.44
3:N:1412:LYS:O	3:N:1414:PRO:HD3	2.18	0.44
5:P:141:VAL:HG22	9:P:496:HOH:O	2.18	0.44
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.99	0.44
2:C:265:ARG:HG2	2:C:267:TYR:N	2.31	0.44
2:C:267:TYR:H	2:C:267:TYR:HD2	1.64	0.44
2:C:278:GLU:HA	2:C:283:ILE:HA	2.00	0.44
2:C:398:THR:O	2:C:635:THR:HG21	2.17	0.44
2:C:588:VAL:HG21	2:C:664:GLY:O	2.18	0.44
3:D:52:PRO:CG	3:D:78:VAL:HG13	2.47	0.44
3:D:1209:LEU:C	3:D:1211:MET:N	2.71	0.44
3:D:1326:THR:HA	9:D:2026:HOH:O	2.17	0.44
1:K:8:ALA:HB2	9:K:1466:HOH:O	2.18	0.44
1:K:64:GLU:O	1:K:64:GLU:HG2	2.17	0.44
2:M:207:LEU:HD22	2:M:221:LEU:HD22	1.99	0.44
2:M:340:MET:SD	2:M:344:PHE:HB2	2.58	0.44
2:M:573:ARG:HB3	2:M:670:GLN:OE1	2.17	0.44
2:M:599:GLU:HB2	9:M:1699:HOH:O	2.18	0.44
2:M:732:ALA:O	2:M:735:ARG:HG3	2.18	0.44
2:M:751:PRO:CG	2:M:796:GLU:HG2	2.48	0.44
2:M:873:PRO:HB3	3:N:949:ILE:HG12	1.99	0.44
2:M:1034:GLU:O	2:M:1037:VAL:HG23	2.17	0.44
3:N:52:PRO:CB	3:N:80:VAL:HG13	2.47	0.44
3:N:118:LEU:O	3:N:119:SER:C	2.56	0.44
3:N:172:PRO:O	3:N:174:GLY:N	2.51	0.44
3:N:421:LEU:HB3	3:N:444:VAL:HG11	2.00	0.44
3:N:643:GLY:CA	3:N:727:GLN:HB2	2.47	0.44
3:N:699:VAL:H	3:N:756:GLN:HE21	1.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:795:VAL:HG12	3:N:796:ARG:N	2.32	0.44
3:N:799:LYS:HE2	3:N:801:GLY:HA3	2.00	0.44
3:N:1231:GLU:HG2	3:N:1232:PRO:N	2.33	0.44
4:O:29:GLN:HE22	4:O:89:MET:HE1	1.83	0.44
4:O:33:HIS:HB3	9:O:1494:HOH:O	2.18	0.44
5:P:385:GLU:O	5:P:397:ILE:HD13	2.18	0.44
1:A:33:GLY:O	1:A:195:LEU:HD22	2.18	0.44
1:A:67:THR:HG23	1:A:67:THR:O	2.17	0.44
1:A:106:PRO:HG3	1:A:133:GLU:O	2.17	0.44
1:A:158:ILE:C	1:A:159:LYS:HG3	2.38	0.44
1:B:158:ILE:HD11	1:B:166:PRO:N	2.33	0.44
2:C:146:VAL:N	9:C:1337:HOH:O	2.50	0.44
2:C:191:PHE:CZ	2:C:238:LEU:HD11	2.52	0.44
2:C:212:GLY:C	2:C:215:GLY:H	2.21	0.44
2:C:1118:LYS:O	2:C:1119:ARG:OXT	2.36	0.44
3:D:204:LEU:HD11	3:D:445:ARG:HH12	1.81	0.44
3:D:508:ARG:CG	3:D:509:PRO:HD2	2.36	0.44
3:D:798:GLU:HB2	3:D:828:LYS:CE	2.40	0.44
3:D:1074:SER:O	3:D:1077:ALA:HB3	2.18	0.44
3:D:1123:PHE:HB3	3:D:1132:LEU:HG	1.98	0.44
3:D:1478:SER:HG	3:D:1481:VAL:H	1.66	0.44
5:F:392:VAL:HG11	5:F:396:ARG:HD2	2.00	0.44
1:L:80:LEU:HD23	3:N:867:ARG:HD2	1.99	0.44
2:M:64:LEU:HB2	2:M:359:MET:SD	2.57	0.44
2:M:176:VAL:HB	9:M:2210:HOH:O	2.18	0.44
2:M:207:LEU:O	2:M:211:LEU:HB3	2.18	0.44
2:M:564:MET:SD	2:M:846:LYS:HE3	2.58	0.44
2:M:942:GLU:O	2:M:945:ARG:HB3	2.17	0.44
3:N:36:THR:O	3:N:38:LYS:N	2.51	0.44
3:N:44:LEU:O	3:N:50:PHE:CE1	2.70	0.44
3:N:528:VAL:HG12	3:N:529:GLN:N	2.33	0.44
5:P:205:ARG:CD	5:P:251:ILE:HG21	2.48	0.44
5:P:226:LYS:HE3	9:P:445:HOH:O	2.18	0.44
2:C:146:VAL:HG11	2:C:306:THR:HG22	1.99	0.44
2:C:264:PRO:HB3	2:C:289:THR:CB	2.47	0.44
2:C:545:ASN:O	2:C:581:THR:HG21	2.17	0.44
2:C:1052:MET:SD	3:D:623:VAL:HG21	2.57	0.44
3:D:162:ARG:HA	3:D:449:SER:OG	2.17	0.44
3:D:554:LEU:HD23	3:D:570:GLU:HG2	2.00	0.44
3:D:569:ASN:HD21	5:F:210:LEU:HD22	1.82	0.44
3:D:937:TYR:HD2	3:D:941:PHE:HE1	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1008:PHE:HB3	9:D:1941:HOH:O	2.17	0.44
3:D:1276:GLU:OE2	3:D:1303:TYR:HE2	2.00	0.44
5:F:151:LEU:HD23	9:F:489:HOH:O	2.17	0.44
5:F:306:GLU:HG3	9:F:582:HOH:O	2.18	0.44
1:L:101:LEU:CD1	9:L:1850:HOH:O	2.64	0.44
2:M:7:GLY:O	2:M:907:ASP:OD1	2.36	0.44
2:M:64:LEU:CD1	2:M:100:LEU:HD13	2.48	0.44
2:M:198:ARG:NE	2:M:228:ALA:HA	2.33	0.44
2:M:207:LEU:HD13	2:M:221:LEU:HD13	2.00	0.44
2:M:564:MET:SD	2:M:846:LYS:HG3	2.58	0.44
3:N:155:ASP:HA	3:N:158:TYR:HB3	2.00	0.44
3:N:195:VAL:HG12	3:N:196:VAL:N	2.32	0.44
3:N:638:LYS:C	3:N:729:HIS:HD2	2.21	0.44
3:N:987:GLU:HA	9:N:2147:HOH:O	2.18	0.44
3:N:996:TRP:HA	3:N:999:THR:CG2	2.46	0.44
4:O:57:ASP:N	4:O:58:PRO:HD3	2.32	0.44
5:P:140:ARG:HG3	5:P:141:VAL:N	2.33	0.44
5:P:396:ARG:HG2	9:P:513:HOH:O	2.18	0.44
1:A:42:ARG:HH12	1:B:34:VAL:CG1	2.28	0.43
2:C:73:LEU:CD2	2:C:94:LEU:HB2	2.47	0.43
2:C:257:VAL:HG12	2:C:263:ASP:OD1	2.17	0.43
2:C:516:ARG:N	9:C:1381:HOH:O	2.50	0.43
2:C:663:ASN:C	2:C:665:PHE:H	2.22	0.43
2:C:813:VAL:HB	9:C:1471:HOH:O	2.18	0.43
2:C:874:LEU:HA	3:D:1023:MET:HE1	1.99	0.43
2:C:979:THR:HG23	2:C:981:GLU:HB2	2.00	0.43
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.53	0.43
3:D:481:MET:CE	3:D:1389:LEU:HG	2.48	0.43
3:D:951:ILE:HD12	3:D:1062:ARG:HG3	1.99	0.43
3:D:1251:ASP:O	3:D:1270:ALA:HB3	2.18	0.43
3:D:1393:GLN:HG3	3:D:1398:TRP:HZ2	1.83	0.43
5:F:115:LYS:HD2	5:F:173:TYR:HE2	1.82	0.43
5:F:185:GLN:O	5:F:189:GLU:HG3	2.17	0.43
5:F:205:ARG:HD3	5:F:251:ILE:HG21	2.00	0.43
1:K:224:TYR:CD1	1:L:9:PRO:HD2	2.53	0.43
1:L:7:LYS:HE3	9:L:1689:HOH:O	2.18	0.43
1:L:125:PRO:HD2	9:L:3251:HOH:O	2.18	0.43
2:M:757:GLY:HA2	2:M:789:SER:CB	2.35	0.43
3:N:15:PRO:HG3	9:N:2008:HOH:O	2.17	0.43
3:N:37:LEU:HD13	3:N:535:PHE:HZ	1.83	0.43
3:N:93:ILE:CD1	3:N:548:ILE:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:615:ARG:NH2	3:N:1089:ALA:HB2	2.23	0.43
3:N:800:LYS:CE	3:N:804:LEU:HD13	2.48	0.43
3:N:1025:GLN:HE21	3:N:1025:GLN:HB3	1.62	0.43
4:O:67:GLU:HG3	4:O:67:GLU:H	1.68	0.43
5:P:82:ARG:O	5:P:86:HIS:HB2	2.18	0.43
5:P:101:GLU:O	5:P:105:LYS:HG3	2.17	0.43
5:P:403:LYS:HB2	9:P:540:HOH:O	2.17	0.43
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.99	0.43
2:C:20:GLU:HB2	9:C:1289:HOH:O	2.18	0.43
2:C:32:ALA:HB2	2:C:73:LEU:CD1	2.47	0.43
2:C:191:PHE:CE2	2:C:238:LEU:HD11	2.54	0.43
2:C:292:ARG:HD2	2:C:299:LYS:CG	2.47	0.43
2:C:352:ALA:C	2:C:355:VAL:HG12	2.39	0.43
2:C:454:SER:HB3	9:C:1409:HOH:O	2.18	0.43
2:C:564:MET:CE	2:C:846:LYS:HE3	2.49	0.43
2:C:599:GLU:CG	2:C:600:ASP:H	2.29	0.43
2:C:720:GLU:HA	9:C:1430:HOH:O	2.18	0.43
2:C:958:THR:HG23	2:C:961:GLU:HB2	2.00	0.43
2:C:1088:LEU:HG	2:C:1092:LEU:HD12	2.00	0.43
3:D:31:THR:HG22	3:D:32:ILE:HB	2.00	0.43
3:D:143:ASN:HD21	3:D:145:VAL:HG12	1.81	0.43
3:D:1147:ARG:HD2	3:D:1188:VAL:CG2	2.48	0.43
3:D:1220:ALA:O	3:D:1224:VAL:HG23	2.18	0.43
5:F:152:ASP:HB3	9:F:665:HOH:O	2.17	0.43
1:K:61:VAL:HG11	1:K:75:VAL:HG21	1.99	0.43
1:K:91:ASN:N	9:K:1900:HOH:O	2.51	0.43
1:L:33:GLY:O	1:L:195:LEU:HD22	2.19	0.43
1:L:77:GLU:O	1:L:77:GLU:HG3	2.15	0.43
2:M:11:GLU:HB3	9:M:2054:HOH:O	2.18	0.43
2:M:133:ASP:N	2:M:133:ASP:OD2	2.51	0.43
2:M:610:ARG:NE	9:M:1664:HOH:O	2.49	0.43
2:M:1082:PRO:C	2:M:1084:SER:N	2.71	0.43
3:N:131:LYS:HE3	3:N:568:ARG:HB3	1.99	0.43
3:N:761:ILE:CD1	4:O:20:THR:HA	2.49	0.43
3:N:938:GLY:O	3:N:942:SER:HB3	2.18	0.43
3:N:1325:LEU:C	9:N:2368:HOH:O	2.57	0.43
4:O:57:ASP:H	4:O:58:PRO:HD3	1.83	0.43
5:P:271:LEU:HD23	5:P:291:ILE:HD11	2.00	0.43
1:A:158:ILE:HD13	1:A:158:ILE:HA	1.88	0.43
2:C:208:ALA:HA	2:C:218:VAL:CG2	2.48	0.43
2:C:230:ARG:HG2	9:C:1514:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:345:ARG:HD2	9:C:1463:HOH:O	2.18	0.43
2:C:561:GLY:HA3	2:C:842:ARG:O	2.19	0.43
2:C:569:VAL:HG12	2:C:996:LYS:O	2.18	0.43
2:C:575:GLN:C	2:C:667:ALA:HB1	2.38	0.43
2:C:601:GLY:HA3	2:C:615:TYR:HA	2.01	0.43
2:C:670:GLN:HE22	2:C:699:PHE:HA	1.81	0.43
2:C:911:GLU:HG2	2:C:915:LYS:NZ	2.33	0.43
2:C:1033:GLY:H	2:C:1036:GLU:HG3	1.83	0.43
3:D:610:LYS:HG2	7:D:1527:MXP:H15A	1.99	0.43
3:D:678:GLU:HB2	9:D:1759:HOH:O	2.18	0.43
3:D:704:ARG:HG2	3:D:705:ALA:N	2.30	0.43
3:D:844:ALA:HB3	3:D:848:GLU:OE2	2.19	0.43
3:D:848:GLU:N	9:D:1677:HOH:O	2.51	0.43
3:D:888:GLU:HB3	9:D:1740:HOH:O	2.18	0.43
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	2.00	0.43
3:D:1095:THR:HG22	9:D:1551:HOH:O	2.16	0.43
3:D:1110:ALA:O	3:D:1112:CYS:N	2.50	0.43
5:F:93:LEU:HD23	5:F:93:LEU:HA	1.81	0.43
1:K:102:LYS:HA	1:K:138:LEU:O	2.18	0.43
1:K:138:LEU:HA	9:K:2460:HOH:O	2.19	0.43
9:K:1685:HOH:O	1:L:219:ARG:HD2	2.18	0.43
2:M:208:ALA:CA	2:M:221:LEU:HD21	2.47	0.43
2:M:278:GLU:HG3	2:M:283:ILE:HA	1.99	0.43
2:M:422:ARG:HG2	9:M:1926:HOH:O	2.18	0.43
2:M:462:ASP:O	2:M:463:GLU:C	2.57	0.43
2:M:537:LYS:HD3	2:M:905:ILE:HD11	2.01	0.43
2:M:1063:ARG:O	2:M:1066:ALA:HB3	2.18	0.43
3:N:961:LYS:HE3	9:N:2153:HOH:O	2.17	0.43
3:N:1066:THR:O	3:N:1070:TYR:HB2	2.18	0.43
9:N:2374:HOH:O	4:O:51:LEU:HD23	2.18	0.43
1:A:227:ASN:HD22	1:A:227:ASN:N	2.15	0.43
2:C:22:GLN:HE22	2:C:135:VAL:CG1	2.30	0.43
2:C:49:ARG:HG2	2:C:266:ARG:HH12	1.83	0.43
2:C:263:ASP:CB	2:C:264:PRO:HD3	2.48	0.43
2:C:313:LEU:HD13	2:C:321:GLU:HB2	1.99	0.43
2:C:413:LEU:HD12	2:C:413:LEU:N	2.24	0.43
2:C:517:ARG:HB2	9:C:1698:HOH:O	2.17	0.43
2:C:610:ARG:NE	9:C:1120:HOH:O	2.52	0.43
2:C:631:SER:HG	2:C:635:THR:H	1.66	0.43
2:C:690:ILE:HD12	2:C:833:LEU:HD21	2.01	0.43
2:C:896:PHE:CE2	2:C:925:TYR:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1009:SER:HB2	3:D:651:GLU:HG2	2.01	0.43
3:D:84:ILE:HG13	3:D:85:VAL:N	2.34	0.43
3:D:86:ARG:HB3	3:D:523:ASP:OD2	2.18	0.43
3:D:420:VAL:HA	9:D:2307:HOH:O	2.19	0.43
3:D:584:ASN:HD21	3:D:590:PRO:HD2	1.81	0.43
3:D:649:ALA:HB3	3:D:691:LEU:HD21	1.98	0.43
3:D:688:TRP:HA	3:D:688:TRP:CE3	2.53	0.43
3:D:1281:VAL:HG21	3:D:1313:VAL:HG21	1.99	0.43
3:D:1304:LYS:HB3	9:D:1723:HOH:O	2.18	0.43
3:D:1354:LYS:HE2	9:D:2358:HOH:O	2.19	0.43
3:D:1395:LEU:HD23	3:D:1396:GLU:N	2.33	0.43
3:D:1426:LYS:HD2	9:D:2086:HOH:O	2.17	0.43
4:E:53:GLY:C	4:E:55:PHE:N	2.70	0.43
5:F:418:LEU:HD12	5:F:418:LEU:N	2.33	0.43
1:L:55:SER:HB2	1:L:158:ILE:HD13	1.96	0.43
1:L:115:LEU:HD12	1:L:115:LEU:O	2.18	0.43
2:M:65:VAL:HB	2:M:101:ILE:HB	2.00	0.43
2:M:199:VAL:HG13	2:M:235:LEU:CG	2.42	0.43
2:M:679:PHE:O	2:M:680:ASP:C	2.56	0.43
2:M:876:VAL:HB	2:M:877:PRO:HD3	2.01	0.43
2:M:881:ASN:N	2:M:881:ASN:ND2	2.66	0.43
2:M:964:LYS:O	2:M:968:LEU:HG	2.18	0.43
2:M:1013:TYR:OH	3:N:624:ASP:OD2	2.33	0.43
3:N:9:ARG:HA	3:N:1434:TRP:CH2	2.52	0.43
3:N:637:LEU:HD11	3:N:641:GLN:HB2	2.00	0.43
3:N:1004:THR:HG21	9:N:2039:HOH:O	2.17	0.43
3:N:1031:ASN:O	3:N:1035:ILE:HG12	2.18	0.43
3:N:1147:ARG:HB3	3:N:1188:VAL:HG23	1.99	0.43
5:P:137:GLY:HA2	9:P:480:HOH:O	2.19	0.43
5:P:163:LEU:HD22	5:P:174:LEU:HB2	2.01	0.43
1:A:63:HIS:HB3	2:C:746:GLY:HA2	1.99	0.43
1:B:72:LYS:HB3	1:B:131:THR:OG1	2.19	0.43
2:C:139:GLN:N	9:C:1322:HOH:O	2.52	0.43
2:C:207:LEU:HD13	2:C:221:LEU:CD1	2.48	0.43
2:C:679:PHE:CE1	2:C:859:PRO:HD3	2.53	0.43
2:C:798:GLY:H	2:C:827:VAL:HG11	1.82	0.43
2:C:971:LYS:HB3	2:C:987:ILE:C	2.39	0.43
2:C:987:ILE:HG12	3:D:948:THR:CG2	2.48	0.43
3:D:111:LYS:NZ	3:D:1449:GLU:HG2	2.34	0.43
3:D:126:VAL:O	3:D:132:TYR:CD1	2.70	0.43
3:D:128:TYR:HB3	3:D:129:PHE:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.47	0.43
3:D:871:LYS:O	3:D:873:LEU:HG	2.18	0.43
3:D:875:THR:HG22	3:D:879:ARG:HB2	1.99	0.43
3:D:1109:GLU:CD	3:D:1202:GLN:HB2	2.39	0.43
3:D:1186:VAL:HA	3:D:1187:PRO:HD3	1.90	0.43
3:D:1195:GLN:CG	3:D:1196:THR:N	2.81	0.43
3:D:1197:ARG:HG3	3:D:1198:TYR:H	1.82	0.43
5:F:209:PHE:O	5:F:213:ILE:HG13	2.18	0.43
1:K:123:MET:HB3	9:K:2581:HOH:O	2.17	0.43
2:M:182:VAL:HB	2:M:193:LEU:HD13	2.00	0.43
2:M:260:LEU:HG	2:M:261:ILE:HG13	2.00	0.43
2:M:437:ARG:HH22	2:M:491:GLU:HB2	1.82	0.43
2:M:687:ALA:C	2:M:688:ILE:HD12	2.38	0.43
3:N:45:PHE:HB3	3:N:86:ARG:NH2	2.33	0.43
3:N:206:ARG:HG2	9:N:2269:HOH:O	2.18	0.43
3:N:561:GLY:HA3	5:P:184:ARG:CZ	2.48	0.43
3:N:715:ALA:O	3:N:764:LEU:HD12	2.17	0.43
3:N:853:VAL:HG22	3:N:858:VAL:HG23	2.00	0.43
3:N:879:ARG:HD3	3:N:902:LEU:O	2.17	0.43
3:N:1171:VAL:O	3:N:1171:VAL:HG12	2.18	0.43
5:P:375:LEU:HB3	9:P:476:HOH:O	2.18	0.43
1:A:67:THR:HG21	2:C:609:ASN:HD21	1.82	0.43
2:C:64:LEU:HD11	2:C:100:LEU:HD13	2.00	0.43
2:C:78:PHE:HB2	2:C:88:LEU:HD21	2.01	0.43
2:C:232:GLU:O	2:C:235:LEU:HB2	2.18	0.43
2:C:280:LYS:HB3	9:C:1547:HOH:O	2.18	0.43
2:C:396:ASP:O	2:C:402:SER:HB3	2.18	0.43
2:C:462:ASP:O	2:C:463:GLU:C	2.56	0.43
2:C:572:ILE:CG2	2:C:703:ILE:HD13	2.48	0.43
3:D:192:ALA:HB2	3:D:393:ILE:CD1	2.48	0.43
3:D:400:VAL:HG21	9:D:2433:HOH:O	2.19	0.43
3:D:417:PRO:HD2	3:D:432:TYR:CE1	2.54	0.43
3:D:614:PHE:O	3:D:615:ARG:O	2.36	0.43
3:D:633:VAL:C	3:D:635:PRO:HD3	2.39	0.43
3:D:1112:CYS:CB	3:D:1195:GLN:HG2	2.42	0.43
3:D:1139:ASP:O	3:D:1142:ALA:HB3	2.18	0.43
5:F:79:ASP:CG	5:F:80:PRO:HD3	2.39	0.43
5:F:196:VAL:HG13	5:F:213:ILE:CD1	2.48	0.43
5:F:226:LYS:HB2	5:F:238:TYR:OH	2.19	0.43
5:F:271:LEU:HD23	5:F:291:ILE:HD11	2.00	0.43
5:F:338:LEU:HA	5:F:339:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:412:GLU:OE1	5:F:418:LEU:HD13	2.19	0.43
5:F:415:THR:HG22	5:F:417:LYS:HG3	2.00	0.43
1:L:44:LEU:CD2	1:L:199:ILE:HD13	2.48	0.43
1:L:107:LYS:HG3	1:L:108:GLU:N	2.34	0.43
2:M:244:PRO:CD	2:M:245:GLY:H	2.31	0.43
2:M:288:ARG:HB3	9:M:1852:HOH:O	2.17	0.43
2:M:816:LYS:O	2:M:819:VAL:HB	2.18	0.43
2:M:897:LEU:HD23	2:M:899:GLN:NE2	2.33	0.43
2:M:969:GLN:HE21	2:M:969:GLN:HB3	1.71	0.43
3:N:403:PHE:CZ	3:N:407:VAL:HG23	2.53	0.43
3:N:611:GLN:NE2	7:N:1527:MXP:C16	2.80	0.43
3:N:1285:GLU:O	3:N:1285:GLU:HG2	2.19	0.43
3:N:1393:GLN:HB2	3:N:1398:TRP:CE2	2.53	0.43
4:O:53:GLY:C	4:O:55:PHE:H	2.22	0.43
5:P:215:GLU:OE2	5:P:254:GLN:NE2	2.49	0.43
2:C:511:GLU:HG3	9:C:1690:HOH:O	2.17	0.43
2:C:762:LYS:HB2	2:C:786:LYS:HD2	2.01	0.43
3:D:724:GLN:N	9:D:1680:HOH:O	2.46	0.43
3:D:799:LYS:O	3:D:829:VAL:HG13	2.19	0.43
3:D:1036:ARG:HH21	3:D:1042:ARG:HA	1.84	0.43
3:D:1065:LEU:CD1	3:D:1069:GLU:HB2	2.48	0.43
3:D:1115:THR:HG21	3:D:1151:ARG:HH21	1.83	0.43
3:D:1119:SER:HA	3:D:1186:VAL:O	2.19	0.43
4:E:39:VAL:HG21	4:E:72:ARG:HD2	2.00	0.43
5:F:225:GLU:HG3	5:F:226:LYS:N	2.32	0.43
5:F:348:SER:OG	5:F:349:LEU:N	2.51	0.43
1:L:57:TYR:HB3	1:L:141:GLU:HG3	2.01	0.43
1:L:86:VAL:HG12	1:L:124:ASN:HB2	2.00	0.43
2:M:17:PRO:O	2:M:20:GLU:HB2	2.18	0.43
2:M:232:GLU:O	2:M:235:LEU:HB2	2.18	0.43
2:M:495:THR:HB	2:M:530:GLU:HG3	2.00	0.43
2:M:532:MET:HG3	2:M:533:ASP:N	2.33	0.43
2:M:551:GLU:HB3	2:M:906:PHE:HD2	1.84	0.43
2:M:601:GLY:O	2:M:649:VAL:HG22	2.18	0.43
2:M:1044:GLY:HA3	4:O:17:TYR:CE1	2.53	0.43
3:N:44:LEU:O	3:N:525:ARG:NH2	2.51	0.43
3:N:47:GLU:HG2	3:N:53:ILE:HG22	2.00	0.43
3:N:133:ILE:HG23	3:N:456:MET:SD	2.58	0.43
3:N:448:GLU:HG3	9:N:1563:HOH:O	2.17	0.43
3:N:1035:ILE:CA	3:N:1038:LEU:HD12	2.49	0.43
3:N:1281:VAL:HG21	3:N:1313:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:94:LEU:HB3	9:P:503:HOH:O	2.18	0.43
1:B:4:SER:HA	1:B:7:LYS:HG2	2.00	0.43
2:C:174:LEU:HB2	2:C:310:LEU:HD22	2.01	0.43
2:C:175:GLU:HB3	2:C:183:SER:OG	2.18	0.43
2:C:419:THR:N	9:C:1152:HOH:O	2.50	0.43
2:C:937:ASP:OD2	2:C:939:ARG:HD2	2.18	0.43
3:D:644:LEU:HD12	3:D:645:PRO:CD	2.48	0.43
3:D:806:PHE:CD1	3:D:813:LEU:HB3	2.53	0.43
3:D:1082:ALA:O	3:D:1086:LEU:HG	2.18	0.43
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.19	0.43
3:D:1154:GLU:HG2	9:D:2105:HOH:O	2.19	0.43
3:D:1166:LEU:HD23	3:D:1166:LEU:H	1.84	0.43
3:D:1495:ILE:HA	4:E:88:GLU:OE2	2.19	0.43
4:E:19:LEU:O	4:E:23:VAL:HG23	2.19	0.43
4:E:54:LEU:HG	4:E:58:PRO:CB	2.49	0.43
1:K:161:ARG:HG2	9:K:1051:HOH:O	2.18	0.43
1:K:176:ARG:HA	9:K:2558:HOH:O	2.18	0.43
1:L:42:ARG:HG2	1:L:42:ARG:HH11	1.83	0.43
1:L:176:ARG:HD3	3:N:884:ARG:CZ	2.48	0.43
2:M:32:ALA:HB2	2:M:73:LEU:HD11	2.00	0.43
2:M:1033:GLY:HA3	9:N:1659:HOH:O	2.18	0.43
3:N:489:ARG:HG3	3:N:1388:ARG:NH2	2.27	0.43
3:N:554:LEU:HD23	3:N:570:GLU:HG2	2.01	0.43
3:N:1031:ASN:O	3:N:1034:GLN:HB2	2.19	0.43
3:N:1209:LEU:C	3:N:1211:MET:N	2.72	0.43
3:N:1352:ILE:CG2	3:N:1368:ILE:HD13	2.49	0.43
5:P:356:LYS:O	5:P:360:LYS:HG3	2.19	0.43
1:B:44:LEU:HD11	1:B:199:ILE:HD11	2.00	0.43
2:C:118:ILE:HG22	2:C:382:ILE:HD13	2.00	0.43
2:C:144:PRO:CG	2:C:165:LEU:HB3	2.48	0.43
2:C:455:LEU:HD12	2:C:456:ALA:N	2.34	0.43
2:C:458:TYR:HB2	2:C:538:GLN:HB2	2.01	0.43
2:C:487:THR:HG22	2:C:488:ALA:N	2.34	0.43
2:C:832:LYS:HG2	9:C:1178:HOH:O	2.17	0.43
2:C:1034:GLU:O	2:C:1037:VAL:N	2.52	0.43
2:C:1070:ILE:HG23	3:D:656:PHE:CE2	2.53	0.43
3:D:116:LEU:CD1	3:D:465:LEU:HG	2.49	0.43
3:D:185:VAL:HG22	3:D:203:ALA:HB2	2.00	0.43
3:D:829:VAL:O	3:D:831:GLY:N	2.52	0.43
3:D:1041:LEU:HD12	3:D:1058:ARG:CA	2.48	0.43
3:D:1147:ARG:NH1	3:D:1190:SER:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:1527:MXP:H15	7:D:1527:MXP:H9	1.89	0.43
5:F:361:LEU:HG	5:F:408:LEU:HD21	2.01	0.43
1:K:101:LEU:HG	1:K:113:ASP:C	2.40	0.43
1:K:161:ARG:HB2	1:K:161:ARG:HH11	1.84	0.43
1:L:81:ASN:ND2	1:L:128:HIS:O	2.52	0.43
2:M:209:ARG:HB2	9:M:2284:HOH:O	2.19	0.43
2:M:309:TYR:HA	2:M:312:ALA:HB3	2.00	0.43
2:M:342:ASP:O	2:M:346:VAL:HG23	2.18	0.43
2:M:350:ARG:HG2	9:M:1970:HOH:O	2.18	0.43
2:M:432:ARG:HD2	9:M:1743:HOH:O	2.19	0.43
2:M:457:ALA:HB3	2:M:538:GLN:HA	2.00	0.43
2:M:520:GLU:HA	2:M:521:PRO:HD3	1.84	0.43
2:M:540:PHE:CE1	2:M:906:PHE:HE1	2.36	0.43
2:M:620:LEU:HD12	2:M:620:LEU:O	2.19	0.43
2:M:640:ARG:HA	2:M:641:PRO:HD3	1.93	0.43
2:M:836:GLY:HA2	3:N:725:SER:OG	2.19	0.43
2:M:837:ASP:OD1	2:M:999:HIS:NE2	2.51	0.43
3:N:126:VAL:HG11	3:N:152:LEU:CD1	2.49	0.43
3:N:131:LYS:HD2	5:P:83:GLN:CD	2.39	0.43
3:N:191:LEU:HD23	3:N:191:LEU:HA	1.75	0.43
3:N:565:ILE:CD1	5:P:84:TYR:HB3	2.49	0.43
3:N:1243:THR:CB	3:N:1253:THR:HB	2.49	0.43
3:N:1467:ILE:HG13	3:N:1467:ILE:H	1.58	0.43
4:O:41:GLU:HB2	4:O:45:ARG:NH1	2.34	0.43
1:A:95:GLN:HA	9:A:395:HOH:O	2.17	0.43
1:A:220:GLU:HG2	9:A:339:HOH:O	2.18	0.43
2:C:144:PRO:HA	2:C:163:ILE:HG13	2.01	0.43
2:C:267:TYR:N	2:C:267:TYR:HD2	2.16	0.43
2:C:313:LEU:HD13	2:C:321:GLU:O	2.19	0.43
2:C:317:VAL:O	2:C:317:VAL:HG12	2.19	0.43
2:C:464:LEU:HD12	2:C:465:GLY:H	1.83	0.43
3:D:32:ILE:HG22	5:F:258:ILE:CD1	2.47	0.43
3:D:145:VAL:HG22	3:D:146:PRO:HD2	2.01	0.43
3:D:478:LEU:HD21	3:D:500:ARG:HH22	1.83	0.43
3:D:522:PRO:N	9:D:1713:HOH:O	2.51	0.43
3:D:583:ASP:OD1	3:D:583:ASP:C	2.57	0.43
3:D:809:PRO:O	3:D:812:ALA:HB3	2.19	0.43
3:D:1045:MET:HG3	3:D:1073:SER:CA	2.46	0.43
3:D:1292:VAL:HB	9:D:2010:HOH:O	2.19	0.43
3:D:1491:THR:HG22	3:D:1495:ILE:HD13	2.01	0.43
5:F:172:ARG:HG3	9:F:453:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:201:LYS:HE2	9:F:724:HOH:O	2.18	0.43
1:K:70:GLY:H	2:M:607:ASP:CG	2.19	0.43
1:K:78:ILE:HG13	1:K:78:ILE:H	1.65	0.43
1:K:106:PRO:HG3	1:K:133:GLU:O	2.19	0.43
1:K:158:ILE:O	1:K:159:LYS:HG3	2.19	0.43
2:M:82:GLU:HG2	2:M:86:LYS:HD2	2.00	0.43
2:M:193:LEU:HD21	9:M:1951:HOH:O	2.18	0.43
2:M:405:ARG:HH11	2:M:566:THR:HG21	1.84	0.43
2:M:495:THR:H	2:M:530:GLU:CD	2.22	0.43
2:M:905:ILE:HD11	9:M:1895:HOH:O	2.19	0.43
3:N:519:VAL:HG13	3:N:544:TYR:CE1	2.54	0.43
3:N:1383:ASP:HB2	3:N:1416:ALA:CB	2.37	0.43
4:O:91:ARG:CZ	9:O:1090:HOH:O	2.67	0.43
1:B:60:ASP:N	1:B:137:ARG:NH2	2.65	0.42
1:B:208:LEU:HD12	1:B:212:ASN:OD1	2.19	0.42
2:C:203:ASP:OD1	2:C:206:THR:HG22	2.19	0.42
2:C:212:GLY:O	2:C:215:GLY:O	2.37	0.42
2:C:271:GLU:HG2	2:C:275:TYR:HE1	1.84	0.42
2:C:286:SER:C	2:C:287:GLY:O	2.56	0.42
2:C:355:VAL:CG2	2:C:372:LEU:HG	2.49	0.42
2:C:408:ARG:NH2	2:C:542:VAL:HG22	2.33	0.42
2:C:431:HIS:HD2	2:C:433:THR:H	1.61	0.42
2:C:585:GLU:HB2	9:C:1331:HOH:O	2.18	0.42
2:C:1082:PRO:C	2:C:1084:SER:N	2.71	0.42
2:C:1085:PHE:CD2	3:D:1468:LEU:HA	2.54	0.42
2:C:1091:GLU:O	2:C:1094:ALA:HB3	2.19	0.42
3:D:732:VAL:HG12	9:D:1673:HOH:O	2.19	0.42
3:D:1109:GLU:HG2	3:D:1201:CYS:CA	2.47	0.42
3:D:1155:VAL:HG11	3:D:1177:ALA:CB	2.49	0.42
3:D:1242:HIS:HE1	3:D:1266:ARG:HB3	1.84	0.42
1:K:128:HIS:CE1	1:K:131:THR:HG23	2.54	0.42
1:K:206:THR:HG22	1:K:209:GLU:CB	2.48	0.42
1:L:13:VAL:HG13	1:L:23:PHE:CD1	2.54	0.42
2:M:16:PRO:HB3	2:M:460:ARG:NH1	2.34	0.42
2:M:98:LEU:HB2	9:M:1972:HOH:O	2.17	0.42
2:M:622:GLU:O	2:M:624:PRO:HD3	2.18	0.42
2:M:874:LEU:HD23	3:N:1023:MET:HE3	2.00	0.42
2:M:1013:TYR:O	5:P:334:PRO:HA	2.19	0.42
3:N:18:ILE:HG23	3:N:518:PRO:CG	2.38	0.42
3:N:393:ILE:HG13	9:N:1934:HOH:O	2.19	0.42
3:N:573:MET:CE	5:P:210:LEU:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:661:MET:CE	3:N:673:ALA:HB1	2.49	0.42
3:N:679:ARG:HB2	3:N:682:ASP:CG	2.39	0.42
3:N:1023:MET:HG2	3:N:1023:MET:H	1.46	0.42
3:N:1114:THR:HG22	3:N:1195:GLN:HB3	1.99	0.42
3:N:1124:GLN:HA	3:N:1125:PRO:HD3	1.72	0.42
4:O:41:GLU:CA	4:O:45:ARG:HD3	2.40	0.42
1:A:67:THR:OG1	2:C:609:ASN:ND2	2.52	0.42
1:B:51:THR:HA	1:B:145:ASP:O	2.20	0.42
1:B:91:ASN:O	1:B:94:LEU:HD12	2.18	0.42
2:C:311:PHE:HB3	9:C:1209:HOH:O	2.18	0.42
2:C:1048:THR:O	2:C:1052:MET:HG2	2.19	0.42
2:C:1103:ASP:HB2	9:C:1226:HOH:O	2.19	0.42
3:D:12:LEU:HD11	3:D:512:MET:HG2	2.01	0.42
3:D:560:GLN:HG2	5:F:221:ILE:HG21	2.01	0.42
3:D:660:LYS:HE2	9:D:1780:HOH:O	2.19	0.42
3:D:795:VAL:CG1	3:D:863:VAL:HG13	2.45	0.42
3:D:853:VAL:HG22	3:D:858:VAL:HG23	2.01	0.42
3:D:996:TRP:O	3:D:999:THR:HG22	2.19	0.42
3:D:1129:THR:HG23	3:D:1130:ARG:H	1.83	0.42
2:M:52:PHE:HB3	2:M:53:PRO:HD3	2.00	0.42
2:M:443:THR:CG2	2:M:450:GLY:H	2.33	0.42
2:M:446:GLY:O	2:M:447:ALA:C	2.57	0.42
2:M:722:ILE:HG13	2:M:757:GLY:O	2.19	0.42
2:M:724:ARG:HD2	2:M:740:GLU:HG2	2.02	0.42
2:M:943:VAL:HG11	2:M:973:VAL:HG13	2.01	0.42
2:M:952:LEU:CD1	2:M:969:GLN:HE22	2.23	0.42
3:N:168:THR:HA	3:N:394:LEU:HA	2.02	0.42
3:N:455:ARG:HH11	3:N:463:GLN:HG3	1.84	0.42
3:N:633:VAL:HG13	3:N:633:VAL:O	2.18	0.42
3:N:1274:ILE:HD12	3:N:1274:ILE:H	1.82	0.42
3:N:1394:VAL:HB	3:N:1397:LYS:HD2	2.02	0.42
4:O:85:LEU:HD23	4:O:86:GLN:N	2.34	0.42
5:P:172:ARG:NH1	9:P:483:HOH:O	2.50	0.42
5:P:217:ASN:O	5:P:221:ILE:HG13	2.20	0.42
5:P:309:LYS:O	5:P:312:GLN:HB2	2.19	0.42
5:P:321:ILE:HD11	5:P:329:TYR:HB2	2.00	0.42
1:A:101:LEU:HD23	1:A:102:LYS:N	2.34	0.42
1:A:206:THR:HG23	1:A:209:GLU:H	1.84	0.42
2:C:52:PHE:HB3	2:C:53:PRO:HD3	1.99	0.42
2:C:78:PHE:HB3	2:C:79:PRO:HD2	2.00	0.42
2:C:144:PRO:HG2	2:C:165:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:TYR:CD2	2:C:267:TYR:N	2.87	0.42
2:C:370:ALA:HB1	9:C:1667:HOH:O	2.18	0.42
2:C:560:MET:O	2:C:564:MET:HE3	2.19	0.42
2:C:627:ARG:HG2	9:C:1753:HOH:O	2.19	0.42
2:C:674:VAL:HG11	2:C:992:MET:HB3	2.02	0.42
2:C:707:ARG:NH2	2:C:824:ARG:CZ	2.82	0.42
2:C:946:ARG:HD2	2:C:984:GLU:HB3	1.99	0.42
2:C:1084:SER:O	2:C:1087:VAL:HG12	2.19	0.42
3:D:15:PRO:HA	3:D:18:ILE:HG12	2.00	0.42
3:D:98:PRO:HG3	3:D:515:GLU:HB3	2.01	0.42
3:D:153:LEU:HD12	3:D:154:THR:N	2.34	0.42
3:D:729:HIS:CE1	3:D:935:LYS:HD3	2.54	0.42
3:D:754:PHE:CG	4:E:24:ALA:HB1	2.55	0.42
3:D:795:VAL:HA	3:D:861:GLN:O	2.19	0.42
3:D:1107:VAL:HG12	3:D:1217:ILE:HA	2.01	0.42
3:D:1428:ALA:O	3:D:1431:THR:CG2	2.66	0.42
5:F:271:LEU:HD22	5:F:304:VAL:HG13	1.99	0.42
1:K:16:GLN:HA	9:K:3198:HOH:O	2.18	0.42
2:M:129:ILE:HG22	2:M:130:ASN:ND2	2.33	0.42
2:M:161:SER:HB3	9:M:2298:HOH:O	2.19	0.42
2:M:173:ASP:O	2:M:184:MET:HA	2.19	0.42
2:M:232:GLU:HG3	2:M:235:LEU:CD1	2.49	0.42
2:M:300:ASP:HA	9:M:1862:HOH:O	2.19	0.42
2:M:412:ALA:HB1	2:M:419:THR:HG23	2.00	0.42
2:M:514:VAL:HG23	9:M:1623:HOH:O	2.18	0.42
2:M:564:MET:CE	2:M:846:LYS:HE3	2.50	0.42
2:M:627:ARG:HG3	2:M:628:PHE:N	2.33	0.42
2:M:674:VAL:HG11	2:M:992:MET:HB3	2.01	0.42
2:M:808:ARG:HA	2:M:815:LEU:HD22	2.00	0.42
2:M:897:LEU:HD23	9:M:1930:HOH:O	2.19	0.42
3:N:399:ARG:NE	9:N:2195:HOH:O	2.52	0.42
3:N:1167:SER:HB3	9:N:1789:HOH:O	2.19	0.42
3:N:1182:GLU:CG	9:N:1552:HOH:O	2.66	0.42
3:N:1216:SER:HB3	4:O:16:LYS:H	1.84	0.42
3:N:1462:LEU:HD22	3:N:1472:ILE:CG2	2.47	0.42
5:P:247:ILE:O	5:P:251:ILE:HG13	2.20	0.42
1:B:24:VAL:HG13	1:B:196:THR:HB	2.01	0.42
1:B:99:LEU:HD21	1:B:122:ILE:HD11	2.00	0.42
2:C:260:LEU:CB	2:C:291:ALA:HB1	2.45	0.42
2:C:549:PHE:HB3	2:C:552:HIS:CD2	2.49	0.42
2:C:840:ALA:HB2	2:C:846:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:897:LEU:HB3	2:C:899:GLN:NE2	2.33	0.42
3:D:133:ILE:HG23	3:D:456:MET:SD	2.60	0.42
3:D:568:ARG:HG3	3:D:572:ARG:HE	1.85	0.42
3:D:820:GLU:HB3	3:D:836:VAL:HG21	2.02	0.42
3:D:1019:PRO:O	3:D:1023:MET:HG2	2.19	0.42
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.54	0.42
3:D:1108:ARG:NH2	3:D:1198:TYR:HB2	2.34	0.42
3:D:1129:THR:HA	9:D:1695:HOH:O	2.18	0.42
3:D:1144:LEU:HA	3:D:1147:ARG:HG3	2.01	0.42
3:D:1382:THR:HG21	3:D:1418:LYS:CE	2.50	0.42
4:E:85:LEU:HD23	4:E:85:LEU:C	2.39	0.42
5:F:363:GLU:CA	5:F:367:MET:HG3	2.49	0.42
1:K:158:ILE:C	1:K:159:LYS:HG3	2.40	0.42
2:M:165:LEU:HD12	2:M:166:PRO:C	2.40	0.42
2:M:612:VAL:HG22	2:M:622:GLU:CB	2.48	0.42
2:M:684:PHE:HD2	3:N:740:PHE:HE1	1.67	0.42
2:M:850:ALA:HA	3:N:632:VAL:HG11	2.01	0.42
3:N:9:ARG:HA	3:N:1434:TRP:HH2	1.83	0.42
3:N:111:LYS:NZ	3:N:1452:ILE:HG21	2.34	0.42
3:N:139:GLY:O	3:N:147:VAL:HB	2.20	0.42
3:N:434:ARG:H	3:N:447:VAL:HG23	1.84	0.42
3:N:799:LYS:CB	3:N:826:PRO:HG2	2.48	0.42
3:N:834:THR:HA	3:N:838:ARG:HD2	2.01	0.42
3:N:892:ASP:O	3:N:895:VAL:N	2.51	0.42
5:P:286:PRO:HD3	9:P:477:HOH:O	2.19	0.42
1:A:55:SER:HB2	1:A:158:ILE:HG13	2.01	0.42
1:B:58:ILE:CG2	1:B:137:ARG:NH2	2.80	0.42
1:B:90:LEU:O	1:B:90:LEU:HG	2.19	0.42
1:B:133:GLU:O	1:B:134:GLU:HG2	2.19	0.42
2:C:91:GLN:HA	2:C:119:PRO:HA	2.01	0.42
2:C:173:ASP:O	2:C:184:MET:HA	2.20	0.42
2:C:263:ASP:HB2	2:C:264:PRO:CD	2.48	0.42
2:C:679:PHE:O	2:C:680:ASP:C	2.57	0.42
2:C:724:ARG:HA	2:C:737:LEU:CD2	2.49	0.42
2:C:769:PRO:HB3	5:F:373:LYS:O	2.19	0.42
2:C:833:LEU:HD12	2:C:834:GLN:N	2.34	0.42
2:C:889:HIS:CD2	9:C:1474:HOH:O	2.72	0.42
2:C:950:LEU:HB3	2:C:952:LEU:HD23	2.01	0.42
2:C:1016:ILE:HG23	3:D:526:PRO:HG2	2.01	0.42
2:C:1033:GLY:O	2:C:1037:VAL:HG23	2.18	0.42
2:C:1109:VAL:HA	3:D:3:LYS:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:671:LYS:N	9:D:1660:HOH:O	2.38	0.42
3:D:796:ARG:NH1	3:D:861:GLN:HE21	2.17	0.42
3:D:1023:MET:HG2	3:D:1023:MET:H	1.42	0.42
3:D:1311:LEU:HB3	9:D:1836:HOH:O	2.20	0.42
3:D:1314:LYS:HA	9:D:1812:HOH:O	2.19	0.42
3:D:1407:LEU:HD11	9:D:2177:HOH:O	2.19	0.42
5:F:111:GLU:O	5:F:115:LYS:HG3	2.20	0.42
5:F:260:ILE:HD12	9:F:458:HOH:O	2.19	0.42
1:L:63:HIS:HB3	9:L:3750:HOH:O	2.20	0.42
1:L:63:HIS:HD2	9:L:3508:HOH:O	2.03	0.42
2:M:212:GLY:C	2:M:215:GLY:H	2.22	0.42
2:M:286:SER:C	2:M:287:GLY:O	2.57	0.42
2:M:742:VAL:HG12	2:M:743:VAL:H	1.85	0.42
2:M:814:GLU:HB2	9:M:1921:HOH:O	2.18	0.42
3:N:152:LEU:H	3:N:152:LEU:CD2	2.24	0.42
3:N:407:VAL:HG22	3:N:422:ALA:CB	2.50	0.42
3:N:829:VAL:H	3:N:835:SER:CB	2.32	0.42
3:N:1223:ILE:HD12	3:N:1223:ILE:N	2.27	0.42
5:P:200:LYS:HD3	9:P:559:HOH:O	2.20	0.42
5:P:416:ARG:HB2	9:P:461:HOH:O	2.18	0.42
1:A:86:VAL:HG13	1:A:124:ASN:HB2	2.01	0.42
2:C:115:LEU:HA	2:C:375:SER:HB3	2.01	0.42
2:C:176:VAL:O	2:C:176:VAL:HG23	2.20	0.42
2:C:253:ALA:O	2:C:256:TYR:HB2	2.19	0.42
2:C:878:SER:OG	3:D:1029:ARG:HD3	2.20	0.42
2:C:953:VAL:HG13	2:C:966:LEU:HD13	2.01	0.42
2:C:971:LYS:HB3	2:C:988:VAL:N	2.35	0.42
2:C:1090:LYS:HD2	3:D:90:MET:CE	2.50	0.42
2:C:1118:LYS:HG3	2:C:1118:LYS:H	1.77	0.42
3:D:38:LYS:N	9:D:1967:HOH:O	2.44	0.42
3:D:118:LEU:O	3:D:119:SER:C	2.58	0.42
3:D:1231:GLU:CB	3:D:1232:PRO:HD3	2.49	0.42
3:D:1481:VAL:HG13	4:E:18:ARG:HE	1.84	0.42
3:D:1503:VAL:HB	9:D:2384:HOH:O	2.18	0.42
5:F:358:LEU:HD22	5:F:370:LYS:HE3	2.02	0.42
1:K:106:PRO:HG3	1:K:134:GLU:HG2	2.01	0.42
1:K:184:THR:HG23	1:K:192:LEU:CD1	2.49	0.42
1:K:227:ASN:HD22	1:K:227:ASN:N	2.16	0.42
1:L:48:ILE:HD13	1:L:210:ALA:HB1	2.02	0.42
1:L:89:PHE:HE2	1:L:146:ARG:HB3	1.83	0.42
2:M:263:ASP:C	2:M:264:PRO:O	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:630:ARG:HB2	2:M:705:ILE:HG21	2.02	0.42
2:M:670:GLN:HE22	2:M:699:PHE:HA	1.84	0.42
2:M:798:GLY:H	2:M:827:VAL:HG11	1.83	0.42
3:N:23:TYR:O	3:N:49:ILE:HG23	2.20	0.42
3:N:500:ARG:HG3	3:N:500:ARG:NH1	2.35	0.42
3:N:610:LYS:CD	7:N:1527:MXP:H15B	2.31	0.42
3:N:1290:LEU:HD23	3:N:1291:SER:H	1.82	0.42
3:N:1425:THR:HG23	3:N:1426:LYS:N	2.35	0.42
4:O:35:PHE:HZ	4:O:60:ALA:HA	1.85	0.42
4:O:54:LEU:HD11	9:O:1151:HOH:O	2.20	0.42
1:B:89:PHE:HE2	1:B:146:ARG:HB3	1.84	0.42
1:B:173:PRO:HB3	1:B:204:SER:HB3	2.02	0.42
2:C:136:ILE:CG2	2:C:336:VAL:HG22	2.49	0.42
2:C:264:PRO:HB3	2:C:289:THR:CG2	2.49	0.42
2:C:265:ARG:HB3	2:C:267:TYR:CE2	2.55	0.42
2:C:411:SER:HA	2:C:452:ILE:HA	2.00	0.42
2:C:446:GLY:O	2:C:447:ALA:C	2.58	0.42
2:C:479:VAL:HG21	2:C:503:LEU:CD1	2.50	0.42
2:C:710:ILE:HB	2:C:790:LEU:HD13	2.00	0.42
2:C:1100:GLN:HE21	2:C:1100:GLN:HB2	1.60	0.42
3:D:131:LYS:HG3	3:D:572:ARG:NH2	2.34	0.42
3:D:185:VAL:HG21	3:D:191:LEU:HD11	2.01	0.42
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.02	0.42
3:D:1382:THR:CG2	3:D:1418:LYS:HE3	2.49	0.42
5:F:152:ASP:O	5:F:156:VAL:HB	2.19	0.42
5:F:249:ARG:HD2	9:F:655:HOH:O	2.19	0.42
1:L:54:THR:HG22	1:L:54:THR:O	2.20	0.42
2:M:62:GLY:HA2	2:M:359:MET:HE1	2.01	0.42
2:M:146:VAL:HG22	2:M:162:ILE:HG23	2.01	0.42
2:M:254:VAL:HA	2:M:257:VAL:HG23	2.01	0.42
2:M:265:ARG:CG	2:M:266:ARG:N	2.82	0.42
2:M:352:ALA:CA	2:M:355:VAL:HG12	2.48	0.42
2:M:599:GLU:CG	2:M:600:ASP:N	2.82	0.42
2:M:916:GLU:O	2:M:919:ALA:HB3	2.19	0.42
2:M:1003:ASP:O	2:M:1005:MET:N	2.53	0.42
3:N:497:GLU:HB2	9:N:1731:HOH:O	2.19	0.42
3:N:670:VAL:O	3:N:674:ARG:HG3	2.19	0.42
3:N:1119:SER:HA	3:N:1186:VAL:O	2.20	0.42
3:N:1242:HIS:CE1	3:N:1266:ARG:HB3	2.54	0.42
3:N:1272:ALA:CB	3:N:1326:THR:HB	2.50	0.42
3:N:1373:ARG:HD3	9:N:1685:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1466:VAL:CG2	3:N:1472:ILE:HD11	2.39	0.42
5:P:114:LYS:HD2	9:P:618:HOH:O	2.20	0.42
1:A:101:LEU:HD12	1:A:114:PHE:CE1	2.55	0.42
1:A:156:HIS:CD2	1:A:157:GLY:H	2.38	0.42
1:B:28:LEU:HA	9:B:395:HOH:O	2.19	0.42
1:B:86:VAL:HG12	1:B:124:ASN:HB2	2.00	0.42
2:C:671:ASN:ND2	2:C:993:PHE:HD2	2.16	0.42
2:C:715:THR:HG22	2:C:717:LEU:H	1.85	0.42
2:C:1081:VAL:HA	2:C:1082:PRO:HD3	1.86	0.42
2:C:1109:VAL:HG11	3:D:5:VAL:HG22	2.01	0.42
2:C:1115:LEU:HD12	2:C:1115:LEU:H	1.83	0.42
3:D:55:ASP:O	3:D:80:VAL:CG1	2.67	0.42
3:D:168:THR:HA	3:D:394:LEU:HA	2.02	0.42
3:D:403:PHE:CE2	3:D:443:VAL:N	2.88	0.42
3:D:481:MET:HE3	3:D:1389:LEU:HG	2.00	0.42
3:D:612:GLY:H	3:D:617:ASN:HD21	1.68	0.42
3:D:749:VAL:HA	3:D:750:PRO:HD3	1.90	0.42
3:D:862:ASP:O	3:D:877:PRO:HD3	2.20	0.42
3:D:932:ASP:O	3:D:935:LYS:HB3	2.20	0.42
3:D:1495:ILE:O	3:D:1498:ALA:HB3	2.20	0.42
5:F:167:PRO:HD2	5:F:170:HIS:HD2	1.84	0.42
5:F:394:ARG:HB3	9:F:575:HOH:O	2.19	0.42
1:L:60:ASP:HB2	1:L:137:ARG:NH1	2.34	0.42
1:L:183:ASP:HA	1:L:192:LEU:O	2.20	0.42
2:M:129:ILE:HG22	2:M:130:ASN:N	2.35	0.42
2:M:171:TRP:HZ3	9:M:2226:HOH:O	2.02	0.42
2:M:267:TYR:CD1	2:M:272:ALA:HB1	2.54	0.42
2:M:443:THR:HG21	2:M:449:ILE:HG13	2.02	0.42
2:M:560:MET:O	2:M:564:MET:HE3	2.19	0.42
3:N:145:VAL:HG22	3:N:146:PRO:HD2	2.02	0.42
3:N:185:VAL:HG21	3:N:191:LEU:HD11	2.00	0.42
3:N:667:ALA:HB1	9:N:1656:HOH:O	2.19	0.42
3:N:820:GLU:HB3	3:N:836:VAL:HG21	2.01	0.42
3:N:1074:SER:O	3:N:1077:ALA:HB3	2.20	0.42
3:N:1082:ALA:O	3:N:1086:LEU:HG	2.19	0.42
3:N:1109:GLU:HG2	3:N:1201:CYS:CA	2.48	0.42
4:O:6:ILE:HG23	4:O:7:ASP:N	2.34	0.42
4:O:77:GLU:HG3	9:O:3449:HOH:O	2.20	0.42
5:P:284:ARG:O	5:P:286:PRO:N	2.53	0.42
1:A:79:ILE:O	1:A:83:LYS:HG3	2.19	0.42
1:B:158:ILE:HD11	1:B:165:ILE:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:ARG:HG2	9:C:1315:HOH:O	2.20	0.42
2:C:839:LEU:HD21	2:C:849:VAL:CG2	2.50	0.42
2:C:911:GLU:HB3	2:C:912:PRO:HD3	2.02	0.42
2:C:967:PHE:CD1	2:C:972:VAL:HG12	2.55	0.42
2:C:1034:GLU:HA	2:C:1037:VAL:CG2	2.47	0.42
3:D:84:ILE:O	3:D:87:ARG:HB3	2.19	0.42
3:D:133:ILE:HD11	3:D:155:ASP:OD1	2.19	0.42
3:D:141:ILE:HG21	3:D:450:TYR:H	1.85	0.42
3:D:544:TYR:N	9:D:1714:HOH:O	2.52	0.42
3:D:729:HIS:ND1	3:D:730:PRO:HD2	2.34	0.42
3:D:957:PRO:HD2	3:D:1007:VAL:HG12	2.00	0.42
3:D:1258:ARG:NE	3:D:1262:LEU:HD11	2.35	0.42
3:D:1311:LEU:H	3:D:1311:LEU:CD2	2.32	0.42
1:K:181:VAL:HG12	9:K:2597:HOH:O	2.20	0.42
2:M:178:PRO:HB3	9:M:1853:HOH:O	2.19	0.42
2:M:183:SER:CB	2:M:190:LYS:HD3	2.50	0.42
2:M:259:GLY:O	2:M:290:LEU:O	2.38	0.42
2:M:289:THR:HG22	2:M:290:LEU:H	1.84	0.42
2:M:461:VAL:HG12	9:M:1945:HOH:O	2.19	0.42
2:M:487:THR:HG22	2:M:488:ALA:N	2.35	0.42
2:M:498:GLN:HA	2:M:498:GLN:NE2	2.34	0.42
2:M:580:MET:HB3	2:M:584:GLU:OE1	2.20	0.42
2:M:676:ILE:O	2:M:676:ILE:CG2	2.68	0.42
2:M:722:ILE:HG23	2:M:805:ARG:HH21	1.85	0.42
3:N:48:ARG:HB2	9:N:2213:HOH:O	2.18	0.42
3:N:421:LEU:HD13	3:N:444:VAL:CG1	2.50	0.42
3:N:500:ARG:O	3:N:504:ASP:HB2	2.20	0.42
3:N:526:PRO:HB2	5:P:317:LEU:HD11	2.02	0.42
3:N:633:VAL:HB	3:N:740:PHE:CE1	2.55	0.42
3:N:704:ARG:HB2	3:N:736:PHE:HB3	2.01	0.42
3:N:1153:VAL:HG12	3:N:1155:VAL:CG2	2.50	0.42
3:N:1205:TYR:CE2	3:N:1366:LYS:HD3	2.54	0.42
3:N:1264:GLU:CG	3:N:1425:THR:H	2.32	0.42
3:N:1382:THR:HG21	3:N:1418:LYS:CE	2.50	0.42
1:A:55:SER:HB2	1:A:158:ILE:HG21	2.01	0.42
1:A:143:ARG:HB2	9:A:331:HOH:O	2.19	0.42
2:C:6:PHE:CE1	2:C:909:ALA:HB2	2.54	0.42
2:C:12:VAL:HB	2:C:472:ARG:CZ	2.50	0.42
2:C:139:GLN:HE22	2:C:415:PRO:HG2	1.85	0.42
2:C:247:PRO:HB2	9:C:1179:HOH:O	2.20	0.42
2:C:254:VAL:HA	2:C:257:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:299:LYS:O	2:C:299:LYS:HG3	2.20	0.42
2:C:443:THR:HG23	2:C:449:ILE:HG13	2.02	0.42
2:C:460:ARG:HG2	2:C:485:TYR:CE2	2.55	0.42
2:C:634:GLY:HA2	9:C:1287:HOH:O	2.20	0.42
3:D:42:ASP:HA	3:D:46:ASP:OD1	2.19	0.42
3:D:112:ILE:CD1	3:D:461:ILE:HG21	2.50	0.42
3:D:119:SER:CB	3:D:123:LEU:HB2	2.40	0.42
3:D:126:VAL:CG1	3:D:132:TYR:HB2	2.49	0.42
3:D:162:ARG:O	3:D:449:SER:OG	2.38	0.42
3:D:897:TRP:HB2	9:D:1776:HOH:O	2.20	0.42
3:D:1066:THR:CG2	3:D:1069:GLU:HG3	2.49	0.42
3:D:1134:LEU:HD22	9:D:1694:HOH:O	2.20	0.42
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.55	0.42
3:D:1467:ILE:HG12	7:D:1527:MXP:H16A	2.02	0.42
4:E:48:MET:N	4:E:54:LEU:HB2	2.34	0.42
5:F:88:ILE:HD13	5:F:193:ARG:CB	2.50	0.42
5:F:88:ILE:HB	5:F:193:ARG:HD2	2.01	0.42
5:F:93:LEU:HG	5:F:190:ALA:HB1	2.02	0.42
5:F:192:LEU:O	5:F:196:VAL:HG23	2.19	0.42
1:K:48:ILE:HG22	1:K:173:PRO:CD	2.49	0.42
1:K:177:VAL:O	2:M:864:GLY:HA3	2.19	0.42
1:L:27:PRO:HB3	1:L:192:LEU:CD2	2.50	0.42
1:L:108:GLU:HG2	9:L:1515:HOH:O	2.19	0.42
1:L:133:GLU:HB3	9:L:1918:HOH:O	2.20	0.42
2:M:146:VAL:HG11	2:M:306:THR:CG2	2.47	0.42
2:M:411:SER:CB	2:M:452:ILE:HG23	2.50	0.42
2:M:479:VAL:CG1	2:M:532:MET:HE2	2.50	0.42
2:M:601:GLY:HA3	2:M:615:TYR:HA	2.02	0.42
2:M:1067:TYR:CE1	3:N:655:PRO:HG3	2.50	0.42
3:N:76:CYS:HA	9:N:1714:HOH:O	2.20	0.42
3:N:563:PRO:HG2	5:P:188:ILE:HG21	2.00	0.42
3:N:959:GLU:H	3:N:959:GLU:HG2	1.24	0.42
3:N:959:GLU:O	3:N:963:TYR:HD1	2.03	0.42
3:N:1066:THR:OG1	3:N:1067:VAL:N	2.51	0.42
3:N:1465:ASN:ND2	3:N:1470:ARG:HD3	2.15	0.42
2:C:124:ASP:HB2	2:C:407:LYS:NZ	2.35	0.41
2:C:204:GLN:NE2	9:C:1386:HOH:O	2.53	0.41
2:C:426:ASP:OD1	2:C:427:VAL:HG22	2.19	0.41
2:C:752:GLY:H	2:C:792:VAL:HB	1.85	0.41
2:C:854:PRO:C	2:C:856:GLU:N	2.72	0.41
2:C:950:LEU:HD12	9:C:1205:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:587:ARG:O	3:D:588:GLY:O	2.38	0.41
3:D:614:PHE:CG	3:D:617:ASN:HB3	2.55	0.41
3:D:661:MET:CE	3:D:673:ALA:HB1	2.50	0.41
3:D:804:LEU:O	3:D:831:GLY:HA2	2.20	0.41
3:D:1065:LEU:HD11	3:D:1070:TYR:N	2.35	0.41
5:F:88:ILE:HD13	5:F:193:ARG:CD	2.47	0.41
1:K:41:ARG:HD2	9:K:1774:HOH:O	2.19	0.41
1:K:54:THR:O	1:K:54:THR:HG22	2.19	0.41
1:K:156:HIS:CD2	1:K:157:GLY:H	2.38	0.41
2:M:170:PRO:HG2	2:M:258:TYR:HD2	1.82	0.41
2:M:202:TYR:OH	2:M:304:LEU:HD22	2.20	0.41
2:M:301:GLU:O	2:M:305:PRO:HG2	2.20	0.41
2:M:756:VAL:HG12	2:M:757:GLY:N	2.35	0.41
2:M:1043:TYR:HE1	3:N:710:ARG:O	2.03	0.41
3:N:584:ASN:OD1	3:N:590:PRO:HD2	2.20	0.41
3:N:840:LYS:HB3	3:N:841:TYR:CE2	2.55	0.41
3:N:984:THR:HG23	3:N:986:ARG:H	1.85	0.41
3:N:1195:GLN:HG3	3:N:1196:THR:N	2.34	0.41
3:N:1274:ILE:HD11	3:N:1334:GLN:HE21	1.82	0.41
3:N:1283:ILE:HD12	3:N:1315:ASP:CG	2.40	0.41
4:O:40:LEU:C	4:O:42:PRO:HD2	2.41	0.41
5:P:271:LEU:CG	5:P:295:MET:HE1	2.50	0.41
5:P:348:SER:OG	5:P:349:LEU:N	2.53	0.41
1:A:124:ASN:OD1	1:A:127:LEU:HB3	2.18	0.41
2:C:86:LYS:CD	9:C:1425:HOH:O	2.69	0.41
2:C:274:ARG:CZ	2:C:285:LEU:H	2.33	0.41
2:C:290:LEU:HD23	2:C:290:LEU:N	2.36	0.41
2:C:328:LEU:HD13	2:C:433:THR:CB	2.47	0.41
2:C:862:PRO:HD3	2:C:973:VAL:O	2.19	0.41
2:C:952:LEU:HD22	2:C:952:LEU:N	2.35	0.41
2:C:969:GLN:HG3	9:C:1350:HOH:O	2.20	0.41
2:C:1039:ALA:HB3	3:D:713:ILE:HD12	2.02	0.41
2:C:1094:ALA:CB	3:D:603:LEU:HD22	2.51	0.41
3:D:172:PRO:O	3:D:174:GLY:N	2.52	0.41
3:D:608:SER:C	3:D:610:LYS:N	2.72	0.41
3:D:804:LEU:N	9:D:1726:HOH:O	2.53	0.41
3:D:1134:LEU:HD21	3:D:1175:ILE:HG23	2.01	0.41
5:F:85:LEU:HA	5:F:88:ILE:CD1	2.44	0.41
5:F:104:ARG:NH1	9:F:673:HOH:O	2.53	0.41
5:F:116:LEU:HB2	5:F:127:ILE:HD12	2.01	0.41
5:F:222:ARG:HG2	9:F:631:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:124:ASN:OD1	1:K:127:LEU:HB3	2.20	0.41
1:L:44:LEU:HD23	1:L:48:ILE:CD1	2.50	0.41
2:M:22:GLN:OE1	2:M:336:VAL:HG21	2.20	0.41
2:M:260:LEU:CB	2:M:291:ALA:HB1	2.42	0.41
2:M:724:ARG:HA	2:M:737:LEU:CD2	2.50	0.41
2:M:926:PHE:O	2:M:929:ARG:HB3	2.20	0.41
3:N:122:GLU:N	9:N:1620:HOH:O	2.52	0.41
3:N:186:VAL:HB	3:N:189:GLN:HB2	2.02	0.41
3:N:432:TYR:O	3:N:448:GLU:HA	2.20	0.41
3:N:633:VAL:O	3:N:635:PRO:HD3	2.20	0.41
3:N:1135:ARG:HH21	3:N:1350:GLU:CD	2.23	0.41
3:N:1323:GLN:HG3	3:N:1324:PRO:CD	2.50	0.41
3:N:1486:VAL:CG1	4:O:73:LEU:HD22	2.50	0.41
5:P:147:LEU:HD23	5:P:147:LEU:HA	1.80	0.41
5:P:220:LEU:O	5:P:223:ALA:HB3	2.20	0.41
1:A:180:GLN:HB3	1:A:180:GLN:HE21	1.62	0.41
1:A:211:LEU:O	1:A:211:LEU:HD12	2.21	0.41
2:C:118:ILE:CG2	2:C:382:ILE:HD13	2.50	0.41
2:C:394:PHE:HB2	9:C:1403:HOH:O	2.19	0.41
2:C:412:ALA:HB1	2:C:419:THR:HG21	2.01	0.41
2:C:709:GLU:HG3	2:C:824:ARG:CG	2.50	0.41
2:C:853:LEU:HG	9:C:1271:HOH:O	2.20	0.41
3:D:103:TRP:HE1	3:D:604:THR:CG2	2.33	0.41
3:D:116:LEU:HD23	3:D:118:LEU:HD21	2.01	0.41
3:D:131:LYS:HD2	5:F:83:GLN:CD	2.40	0.41
3:D:835:SER:O	3:D:837:GLY:N	2.53	0.41
3:D:874:GLU:HG3	9:D:1855:HOH:O	2.20	0.41
3:D:1283:ILE:HG22	3:D:1284:GLU:N	2.35	0.41
3:D:1350:GLU:O	3:D:1350:GLU:HG3	2.21	0.41
5:F:76:SER:O	5:F:80:PRO:HG2	2.20	0.41
1:K:18:ARG:HH12	1:K:88:ARG:CD	2.33	0.41
1:K:79:ILE:O	1:K:83:LYS:HG3	2.19	0.41
2:M:557:ARG:CZ	2:M:879:ARG:HG2	2.50	0.41
3:N:119:SER:CB	3:N:123:LEU:HB2	2.40	0.41
3:N:131:LYS:O	3:N:133:ILE:HD13	2.21	0.41
3:N:405:ASP:HB3	9:N:1860:HOH:O	2.20	0.41
3:N:688:TRP:HA	3:N:688:TRP:CE3	2.56	0.41
2:C:64:LEU:HG	2:C:65:VAL:N	2.34	0.41
2:C:540:PHE:HE1	2:C:906:PHE:HE1	1.68	0.41
2:C:815:LEU:HD12	9:C:1534:HOH:O	2.20	0.41
3:D:501:ALA:HB2	9:D:2147:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:560:GLN:O	5:F:132:ARG:NH1	2.47	0.41
3:D:633:VAL:O	3:D:635:PRO:HD3	2.20	0.41
3:D:1057:VAL:HG22	3:D:1069:GLU:HB3	2.02	0.41
3:D:1217:ILE:N	9:D:2106:HOH:O	2.52	0.41
3:D:1490:LYS:HG2	9:D:2098:HOH:O	2.19	0.41
5:F:117:SER:HB3	5:F:122:LEU:O	2.19	0.41
1:K:115:LEU:HA	1:K:116:PRO:HD3	1.90	0.41
1:K:159:LYS:HA	9:K:1082:HOH:O	2.19	0.41
2:M:597:ALA:O	2:M:652:GLY:N	2.53	0.41
2:M:875:GLY:HA2	2:M:879:ARG:HH11	1.85	0.41
2:M:1100:GLN:HE21	2:M:1100:GLN:HB2	1.65	0.41
3:N:686:GLU:HA	3:N:689:ASP:OD2	2.21	0.41
3:N:696:HIS:HB3	9:N:1565:HOH:O	2.19	0.41
5:P:172:ARG:HD3	9:P:483:HOH:O	2.21	0.41
5:P:315:VAL:HG11	9:P:467:HOH:O	2.20	0.41
1:A:11:PHE:CD1	1:B:225:PHE:HA	2.55	0.41
1:A:47:SER:OG	1:B:32:PHE:HZ	2.03	0.41
1:B:23:PHE:CD2	1:B:211:LEU:HD22	2.56	0.41
2:C:127:PHE:O	2:C:133:ASP:HA	2.21	0.41
2:C:396:ASP:HA	2:C:633:GLN:CD	2.40	0.41
2:C:1034:GLU:O	2:C:1037:VAL:HG23	2.21	0.41
3:D:90:MET:HE2	3:D:521:PRO:HD3	2.01	0.41
3:D:196:VAL:HG13	9:D:1768:HOH:O	2.20	0.41
3:D:688:TRP:HA	3:D:688:TRP:HE3	1.86	0.41
3:D:693:GLU:HG2	9:D:1780:HOH:O	2.21	0.41
3:D:699:VAL:HG12	3:D:717:GLN:CA	2.51	0.41
3:D:767:HIS:NE2	4:E:6:ILE:HG12	2.36	0.41
3:D:850:LEU:H	3:D:850:LEU:CD1	2.24	0.41
3:D:1171:VAL:HG12	3:D:1171:VAL:O	2.21	0.41
3:D:1191:PRO:HD3	3:D:1204:CYS:O	2.21	0.41
3:D:1192:LEU:HD22	3:D:1345:GLU:HG2	2.02	0.41
1:L:147:GLY:N	1:L:171:PHE:CE1	2.88	0.41
2:M:22:GLN:HE22	2:M:135:VAL:CG1	2.33	0.41
2:M:113:VAL:HB	2:M:115:LEU:HD23	2.02	0.41
2:M:475:VAL:O	2:M:478:VAL:HB	2.20	0.41
3:N:50:PHE:CD2	3:N:522:PRO:HG3	2.56	0.41
3:N:87:ARG:HB2	3:N:523:ASP:HB2	2.03	0.41
3:N:570:GLU:HB2	5:P:214:GLN:NE2	2.35	0.41
3:N:852:ALA:HB1	3:N:857:ILE:HB	2.02	0.41
3:N:1364:HIS:ND1	3:N:1366:LYS:HB2	2.36	0.41
5:P:163:LEU:HD13	5:P:174:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:24:GLU:HG2	2:C:27:ARG:CD	2.50	0.41
2:C:118:ILE:H	2:C:118:ILE:HG13	1.64	0.41
2:C:462:ASP:HB3	2:C:468:ARG:CD	2.50	0.41
2:C:479:VAL:HG13	2:C:508:ILE:HD12	2.03	0.41
2:C:592:LEU:HD23	2:C:592:LEU:HA	1.90	0.41
2:C:620:LEU:HD12	2:C:620:LEU:O	2.21	0.41
2:C:742:VAL:HG21	9:C:1160:HOH:O	2.19	0.41
3:D:29:PRO:HG2	3:D:549:ASN:HD21	1.84	0.41
3:D:204:LEU:HD21	3:D:445:ARG:HH12	1.86	0.41
3:D:766:ALA:O	3:D:769:LEU:HD21	2.19	0.41
3:D:832:ARG:HB2	9:D:1797:HOH:O	2.19	0.41
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.02	0.41
3:D:1122:LEU:O	3:D:1134:LEU:HA	2.20	0.41
3:D:1209:LEU:HD12	3:D:1219:GLU:CD	2.41	0.41
4:E:41:GLU:HB2	4:E:45:ARG:NH1	2.36	0.41
5:F:75:ILE:HG13	9:F:645:HOH:O	2.20	0.41
5:F:196:VAL:HG22	5:F:213:ILE:HD13	2.01	0.41
5:F:215:GLU:OE2	5:F:254:GLN:NE2	2.50	0.41
1:L:127:LEU:HD12	9:L:1125:HOH:O	2.20	0.41
2:M:292:ARG:NH1	2:M:299:LYS:HD3	2.35	0.41
2:M:327:HIS:O	2:M:330:ASN:HB2	2.21	0.41
2:M:374:ASN:O	2:M:377:PRO:HD2	2.20	0.41
2:M:663:ASN:C	2:M:665:PHE:H	2.24	0.41
2:M:1034:GLU:HA	2:M:1037:VAL:CG2	2.49	0.41
3:N:570:GLU:HB2	5:P:214:GLN:HE22	1.85	0.41
3:N:637:LEU:HD12	3:N:641:GLN:HB2	2.02	0.41
3:N:775:GLY:C	9:N:1689:HOH:O	2.58	0.41
3:N:806:PHE:O	3:N:808:THR:N	2.53	0.41
3:N:1276:GLU:OE2	3:N:1303:TYR:HE2	2.04	0.41
3:N:1389:LEU:HD12	3:N:1390:LEU:N	2.32	0.41
5:P:169:GLU:H	5:P:169:GLU:HG3	1.67	0.41
5:P:305:GLU:HG2	5:P:309:LYS:HE3	2.01	0.41
9:A:432:HOH:O	2:C:832:LYS:HE3	2.20	0.41
1:B:57:TYR:CE2	1:B:59:GLU:HA	2.55	0.41
2:C:162:ILE:CD1	2:C:306:THR:HG21	2.50	0.41
2:C:274:ARG:HB2	2:C:285:LEU:HB3	2.02	0.41
2:C:437:ARG:HG2	2:C:467:ILE:O	2.21	0.41
2:C:914:ILE:HA	2:C:914:ILE:HD12	1.74	0.41
2:C:1002:GLU:O	2:C:1003:ASP:C	2.58	0.41
2:C:1013:TYR:OH	3:D:624:ASP:OD2	2.37	0.41
9:C:1734:HOH:O	3:D:1471:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:165:LYS:HG2	9:D:1699:HOH:O	2.21	0.41
3:D:596:SER:C	3:D:598:ARG:H	2.24	0.41
3:D:601:ARG:HG3	9:D:2091:HOH:O	2.21	0.41
3:D:771:SER:HA	3:D:772:PRO:HD3	1.91	0.41
5:F:321:ILE:HG13	5:F:329:TYR:HA	2.01	0.41
1:K:101:LEU:HD23	1:K:102:LYS:N	2.35	0.41
1:K:158:ILE:HG22	1:K:159:LYS:N	2.35	0.41
1:L:172:SER:OG	1:L:174:VAL:HB	2.21	0.41
2:M:22:GLN:HE22	2:M:135:VAL:HG12	1.85	0.41
2:M:264:PRO:HB3	2:M:289:THR:CB	2.50	0.41
2:M:299:LYS:O	2:M:299:LYS:HG3	2.21	0.41
2:M:663:ASN:HD22	2:M:663:ASN:HA	1.52	0.41
2:M:724:ARG:HB2	2:M:740:GLU:HA	2.01	0.41
2:M:968:LEU:HD13	9:M:2164:HOH:O	2.21	0.41
3:N:611:GLN:N	9:N:1557:HOH:O	2.54	0.41
3:N:637:LEU:HD11	3:N:642:CYS:CA	2.51	0.41
3:N:818:ARG:O	3:N:821:VAL:HB	2.20	0.41
3:N:911:LEU:O	3:N:915:VAL:HG23	2.20	0.41
3:N:1007:VAL:CG2	3:N:1008:PHE:N	2.84	0.41
3:N:1333:HIS:O	3:N:1336:LEU:HB3	2.19	0.41
4:O:49:GLN:C	4:O:51:LEU:N	2.74	0.41
1:A:46:SER:HB3	2:C:856:GLU:CD	2.41	0.41
2:C:96:ALA:HB2	9:C:1545:HOH:O	2.20	0.41
2:C:172:ILE:HD12	2:C:172:ILE:N	2.34	0.41
2:C:313:LEU:HD12	2:C:313:LEU:O	2.21	0.41
2:C:414:GLY:O	2:C:416:GLY:N	2.54	0.41
2:C:469:THR:HG23	2:C:471:TYR:CE1	2.56	0.41
2:C:511:GLU:N	9:C:1690:HOH:O	2.53	0.41
2:C:952:LEU:CD1	2:C:969:GLN:HE22	2.19	0.41
3:D:415:VAL:HG13	3:D:419:ASP:HB2	2.01	0.41
3:D:925:GLU:OE1	4:E:6:ILE:HG22	2.20	0.41
3:D:998:GLU:HB3	9:D:2202:HOH:O	2.20	0.41
3:D:1326:THR:HG22	3:D:1327:ARG:H	1.85	0.41
3:D:1339:LYS:HB3	3:D:1343:ALA:HB2	2.02	0.41
3:D:1459:LEU:HB2	3:D:1470:ARG:NH1	2.35	0.41
4:E:50:THR:HA	9:E:107:HOH:O	2.20	0.41
5:F:280:GLN:NE2	9:F:601:HOH:O	2.54	0.41
5:F:284:ARG:O	5:F:286:PRO:N	2.53	0.41
1:K:16:GLN:HB2	9:K:3198:HOH:O	2.20	0.41
1:L:101:LEU:HD12	1:L:114:PHE:CA	2.50	0.41
1:L:117:VAL:HB	1:L:120:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:142:VAL:O	1:L:142:VAL:HG23	2.21	0.41
2:M:140:ILE:H	2:M:140:ILE:HD12	1.86	0.41
2:M:278:GLU:HA	2:M:283:ILE:HA	2.03	0.41
2:M:676:ILE:HG21	2:M:988:VAL:HG22	2.01	0.41
2:M:1008:ARG:CZ	2:M:1020:PRO:HB3	2.51	0.41
2:M:1054:THR:HB	2:M:1055:LEU:H	1.61	0.41
3:N:105:VAL:HG12	3:N:106:LYS:HG3	2.02	0.41
3:N:165:LYS:CG	3:N:397:LYS:HD3	2.50	0.41
3:N:206:ARG:HA	9:N:2058:HOH:O	2.20	0.41
3:N:489:ARG:HD3	9:N:1694:HOH:O	2.20	0.41
3:N:804:LEU:O	3:N:831:GLY:HA2	2.21	0.41
3:N:899:LEU:HD12	3:N:900:ILE:HG23	2.02	0.41
3:N:1051:GLU:HG3	3:N:1051:GLU:H	1.53	0.41
3:N:1147:ARG:NH1	9:N:2122:HOH:O	2.52	0.41
3:N:1223:ILE:O	3:N:1224:VAL:C	2.59	0.41
3:N:1341:PRO:HB2	9:N:1945:HOH:O	2.19	0.41
5:P:350:LEU:O	5:P:354:LEU:HB2	2.21	0.41
5:P:371:LEU:HB2	5:P:372:ARG:HH11	1.86	0.41
1:A:18:ARG:HH12	1:A:88:ARG:HD3	1.86	0.41
1:A:170:VAL:HA	9:A:399:HOH:O	2.21	0.41
1:A:227:ASN:ND2	1:A:227:ASN:N	2.65	0.41
1:B:111:ALA:HB3	1:B:124:ASN:O	2.21	0.41
2:C:7:GLY:O	2:C:907:ASP:OD1	2.38	0.41
2:C:35:PRO:HB3	9:C:1537:HOH:O	2.21	0.41
2:C:36:PRO:CB	2:C:70:GLU:HG2	2.51	0.41
2:C:45:GLN:NE2	9:C:1426:HOH:O	2.52	0.41
2:C:149:THR:HA	2:C:150:PRO:HD3	1.92	0.41
2:C:317:VAL:HB	9:C:1324:HOH:O	2.20	0.41
2:C:612:VAL:HG22	2:C:622:GLU:CB	2.51	0.41
2:C:612:VAL:HG22	2:C:622:GLU:HG3	2.02	0.41
2:C:724:ARG:HB2	2:C:740:GLU:HA	2.02	0.41
2:C:807:ARG:HA	2:C:821:GLU:HB2	2.02	0.41
2:C:815:LEU:HG	2:C:819:VAL:HG11	2.00	0.41
2:C:818:GLY:N	5:F:309:LYS:CE	2.82	0.41
2:C:969:GLN:HE21	2:C:969:GLN:HB3	1.72	0.41
2:C:1063:ARG:O	2:C:1066:ALA:HB3	2.21	0.41
2:C:1067:TYR:CE1	2:C:1071:ILE:HD11	2.56	0.41
3:D:29:PRO:CB	3:D:545:ARG:HG2	2.49	0.41
3:D:33:ASN:HB3	9:D:2304:HOH:O	2.21	0.41
3:D:44:LEU:HD21	3:D:544:TYR:HB3	2.03	0.41
3:D:85:VAL:HG11	3:D:89:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:93:ILE:HD13	3:D:547:LEU:HD23	2.03	0.41
3:D:119:SER:N	3:D:123:LEU:HD22	2.26	0.41
3:D:482:LYS:HB2	9:D:1744:HOH:O	2.20	0.41
3:D:647:ARG:HB2	9:D:1878:HOH:O	2.21	0.41
3:D:704:ARG:HB2	3:D:736:PHE:HB3	2.03	0.41
3:D:899:LEU:HD12	3:D:900:ILE:HG23	2.03	0.41
3:D:1361:VAL:HG23	9:D:1625:HOH:O	2.21	0.41
4:E:53:GLY:C	4:E:55:PHE:H	2.24	0.41
1:K:48:ILE:HD11	1:K:210:ALA:O	2.21	0.41
1:K:49:PRO:HB3	1:K:148:VAL:CG2	2.51	0.41
1:K:198:ARG:NH2	9:K:1749:HOH:O	2.54	0.41
1:L:75:VAL:O	1:L:79:ILE:HG23	2.20	0.41
2:M:34:VAL:CG2	2:M:38:LYS:HD3	2.49	0.41
2:M:56:GLU:OE2	2:M:356:ARG:HG2	2.20	0.41
2:M:129:ILE:CD1	2:M:386:PHE:HB3	2.51	0.41
2:M:131:GLY:HA2	9:M:1651:HOH:O	2.20	0.41
2:M:190:LYS:H	2:M:190:LYS:HG3	1.56	0.41
2:M:218:VAL:CA	2:M:221:LEU:HD23	2.50	0.41
2:M:255:ALA:HB3	2:M:298:PHE:CZ	2.56	0.41
2:M:280:LYS:HA	9:M:1935:HOH:O	2.20	0.41
2:M:408:ARG:HH11	2:M:408:ARG:HD2	1.74	0.41
2:M:535:SER:HB2	2:M:537:LYS:HG3	2.03	0.41
2:M:911:GLU:HB3	2:M:912:PRO:HD3	2.03	0.41
2:M:958:THR:HG23	2:M:961:GLU:HB2	2.03	0.41
2:M:971:LYS:HB3	2:M:988:VAL:N	2.36	0.41
2:M:1090:LYS:HD2	3:N:90:MET:CE	2.51	0.41
3:N:60:CYS:N	3:N:76:CYS:SG	2.91	0.41
3:N:192:ALA:HB2	3:N:393:ILE:CD1	2.51	0.41
3:N:398:ALA:HB2	9:N:1561:HOH:O	2.21	0.41
3:N:417:PRO:HG3	3:N:430:ASP:O	2.21	0.41
3:N:562:ALA:HB3	9:P:599:HOH:O	2.20	0.41
3:N:572:ARG:HH11	3:N:572:ARG:HD3	1.63	0.41
3:N:591:VAL:CG1	3:N:597:ASP:HA	2.50	0.41
3:N:611:GLN:CG	3:N:619:LEU:CG	2.91	0.41
3:N:705:ALA:CB	3:N:706:PRO:CD	2.94	0.41
3:N:711:LEU:C	3:N:713:ILE:N	2.74	0.41
3:N:771:SER:HA	3:N:772:PRO:HD3	1.86	0.41
3:N:889:ALA:HB1	3:N:930:LEU:HA	2.03	0.41
3:N:1000:THR:CG2	3:N:1001:GLU:N	2.84	0.41
3:N:1075:HIS:CE1	9:N:1553:HOH:O	2.74	0.41
3:N:1148:VAL:HG21	3:N:1203:LYS:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1155:VAL:CG1	3:N:1177:ALA:HB1	2.50	0.41
3:N:1264:GLU:HA	3:N:1423:GLY:CA	2.51	0.41
3:N:1369:GLU:HA	3:N:1372:VAL:HG12	2.02	0.41
3:N:1441:GLN:N	9:N:1579:HOH:O	2.54	0.41
3:N:1442:ASN:N	9:N:1579:HOH:O	2.53	0.41
4:O:16:LYS:HD3	4:O:17:TYR:CE2	2.56	0.41
4:O:36:LYS:HG2	9:O:3235:HOH:O	2.20	0.41
4:O:54:LEU:HA	4:O:58:PRO:CG	2.50	0.41
5:P:207:LEU:HD23	5:P:207:LEU:HA	1.95	0.41
5:P:277:GLN:HA	9:P:458:HOH:O	2.21	0.41
1:B:158:ILE:CG2	1:B:159:LYS:N	2.83	0.41
2:C:162:ILE:HD12	2:C:172:ILE:HB	2.03	0.41
2:C:166:PRO:HD3	2:C:265:ARG:CB	2.51	0.41
2:C:663:ASN:HD22	2:C:663:ASN:HA	1.51	0.41
2:C:707:ARG:CZ	2:C:824:ARG:CZ	2.98	0.41
2:C:818:GLY:CA	5:F:309:LYS:NZ	2.83	0.41
2:C:1097:LEU:N	2:C:1097:LEU:CD1	2.84	0.41
3:D:155:ASP:HA	3:D:158:TYR:HB3	2.03	0.41
3:D:687:VAL:CG1	9:D:2185:HOH:O	2.67	0.41
3:D:729:HIS:ND1	3:D:730:PRO:CD	2.84	0.41
3:D:1035:ILE:CA	3:D:1038:LEU:HD12	2.50	0.41
3:D:1116:ASN:HB3	9:D:2418:HOH:O	2.20	0.41
3:D:1243:THR:CB	3:D:1253:THR:HB	2.50	0.41
3:D:1384:PRO:HB3	3:D:1387:SER:O	2.20	0.41
4:E:49:GLN:C	4:E:51:LEU:N	2.73	0.41
1:K:85:LEU:HB2	1:K:127:LEU:HD21	2.03	0.41
1:K:198:ARG:HB2	1:K:200:TRP:CH2	2.55	0.41
1:L:41:ARG:NH1	1:L:177:VAL:HG23	2.36	0.41
2:M:182:VAL:HG12	2:M:193:LEU:HD13	2.02	0.41
2:M:271:GLU:HA	2:M:275:TYR:CD1	2.56	0.41
2:M:474:VAL:HG23	2:M:478:VAL:O	2.21	0.41
3:N:601:ARG:HG2	3:N:605:ASP:OD1	2.21	0.41
3:N:712:GLY:O	3:N:713:ILE:HG13	2.21	0.41
3:N:907:GLU:HG2	3:N:908:LYS:H	1.85	0.41
3:N:937:TYR:HD2	3:N:941:PHE:HE1	1.69	0.41
3:N:1404:ASN:HA	9:N:1794:HOH:O	2.19	0.41
5:P:132:ARG:NH2	5:P:184:ARG:NH1	2.69	0.41
2:C:91:GLN:HG2	2:C:119:PRO:HG3	2.03	0.40
2:C:234:ALA:HA	2:C:237:ARG:HB2	2.02	0.40
2:C:269:LEU:O	2:C:269:LEU:HD23	2.22	0.40
2:C:292:ARG:NH1	9:C:1267:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:442:GLU:O	2:C:442:GLU:HG3	2.21	0.40
2:C:495:THR:HG21	2:C:524:VAL:HG21	2.02	0.40
2:C:518:LYS:N	9:C:1698:HOH:O	2.52	0.40
2:C:836:GLY:HA3	3:D:724:GLN:OE1	2.20	0.40
2:C:874:LEU:HD23	3:D:1023:MET:HE1	2.03	0.40
2:C:966:LEU:HD21	2:C:986:PRO:CG	2.51	0.40
3:D:674:ARG:HH11	3:D:674:ARG:HG2	1.86	0.40
3:D:684:LYS:HG2	9:D:2411:HOH:O	2.20	0.40
3:D:717:GLN:CG	9:D:1581:HOH:O	2.68	0.40
3:D:760:ARG:HD2	4:E:3:GLU:CD	2.41	0.40
3:D:820:GLU:CB	3:D:836:VAL:HG21	2.51	0.40
3:D:1412:LYS:O	3:D:1414:PRO:HD3	2.21	0.40
3:D:1447:LEU:O	3:D:1448:THR:C	2.60	0.40
5:F:90:GLN:HE21	5:F:90:GLN:HB3	1.73	0.40
1:L:71:VAL:HG22	1:L:132:LEU:CD1	2.50	0.40
1:L:101:LEU:HD12	1:L:113:ASP:C	2.40	0.40
2:M:242:LEU:HD23	2:M:242:LEU:HA	1.78	0.40
2:M:414:GLY:O	2:M:416:GLY:N	2.54	0.40
2:M:437:ARG:NH1	2:M:488:ALA:HA	2.35	0.40
2:M:471:TYR:CD2	2:M:496:ILE:HG21	2.55	0.40
2:M:512:ARG:HB3	2:M:523:ILE:HD11	2.03	0.40
2:M:840:ALA:HB2	2:M:846:LYS:HA	2.02	0.40
2:M:861:LEU:CD2	2:M:925:TYR:HE2	2.33	0.40
2:M:929:ARG:HH22	2:M:940:GLU:CD	2.24	0.40
3:N:106:LYS:HZ2	3:N:587:ARG:HH11	1.69	0.40
3:N:515:GLU:HG3	9:N:1827:HOH:O	2.20	0.40
3:N:516:ALA:HB1	9:N:2118:HOH:O	2.21	0.40
3:N:729:HIS:CE1	3:N:935:LYS:HD3	2.56	0.40
3:N:850:LEU:H	3:N:850:LEU:CD1	2.24	0.40
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.56	0.40
3:N:1223:ILE:O	3:N:1227:GLN:HG3	2.22	0.40
3:N:1396:GLU:O	3:N:1396:GLU:HG2	2.22	0.40
5:P:256:ARG:HA	9:P:486:HOH:O	2.21	0.40
5:P:321:ILE:HB	5:P:327:SER:OG	2.21	0.40
2:C:15:LEU:HA	2:C:16:PRO:HD3	1.95	0.40
2:C:181:VAL:HG12	2:C:182:VAL:N	2.36	0.40
2:C:464:LEU:HD12	2:C:465:GLY:N	2.36	0.40
2:C:468:ARG:NH1	9:C:1743:HOH:O	2.54	0.40
2:C:708:TYR:CD1	2:C:708:TYR:N	2.89	0.40
2:C:858:MET:HB2	2:C:859:PRO:CD	2.51	0.40
2:C:958:THR:HA	9:C:1402:HOH:O	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:152:LEU:HD23	3:D:152:LEU:N	2.27	0.40
3:D:400:VAL:HG13	3:D:402:PRO:CD	2.51	0.40
3:D:610:LYS:HB3	7:D:1527:MXP:H15	2.03	0.40
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.56	0.40
3:D:840:LYS:NZ	9:D:2398:HOH:O	2.55	0.40
3:D:1007:VAL:CG2	3:D:1008:PHE:N	2.84	0.40
3:D:1114:THR:HG23	3:D:1116:ASN:ND2	2.36	0.40
3:D:1310:ARG:HG3	3:D:1327:ARG:CB	2.48	0.40
3:D:1394:VAL:HG23	9:D:2328:HOH:O	2.21	0.40
5:F:94:LEU:HB2	5:F:98:GLU:CG	2.52	0.40
5:F:270:LYS:N	9:F:511:HOH:O	2.54	0.40
5:F:364:ARG:HH12	5:F:396:ARG:CZ	2.34	0.40
1:K:107:LYS:HE3	1:K:113:ASP:OD2	2.19	0.40
1:K:176:ARG:HG3	1:K:200:TRP:CE3	2.57	0.40
1:K:201:THR:HG21	1:K:205:VAL:O	2.20	0.40
1:L:158:ILE:CG2	1:L:159:LYS:N	2.84	0.40
1:L:197:LEU:HD21	1:L:199:ILE:CD1	2.47	0.40
2:M:75:GLU:HA	2:M:76:PRO:HD3	1.97	0.40
2:M:143:SER:HB2	2:M:276:LYS:HZ1	1.83	0.40
2:M:308:ARG:HG2	9:M:1753:HOH:O	2.21	0.40
2:M:361:MET:HE2	9:M:2183:HOH:O	2.20	0.40
2:M:400:PRO:O	2:M:401:LEU:C	2.58	0.40
2:M:443:THR:HA	2:M:444:PRO:HD3	1.80	0.40
2:M:606:VAL:HG21	2:M:645:VAL:HG22	2.03	0.40
2:M:674:VAL:O	2:M:989:VAL:HA	2.20	0.40
2:M:929:ARG:HH12	2:M:940:GLU:CD	2.24	0.40
2:M:1060:ILE:O	2:M:1063:ARG:HG2	2.20	0.40
3:N:489:ARG:NH2	3:N:1389:LEU:HD11	2.32	0.40
3:N:530:VAL:HG23	3:N:534:ARG:O	2.21	0.40
3:N:596:SER:C	3:N:598:ARG:H	2.24	0.40
3:N:951:ILE:HD12	3:N:1062:ARG:HG3	2.02	0.40
3:N:1087:ARG:HD3	3:N:1238:MET:H	1.86	0.40
3:N:1161:GLU:H	3:N:1161:GLU:HG2	1.37	0.40
1:B:61:VAL:N	1:B:137:ARG:NH2	2.67	0.40
2:C:263:ASP:C	2:C:264:PRO:O	2.59	0.40
2:C:491:GLU:HG2	9:C:1297:HOH:O	2.21	0.40
2:C:721:ARG:NE	9:C:1244:HOH:O	2.55	0.40
2:C:773:LEU:HG	2:C:777:ILE:HD11	2.03	0.40
2:C:865:THR:O	2:C:865:THR:HG23	2.21	0.40
2:C:1010:THR:HG22	2:C:1011:GLY:N	2.36	0.40
3:D:93:ILE:HD13	3:D:548:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:521:PRO:O	3:D:525:ARG:NH1	2.52	0.40
3:D:638:LYS:C	3:D:729:HIS:HD2	2.25	0.40
3:D:797:LYS:HA	3:D:828:LYS:HB2	2.04	0.40
3:D:1066:THR:OG1	3:D:1067:VAL:N	2.53	0.40
3:D:1335:LEU:HD23	3:D:1344:VAL:CA	2.28	0.40
3:D:1353:GLN:OE1	3:D:1365:ASP:OD2	2.39	0.40
3:D:1372:VAL:CG1	3:D:1373:ARG:N	2.84	0.40
5:F:205:ARG:NH1	5:F:248:ASN:OD1	2.54	0.40
5:F:272:SER:O	5:F:276:ARG:HG3	2.22	0.40
1:K:28:LEU:HD23	1:K:28:LEU:HA	1.77	0.40
1:L:10:VAL:HG12	1:L:12:THR:HG23	2.02	0.40
2:M:110:GLU:HB3	2:M:369:PRO:HG3	2.02	0.40
2:M:118:ILE:H	2:M:118:ILE:HG13	1.63	0.40
2:M:221:LEU:HG	2:M:222:MET:N	2.37	0.40
2:M:234:ALA:HA	2:M:237:ARG:HB2	2.02	0.40
2:M:420:ARG:H	2:M:420:ARG:HG2	1.44	0.40
2:M:424:GLY:N	9:M:1722:HOH:O	2.54	0.40
2:M:480:THR:CG2	2:M:481:ASP:H	2.34	0.40
2:M:586:ARG:NE	2:M:590:ASP:OD2	2.53	0.40
2:M:742:VAL:CG1	2:M:743:VAL:N	2.83	0.40
2:M:950:LEU:HB3	2:M:952:LEU:HD23	2.02	0.40
2:M:1017:THR:OG1	2:M:1019:GLN:HG3	2.22	0.40
3:N:46:ASP:O	3:N:48:ARG:N	2.54	0.40
3:N:776:GLU:HB3	3:N:912:LYS:HE2	2.03	0.40
3:N:793:THR:HG22	3:N:879:ARG:HA	2.03	0.40
3:N:862:ASP:O	3:N:876:SER:HB2	2.21	0.40
3:N:932:ASP:O	3:N:935:LYS:HB3	2.22	0.40
3:N:1366:LYS:O	3:N:1369:GLU:HB2	2.22	0.40
3:N:1435:LEU:HD23	3:N:1467:ILE:HD12	2.02	0.40
4:O:26:ARG:HG2	4:O:67:GLU:OE1	2.22	0.40
1:A:13:VAL:CG1	1:A:15:THR:HG22	2.49	0.40
1:A:95:GLN:HG2	9:A:325:HOH:O	2.21	0.40
1:A:96:THR:N	9:A:349:HOH:O	2.54	0.40
2:C:54:ILE:HD13	9:C:1578:HOH:O	2.21	0.40
2:C:166:PRO:HG2	9:C:1175:HOH:O	2.21	0.40
2:C:378:LEU:O	2:C:382:ILE:HG13	2.22	0.40
2:C:400:PRO:O	2:C:401:LEU:C	2.58	0.40
2:C:410:ILE:N	2:C:453:THR:O	2.53	0.40
2:C:549:PHE:HE2	2:C:887:GLU:N	2.20	0.40
2:C:686:ASP:N	9:C:1222:HOH:O	2.54	0.40
2:C:897:LEU:CD1	2:C:921:ALA:HA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:46:ASP:O	3:D:48:ARG:N	2.54	0.40
3:D:97:THR:O	3:D:98:PRO:O	2.40	0.40
3:D:500:ARG:O	3:D:504:ASP:HB2	2.21	0.40
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.91	0.40
3:D:778:LEU:HD11	9:D:1940:HOH:O	2.21	0.40
3:D:898:GLU:OE2	3:D:921:ARG:NH1	2.54	0.40
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	2.03	0.40
3:D:1256:LEU:N	3:D:1257:PRO:CD	2.85	0.40
3:D:1305:LEU:HD22	3:D:1309:ALA:CB	2.52	0.40
5:F:280:GLN:O	5:F:280:GLN:HG2	2.22	0.40
1:K:42:ARG:NH1	1:L:34:VAL:HB	2.14	0.40
1:K:180:GLN:HE21	1:K:180:GLN:HB3	1.65	0.40
2:M:172:ILE:HG22	2:M:173:ASP:N	2.36	0.40
2:M:176:VAL:O	2:M:176:VAL:HG23	2.22	0.40
2:M:284:ARG:HD2	9:M:2219:HOH:O	2.21	0.40
2:M:443:THR:HG21	2:M:450:GLY:H	1.85	0.40
2:M:713:ARG:HB2	2:M:720:GLU:OE1	2.21	0.40
2:M:1008:ARG:HD2	2:M:1028:GLY:H	1.85	0.40
3:N:565:ILE:HD12	5:P:192:LEU:CD1	2.50	0.40
3:N:610:LYS:CG	7:N:1527:MXP:H15A	2.47	0.40
3:N:935:LYS:HB3	3:N:935:LYS:HE2	1.94	0.40
3:N:982:PHE:HA	9:N:1762:HOH:O	2.21	0.40
3:N:1109:GLU:CD	3:N:1202:GLN:HB2	2.42	0.40
3:N:1144:LEU:HD12	3:N:1171:VAL:HG13	2.04	0.40
3:N:1161:GLU:CG	3:N:1164:ARG:HD2	2.52	0.40
3:N:1384:PRO:C	3:N:1413:THR:HG21	2.42	0.40
3:N:1399:ASP:O	3:N:1403:LEU:HB2	2.21	0.40
5:P:363:GLU:CA	5:P:367:MET:HG3	2.51	0.40
5:P:399:GLN:O	5:P:403:LYS:HB2	2.21	0.40
1:A:42:ARG:HD3	1:B:35:THR:OG1	2.21	0.40
1:A:43:ILE:HG21	1:A:214:ALA:HA	2.04	0.40
1:A:44:LEU:O	1:A:174:VAL:HG21	2.21	0.40
2:C:207:LEU:HD13	2:C:221:LEU:HD13	2.03	0.40
2:C:861:LEU:CD2	2:C:925:TYR:HE2	2.34	0.40
2:C:1005:MET:HB2	3:D:629:SER:HB2	2.02	0.40
2:C:1059:ASP:CG	2:C:1062:GLY:HA3	2.42	0.40
2:C:1097:LEU:HD12	2:C:1097:LEU:H	1.86	0.40
3:D:99:ALA:HA	3:D:575:GLN:NE2	2.37	0.40
3:D:659:LYS:O	3:D:659:LYS:HG2	2.21	0.40
3:D:758:GLU:O	3:D:762:GLN:HG3	2.20	0.40
3:D:1209:LEU:HD23	3:D:1211:MET:CG	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.36	0.40
3:D:1476:THR:C	3:D:1478:SER:H	2.24	0.40
5:F:220:LEU:HB2	5:F:243:ILE:HD11	2.02	0.40
5:F:364:ARG:HD3	9:F:425:HOH:O	2.21	0.40
1:K:20:TYR:HE2	1:K:22:GLU:HG3	1.85	0.40
1:K:41:ARG:NH2	2:M:860:HIS:HB3	2.37	0.40
1:L:145:ASP:O	1:L:171:PHE:HE1	2.04	0.40
2:M:73:LEU:HD23	2:M:94:LEU:HD13	2.04	0.40
2:M:174:LEU:CD2	2:M:184:MET:HG3	2.52	0.40
2:M:183:SER:HB3	2:M:190:LYS:HD3	2.03	0.40
2:M:351:LEU:HD11	2:M:373:VAL:HG13	2.03	0.40
2:M:890:LEU:HD12	2:M:914:ILE:CD1	2.46	0.40
3:N:153:LEU:HB3	9:N:1717:HOH:O	2.20	0.40
3:N:199:LEU:H	3:N:199:LEU:HG	1.60	0.40
3:N:397:LYS:HE3	3:N:448:GLU:HB3	2.04	0.40
3:N:447:VAL:HG11	9:N:1573:HOH:O	2.21	0.40
3:N:478:LEU:HD21	3:N:500:ARG:HH21	1.84	0.40
3:N:489:ARG:HG2	3:N:490:ALA:N	2.37	0.40
3:N:733:CYS:HG	3:N:740:PHE:HZ	1.66	0.40
3:N:835:SER:O	3:N:837:GLY:N	2.54	0.40
3:N:1095:THR:O	3:N:1096:ARG:C	2.60	0.40
3:N:1148:VAL:HG13	3:N:1163:GLY:O	2.21	0.40
3:N:1500:LYS:O	3:N:1503:VAL:HG23	2.22	0.40
4:O:85:LEU:HD23	4:O:85:LEU:C	2.42	0.40
5:P:295:MET:HB3	5:P:299:TRP:CG	2.57	0.40
5:P:368:VAL:HA	9:P:506:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/315 (72%)	200 (88%)	24 (11%)	3 (1%)	12	30
1	B	227/315 (72%)	195 (86%)	29 (13%)	3 (1%)	12	30
1	K	227/315 (72%)	201 (88%)	22 (10%)	4 (2%)	8	21
1	L	227/315 (72%)	199 (88%)	25 (11%)	3 (1%)	12	30
2	C	1117/1119 (100%)	905 (81%)	154 (14%)	58 (5%)	2	3
2	M	1117/1119 (100%)	904 (81%)	153 (14%)	60 (5%)	2	3
3	D	1317/1524 (86%)	1098 (83%)	170 (13%)	49 (4%)	3	7
3	N	1317/1524 (86%)	1089 (83%)	176 (13%)	52 (4%)	3	6
4	E	93/99 (94%)	77 (83%)	12 (13%)	4 (4%)	2	5
4	O	93/99 (94%)	77 (83%)	10 (11%)	6 (6%)	1	2
5	F	341/423 (81%)	285 (84%)	37 (11%)	19 (6%)	2	3
5	P	341/423 (81%)	287 (84%)	36 (11%)	18 (5%)	2	3
All	All	6644/7590 (88%)	5517 (83%)	848 (13%)	279 (4%)	3	5

All (279) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
2	C	7	GLY
2	C	178	PRO
2	C	231	PRO
2	C	244	PRO
2	C	262	ALA
2	C	290	LEU
2	C	363	SER
2	C	369	PRO
2	C	465	GLY
2	C	517	ARG
2	C	548	PRO
2	C	598	GLU
2	C	627	ARG
2	C	767	PRO
2	C	864	GLY
2	C	908	GLY
2	C	1079	PRO
2	C	1106	ASP
3	D	55	ASP
3	D	82	LYS

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Mol	Chain	Res	Type
3	D	136	ASP
3	D	199	LEU
3	D	610	LYS
3	D	822	ALA
3	D	1129	THR
3	D	1208	ASP
3	D	1243	THR
3	D	1441	GLN
4	E	42	PRO
4	E	58	PRO
5	F	76	SER
5	F	95	THR
5	F	147	LEU
5	F	232	ARG
5	F	325	LYS
5	F	390	PHE
1	K	29	GLU
1	L	29	GLU
2	M	7	GLY
2	M	178	PRO
2	M	231	PRO
2	M	244	PRO
2	M	262	ALA
2	M	290	LEU
2	M	369	PRO
2	M	465	GLY
2	M	548	PRO
2	M	598	GLU
2	M	627	ARG
2	M	767	PRO
2	M	864	GLY
2	M	908	GLY
2	M	1079	PRO
2	M	1106	ASP
3	N	55	ASP
3	N	82	LYS
3	N	136	ASP
3	N	199	LEU
3	N	705	ALA
3	N	822	ALA
3	N	1129	THR
3	N	1208	ASP

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Mol	Chain	Res	Type
3	N	1243	THR
4	O	42	PRO
4	O	58	PRO
5	P	76	SER
5	P	95	THR
5	P	147	LEU
5	P	232	ARG
5	P	325	LYS
5	P	390	PHE
1	A	187	GLY
1	B	187	GLY
2	C	59	LYS
2	C	156	GLY
2	C	251	ASP
2	C	282	GLY
2	C	626	ARG
2	C	680	ASP
2	C	738	ASP
2	C	777	ILE
2	C	807	ARG
2	C	809	GLY
2	C	811	PRO
2	C	1004	LYS
3	D	24	GLY
3	D	98	PRO
3	D	137	PRO
3	D	504	ASP
3	D	588	GLY
3	D	616	GLN
3	D	705	ALA
3	D	803	GLY
3	D	1064	GLY
3	D	1196	THR
3	D	1265	ALA
4	E	4	PRO
5	F	153	PRO
5	F	255	ALA
5	F	416	ARG
1	K	187	GLY
1	L	187	GLY
2	M	59	LYS
2	M	156	GLY

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Mol	Chain	Res	Type
2	M	251	ASP
2	M	282	GLY
2	M	363	SER
2	M	517	ARG
2	M	626	ARG
2	M	680	ASP
2	M	738	ASP
2	M	777	ILE
2	M	807	ARG
2	M	809	GLY
2	M	811	PRO
2	M	1004	LYS
3	N	24	GLY
3	N	137	PRO
3	N	504	ASP
3	N	588	GLY
3	N	803	GLY
3	N	1064	GLY
3	N	1125	PRO
3	N	1197	ARG
3	N	1265	ALA
3	N	1342	GLU
3	N	1441	GLN
4	O	4	PRO
5	P	153	PRO
5	P	255	ALA
5	P	416	ARG
2	C	40	GLU
2	C	74	GLY
2	C	164	PRO
2	C	727	PRO
2	C	812	GLY
2	C	874	LEU
2	C	911	GLU
3	D	31	THR
3	D	47	GLU
3	D	96	ALA
3	D	119	SER
3	D	592	THR
3	D	594	PRO
3	D	807	ALA
3	D	844	ALA

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Mol	Chain	Res	Type
3	D	1125	PRO
3	D	1197	ARG
3	D	1241	PHE
3	D	1388	ARG
4	E	82	GLU
5	F	167	PRO
5	F	203	THR
5	F	286	PRO
5	F	297	PRO
5	F	341	PRO
5	F	393	THR
2	M	40	GLU
2	M	74	GLY
2	M	164	PRO
2	M	699	PHE
2	M	727	PRO
2	M	911	GLU
2	M	1045	ALA
3	N	31	THR
3	N	96	ALA
3	N	98	PRO
3	N	119	SER
3	N	592	THR
3	N	594	PRO
3	N	807	ALA
3	N	844	ALA
3	N	1111	ASP
3	N	1196	THR
3	N	1241	PHE
3	N	1388	ARG
4	O	82	GLU
5	P	167	PRO
5	P	203	THR
5	P	286	PRO
5	P	297	PRO
5	P	364	ARG
5	P	393	THR
1	A	26	GLU
2	C	111	ASP
2	C	170	PRO
2	C	250	ARG
2	C	699	PHE

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Mol	Chain	Res	Type
2	C	1045	ALA
3	D	484	PRO
3	D	1111	ASP
3	D	1432	LYS
5	F	421	PHE
2	M	111	ASP
2	M	170	PRO
2	M	188	LYS
2	M	250	ARG
2	M	268	ASP
2	M	812	GLY
3	N	484	PRO
3	N	526	PRO
3	N	617	ASN
3	N	892	ASP
3	N	1066	THR
3	N	1341	PRO
3	N	1432	LYS
5	P	421	PHE
2	C	53	PRO
2	C	188	LYS
2	C	268	ASP
2	C	400	PRO
2	C	1113	GLU
3	D	173	PRO
3	D	483	HIS
3	D	522	PRO
3	D	530	VAL
3	D	533	GLY
3	D	808	THR
3	D	892	ASP
3	D	1306	PRO
5	F	138	SER
1	K	26	GLU
2	M	10	ARG
2	M	53	PRO
2	M	90	TYR
2	M	292	ARG
2	M	984	GLU
2	M	1113	GLU
3	N	47	GLU
3	N	173	PRO

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Mol	Chain	Res	Type
3	N	483	HIS
3	N	522	PRO
3	N	766	ALA
3	N	808	THR
3	N	1306	PRO
5	P	341	PRO
2	C	10	ARG
2	C	90	TYR
2	C	180	GLY
2	C	377	PRO
2	C	1059	ASP
5	F	293	GLU
5	F	375	LEU
2	M	180	GLY
2	M	377	PRO
2	M	874	LEU
2	M	1005	MET
3	N	530	VAL
3	N	787	LEU
5	P	138	SER
2	C	336	VAL
3	D	526	PRO
3	D	1385	GLY
3	N	1385	GLY
2	C	264	PRO
2	C	415	PRO
1	K	9	PRO
2	M	261	ILE
2	M	336	VAL
2	M	415	PRO
2	M	505	GLY
3	N	1248	GLY
2	C	261	ILE
2	C	505	GLY
3	D	1248	GLY
1	L	9	PRO
2	M	264	PRO
2	M	529	VAL
3	N	1349	VAL
2	C	450	GLY
3	D	108	VAL
3	D	1267	ARG

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Mol	Chain	Res	Type
2	M	905	ILE
3	N	108	VAL
4	O	5	GLY
4	O	57	ASP
1	B	9	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/273 (74%)	161 (80%)	41 (20%)	1	3
1	B	202/273 (74%)	163 (81%)	39 (19%)	1	3
1	K	202/273 (74%)	159 (79%)	43 (21%)	1	3
1	L	202/273 (74%)	166 (82%)	36 (18%)	2	4
2	C	941/941 (100%)	755 (80%)	186 (20%)	1	3
2	M	941/941 (100%)	757 (80%)	184 (20%)	1	3
3	D	1112/1279 (87%)	935 (84%)	177 (16%)	2	6
3	N	1112/1279 (87%)	934 (84%)	178 (16%)	2	6
4	E	84/88 (96%)	68 (81%)	16 (19%)	1	4
4	O	84/88 (96%)	68 (81%)	16 (19%)	1	4
5	F	295/370 (80%)	252 (85%)	43 (15%)	3	7
5	P	295/370 (80%)	254 (86%)	41 (14%)	3	8
All	All	5672/6448 (88%)	4672 (82%)	1000 (18%)	2	4

All (1000) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	9	PRO
1	A	12	THR
1	A	15	THR
1	A	16	GLN

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Mol	Chain	Res	Type
1	A	20	TYR
1	A	44	LEU
1	A	45	LEU
1	A	47	SER
1	A	67	THR
1	A	73	GLU
1	A	74	ASP
1	A	77	GLU
1	A	84	GLU
1	A	88	ARG
1	A	89	PHE
1	A	92	PRO
1	A	96	THR
1	A	101	LEU
1	A	115	LEU
1	A	120	VAL
1	A	121	GLU
1	A	127	LEU
1	A	133	GLU
1	A	142	VAL
1	A	145	ASP
1	A	154	GLU
1	A	167	VAL
1	A	170	VAL
1	A	180	GLN
1	A	184	THR
1	A	190	THR
1	A	196	THR
1	A	197	LEU
1	A	198	ARG
1	A	205	VAL
1	A	211	LEU
1	A	216	GLU
1	A	223	THR
1	A	227	ASN
1	A	229	GLN
1	B	1	MET
1	B	3	ASP
1	B	25	LEU
1	B	26	GLU
1	B	27	PRO
1	B	38	ASN

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Mol	Chain	Res	Type
1	B	47	SER
1	B	62	LEU
1	B	67	THR
1	B	69	PRO
1	B	73	GLU
1	B	74	ASP
1	B	77	GLU
1	B	82	LEU
1	B	89	PHE
1	B	96	THR
1	B	112	ARG
1	B	119	ASP
1	B	123	MET
1	B	124	ASN
1	B	126	ASP
1	B	137	ARG
1	B	140	MET
1	B	154	GLU
1	B	162	ILE
1	B	170	VAL
1	B	184	THR
1	B	188	GLN
1	B	190	THR
1	B	192	LEU
1	B	196	THR
1	B	197	LEU
1	B	200	TRP
1	B	206	THR
1	B	208	LEU
1	B	209	GLU
1	B	213	GLN
1	B	220	GLU
1	B	227	ASN
2	C	6	PHE
2	C	11	GLU
2	C	15	LEU
2	C	24	GLU
2	C	26	TYR
2	C	30	LEU
2	C	34	VAL
2	C	35	PRO
2	C	36	PRO

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Mol	Chain	Res	Type
2	C	37	GLU
2	C	41	ASN
2	C	44	ILE
2	C	48	PHE
2	C	52	PHE
2	C	58	ASP
2	C	73	LEU
2	C	81	ASP
2	C	89	THR
2	C	94	LEU
2	C	95	TYR
2	C	98	LEU
2	C	100	LEU
2	C	104	ASP
2	C	108	ILE
2	C	112	GLU
2	C	114	PHE
2	C	115	LEU
2	C	117	HIS
2	C	129	ILE
2	C	133	ASP
2	C	140	ILE
2	C	141	HIS
2	C	149	THR
2	C	151	ASP
2	C	158	TYR
2	C	163	ILE
2	C	178	PRO
2	C	182	VAL
2	C	186	VAL
2	C	194	VAL
2	C	196	LEU
2	C	205	GLU
2	C	209	ARG
2	C	221	LEU
2	C	223	ASP
2	C	229	MET
2	C	238	LEU
2	C	239	PHE
2	C	241	LEU
2	C	254	VAL
2	C	257	VAL

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Mol	Chain	Res	Type
2	C	260	LEU
2	C	264	PRO
2	C	267	TYR
2	C	275	TYR
2	C	279	GLU
2	C	281	LEU
2	C	285	LEU
2	C	286	SER
2	C	297	GLU
2	C	303	PHE
2	C	304	LEU
2	C	309	TYR
2	C	321	GLU
2	C	332	ARG
2	C	339	LEU
2	C	343	GLN
2	C	359	MET
2	C	360	LEU
2	C	365	ASP
2	C	366	SER
2	C	367	LEU
2	C	392	SER
2	C	393	GLN
2	C	394	PHE
2	C	396	ASP
2	C	398	THR
2	C	402	SER
2	C	413	LEU
2	C	415	PRO
2	C	420	ARG
2	C	425	PHE
2	C	426	ASP
2	C	427	VAL
2	C	443	THR
2	C	448	ASN
2	C	451	LEU
2	C	452	ILE
2	C	454	SER
2	C	463	GLU
2	C	469	THR
2	C	479	VAL
2	C	486	MET

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Mol	Chain	Res	Type
2	C	508	ILE
2	C	516	ARG
2	C	528	GLU
2	C	533	ASP
2	C	542	VAL
2	C	543	ASN
2	C	557	ARG
2	C	559	LEU
2	C	564	MET
2	C	566	THR
2	C	578	VAL
2	C	583	LEU
2	C	584	GLU
2	C	605	LYS
2	C	607	ASP
2	C	614	ARG
2	C	619	ARG
2	C	633	GLN
2	C	645	VAL
2	C	657	ASP
2	C	661	SER
2	C	663	ASN
2	C	668	LEU
2	C	671	ASN
2	C	672	VAL
2	C	674	VAL
2	C	679	PHE
2	C	685	GLU
2	C	690	ILE
2	C	693	GLU
2	C	698	ASP
2	C	699	PHE
2	C	701	THR
2	C	725	ASP
2	C	727	PRO
2	C	729	LEU
2	C	734	LEU
2	C	737	LEU
2	C	758	ARG
2	C	760	SER
2	C	765	SER
2	C	769	PRO

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Mol	Chain	Res	Type
2	C	775	ARG
2	C	780	GLU
2	C	785	VAL
2	C	799	ILE
2	C	821	GLU
2	C	839	LEU
2	C	841	ASN
2	C	853	LEU
2	C	861	LEU
2	C	862	PRO
2	C	863	ASP
2	C	868	ASP
2	C	870	ILE
2	C	881	ASN
2	C	890	LEU
2	C	901	TYR
2	C	904	PRO
2	C	905	ILE
2	C	907	ASP
2	C	916	GLU
2	C	923	GLU
2	C	925	TYR
2	C	937	ASP
2	C	950	LEU
2	C	953	VAL
2	C	959	PRO
2	C	971	LYS
2	C	981	GLU
2	C	984	GLU
2	C	995	MET
2	C	1002	GLU
2	C	1016	ILE
2	C	1017	THR
2	C	1018	GLN
2	C	1030	GLN
2	C	1034	GLU
2	C	1035	MET
2	C	1036	GLU
2	C	1054	THR
2	C	1060	ILE
2	C	1079	PRO
2	C	1087	VAL

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Mol	Chain	Res	Type
2	C	1092	LEU
2	C	1095	LEU
2	C	1098	ASP
2	C	1100	GLN
2	C	1109	VAL
2	C	1110	ASP
2	C	1117	SER
2	C	1118	LYS
2	C	1119	ARG
3	D	12	LEU
3	D	14	SER
3	D	15	PRO
3	D	32	ILE
3	D	40	GLU
3	D	56	TYR
3	D	80	VAL
3	D	85	VAL
3	D	101	HIS
3	D	102	ILE
3	D	112	ILE
3	D	115	LEU
3	D	116	LEU
3	D	117	ASP
3	D	128	TYR
3	D	133	ILE
3	D	135	LEU
3	D	136	ASP
3	D	141	ILE
3	D	145	VAL
3	D	153	LEU
3	D	155	ASP
3	D	160	GLU
3	D	166	GLN
3	D	171	LEU
3	D	187	LYS
3	D	189	GLN
3	D	190	GLU
3	D	197	SER
3	D	205	TYR
3	D	394	LEU
3	D	400	VAL
3	D	402	PRO

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Mol	Chain	Res	Type
3	D	405	ASP
3	D	406	ASP
3	D	438	ASP
3	D	456	MET
3	D	465	LEU
3	D	489	ARG
3	D	493	ARG
3	D	504	ASP
3	D	505	SER
3	D	508	ARG
3	D	521	PRO
3	D	554	LEU
3	D	565	ILE
3	D	569	ASN
3	D	573	MET
3	D	581	LEU
3	D	591	VAL
3	D	594	PRO
3	D	605	ASP
3	D	608	SER
3	D	615	ARG
3	D	617	ASN
3	D	619	LEU
3	D	624	ASP
3	D	625	TYR
3	D	636	GLN
3	D	641	GLN
3	D	660	LYS
3	D	695	ILE
3	D	704	ARG
3	D	719	VAL
3	D	724	GLN
3	D	726	ILE
3	D	736	PHE
3	D	739	ASP
3	D	741	ASP
3	D	749	VAL
3	D	754	PHE
3	D	756	GLN
3	D	781	PRO
3	D	783	ARG
3	D	792	ILE

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Mol	Chain	Res	Type
3	D	810	GLU
3	D	824	ASN
3	D	832	ARG
3	D	839	LEU
3	D	845	ASN
3	D	847	ASP
3	D	861	GLN
3	D	863	VAL
3	D	864	VAL
3	D	865	THR
3	D	868	TYR
3	D	876	SER
3	D	880	ILE
3	D	888	GLU
3	D	892	ASP
3	D	899	LEU
3	D	901	GLN
3	D	914	LEU
3	D	915	VAL
3	D	942	SER
3	D	944	THR
3	D	948	THR
3	D	951	ILE
3	D	958	GLU
3	D	959	GLU
3	D	968	ASP
3	D	972	LEU
3	D	975	GLU
3	D	984	THR
3	D	985	ASP
3	D	999	THR
3	D	1001	GLU
3	D	1003	VAL
3	D	1023	MET
3	D	1025	GLN
3	D	1032	PRO
3	D	1033	GLN
3	D	1038	LEU
3	D	1041	LEU
3	D	1051	GLU
3	D	1052	THR
3	D	1065	LEU

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Mol	Chain	Res	Type
3	D	1068	LEU
3	D	1074	SER
3	D	1083	ASP
3	D	1090	ASP
3	D	1093	TYR
3	D	1095	THR
3	D	1109	GLU
3	D	1111	ASP
3	D	1112	CYS
3	D	1115	THR
3	D	1116	ASN
3	D	1129	THR
3	D	1132	LEU
3	D	1134	LEU
3	D	1151	ARG
3	D	1166	LEU
3	D	1173	LEU
3	D	1183	ILE
3	D	1198	TYR
3	D	1207	TYR
3	D	1228	SER
3	D	1234	THR
3	D	1243	THR
3	D	1251	ASP
3	D	1252	ILE
3	D	1258	ARG
3	D	1260	ILE
3	D	1274	ILE
3	D	1280	VAL
3	D	1290	LEU
3	D	1299	PHE
3	D	1302	GLU
3	D	1305	LEU
3	D	1315	ASP
3	D	1320	GLU
3	D	1344	VAL
3	D	1345	GLU
3	D	1348	LEU
3	D	1359	GLN
3	D	1363	LEU
3	D	1382	THR
3	D	1383	ASP

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Mol	Chain	Res	Type
3	D	1387	SER
3	D	1407	LEU
3	D	1415	VAL
3	D	1420	LEU
3	D	1431	THR
3	D	1433	SER
3	D	1439	SER
3	D	1440	PHE
3	D	1441	GLN
3	D	1460	ILE
3	D	1465	ASN
3	D	1466	VAL
3	D	1468	LEU
3	D	1478	SER
3	D	1485	GLN
3	D	1488	ASP
3	D	1491	THR
3	D	1496	GLU
4	E	4	PRO
4	E	20	THR
4	E	30	LEU
4	E	41	GLU
4	E	42	PRO
4	E	43	GLU
4	E	46	PRO
4	E	51	LEU
4	E	56	ASP
4	E	57	ASP
4	E	62	THR
4	E	67	GLU
4	E	72	ARG
4	E	79	LEU
4	E	81	PRO
4	E	94	PRO
5	F	79	ASP
5	F	83	GLN
5	F	84	TYR
5	F	86	HIS
5	F	91	VAL
5	F	94	LEU
5	F	117	SER
5	F	122	LEU

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Mol	Chain	Res	Type
5	F	123	ASP
5	F	125	ASP
5	F	127	ILE
5	F	135	ILE
5	F	145	PRO
5	F	149	GLU
5	F	150	THR
5	F	169	GLU
5	F	174	LEU
5	F	178	ARG
5	F	192	LEU
5	F	194	LEU
5	F	225	GLU
5	F	240	THR
5	F	245	GLN
5	F	249	ARG
5	F	262	VAL
5	F	281	GLU
5	F	282	LEU
5	F	291	ILE
5	F	297	PRO
5	F	317	LEU
5	F	335	ASP
5	F	336	GLU
5	F	341	PRO
5	F	348	SER
5	F	351	SER
5	F	353	GLU
5	F	362	SER
5	F	372	ARG
5	F	393	THR
5	F	399	GLN
5	F	408	LEU
5	F	410	TYR
5	F	420	ASP
1	K	3	ASP
1	K	9	PRO
1	K	12	THR
1	K	15	THR
1	K	16	GLN
1	K	20	TYR
1	K	44	LEU

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Mol	Chain	Res	Type
1	K	45	LEU
1	K	47	SER
1	K	67	THR
1	K	73	GLU
1	K	74	ASP
1	K	80	LEU
1	K	82	LEU
1	K	84	GLU
1	K	86	VAL
1	K	88	ARG
1	K	89	PHE
1	K	92	PRO
1	K	96	THR
1	K	101	LEU
1	K	115	LEU
1	K	120	VAL
1	K	121	GLU
1	K	127	LEU
1	K	133	GLU
1	K	142	VAL
1	K	154	GLU
1	K	167	VAL
1	K	170	VAL
1	K	180	GLN
1	K	184	THR
1	K	190	THR
1	K	196	THR
1	K	197	LEU
1	K	198	ARG
1	K	206	THR
1	K	211	LEU
1	K	216	GLU
1	K	222	LEU
1	K	223	THR
1	K	227	ASN
1	K	229	GLN
1	L	1	MET
1	L	9	PRO
1	L	25	LEU
1	L	26	GLU
1	L	27	PRO
1	L	38	ASN

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Mol	Chain	Res	Type
1	L	62	LEU
1	L	67	THR
1	L	69	PRO
1	L	73	GLU
1	L	74	ASP
1	L	77	GLU
1	L	89	PHE
1	L	96	THR
1	L	112	ARG
1	L	119	ASP
1	L	124	ASN
1	L	126	ASP
1	L	137	ARG
1	L	140	MET
1	L	154	GLU
1	L	162	ILE
1	L	173	PRO
1	L	184	THR
1	L	188	GLN
1	L	190	THR
1	L	192	LEU
1	L	193	ASP
1	L	196	THR
1	L	197	LEU
1	L	200	TRP
1	L	206	THR
1	L	207	PRO
1	L	208	LEU
1	L	209	GLU
1	L	227	ASN
2	M	11	GLU
2	M	24	GLU
2	M	26	TYR
2	M	30	LEU
2	M	34	VAL
2	M	35	PRO
2	M	37	GLU
2	M	41	ASN
2	M	44	ILE
2	M	48	PHE
2	M	52	PHE
2	M	73	LEU

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Mol	Chain	Res	Type
2	M	79	PRO
2	M	81	ASP
2	M	89	THR
2	M	94	LEU
2	M	95	TYR
2	M	98	LEU
2	M	100	LEU
2	M	104	ASP
2	M	108	ILE
2	M	112	GLU
2	M	114	PHE
2	M	115	LEU
2	M	117	HIS
2	M	133	ASP
2	M	140	ILE
2	M	141	HIS
2	M	149	THR
2	M	150	PRO
2	M	151	ASP
2	M	158	TYR
2	M	163	ILE
2	M	182	VAL
2	M	186	VAL
2	M	191	PHE
2	M	194	VAL
2	M	205	GLU
2	M	209	ARG
2	M	219	GLN
2	M	221	LEU
2	M	222	MET
2	M	229	MET
2	M	235	LEU
2	M	238	LEU
2	M	239	PHE
2	M	241	LEU
2	M	254	VAL
2	M	256	TYR
2	M	257	VAL
2	M	260	LEU
2	M	264	PRO
2	M	267	TYR
2	M	275	TYR

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Mol	Chain	Res	Type
2	M	279	GLU
2	M	281	LEU
2	M	285	LEU
2	M	286	SER
2	M	290	LEU
2	M	297	GLU
2	M	303	PHE
2	M	304	LEU
2	M	309	TYR
2	M	321	GLU
2	M	332	ARG
2	M	339	LEU
2	M	343	GLN
2	M	359	MET
2	M	360	LEU
2	M	365	ASP
2	M	366	SER
2	M	367	LEU
2	M	384	GLU
2	M	392	SER
2	M	393	GLN
2	M	394	PHE
2	M	396	ASP
2	M	402	SER
2	M	413	LEU
2	M	415	PRO
2	M	420	ARG
2	M	425	PHE
2	M	426	ASP
2	M	427	VAL
2	M	443	THR
2	M	448	ASN
2	M	451	LEU
2	M	452	ILE
2	M	454	SER
2	M	463	GLU
2	M	469	THR
2	M	474	VAL
2	M	479	VAL
2	M	502	PRO
2	M	508	ILE
2	M	516	ARG

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Mol	Chain	Res	Type
2	M	524	VAL
2	M	527	GLU
2	M	528	GLU
2	M	533	ASP
2	M	537	LYS
2	M	542	VAL
2	M	543	ASN
2	M	559	LEU
2	M	564	MET
2	M	566	THR
2	M	583	LEU
2	M	588	VAL
2	M	605	LYS
2	M	607	ASP
2	M	614	ARG
2	M	619	ARG
2	M	633	GLN
2	M	645	VAL
2	M	657	ASP
2	M	661	SER
2	M	663	ASN
2	M	668	LEU
2	M	671	ASN
2	M	672	VAL
2	M	674	VAL
2	M	679	PHE
2	M	684	PHE
2	M	690	ILE
2	M	693	GLU
2	M	697	ARG
2	M	698	ASP
2	M	699	PHE
2	M	701	THR
2	M	725	ASP
2	M	727	PRO
2	M	729	LEU
2	M	734	LEU
2	M	737	LEU
2	M	758	ARG
2	M	760	SER
2	M	765	SER
2	M	775	ARG

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Mol	Chain	Res	Type
2	M	785	VAL
2	M	794	PRO
2	M	799	ILE
2	M	821	GLU
2	M	822	VAL
2	M	839	LEU
2	M	841	ASN
2	M	853	LEU
2	M	861	LEU
2	M	862	PRO
2	M	863	ASP
2	M	870	ILE
2	M	881	ASN
2	M	890	LEU
2	M	901	TYR
2	M	904	PRO
2	M	905	ILE
2	M	907	ASP
2	M	916	GLU
2	M	917	LEU
2	M	923	GLU
2	M	937	ASP
2	M	950	LEU
2	M	953	VAL
2	M	959	PRO
2	M	981	GLU
2	M	984	GLU
2	M	995	MET
2	M	1002	GLU
2	M	1016	ILE
2	M	1017	THR
2	M	1018	GLN
2	M	1030	GLN
2	M	1035	MET
2	M	1036	GLU
2	M	1054	THR
2	M	1060	ILE
2	M	1075	ASP
2	M	1079	PRO
2	M	1087	VAL
2	M	1092	LEU
2	M	1098	ASP

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Mol	Chain	Res	Type
2	M	1109	VAL
2	M	1110	ASP
2	M	1117	SER
2	M	1118	LYS
3	N	3	LYS
3	N	12	LEU
3	N	14	SER
3	N	15	PRO
3	N	20	SER
3	N	32	ILE
3	N	40	GLU
3	N	80	VAL
3	N	82	LYS
3	N	85	VAL
3	N	102	ILE
3	N	115	LEU
3	N	116	LEU
3	N	117	ASP
3	N	128	TYR
3	N	133	ILE
3	N	135	LEU
3	N	136	ASP
3	N	141	ILE
3	N	145	VAL
3	N	153	LEU
3	N	155	ASP
3	N	160	GLU
3	N	166	GLN
3	N	171	LEU
3	N	181	ASP
3	N	187	LYS
3	N	189	GLN
3	N	190	GLU
3	N	193	PRO
3	N	197	SER
3	N	205	TYR
3	N	394	LEU
3	N	400	VAL
3	N	402	PRO
3	N	405	ASP
3	N	406	ASP
3	N	431	VAL

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Mol	Chain	Res	Type
3	N	438	ASP
3	N	449	SER
3	N	456	MET
3	N	461	ILE
3	N	465	LEU
3	N	489	ARG
3	N	493	ARG
3	N	504	ASP
3	N	505	SER
3	N	521	PRO
3	N	565	ILE
3	N	569	ASN
3	N	581	LEU
3	N	590	PRO
3	N	591	VAL
3	N	594	PRO
3	N	605	ASP
3	N	614	PHE
3	N	615	ARG
3	N	617	ASN
3	N	619	LEU
3	N	624	ASP
3	N	636	GLN
3	N	639	LEU
3	N	641	GLN
3	N	642	CYS
3	N	660	LYS
3	N	682	ASP
3	N	688	TRP
3	N	704	ARG
3	N	719	VAL
3	N	724	GLN
3	N	726	ILE
3	N	736	PHE
3	N	739	ASP
3	N	741	ASP
3	N	749	VAL
3	N	754	PHE
3	N	781	PRO
3	N	783	ARG
3	N	792	ILE
3	N	810	GLU

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Mol	Chain	Res	Type
3	N	824	ASN
3	N	832	ARG
3	N	839	LEU
3	N	847	ASP
3	N	863	VAL
3	N	864	VAL
3	N	865	THR
3	N	880	ILE
3	N	888	GLU
3	N	892	ASP
3	N	899	LEU
3	N	901	GLN
3	N	910	SER
3	N	915	VAL
3	N	942	SER
3	N	944	THR
3	N	948	THR
3	N	951	ILE
3	N	958	GLU
3	N	959	GLU
3	N	968	ASP
3	N	972	LEU
3	N	975	GLU
3	N	985	ASP
3	N	1001	GLU
3	N	1003	VAL
3	N	1023	MET
3	N	1025	GLN
3	N	1032	PRO
3	N	1033	GLN
3	N	1038	LEU
3	N	1041	LEU
3	N	1051	GLU
3	N	1052	THR
3	N	1065	LEU
3	N	1068	LEU
3	N	1083	ASP
3	N	1090	ASP
3	N	1095	THR
3	N	1109	GLU
3	N	1112	CYS
3	N	1115	THR

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Mol	Chain	Res	Type
3	N	1116	ASN
3	N	1129	THR
3	N	1133	ARG
3	N	1134	LEU
3	N	1151	ARG
3	N	1166	LEU
3	N	1173	LEU
3	N	1183	ILE
3	N	1198	TYR
3	N	1207	TYR
3	N	1210	SER
3	N	1228	SER
3	N	1243	THR
3	N	1251	ASP
3	N	1252	ILE
3	N	1258	ARG
3	N	1260	ILE
3	N	1274	ILE
3	N	1280	VAL
3	N	1290	LEU
3	N	1299	PHE
3	N	1300	SER
3	N	1302	GLU
3	N	1305	LEU
3	N	1306	PRO
3	N	1311	LEU
3	N	1315	ASP
3	N	1320	GLU
3	N	1344	VAL
3	N	1345	GLU
3	N	1348	LEU
3	N	1350	GLU
3	N	1363	LEU
3	N	1382	THR
3	N	1383	ASP
3	N	1403	LEU
3	N	1407	LEU
3	N	1415	VAL
3	N	1419	PRO
3	N	1420	LEU
3	N	1424	VAL
3	N	1431	THR

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Mol	Chain	Res	Type
3	N	1433	SER
3	N	1440	PHE
3	N	1441	GLN
3	N	1460	ILE
3	N	1462	LEU
3	N	1465	ASN
3	N	1466	VAL
3	N	1468	LEU
3	N	1478	SER
3	N	1481	VAL
3	N	1485	GLN
3	N	1488	ASP
3	N	1491	THR
3	N	1496	GLU
4	O	4	PRO
4	O	15	SER
4	O	20	THR
4	O	30	LEU
4	O	41	GLU
4	O	42	PRO
4	O	43	GLU
4	O	46	PRO
4	O	51	LEU
4	O	56	ASP
4	O	57	ASP
4	O	62	THR
4	O	67	GLU
4	O	79	LEU
4	O	81	PRO
4	O	94	PRO
5	P	80	PRO
5	P	83	GLN
5	P	84	TYR
5	P	86	HIS
5	P	91	VAL
5	P	94	LEU
5	P	117	SER
5	P	122	LEU
5	P	123	ASP
5	P	125	ASP
5	P	127	ILE
5	P	135	ILE

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Mol	Chain	Res	Type
5	P	149	GLU
5	P	174	LEU
5	P	178	ARG
5	P	194	LEU
5	P	225	GLU
5	P	240	THR
5	P	245	GLN
5	P	249	ARG
5	P	259	ARG
5	P	261	PRO
5	P	262	VAL
5	P	281	GLU
5	P	282	LEU
5	P	297	PRO
5	P	317	LEU
5	P	335	ASP
5	P	336	GLU
5	P	338	LEU
5	P	341	PRO
5	P	342	VAL
5	P	348	SER
5	P	350	LEU
5	P	351	SER
5	P	353	GLU
5	P	362	SER
5	P	393	THR
5	P	408	LEU
5	P	410	TYR
5	P	420	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	63	HIS
1	A	81	ASN
1	A	124	ASN
1	A	139	ASN
1	A	156	HIS
1	A	180	GLN
1	A	221	HIS
1	A	227	ASN

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Mol	Chain	Res	Type
1	A	229	GLN
1	B	38	ASN
1	B	95	GLN
1	B	124	ASN
1	B	128	HIS
1	B	163	ASN
1	B	180	GLN
1	B	227	ASN
2	C	31	GLN
2	C	41	ASN
2	C	117	HIS
2	C	130	ASN
2	C	139	GLN
2	C	204	GLN
2	C	343	GLN
2	C	393	GLN
2	C	431	HIS
2	C	434	HIS
2	C	498	GLN
2	C	609	ASN
2	C	632	ASN
2	C	639	GLN
2	C	663	ASN
2	C	670	GLN
2	C	671	ASN
2	C	834	GLN
2	C	841	ASN
2	C	881	ASN
2	C	889	HIS
2	C	899	GLN
2	C	969	GLN
2	C	1018	GLN
2	C	1019	GLN
2	C	1047	HIS
2	C	1107	ASN
3	D	66	GLN
3	D	143	ASN
3	D	151	GLN
3	D	166	GLN
3	D	507	ASN
3	D	549	ASN
3	D	611	GLN

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Mol	Chain	Res	Type
3	D	727	GLN
3	D	756	GLN
3	D	816	HIS
3	D	824	ASN
3	D	861	GLN
3	D	1005	GLN
3	D	1025	GLN
3	D	1116	ASN
3	D	1195	GLN
3	D	1202	GLN
3	D	1323	GLN
3	D	1441	GLN
3	D	1465	ASN
3	D	1485	GLN
4	E	28	GLN
4	E	29	GLN
4	E	37	ASN
4	E	59	ASN
4	E	86	GLN
5	F	83	GLN
5	F	86	HIS
5	F	90	GLN
5	F	245	GLN
5	F	312	GLN
5	F	337	HIS
5	F	402	ASN
1	K	63	HIS
1	K	124	ASN
1	K	128	HIS
1	K	139	ASN
1	K	156	HIS
1	K	163	ASN
1	K	180	GLN
1	K	227	ASN
1	K	229	GLN
1	L	38	ASN
1	L	95	GLN
1	L	124	ASN
1	L	128	HIS
1	L	163	ASN
1	L	180	GLN
1	L	227	ASN

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Mol	Chain	Res	Type
2	M	22	GLN
2	M	31	GLN
2	M	41	ASN
2	M	117	HIS
2	M	130	ASN
2	M	139	GLN
2	M	204	GLN
2	M	343	GLN
2	M	374	ASN
2	M	393	GLN
2	M	431	HIS
2	M	434	HIS
2	M	498	GLN
2	M	609	ASN
2	M	632	ASN
2	M	639	GLN
2	M	663	ASN
2	M	670	GLN
2	M	671	ASN
2	M	834	GLN
2	M	841	ASN
2	M	881	ASN
2	M	889	HIS
2	M	969	GLN
2	M	1019	GLN
2	M	1100	GLN
3	N	143	ASN
3	N	151	GLN
3	N	166	GLN
3	N	507	ASN
3	N	549	ASN
3	N	611	GLN
3	N	640	HIS
3	N	696	HIS
3	N	703	ASN
3	N	709	HIS
3	N	727	GLN
3	N	744	GLN
3	N	756	GLN
3	N	768	ASN
3	N	824	ASN
3	N	861	GLN

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Mol	Chain	Res	Type
3	N	994	GLN
3	N	1025	GLN
3	N	1046	GLN
3	N	1116	ASN
3	N	1195	GLN
3	N	1202	GLN
3	N	1323	GLN
3	N	1333	HIS
3	N	1334	GLN
3	N	1359	GLN
3	N	1404	ASN
3	N	1465	ASN
3	N	1485	GLN
4	O	28	GLN
4	O	29	GLN
4	O	37	ASN
4	O	59	ASN
4	O	86	GLN
5	P	83	GLN
5	P	86	HIS
5	P	90	GLN
5	P	214	GLN
5	P	312	GLN
5	P	402	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	$\#\|Z\| > 2$
7	MXP	D	1527	-	30,30,30	2.35	13 (43%)	32,38,38	3.46	13 (40%)
7	MXP	N	1527	-	30,30,30	2.62	13 (43%)	32,38,38	3.63	14 (43%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MXP	D	1527	-	-	6/27/28/28	0/1/1/1
7	MXP	N	1527	-	-	7/27/28/28	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	1527	MXP	C9-C10	7.23	1.41	1.34
7	D	1527	MXP	C9-C10	6.34	1.40	1.34
7	N	1527	MXP	C1-C5	4.42	1.45	1.34
7	N	1527	MXP	C21-C20	4.32	1.38	1.32
7	D	1527	MXP	O6-C22	4.26	1.29	1.21
7	N	1527	MXP	O5-C22	-4.05	1.27	1.34
7	D	1527	MXP	C21-C20	3.96	1.38	1.32
7	D	1527	MXP	C9-C8	3.90	1.56	1.42
7	N	1527	MXP	C9-C8	3.82	1.56	1.42
7	N	1527	MXP	O2-C2	3.68	1.43	1.34
7	N	1527	MXP	O6-C22	3.52	1.28	1.21
7	D	1527	MXP	O5-C22	-3.38	1.28	1.34
7	N	1527	MXP	C8-C7	3.03	1.43	1.34
7	D	1527	MXP	O5-C23	-3.02	1.38	1.45
7	N	1527	MXP	C7-C6	3.02	1.55	1.48
7	D	1527	MXP	O1-C5	2.98	1.43	1.37
7	N	1527	MXP	O1-C5	2.97	1.43	1.37
7	D	1527	MXP	C1-C5	2.70	1.41	1.34
7	D	1527	MXP	C8-C7	2.65	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	1527	MXP	O5-C23	-2.63	1.39	1.45
7	N	1527	MXP	O1-C4	2.35	1.44	1.39
7	D	1527	MXP	C3-C6	2.28	1.59	1.46
7	D	1527	MXP	C7-C6	2.26	1.53	1.48
7	N	1527	MXP	C3-C6	2.15	1.58	1.46
7	D	1527	MXP	O2-C2	2.02	1.39	1.34
7	D	1527	MXP	C3-C2	2.02	1.45	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	1527	MXP	O4-C6-C7	10.94	138.42	121.07
7	D	1527	MXP	O4-C6-C7	10.20	137.24	121.07
7	D	1527	MXP	O1-C5-C17	7.10	119.05	111.05
7	N	1527	MXP	O1-C5-C1	-7.04	117.16	121.94
7	D	1527	MXP	C8-C9-C10	-6.76	116.93	127.30
7	N	1527	MXP	O1-C5-C17	6.58	118.46	111.05
7	N	1527	MXP	C8-C9-C10	-6.57	117.22	127.30
7	D	1527	MXP	C23-O5-C22	6.10	122.86	115.66
7	N	1527	MXP	C23-O5-C22	5.90	122.63	115.66
7	N	1527	MXP	O5-C22-N1	5.55	115.04	109.16
7	N	1527	MXP	C15-C7-C6	5.26	124.54	115.62
7	D	1527	MXP	O1-C5-C1	-5.15	118.44	121.94
7	D	1527	MXP	O5-C22-N1	5.12	114.59	109.16
7	D	1527	MXP	C15-C7-C6	4.84	123.84	115.62
7	N	1527	MXP	O6-C22-N1	-3.84	120.10	125.41
7	D	1527	MXP	O6-C22-N1	-3.71	120.27	125.41
7	D	1527	MXP	C4-C3-C6	3.20	127.17	115.67
7	N	1527	MXP	O2-C2-C3	-2.85	118.35	121.77
7	N	1527	MXP	C4-C3-C6	2.78	125.67	115.67
7	D	1527	MXP	O1-C4-C3	2.68	121.19	117.24
7	D	1527	MXP	O1-C4-O3	2.56	119.82	115.20
7	N	1527	MXP	O1-C4-C3	2.55	121.00	117.24
7	D	1527	MXP	O3-C4-C3	-2.42	118.99	126.60
7	D	1527	MXP	C12-C11-C10	2.29	119.46	113.45
7	N	1527	MXP	C12-C11-C10	2.27	119.42	113.45
7	N	1527	MXP	C4-O1-C5	-2.07	120.79	122.28
7	N	1527	MXP	C2-C3-C4	-2.02	116.85	118.43

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	1527	MXP	C10-C11-C12-C13
7	D	1527	MXP	C18-C17-C5-O1
7	N	1527	MXP	C18-C17-C5-O1
7	N	1527	MXP	C10-C11-C12-C13
7	D	1527	MXP	C18-C17-C5-C1
7	N	1527	MXP	C18-C17-C5-C1
7	N	1527	MXP	C18-C19-C20-C21
7	D	1527	MXP	C18-C19-C20-C21
7	D	1527	MXP	C16-C10-C11-C12
7	N	1527	MXP	C16-C10-C11-C12
7	N	1527	MXP	C9-C10-C11-C12
7	D	1527	MXP	C9-C10-C11-C12
7	N	1527	MXP	C5-C17-C18-C19

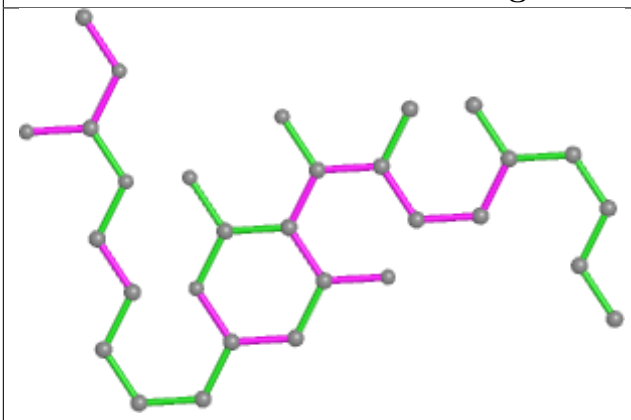
There are no ring outliers.

2 monomers are involved in 36 short contacts:

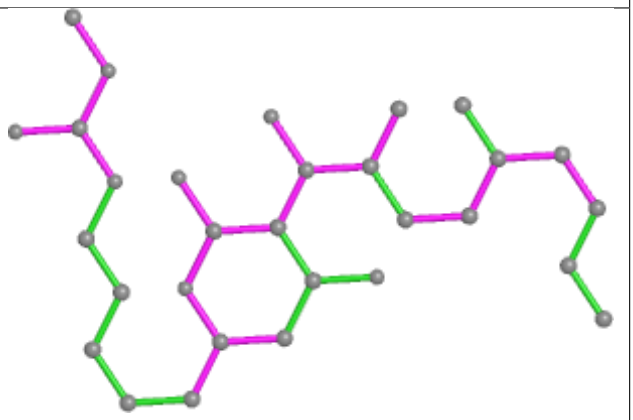
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1527	MXP	18	0
7	N	1527	MXP	18	0

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 then 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.

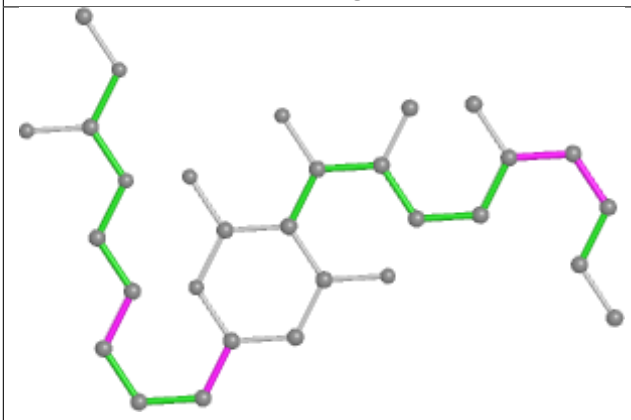
Ligand MXP D 1527



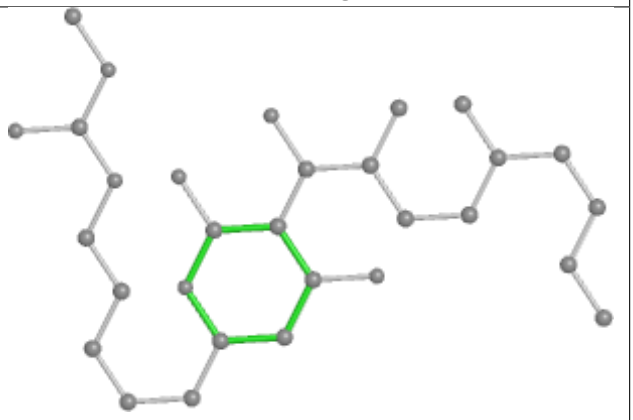
Bond lengths



Bond angles

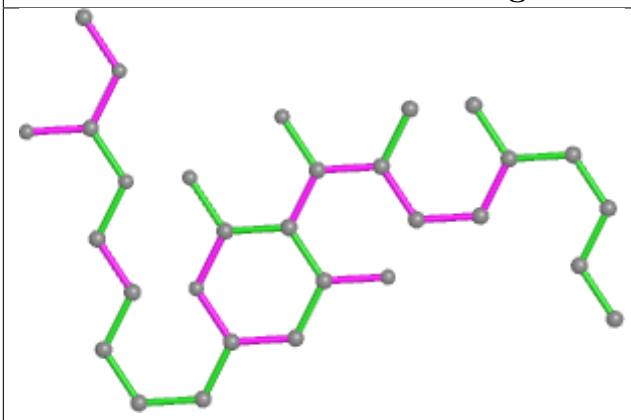


Torsions

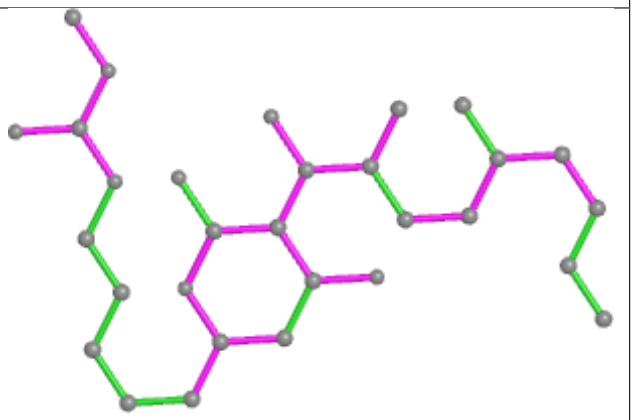


Rings

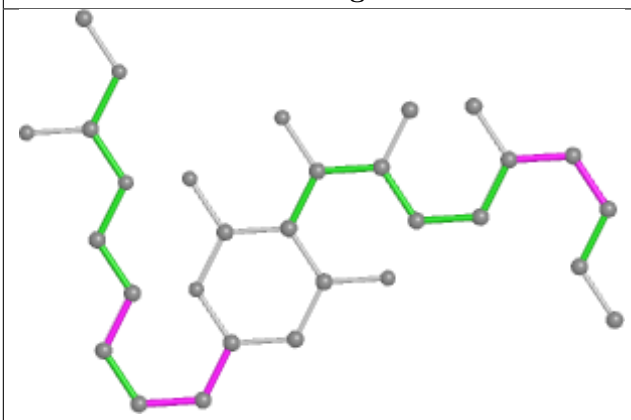
Ligand MXP N 1527



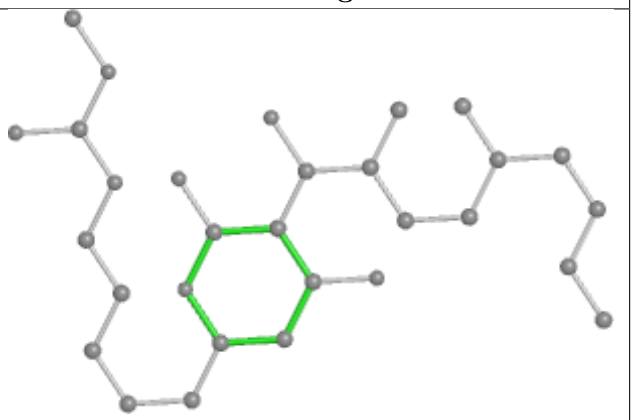
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.06	3 (1%)	77	78	28, 50, 78, 101	0
1	B	229/315 (72%)	-0.06	8 (3%)	44	44	36, 71, 86, 104	0
1	K	229/315 (72%)	-0.08	2 (0%)	84	85	25, 52, 81, 93	0
1	L	229/315 (72%)	-0.05	6 (2%)	56	57	47, 73, 86, 104	0
2	C	1119/1119 (100%)	-0.06	27 (2%)	59	60	14, 62, 88, 96	0
2	M	1119/1119 (100%)	-0.09	14 (1%)	77	78	11, 60, 86, 101	0
3	D	1321/1524 (86%)	-0.08	20 (1%)	73	76	10, 53, 85, 107	0
3	N	1321/1524 (86%)	-0.10	21 (1%)	72	74	11, 54, 84, 109	0
4	E	95/99 (95%)	-0.13	2 (2%)	63	65	30, 64, 90, 95	0
4	O	95/99 (95%)	-0.19	2 (2%)	63	65	29, 61, 83, 100	0
5	F	345/423 (81%)	-0.10	5 (1%)	75	77	27, 68, 89, 100	0
5	P	345/423 (81%)	-0.07	9 (2%)	56	57	23, 68, 91, 103	0
All	All	6676/7590 (87%)	-0.09	119 (1%)	68	70	10, 59, 87, 109	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1241	PHE	8.6
3	N	1240	THR	6.2
3	N	1243	THR	6.1
2	C	186	VAL	6.0
2	M	186	VAL	5.8
3	D	1240	THR	5.7
3	D	1248	GLY	4.8
3	D	407	VAL	4.5
5	P	145	PRO	4.4
2	C	207	LEU	4.4
5	P	90	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
2	C	307	LEU	4.2
3	N	1247	ALA	4.2
2	M	372	LEU	4.2
3	N	191	LEU	4.0
4	E	95	VAL	4.0
2	C	164	PRO	3.8
3	D	1245	GLY	3.8
1	L	1	MET	3.7
2	C	372	LEU	3.6
4	O	95	VAL	3.6
3	N	1398	TRP	3.6
2	M	418	LEU	3.6
3	N	1248	GLY	3.6
3	D	409	VAL	3.5
5	P	405	LEU	3.4
3	D	1398	TRP	3.4
3	D	1242	HIS	3.4
3	D	1246	VAL	3.4
3	N	802	ALA	3.4
3	D	1247	ALA	3.4
2	C	211	LEU	3.4
3	D	43	GLY	3.4
1	A	158	ILE	3.4
3	D	1243	THR	3.3
4	E	56	ASP	3.3
2	C	260	LEU	3.3
2	C	226	VAL	3.3
3	N	1238	MET	3.3
1	A	1	MET	3.2
3	N	1242	HIS	3.2
3	N	839	LEU	3.2
1	B	6	LEU	3.1
3	N	611	GLN	3.1
3	N	1246	VAL	3.1
5	P	88	ILE	3.1
2	C	306	THR	3.1
5	F	142	ARG	3.0
1	B	1	MET	3.0
1	K	5	LYS	2.9
1	K	6	LEU	2.8
2	M	615	TYR	2.8
2	M	269	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	N	1241	PHE	2.8
3	D	422	ALA	2.7
5	F	150	THR	2.7
1	L	2	LEU	2.7
3	N	203	ALA	2.7
1	B	71	VAL	2.7
1	B	138	LEU	2.6
2	C	208	ALA	2.5
5	P	354	LEU	2.5
2	C	65	VAL	2.5
2	M	417	GLY	2.4
3	N	119	SER	2.4
2	M	105	THR	2.4
2	C	333	ILE	2.4
3	D	395	VAL	2.4
2	M	207	LEU	2.4
3	N	816	HIS	2.4
3	D	801	GLY	2.4
3	N	450	TYR	2.4
2	C	170	PRO	2.4
1	L	82	LEU	2.3
2	C	475	VAL	2.3
2	C	529	VAL	2.3
1	B	117	VAL	2.3
2	C	303	PHE	2.3
1	B	5	LYS	2.3
1	A	93	SER	2.3
3	D	1249	ALA	2.3
5	P	369	LEU	2.3
4	O	94	PRO	2.3
2	M	307	LEU	2.3
1	B	68	ILE	2.3
2	C	726	ILE	2.3
3	D	802	ALA	2.3
2	C	417	GLY	2.2
3	D	1407	LEU	2.2
2	C	373	VAL	2.2
5	P	144	ILE	2.2
2	C	183	SER	2.2
5	F	90	GLN	2.2
5	P	357	ALA	2.2
5	F	397	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2	LEU	2.2
2	M	280	LYS	2.2
2	M	208	ALA	2.2
2	C	344	PHE	2.2
3	N	185	VAL	2.2
1	L	131	THR	2.2
1	L	5	LYS	2.1
3	D	1244	GLY	2.1
2	C	116	GLY	2.1
1	L	144	VAL	2.1
2	C	479	VAL	2.1
2	C	155	PRO	2.1
3	N	501	ALA	2.1
2	C	513	VAL	2.1
2	C	125	GLY	2.1
2	M	313	LEU	2.1
5	F	139	ALA	2.0
5	P	384	GLU	2.0
2	C	99	GLN	2.0
2	M	115	LEU	2.0
2	M	243	ARG	2.0
3	D	1401	GLU	2.0
3	N	806	PHE	2.0
3	N	489	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

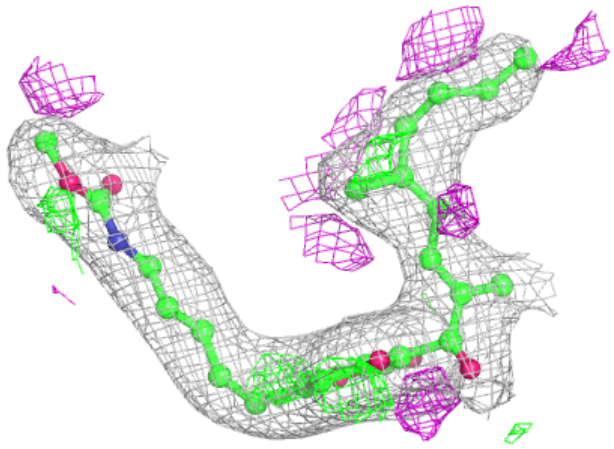
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

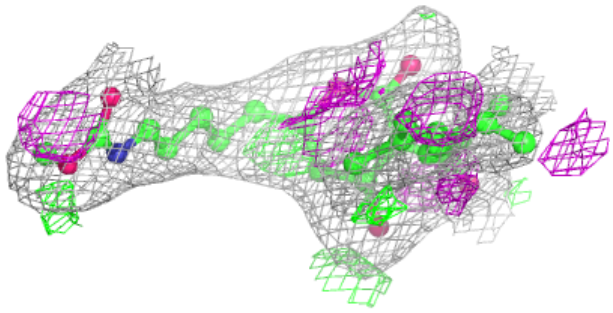
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MXP	D	1527	30/30	0.96	0.19	13,20,27,34	0
7	MXP	N	1527	30/30	0.96	0.17	17,30,38,40	0
6	ZN	D	1525	1/1	0.97	0.14	62,62,62,62	0
6	ZN	N	1526	1/1	0.97	0.18	66,66,66,66	0
8	MG	N	1528	1/1	0.97	0.07	41,41,41,41	0
8	MG	D	1528	1/1	0.98	0.09	35,35,35,35	0
6	ZN	N	1525	1/1	0.99	0.17	58,58,58,58	0
6	ZN	D	1526	1/1	0.99	0.21	48,48,48,48	0

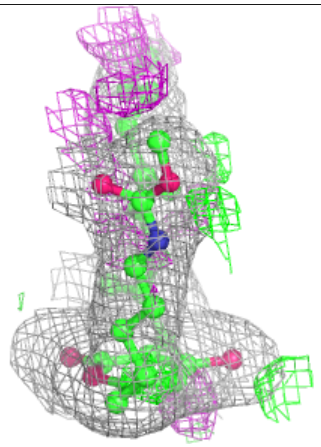
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MXP D 1527:

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

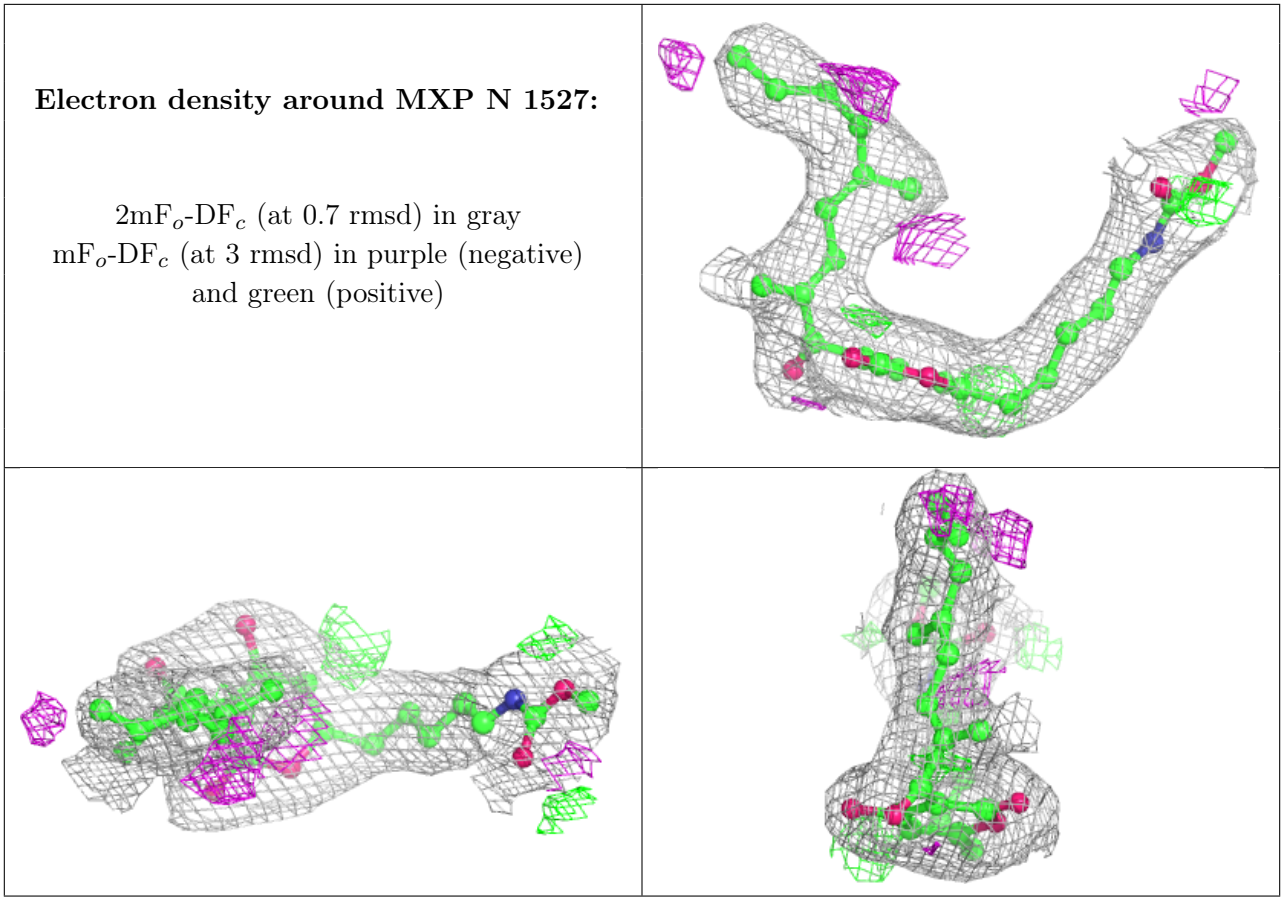






Electron density around MXP N 1527:

$2mF_o$-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

There are no such residues in this entry.