



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 08:52 PM EDT

PDB ID : 6TIW / pdb_00006tiw
EMDB ID : EMD-10421
Title : Human kinesin-5 motor domain in the GSK state bound to microtubules (Conformation 2)
Authors : Pena, A.; Sweeney, A.; Cook, A.D.; Moores, C.A.; Topf, M.
Deposited on : 2019-11-22
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

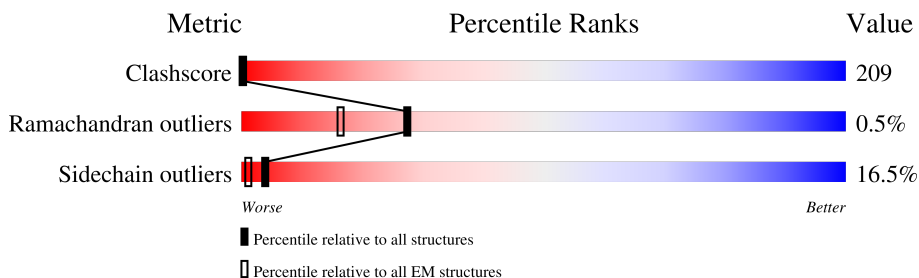
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	K	391	
2	B	429	
3	A	438	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MZK	K	501	-	-	X	-
5	G2P	A	501	-	-	X	-
5	G2P	B	501	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9491 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Kinesin-like protein KIF11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	334	Total	C	N	O	S	0	0
			2607	1630	466	501	10		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-21	MET	-	initiating methionine	UNP P52732
K	-20	HIS	-	expression tag	UNP P52732
K	-19	HIS	-	expression tag	UNP P52732
K	-18	HIS	-	expression tag	UNP P52732
K	-17	HIS	-	expression tag	UNP P52732
K	-16	HIS	-	expression tag	UNP P52732
K	-15	HIS	-	expression tag	UNP P52732
K	-14	SER	-	expression tag	UNP P52732
K	-13	SER	-	expression tag	UNP P52732
K	-12	GLY	-	expression tag	UNP P52732
K	-11	VAL	-	expression tag	UNP P52732
K	-10	ASP	-	expression tag	UNP P52732
K	-9	LEU	-	expression tag	UNP P52732
K	-8	GLY	-	expression tag	UNP P52732
K	-7	THR	-	expression tag	UNP P52732
K	-6	GLU	-	expression tag	UNP P52732
K	-5	ASN	-	expression tag	UNP P52732
K	-4	LEU	-	expression tag	UNP P52732
K	-3	TYR	-	expression tag	UNP P52732
K	-2	PHE	-	expression tag	UNP P52732
K	-1	GLN	-	expression tag	UNP P52732
K	0	SER	-	expression tag	UNP P52732

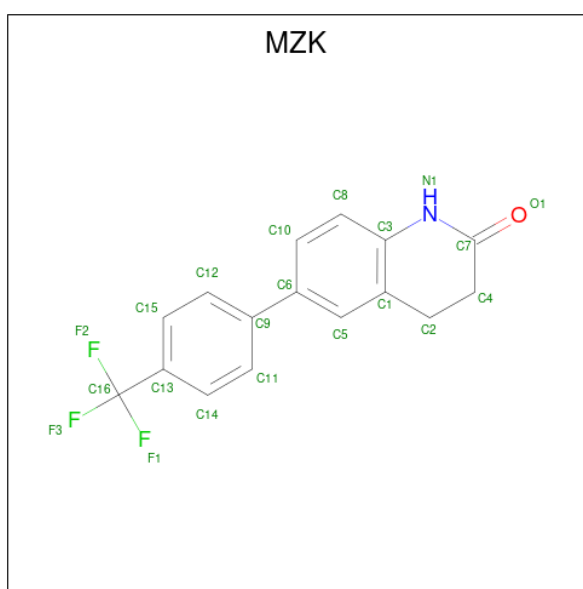
- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	429	Total	C	N	O	S	0	0
			3372	2117	578	651	26		

- Molecule 3 is a protein called Tubulin alpha-1B chain.

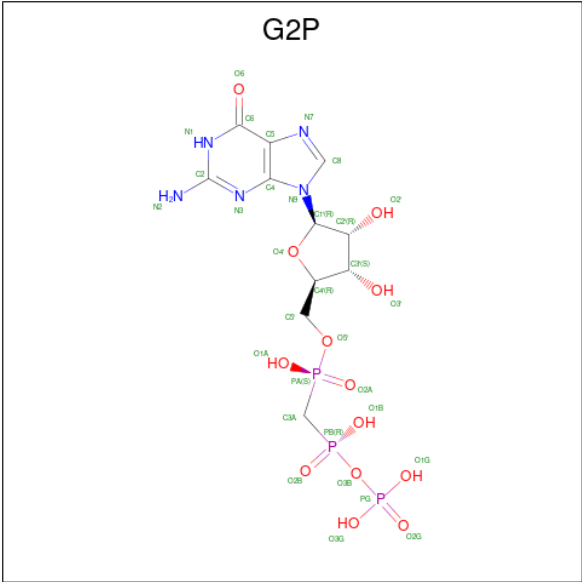
Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	438	Total	C	N	O	S	0	0
			3425	2167	582	654	22		

- Molecule 4 is 6-[4-(trifluoromethyl)phenyl]-3,4-dihydro-1 {H}-quinolin-2-one (CCD ID: MZK) (formula: C₁₆H₁₂F₃NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	K	1	Total	C	F	N	O	0
			21	16	3	1	1	

- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			32	11	5	13	3	
5	A	1	Total	C	N	O	P	0
			32	11	5	13	3	

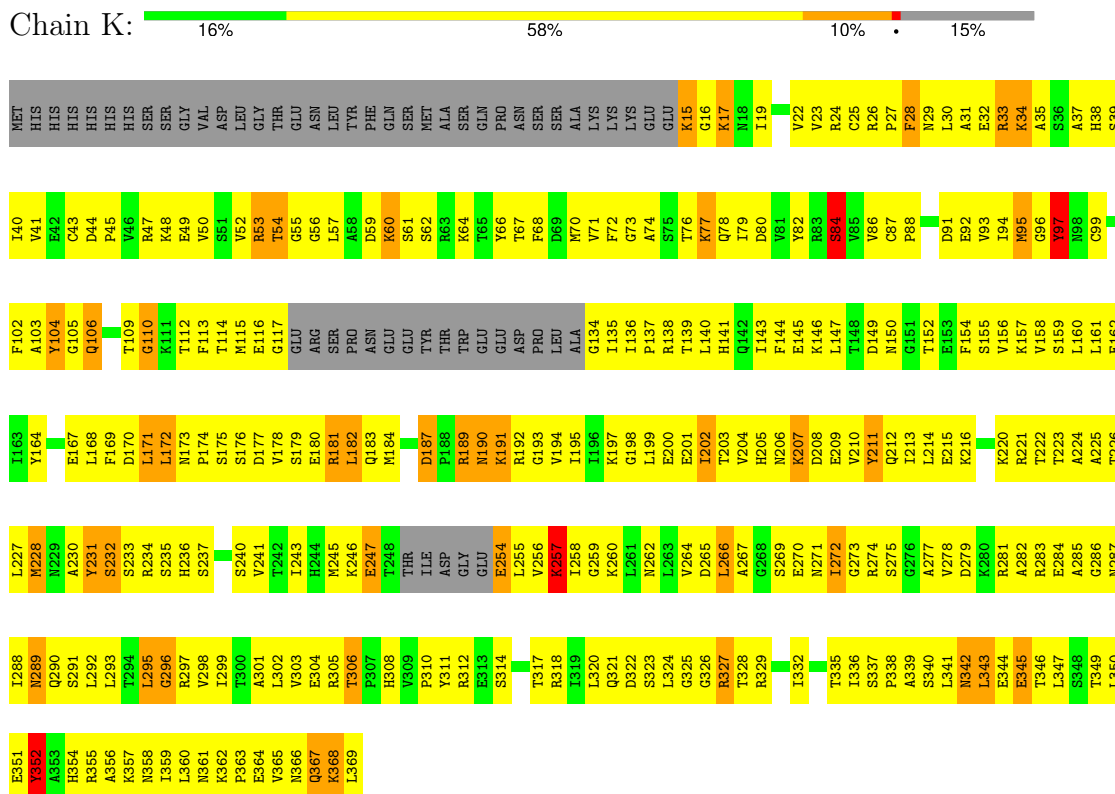
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	
6	A	1	Total	Mg	0
			1	1	

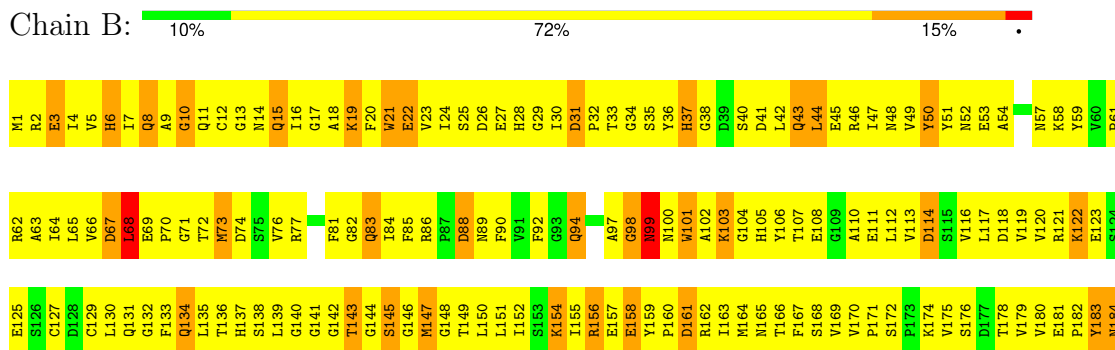
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Kinesin-like protein KIF11



• Molecule 2: Tubulin beta chain



A185	N247	H307	I368	A428
T186	A248	G308	G369	T429
L187	D249	R309	C370	
L250	L250	Y310	S371	
V189	L251	L311	T372	
H190	K252	T312	A373	
Q191	L253	V313	I374	
L192	A254	A314	Q375	
V193	V255	A315	E376	
E194	N256	V316	L377	
N195	M257	F317	F378	
T196	V258	R318	K379	
D197	P259	G319	R380	
E198	F260	R320	I381	
T199	P261	M321	S382	
Y200	R262	S322	E383	
C201	L263	M323	Q384	
I202	H264	F385	F386	
D203	F265	E325	T386	
N204	F266	V326	A387	
E205	M267	M388	N388	
A206	G268	E328	F389	
L207	P269	R329	R390	
F270	F270	M330	K391	
Y208	A271	L331	K392	
D209	P272		A393	
I210	L273	Q334	F394	
C211	T274	N335	L395	
R212	S275	K336	H396	
T214	R276	W397	W397	
L215	G277	S338	Y398	
K216	S278	S339	T399	
L217	Q279	G400	G400	
T218	Q280	E401	E401	
T219	Y281	F342	G402	
P220	R282	M403	M403	
T221	A283	W444	D404	
Y222	L284	E345	E405	
G223	T285	P346	M406	
D224	V286	K347	E407	
L225	P287	N348	F408	
N226	E288	V349	T409	
H227	L289	K350	E410	
L228	T290	T351	A411	
V229	Q291	A352	E412	
S230	Q292	V353	S413	
A231	M293	C354	N414	
T232	F294	D355	M415	
M233	D295	I356	M416	
S234	A296	P357	D417	
	K297	P358	L418	
	N298	R359	V419	
T238	M299	G360	S420	
C239	M300	E421	E421	
L240	A301	K362	Y422	
R241	F242	M363	Q423	
P243	C303	S364	Q424	
G244	D304	A365	Y425	
Q245	P305	T366	Q426	
L246	R306	F367	D427	

• Molecule 3: Tubulin alpha-1B chain

Chain A:  8% 75% 14%

M1	V62	I122	V182	L242	M302	V362	E423
R2	P63	R123	E183	R243	V303	V363	D424
E3	R64	E184	P184	F244	C304	P364	M425
C4	A65	L125	Y185	D245	C305	A426	A426
I5	V66	A126	G246	G246	D306	L367	L427
S6	F67	D127	N186	G247	P307	A368	L428
T7	V68	Q128	I188	L248	R308	A369	A429
H8	D69	C129	L189	N249	H309	K370	K430
V9	L70	T130	T190	V250	G310	V371	D431
G10	E71	G131	T191	D251	K311	Q372	Y432
Q11	P72	L132	H192	L252	K312	R373	E433
A12	T73	Q133	T193	T253	M313	A374	E434
G13	V74	G134	T194	E254	A314	V375	V435
V14	I75	F135	L195	F255	C315	C376	G436
Q15	D76	L136	E196	Q256	C316	M377	V437
I16	E77	L137	T257	T257	L317	L378	D438
G17	F78	F138	S198	N258	L318	S379	
N18	R79	R139	D199	L259	Y319	T381	N380
A19	T80	S140	C200	V260	R320	T382	T381
C20	G81	F141	A201	P261	G321	T383	T382
W21	T82	G142	F202	Y262	D322	A383	A383
L23	Y83	G143	M203	P263	V323	I384	I384
L23	R84	G144	V204	R264	V324	A385	A385
Y24	Q85	T145	D205	I265	P325	E386	E386
C25	L86	G146	N206	H266	K326	A387	A387
L26	F87	S147	E207	F267	D327	W388	W388
E27	H88	G148	A208	P268	V328	A389	A389
R28	F89	F149	L209	L269	N329	R390	R390
Q29	E90	T150	D210	A270	A330	L391	L391
Q30	Q91	S151	Y211	T271	A331	D392	D392
L31	L92	L152	T212	Y272	I332	H393	H393
P32	T93	L153	C213	A273	A333	K394	K394
D33	T94	M154	R214	P274	T334	F395	F395
G34	G95	E155	R215	V275	I335	D396	D396
Q35	K96	R156	N216	L276	K336	L397	L397
M36	E97	L157	D217	S277	T337	M398	M398
P37	D98	S158	D218	A278	K338	Y399	Y399
S38	S99	V159	I219	E279	R339	A400	A400
D39	A100	D160	E220	K280	S340	K401	K401
K40	N101	Y161	R221	A281	I341	R402	R402
T41	N102	Q162	P222	Y282	Q342	A403	A403
L42	Y103	K163	T223	H283	F343	F404	F404
	A104	K164	Y224	E284	V344	V405	V405
G45	E105	S165	T225	Q285	D345	H406	H406
D46	G106	K166	N226	L286	W346	W407	W407
D47	H107	L167	L227	S287	C347	Y408	Y408
S48	Y108	E168	N228	P288	P348	V409	V409
F49	T109	F169	R229	A289	T349	G410	G410
N50	T110	S170	L230	E290	G350	E411	E411
T51	G111	I171	I231	I291	F351	G412	G412
F52	K112	Y172	S232	T292	K352	M413	M413
F53	E113	F173	Q233	N293	V353	E414	E414
S54	T114	A174	I234	A294	G354	E415	E415
E55	T115	P175	V235	C295	I355	G416	G416
T56	D116	Q176	S236	F296	N356	E417	E417
Q57	L117	T177	S237	E297	Y357	F418	F418
A58	V118	S178	T338	P298	Q358	S419	S419
G59	L119	T179	T239	A299	P359	E420	E420
K60	D120	A180	A240	N300	R360	A421	A421
H61	R121	V181	S241	Q301	T361	R422	R422

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.7°, rise=8.9 Å, axial sym=C1	Depositor
Number of segments used	507219	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G2P, MG, MZK

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	K	1.68	13/2640 (0.5%)	1.27	18/3557 (0.5%)
2	B	1.20	5/3447 (0.1%)	1.57	40/4669 (0.9%)
3	A	1.23	12/3503 (0.3%)	1.41	41/4754 (0.9%)
All	All	1.36	30/9590 (0.3%)	1.44	99/12980 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	5
2	B	0	10
3	A	1	18
All	All	1	33

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	84	SER	CB-OG	-56.93	0.68	1.42
2	B	324	LYS	CE-NZ	25.12	2.11	1.49
1	K	254	GLU	CB-CG	-24.02	1.06	1.52
3	A	221	ARG	CB-CG	19.21	2.04	1.52
3	A	221	ARG	CG-CD	16.02	1.92	1.51
3	A	221	ARG	CA-CB	14.49	1.85	1.53
1	K	247	GLU	CB-CG	-13.94	1.25	1.52
2	B	324	LYS	CD-CE	13.73	1.85	1.51
1	K	247	GLU	CD-OE1	-11.45	1.13	1.25
1	K	257	LYS	CB-CG	-10.64	1.23	1.52
1	K	260	LYS	CG-CD	-9.29	1.20	1.52
3	A	221	ARG	C-N	8.93	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	409	VAL	CA-CB	-8.05	1.37	1.54
1	K	306	THR	C-O	-7.66	1.08	1.23
1	K	97	TYR	CE1-CZ	-7.65	1.28	1.38
3	A	221	ARG	CD-NE	-6.99	1.34	1.46
3	A	179	THR	CA-C	6.87	1.70	1.52
2	B	350	LYS	CD-CE	-6.74	1.34	1.51
3	A	404	PHE	N-CA	6.59	1.59	1.46
1	K	97	TYR	CE2-CZ	-6.52	1.30	1.38
2	B	260	PHE	CB-CG	-6.03	1.41	1.51
3	A	221	ARG	CZ-NH2	-6.00	1.25	1.33
1	K	352	TYR	CG-CD2	5.90	1.46	1.39
1	K	97	TYR	CG-CD2	5.89	1.46	1.39
3	A	406	HIS	CB-CG	-5.73	1.39	1.50
1	K	352	TYR	CB-CG	5.71	1.60	1.51
3	A	221	ARG	CA-C	5.58	1.67	1.52
1	K	254	GLU	CD-OE2	-5.46	1.19	1.25
2	B	252	LYS	CB-CG	-5.38	1.38	1.52
3	A	99	ALA	CA-C	-5.03	1.39	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	251	ARG	NE-CZ-NH2	35.87	138.24	120.30
2	B	251	ARG	NH1-CZ-NH2	-24.10	92.89	119.40
2	B	10	GLY	O-C-N	-19.90	90.86	122.70
3	A	403	ALA	O-C-N	-17.81	94.20	122.70
2	B	260	PHE	CB-CG-CD2	-15.53	109.93	120.80
2	B	10	GLY	CA-C-N	14.42	148.93	117.20
2	B	251	ARG	NE-CZ-NH1	14.10	127.35	120.30
2	B	68	LEU	CB-CG-CD2	13.45	133.86	111.00
2	B	98	GLY	O-C-N	-13.29	101.44	122.70
1	K	352	TYR	CB-CG-CD2	-12.31	113.62	121.00
1	K	254	GLU	CA-CB-CG	11.92	139.62	113.40
2	B	68	LEU	CB-CG-CD1	-11.21	91.94	111.00
3	A	409	VAL	CG1-CB-CG2	11.14	128.72	110.90
3	A	221	ARG	CG-CD-NE	10.88	134.66	111.80
1	K	352	TYR	CB-CG-CD1	-10.71	114.58	121.00
2	B	99	ASN	N-CA-CB	10.69	129.84	110.60
1	K	84	SER	CA-CB-OG	10.40	139.29	111.20
3	A	99	ALA	N-CA-CB	10.27	124.47	110.10
3	A	100	ALA	O-C-N	-10.24	106.32	122.70
2	B	323	MET	O-C-N	-10.14	106.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	257	LYS	CA-CB-CG	9.90	135.18	113.40
3	A	221	ARG	CD-NE-CZ	-9.90	109.74	123.60
3	A	403	ALA	CA-C-N	9.85	138.88	117.20
3	A	405	VAL	CA-CB-CG2	9.80	125.60	110.90
2	B	261	PRO	N-CD-CG	9.69	117.73	103.20
3	A	101	ASN	N-CA-CB	9.58	127.85	110.60
1	K	231	TYR	CZ-CE2-CD2	-9.46	111.28	119.80
2	B	98	GLY	CA-C-N	8.83	136.62	117.20
1	K	97	TYR	CG-CD2-CE2	-8.82	114.25	121.30
3	A	220	GLU	N-CA-CB	8.81	126.46	110.60
1	K	257	LYS	CB-CG-CD	8.78	134.43	111.60
3	A	221	ARG	CB-CA-C	8.61	127.61	110.40
3	A	181	VAL	CA-CB-CG2	8.45	123.57	110.90
1	K	231	TYR	CG-CD2-CE2	8.33	127.97	121.30
3	A	179	THR	CA-CB-CG2	8.24	123.94	112.40
2	B	259	PRO	N-CA-CB	8.02	112.93	103.30
3	A	404	PHE	CB-CG-CD1	7.99	126.39	120.80
3	A	221	ARG	CB-CG-CD	7.88	132.10	111.60
2	B	261	PRO	CA-N-CD	-7.79	100.60	111.50
2	B	99	ASN	C-N-CA	-7.67	102.53	121.70
3	A	221	ARG	N-CA-C	7.50	131.24	111.00
2	B	324	LYS	CD-CE-NZ	7.49	128.92	111.70
2	B	345	ILE	CA-CB-CG1	-7.47	96.81	111.00
3	A	161	TYR	CA-CB-CG	-7.43	99.28	113.40
2	B	324	LYS	N-CA-CB	7.42	123.96	110.60
2	B	324	LYS	CA-CB-CG	7.42	129.71	113.40
2	B	252	LYS	CA-CB-CG	-7.25	97.46	113.40
2	B	324	LYS	CB-CG-CD	7.20	130.32	111.60
3	A	220	GLU	CA-C-O	-7.18	105.03	120.10
3	A	427	ALA	CB-CA-C	-7.15	99.37	110.10
1	K	295	LEU	O-C-N	-7.12	111.10	123.20
3	A	221	ARG	CA-CB-CG	6.81	128.39	113.40
3	A	178	SER	CB-CA-C	6.78	122.98	110.10
3	A	409	VAL	CA-CB-CG2	-6.77	100.75	110.90
2	B	259	PRO	CA-N-CD	-6.74	102.06	111.50
2	B	260	PHE	CA-C-O	-6.71	106.01	120.10
3	A	99	ALA	CA-C-O	-6.71	106.02	120.10
3	A	405	VAL	CA-C-N	6.68	131.91	117.20
2	B	260	PHE	CB-CG-CD1	6.55	125.38	120.80
2	B	252	LYS	CB-CA-C	-6.49	97.43	110.40
3	A	11	GLN	O-C-N	-6.47	112.35	122.70
3	A	409	VAL	C-N-CA	-6.36	108.95	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	251	ARG	CG-CD-NE	6.33	125.10	111.80
1	K	260	LYS	CG-CD-CE	6.25	130.64	111.90
3	A	105	ARG	NE-CZ-NH2	-6.25	117.18	120.30
3	A	100	ALA	CA-C-N	6.20	130.84	117.20
2	B	252	LYS	CG-CD-CE	6.13	130.29	111.90
1	K	211	TYR	CA-CB-CG	-6.12	101.77	113.40
1	K	232	SER	N-CA-CB	6.10	119.65	110.50
1	K	260	LYS	CB-CG-CD	5.96	127.11	111.60
2	B	99	ASN	O-C-N	5.89	132.13	122.70
2	B	259	PRO	N-CD-CG	5.83	111.95	103.20
2	B	324	LYS	N-CA-C	-5.83	95.26	111.00
3	A	220	GLU	CB-CA-C	-5.83	98.74	110.40
3	A	181	VAL	CA-CB-CG1	-5.66	102.41	110.90
3	A	427	ALA	CA-C-N	-5.65	104.77	117.20
2	B	347	ASN	CA-CB-CG	-5.64	101.00	113.40
3	A	102	ASN	N-CA-CB	5.58	120.65	110.60
2	B	143	THR	N-CA-CB	5.56	120.87	110.30
3	A	405	VAL	N-CA-C	5.54	125.96	111.00
2	B	261	PRO	N-CA-CB	5.52	109.93	103.30
2	B	251	ARG	CD-NE-CZ	-5.51	115.89	123.60
1	K	247	GLU	CA-CB-CG	5.50	125.51	113.40
1	K	254	GLU	CB-CG-CD	5.49	129.03	114.20
1	K	211	TYR	CG-CD2-CE2	-5.49	116.91	121.30
1	K	295	LEU	CA-C-N	5.43	127.06	116.20
3	A	221	ARG	N-CA-CB	-5.43	100.83	110.60
3	A	178	SER	O-C-N	-5.42	114.04	122.70
3	A	179	THR	OG1-CB-CG2	-5.41	97.55	110.00
3	A	406	HIS	N-CA-CB	5.29	120.12	110.60
3	A	405	VAL	CA-CB-CG1	-5.24	103.05	110.90
2	B	67	ASP	C-N-CA	-5.22	108.64	121.70
2	B	350	LYS	C-N-CA	-5.21	108.67	121.70
2	B	323	MET	CA-C-N	5.16	128.54	117.20
2	B	324	LYS	CG-CD-CE	5.12	127.27	111.90
3	A	178	SER	CA-C-N	5.05	128.31	117.20
3	A	427	ALA	O-C-N	5.03	130.75	122.70
2	B	260	PHE	CA-C-N	5.01	131.13	117.10
3	A	180	ALA	N-CA-CB	-5.00	103.09	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	221	ARG	CA

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	100	ALA	Mainchain
3	A	101	ASN	Sidechain,Mainchain
3	A	11	GLN	Sidechain
3	A	178	SER	Peptide,Mainchain
3	A	179	THR	Mainchain
3	A	219	ILE	Mainchain
3	A	220	GLU	Sidechain,Mainchain
3	A	221	ARG	Mainchain
3	A	224	TYR	Mainchain
3	A	403	ALA	Mainchain
3	A	404	PHE	Sidechain,Peptide,Mainchain
3	A	99	ALA	Peptide,Mainchain
2	B	15	GLN	Peptide
2	B	252	LYS	Mainchain
2	B	259	PRO	Peptide
2	B	260	PHE	Sidechain,Mainchain
2	B	323	MET	Mainchain
2	B	345	ILE	Mainchain
2	B	346	PRO	Mainchain
2	B	420	SER	Mainchain
2	B	99	ASN	Mainchain
1	K	106	GLN	Sidechain
1	K	110	GLY	Peptide
1	K	296	GLY	Mainchain
1	K	352	TYR	Sidechain
1	K	53	ARG	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2607	0	2670	967	0
2	B	3372	0	3253	1554	0
3	A	3425	0	3334	1601	0
4	K	21	0	0	14	0
5	A	32	0	14	18	0
5	B	32	0	14	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	9491	0	9285	3916	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 209.

All (3916) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:LYS:CD	2:B:324:LYS:CE	1.85	1.55
3:A:221:ARG:CA	3:A:221:ARG:CB	1.85	1.51
1:K:181:ARG:HH21	1:K:197:LYS:CG	1.19	1.51
3:A:221:ARG:CD	3:A:221:ARG:CG	1.92	1.47
1:K:95:MET:CE	1:K:97:TYR:HB2	1.45	1.43
1:K:181:ARG:NH2	1:K:197:LYS:HG3	1.27	1.42
1:K:95:MET:HE2	1:K:97:TYR:CB	1.53	1.38
3:A:221:ARG:CB	3:A:221:ARG:CG	2.04	1.35
1:K:82:TYR:CE2	1:K:86:VAL:HG21	1.69	1.26
1:K:162:GLU:CG	1:K:235:SER:HB2	1.68	1.24
1:K:82:TYR:CD2	1:K:86:VAL:HG21	1.73	1.23
1:K:297:ARG:HH12	2:B:262:ARG:CD	1.50	1.23
1:K:162:GLU:HG2	1:K:235:SER:CB	1.70	1.21
1:K:162:GLU:OE2	1:K:223:THR:CG2	1.89	1.20
2:B:64:ILE:HD11	2:B:119:VAL:HG11	1.23	1.20
1:K:187:ASP:OD1	1:K:195:ILE:HG13	1.33	1.20
1:K:157:LYS:CG	1:K:203:THR:OG1	1.89	1.19
1:K:162:GLU:CG	1:K:235:SER:CB	2.19	1.19
3:A:319:TYR:HD1	3:A:355:ILE:HG12	1.08	1.19
3:A:278:ALA:HA	3:A:368:LEU:HA	1.24	1.19
3:A:23:LEU:HD12	3:A:363:VAL:HA	1.24	1.18
3:A:268:PRO:HG2	3:A:378:LEU:HD13	1.26	1.17
1:K:162:GLU:HG2	1:K:235:SER:HB3	1.26	1.17
3:A:247:ALA:HB3	3:A:355:ILE:HB	1.20	1.16
1:K:82:TYR:CZ	1:K:86:VAL:HG11	1.80	1.16
1:K:157:LYS:HG3	1:K:203:THR:OG1	1.45	1.15
3:A:48:SER:HB2	3:A:243:ARG:HD3	1.20	1.15
3:A:176:GLN:HG2	3:A:207:GLU:HB2	1.29	1.15
2:B:326:VAL:HG12	2:B:330:MET:HE1	1.15	1.14
3:A:172:TYR:HB2	3:A:203:MET:HB2	1.25	1.14
3:A:286:LEU:HD13	3:A:291:ILE:HD11	1.30	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:162:GLU:OE2	1:K:223:THR:HG22	1.47	1.14
2:B:285:THR:HG22	2:B:288:GLU:HB2	1.28	1.13
2:B:41:ASP:HA	2:B:44:LEU:HD23	1.15	1.12
3:A:274:PRO:HG3	3:A:291:ILE:HG12	1.32	1.12
1:K:312:ARG:HA	1:K:318:ARG:CG	1.79	1.12
3:A:166:LYS:HD2	3:A:198:SER:HA	1.28	1.12
2:B:324:LYS:CE	2:B:324:LYS:NZ	2.11	1.12
1:K:181:ARG:NH2	1:K:197:LYS:HE2	1.63	1.11
2:B:324:LYS:NZ	3:A:221:ARG:CG	2.14	1.11
3:A:216:ASN:HB3	3:A:277:SER:HB2	1.29	1.11
2:B:324:LYS:HE2	3:A:221:ARG:CA	1.81	1.10
1:K:84:SER:OG	1:K:84:SER:HB2	1.29	1.10
1:K:55:GLY:HA3	1:K:60:LYS:HE3	1.11	1.10
1:K:157:LYS:HB3	1:K:201:GLU:HB3	1.33	1.10
3:A:251:ASP:HB3	3:A:254:GLU:HB3	1.33	1.10
1:K:162:GLU:CD	1:K:235:SER:HB2	1.73	1.09
1:K:181:ARG:NH2	1:K:197:LYS:CE	2.15	1.09
3:A:319:TYR:HB2	3:A:355:ILE:HA	1.12	1.09
3:A:3:GLU:HG2	3:A:50:ASN:HB3	1.16	1.09
3:A:30:ILE:HA	3:A:36:MET:HB3	1.15	1.09
3:A:70:LEU:HD13	3:A:145:THR:HG23	1.25	1.09
3:A:246:GLY:HA3	3:A:356:ASN:HA	1.25	1.09
2:B:250:LEU:HD12	2:B:253:LEU:HD11	1.10	1.09
3:A:70:LEU:HG	3:A:110:ILE:HG21	1.28	1.09
3:A:242:LEU:HD23	3:A:252:LEU:HG	1.24	1.09
2:B:274:THR:HB	2:B:279:GLN:HB2	1.15	1.09
3:A:181:VAL:HG11	3:A:404:PHE:CE1	1.87	1.09
1:K:53:ARG:HB3	1:K:60:LYS:HB3	1.14	1.09
2:B:309:ARG:HB2	2:B:426:GLN:HA	1.30	1.09
1:K:16:GLY:HA3	1:K:362:LYS:HA	1.33	1.08
3:A:34:GLY:HA3	3:A:86:LEU:HD13	1.35	1.08
1:K:181:ARG:NH2	1:K:197:LYS:CG	1.95	1.08
1:K:344:GLU:HB3	3:A:414:GLU:HG2	1.23	1.08
1:K:169:PHE:HA	1:K:179:SER:HA	1.32	1.08
1:K:160:LEU:HG	1:K:171:LEU:HD12	1.20	1.08
3:A:268:PRO:HB2	3:A:378:LEU:HB3	1.35	1.08
3:A:320:ARG:HG3	3:A:374:ALA:HB3	1.25	1.08
2:B:1:MET:HE2	2:B:49:VAL:HB	1.26	1.07
3:A:317:LEU:HB2	3:A:353:VAL:HB	1.36	1.07
2:B:172:SER:HB2	2:B:205:GLU:HB3	1.34	1.07
1:K:155:SER:HB3	1:K:203:THR:HG21	1.13	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:171:LEU:HD13	1:K:221:ARG:HA	1.36	1.07
2:B:273:LEU:HD11	2:B:297:LYS:HD2	1.11	1.07
2:B:392:LYS:HB3	2:B:395:LEU:HD11	1.24	1.07
2:B:54:ALA:HB3	2:B:58:LYS:HB3	1.37	1.07
2:B:252:LYS:HD2	3:A:101:ASN:HB3	1.36	1.07
1:K:159:SER:HA	1:K:172:LEU:HD13	1.18	1.06
2:B:212:PHE:HB2	2:B:220:PRO:HD3	1.37	1.06
1:K:187:ASP:OD1	1:K:195:ILE:CG1	2.02	1.06
1:K:84:SER:OG	1:K:84:SER:HB3	1.29	1.06
1:K:290:GLN:HE21	3:A:410:GLY:HA3	1.16	1.06
3:A:31:GLN:HG2	3:A:32:PRO:HD2	1.32	1.06
1:K:159:SER:HB2	1:K:199:LEU:HD21	1.35	1.05
1:K:246:LYS:CE	1:K:254:GLU:CD	2.24	1.05
2:B:269:GLY:HA3	2:B:367:PHE:HB3	1.38	1.05
3:A:68:VAL:HG12	3:A:93:ILE:HD11	1.38	1.05
3:A:313:MET:HE2	3:A:344:VAL:HG11	1.31	1.05
2:B:324:LYS:CE	3:A:221:ARG:HD3	1.85	1.04
1:K:47:ARG:NE	1:K:49:GLU:OE2	1.89	1.04
3:A:4:CYS:HA	3:A:132:LEU:HG	1.08	1.04
1:K:297:ARG:HH12	2:B:262:ARG:HD2	0.90	1.04
2:B:258:VAL:HG12	2:B:263:LEU:HD12	1.37	1.04
2:B:286:VAL:HG11	2:B:325:GLU:HB3	1.37	1.04
1:K:17:LYS:HG2	1:K:363:PRO:HG2	1.35	1.03
2:B:130:LEU:HD22	2:B:133:PHE:HE1	1.24	1.03
2:B:154:LYS:HE2	2:B:157:GLU:HB3	1.39	1.03
2:B:97:ALA:CB	2:B:143:THR:HA	1.88	1.03
2:B:274:THR:HG22	2:B:278:SER:HB2	1.39	1.03
1:K:246:LYS:HE3	1:K:254:GLU:CD	1.79	1.02
2:B:324:LYS:CE	3:A:221:ARG:CG	2.36	1.02
3:A:171:ILE:HA	3:A:204:VAL:HG12	1.36	1.02
2:B:246:LEU:HD12	2:B:352:ALA:HA	1.35	1.02
3:A:200:CYS:HA	3:A:266:HIS:HB3	1.02	1.02
1:K:84:SER:OG	1:K:84:SER:CA	2.08	1.02
2:B:215:LEU:HD22	2:B:217:LEU:HB2	1.38	1.02
1:K:95:MET:HG3	1:K:365:VAL:HG13	1.40	1.01
1:K:157:LYS:CE	1:K:203:THR:OG1	2.08	1.01
2:B:314:ALA:H	2:B:368:ILE:HB	1.22	1.01
1:K:297:ARG:NH1	2:B:262:ARG:HD2	1.74	1.01
3:A:217:LEU:HB3	3:A:219:ILE:HG12	1.38	1.01
2:B:149:THR:HA	2:B:191:GLN:HE22	1.25	1.01
1:K:31:ALA:HA	1:K:34:LYS:HD3	1.38	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:290:GLN:HE21	3:A:410:GLY:CA	1.74	1.00
3:A:115:ILE:HG12	3:A:119:LEU:HD23	1.41	1.00
2:B:100:ASN:HB2	2:B:103:LYS:HB2	1.43	1.00
1:K:48:LYS:HE3	1:K:70:MET:HA	1.42	1.00
1:K:312:ARG:HA	1:K:318:ARG:CD	1.90	1.00
2:B:4:ILE:HG23	2:B:133:PHE:HA	1.39	1.00
2:B:273:LEU:HG	2:B:298:ASN:HA	1.39	1.00
2:B:345:ILE:HD13	3:A:181:VAL:HG22	1.40	0.99
3:A:226:ASN:HA	3:A:229:ARG:HG3	1.41	0.99
1:K:17:LYS:HE3	1:K:329:ARG:HD3	1.43	0.99
2:B:120:VAL:HG23	2:B:121:ARG:HE	1.26	0.99
2:B:97:ALA:HB3	2:B:143:THR:HA	1.43	0.99
2:B:178:THR:HG23	2:B:181:GLU:H	1.25	0.99
2:B:324:LYS:HZ2	3:A:221:ARG:CG	1.71	0.99
3:A:70:LEU:HD23	3:A:110:ILE:HG13	1.45	0.99
1:K:187:ASP:HB3	1:K:195:ILE:HD11	1.44	0.99
1:K:26:ARG:HD2	1:K:29:ASN:HD21	1.28	0.99
1:K:293:LEU:HG	3:A:409:VAL:HG21	1.40	0.99
1:K:320:LEU:HD12	1:K:323:SER:HB2	1.44	0.99
2:B:103:LYS:HD2	2:B:401:GLU:HA	1.44	0.99
2:B:321:MET:HE3	2:B:326:VAL:HG22	1.44	0.99
3:A:319:TYR:CD1	3:A:355:ILE:HG12	1.98	0.99
1:K:77:LYS:HZ2	1:K:78:GLN:HG3	1.21	0.98
3:A:5:ILE:HG12	3:A:64:ARG:HB3	1.45	0.98
2:B:324:LYS:HG2	3:A:221:ARG:HB2	1.46	0.98
2:B:316:VAL:H	2:B:366:THR:HG22	1.28	0.98
2:B:422:TYR:HA	2:B:425:TYR:CE2	1.99	0.98
3:A:383:ALA:HA	3:A:386:GLU:HG2	1.44	0.98
2:B:376:GLU:HB3	2:B:380:ARG:HH12	1.27	0.97
2:B:324:LYS:CE	3:A:221:ARG:CD	2.42	0.97
1:K:84:SER:OG	1:K:84:SER:CB	0.68	0.97
3:A:195:LEU:HD13	3:A:201:ALA:HB2	1.45	0.97
1:K:82:TYR:OH	1:K:86:VAL:HG11	1.63	0.97
1:K:297:ARG:NH1	2:B:262:ARG:CD	2.27	0.97
1:K:223:THR:HG21	1:K:235:SER:H	1.29	0.97
3:A:5:ILE:H	3:A:132:LEU:HD21	1.27	0.97
2:B:324:LYS:CE	3:A:221:ARG:CB	2.43	0.97
2:B:4:ILE:HD11	2:B:131:GLN:HB3	1.44	0.96
3:A:181:VAL:HG11	3:A:404:PHE:HE1	1.24	0.96
1:K:343:LEU:HD23	1:K:343:LEU:H	1.29	0.96
2:B:182:PRO:HB2	2:B:385:PHE:HZ	1.26	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:262:TYR:HB3	3:A:264:ARG:HD3	1.47	0.96
1:K:283:ARG:NH2	2:B:160:PRO:HB2	1.81	0.96
1:K:312:ARG:HA	1:K:318:ARG:HD2	1.46	0.96
1:K:95:MET:CG	1:K:365:VAL:HG13	1.96	0.96
2:B:324:LYS:HE3	3:A:222:PRO:CD	1.94	0.96
1:K:329:ARG:HB2	1:K:363:PRO:HB3	1.48	0.95
1:K:172:LEU:HD11	1:K:199:LEU:HD11	1.46	0.95
3:A:185:TYR:HA	3:A:395:PHE:CZ	2.01	0.95
2:B:77:ARG:HH11	2:B:82:GLY:HA2	1.29	0.95
3:A:154:MET:HE1	3:A:166:LYS:HE2	1.46	0.95
2:B:419:VAL:HA	2:B:422:TYR:CD2	2.00	0.95
2:B:277:GLY:HA2	2:B:280:GLN:HE21	1.28	0.95
3:A:81:GLY:HA3	3:A:83:TYR:CE2	2.01	0.95
3:A:204:VAL:HG23	3:A:209:ILE:HD12	1.48	0.95
2:B:46:ARG:HB3	2:B:241:ARG:HD3	1.46	0.95
1:K:29:ASN:HB2	1:K:32:GLU:HG2	1.47	0.95
2:B:324:LYS:NZ	3:A:221:ARG:CB	2.29	0.95
3:A:296:PHE:CE1	3:A:335:ILE:HD12	2.01	0.95
2:B:152:ILE:HG13	2:B:192:LEU:HD23	1.47	0.94
2:B:376:GLU:HA	2:B:379:LYS:HE2	1.49	0.94
3:A:288:VAL:HG12	3:A:331:ALA:HB2	1.48	0.94
3:A:296:PHE:HE1	3:A:335:ILE:HD12	1.31	0.94
2:B:33:THR:HG23	2:B:35:SER:H	1.28	0.94
3:A:414:GLU:HG3	3:A:416:GLY:H	1.32	0.94
1:K:26:ARG:HG2	1:K:109:THR:HG23	1.49	0.94
1:K:190:ASN:HB3	1:K:193:GLY:HA3	1.50	0.94
3:A:63:PRO:HD3	3:A:86:LEU:HD11	1.49	0.94
3:A:200:CYS:HB2	3:A:267:PHE:HB3	1.49	0.94
1:K:178:VAL:HA	1:K:220:LYS:HE2	1.48	0.94
2:B:20:PHE:HD1	2:B:230:SER:HB2	1.32	0.94
2:B:250:LEU:CD1	2:B:253:LEU:HD11	1.99	0.93
2:B:267:MET:HG3	2:B:370:ASN:HA	1.51	0.93
3:A:313:MET:HG3	3:A:344:VAL:HG21	1.48	0.93
2:B:215:LEU:HA	2:B:276:ARG:HB3	1.49	0.93
3:A:116:ASP:HA	3:A:119:LEU:HD21	1.49	0.93
3:A:216:ASN:CB	3:A:277:SER:HB2	1.99	0.93
3:A:277:SER:H	3:A:280:LYS:HB2	1.33	0.93
2:B:73:MET:HG2	2:B:92:PHE:CE1	2.04	0.93
2:B:324:LYS:CE	3:A:221:ARG:CA	2.46	0.93
3:A:34:GLY:CA	3:A:86:LEU:HD13	1.98	0.93
2:B:284:LEU:HD13	2:B:289:LEU:HG	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:ALA:HB3	2:B:368:ILE:HG13	1.51	0.93
2:B:326:VAL:HG12	2:B:330:MET:CE	1.99	0.93
3:A:79:ARG:HD3	3:A:92:LEU:HD23	1.51	0.92
2:B:112:LEU:HD11	2:B:151:LEU:HB3	1.50	0.92
3:A:31:GLN:HB2	3:A:37:PRO:HD3	1.51	0.92
3:A:351:PHE:HD2	3:A:352:LYS:HB2	1.34	0.92
2:B:64:ILE:HD11	2:B:119:VAL:CG1	2.00	0.92
3:A:229:ARG:HB3	3:A:363:VAL:HG21	1.51	0.92
2:B:290:THR:HB	2:B:294:PHE:CZ	2.05	0.92
3:A:9:VAL:HB	3:A:139:HIS:CB	1.99	0.92
2:B:304:ASP:HB3	2:B:307:HIS:CG	2.05	0.92
1:K:187:ASP:HB2	1:K:189:ARG:CD	2.00	0.91
1:K:293:LEU:CG	3:A:409:VAL:HG21	2.00	0.91
3:A:286:LEU:HD11	3:A:373:ARG:HG3	1.49	0.91
1:K:320:LEU:HG	1:K:324:LEU:CD2	2.00	0.91
2:B:273:LEU:CD1	2:B:297:LYS:HD2	1.99	0.91
2:B:321:MET:CE	2:B:326:VAL:HG22	2.01	0.91
1:K:171:LEU:HA	1:K:220:LYS:CG	2.01	0.91
2:B:186:THR:HG23	2:B:187:LEU:HD22	1.51	0.91
1:K:47:ARG:HB3	1:K:49:GLU:HG3	1.51	0.91
1:K:320:LEU:HG	1:K:324:LEU:HD21	1.52	0.91
2:B:273:LEU:CG	2:B:298:ASN:HA	2.00	0.91
2:B:284:LEU:HD11	2:B:361:LEU:HD12	1.53	0.91
3:A:385:ALA:HA	3:A:388:TRP:CE2	2.06	0.91
1:K:144:PHE:CD2	1:K:207:LYS:HG3	2.06	0.90
3:A:171:ILE:CD1	5:A:501:G2P:H1'	1.99	0.90
2:B:102:ALA:CB	2:B:401:GLU:HB3	2.02	0.90
2:B:322:SER:OG	3:A:221:ARG:HB3	1.69	0.90
2:B:421:GLU:HG3	2:B:425:TYR:HE1	1.36	0.90
2:B:324:LYS:CE	3:A:222:PRO:CD	2.49	0.90
3:A:287:SER:HA	3:A:373:ARG:HH21	1.36	0.90
2:B:215:LEU:CD2	2:B:217:LEU:HB2	2.01	0.90
3:A:319:TYR:HB2	3:A:355:ILE:CA	1.99	0.90
1:K:82:TYR:CD2	1:K:86:VAL:CG2	2.54	0.90
1:K:157:LYS:HE3	1:K:203:THR:OG1	1.69	0.90
1:K:325:GLY:HA2	1:K:361:ASN:HA	1.54	0.90
3:A:153:LEU:HD12	3:A:156:ARG:HH12	1.37	0.90
1:K:159:SER:CA	1:K:172:LEU:HD13	2.02	0.90
3:A:3:GLU:HG2	3:A:50:ASN:CB	2.00	0.90
3:A:346:TRP:HE1	3:A:438:ASP:HA	1.34	0.90
2:B:250:LEU:HA	2:B:253:LEU:HD21	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:82:TYR:CE2	1:K:86:VAL:CG2	2.54	0.90
1:K:206:ASN:HD21	1:K:209:GLU:HG3	1.37	0.90
2:B:28:HIS:CD2	2:B:47:ILE:HD12	2.07	0.90
1:K:293:LEU:CD2	3:A:409:VAL:HG21	2.02	0.89
1:K:66:TYR:CE2	1:K:67:THR:O	2.25	0.89
1:K:144:PHE:CE2	1:K:207:LYS:HA	2.06	0.89
1:K:160:LEU:CG	1:K:171:LEU:HD12	2.01	0.89
2:B:148:GLY:HA2	2:B:151:LEU:HD21	1.54	0.89
2:B:345:ILE:CD1	3:A:181:VAL:HG22	2.03	0.89
3:A:286:LEU:CD1	3:A:291:ILE:HD11	2.02	0.89
1:K:215:GLU:CG	1:K:216:LYS:HE3	2.03	0.89
3:A:9:VAL:CG1	3:A:146:GLY:HA2	2.03	0.89
3:A:41:THR:HG21	3:A:49:PHE:HB2	1.54	0.89
3:A:262:TYR:HB3	3:A:264:ARG:CD	2.01	0.89
2:B:9:ALA:HB1	2:B:147:MET:CE	2.02	0.89
2:B:102:ALA:HB3	2:B:401:GLU:HB3	1.51	0.89
2:B:260:PHE:CE1	3:A:404:PHE:HA	2.08	0.89
1:K:55:GLY:CA	1:K:60:LYS:HE3	2.00	0.89
1:K:352:TYR:HB2	4:K:501:MZK:C15	2.03	0.89
3:A:200:CYS:CA	3:A:266:HIS:HB3	1.98	0.89
3:A:286:LEU:CD2	3:A:371:VAL:HB	2.02	0.89
3:A:344:VAL:HB	3:A:346:TRP:CD1	2.08	0.89
1:K:82:TYR:CZ	1:K:86:VAL:CG1	2.55	0.89
2:B:103:LYS:HD2	2:B:401:GLU:CA	2.02	0.89
3:A:278:ALA:CA	3:A:368:LEU:HA	2.01	0.89
3:A:318:LEU:HD22	3:A:319:TYR:H	1.37	0.89
3:A:351:PHE:CD2	3:A:352:LYS:HB2	2.08	0.89
1:K:53:ARG:CB	1:K:60:LYS:HB3	2.02	0.89
1:K:223:THR:HB	1:K:234:ARG:HB2	1.53	0.89
2:B:253:LEU:HB2	2:B:257:MET:CE	2.02	0.88
3:A:384:ILE:HD11	3:A:432:TYR:HE2	1.36	0.88
1:K:109:THR:CG2	1:K:335:THR:HB	2.03	0.88
1:K:170:ASP:HB2	1:K:180:GLU:HB2	1.54	0.88
1:K:181:ARG:CZ	1:K:197:LYS:HG3	2.02	0.88
3:A:189:LEU:HD13	3:A:418:PHE:CD2	2.07	0.88
1:K:187:ASP:HB3	1:K:195:ILE:CD1	2.04	0.88
2:B:392:LYS:CB	2:B:395:LEU:HD11	2.03	0.88
3:A:259:LEU:HD13	3:A:378:LEU:HD12	1.53	0.88
2:B:9:ALA:HB1	2:B:147:MET:HE2	1.54	0.88
2:B:51:TYR:HD2	2:B:59:TYR:HB3	1.38	0.88
3:A:276:ILE:HG13	3:A:371:VAL:HG11	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:16:ILE:HA	3:A:228:ASN:HD22	1.39	0.88
1:K:181:ARG:CZ	1:K:197:LYS:HE2	2.02	0.88
1:K:53:ARG:HB3	1:K:60:LYS:CB	2.01	0.88
2:B:20:PHE:HA	2:B:230:SER:HB2	1.53	0.88
3:A:4:CYS:HA	3:A:132:LEU:CG	2.01	0.88
3:A:107:HIS:HB2	3:A:148:GLY:HA2	1.56	0.88
2:B:162:ARG:CZ	2:B:162:ARG:HA	2.03	0.88
3:A:216:ASN:HB3	3:A:280:LYS:HD2	1.55	0.88
1:K:169:PHE:CD1	1:K:179:SER:HB2	2.09	0.88
2:B:371:SER:HB2	2:B:374:ILE:HG22	1.55	0.88
3:A:3:GLU:CG	3:A:50:ASN:HB3	2.04	0.88
3:A:286:LEU:HD23	3:A:371:VAL:HB	1.56	0.88
1:K:91:ASP:O	1:K:95:MET:SD	2.32	0.87
3:A:237:SER:HA	3:A:320:ARG:HH11	1.37	0.87
1:K:95:MET:HE2	1:K:97:TYR:CG	2.08	0.87
3:A:269:LEU:HD23	3:A:384:ILE:HD12	1.56	0.87
1:K:327:ARG:H	1:K:327:ARG:HH21	1.21	0.87
2:B:324:LYS:CD	3:A:221:ARG:CG	2.52	0.87
3:A:1:MET:HG2	3:A:47:ASP:N	1.89	0.87
3:A:232:SER:HB3	3:A:363:VAL:HG11	1.56	0.87
3:A:272:TYR:HE1	3:A:374:ALA:HB1	1.37	0.87
1:K:94:ILE:O	1:K:245:MET:HE3	1.73	0.87
2:B:339:SER:HA	2:B:429:THR:CG2	2.04	0.87
2:B:371:SER:HB2	2:B:374:ILE:CG2	2.04	0.87
3:A:103:TYR:HB2	3:A:147:SER:HB3	1.56	0.87
2:B:216:LYS:HE2	2:B:277:GLY:HA3	1.57	0.87
1:K:160:LEU:H	1:K:172:LEU:HD22	1.39	0.87
1:K:269:SER:HB3	1:K:288:ILE:HD11	1.56	0.87
1:K:298:VAL:HG23	1:K:310:PRO:HD2	1.54	0.87
3:A:68:VAL:HG21	3:A:149:PHE:CE1	2.08	0.87
3:A:70:LEU:CD2	3:A:110:ILE:HG13	2.04	0.87
3:A:275:VAL:HB	3:A:300:ASN:HD22	1.40	0.87
1:K:16:GLY:HA3	1:K:362:LYS:CA	2.05	0.86
2:B:244:GLY:HA2	2:B:355:ASP:N	1.90	0.86
3:A:282:TYR:CE1	3:A:369:ALA:HB2	2.10	0.86
2:B:1:MET:HE2	2:B:49:VAL:CB	2.04	0.86
2:B:45:GLU:HG3	2:B:46:ARG:HE	1.37	0.86
2:B:324:LYS:HE3	3:A:222:PRO:HD3	1.57	0.86
2:B:253:LEU:HB2	2:B:257:MET:HE1	1.57	0.86
2:B:142:GLY:HA2	2:B:184:ASN:CG	1.96	0.86
2:B:286:VAL:HB	2:B:287:PRO:HD3	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:209:ILE:HG12	3:A:302:MET:HB2	1.57	0.86
3:A:246:GLY:HA2	3:A:357:TYR:H	1.41	0.86
1:K:181:ARG:HB2	1:K:181:ARG:HH11	1.40	0.86
2:B:324:LYS:HZ1	3:A:222:PRO:N	1.73	0.86
2:B:376:GLU:CA	2:B:379:LYS:HE2	2.05	0.86
3:A:107:HIS:CD2	3:A:152:LEU:HB2	2.10	0.86
3:A:172:TYR:CB	3:A:203:MET:HB2	2.05	0.86
2:B:324:LYS:HZ3	3:A:221:ARG:CB	1.89	0.86
3:A:264:ARG:HD3	3:A:264:ARG:H	1.39	0.86
1:K:206:ASN:ND2	1:K:209:GLU:HG3	1.91	0.86
3:A:54:SER:HB3	3:A:64:ARG:HH11	1.40	0.86
3:A:233:GLN:HE21	3:A:234:ILE:HG22	1.41	0.86
3:A:320:ARG:HB2	3:A:374:ALA:H	1.37	0.85
2:B:24:ILE:HA	2:B:27:GLU:HG2	1.58	0.85
2:B:130:LEU:HD22	2:B:133:PHE:CE1	2.10	0.85
2:B:242:PHE:CD2	2:B:356:ILE:HD11	2.10	0.85
2:B:314:ALA:N	2:B:368:ILE:HB	1.92	0.85
3:A:166:LYS:CD	3:A:198:SER:HA	2.04	0.85
1:K:26:ARG:HH12	1:K:28:PHE:HA	1.41	0.85
1:K:109:THR:HG21	1:K:336:ILE:N	1.92	0.85
1:K:162:GLU:OE2	1:K:221:ARG:NH1	2.10	0.85
2:B:116:VAL:HG23	2:B:117:LEU:HD22	1.58	0.85
3:A:280:LYS:HA	3:A:283:HIS:CD2	2.11	0.85
1:K:26:ARG:CZ	1:K:338:PRO:HD2	2.06	0.85
1:K:37:ALA:HA	1:K:341:LEU:HD11	1.57	0.85
1:K:55:GLY:HA2	1:K:60:LYS:HA	1.58	0.85
2:B:1:MET:HG3	2:B:127:CYS:HB2	1.56	0.85
3:A:279:GLU:HA	3:A:282:TYR:CD2	2.12	0.85
3:A:385:ALA:HA	3:A:388:TRP:CD2	2.11	0.85
1:K:160:LEU:N	1:K:172:LEU:HB3	1.92	0.85
1:K:17:LYS:HD3	1:K:363:PRO:HB2	1.58	0.85
3:A:6:SER:HB3	3:A:138:PHE:CE1	2.11	0.85
2:B:152:ILE:HD13	2:B:155:ILE:HD11	1.58	0.85
2:B:170:VAL:CG2	2:B:203:ASP:HA	2.05	0.85
2:B:215:LEU:HA	2:B:276:ARG:CB	2.06	0.85
3:A:4:CYS:H	3:A:51:THR:HA	1.42	0.85
3:A:313:MET:CE	3:A:344:VAL:HG11	2.06	0.85
1:K:92:GLU:OE1	1:K:329:ARG:HG2	1.76	0.84
2:B:179:VAL:HG21	2:B:388:MET:HG3	1.56	0.84
2:B:377:LEU:HA	2:B:380:ARG:NE	1.92	0.84
2:B:398:TYR:HA	2:B:401:GLU:HG3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:PRO:HB2	2:B:385:PHE:CZ	2.12	0.84
2:B:330:MET:HG3	2:B:331:LEU:HD13	1.59	0.84
1:K:170:ASP:HB2	1:K:180:GLU:CB	2.06	0.84
1:K:352:TYR:HA	4:K:501:MZK:F3	1.66	0.84
2:B:308:GLY:HA2	2:B:372:THR:CB	2.07	0.84
2:B:12:CYS:O	2:B:16:ILE:HG13	1.76	0.84
3:A:12:ALA:HA	3:A:15:GLN:NE2	1.92	0.84
2:B:21:TRP:CE3	2:B:21:TRP:HA	2.10	0.84
2:B:324:LYS:HE3	3:A:221:ARG:HD3	1.60	0.84
3:A:223:THR:HG22	3:A:225:THR:H	1.43	0.84
1:K:162:GLU:OE2	1:K:223:THR:HG23	1.77	0.84
3:A:48:SER:HB2	3:A:243:ARG:CD	2.06	0.84
3:A:310:GLY:HA3	3:A:381:THR:HB	1.56	0.84
1:K:269:SER:HB3	1:K:288:ILE:CD1	2.07	0.84
2:B:274:THR:HB	2:B:279:GLN:CB	2.04	0.84
2:B:286:VAL:HG11	2:B:325:GLU:CB	2.07	0.84
2:B:323:MET:HB2	3:A:221:ARG:CD	2.07	0.84
1:K:17:LYS:CG	1:K:363:PRO:HG2	2.07	0.84
2:B:292:GLN:O	2:B:298:ASN:HB2	1.78	0.84
2:B:12:CYS:SG	2:B:138:SER:HB3	2.17	0.84
3:A:320:ARG:CG	3:A:374:ALA:HB3	2.07	0.84
1:K:224:ALA:HB3	1:K:234:ARG:HG2	1.59	0.84
1:K:293:LEU:HD12	3:A:405:VAL:HG11	1.58	0.84
3:A:24:TYR:HB3	3:A:52:PHE:CD1	2.13	0.84
2:B:293:MET:HE1	2:B:367:PHE:HA	1.58	0.83
3:A:23:LEU:HD12	3:A:363:VAL:CA	2.06	0.83
1:K:234:ARG:NH2	1:K:284:GLU:HG3	1.92	0.83
3:A:36:MET:HE3	3:A:38:SER:HB3	1.59	0.83
3:A:81:GLY:HA3	3:A:83:TYR:CZ	2.12	0.83
3:A:163:LYS:HE3	3:A:164:LYS:H	1.43	0.83
1:K:292:LEU:HD23	4:K:501:MZK:C3	2.07	0.83
2:B:17:GLY:N	2:B:136:THR:HG21	1.93	0.83
2:B:323:MET:HB2	3:A:221:ARG:HG3	1.60	0.83
3:A:71:GLU:HB3	3:A:98:ASP:CG	1.99	0.83
3:A:215:ARG:NH1	3:A:216:ASN:HA	1.93	0.83
3:A:216:ASN:CB	3:A:280:LYS:HD2	2.08	0.83
1:K:162:GLU:CD	1:K:235:SER:CB	2.44	0.83
1:K:269:SER:HB3	1:K:288:ILE:CG1	2.09	0.83
2:B:21:TRP:CD1	2:B:63:ALA:HB2	2.13	0.83
1:K:160:LEU:HG	1:K:171:LEU:CD1	2.07	0.83
1:K:168:LEU:HD12	1:K:182:LEU:HB3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:180:GLU:HG3	1:K:199:LEU:HD13	1.60	0.83
1:K:321:GLN:HA	1:K:324:LEU:HD23	1.59	0.83
2:B:64:ILE:HD12	2:B:119:VAL:HG21	1.61	0.83
3:A:70:LEU:HD13	3:A:145:THR:CG2	2.07	0.83
3:A:125:LEU:O	3:A:128:GLN:HG3	1.78	0.83
3:A:434:GLU:O	3:A:437:VAL:HG22	1.79	0.83
2:B:42:LEU:HA	2:B:45:GLU:OE1	1.79	0.83
2:B:252:LYS:HD2	3:A:101:ASN:CB	2.09	0.83
1:K:94:ILE:HG12	1:K:147:LEU:HD21	1.61	0.83
1:K:26:ARG:HD2	1:K:29:ASN:ND2	1.94	0.83
1:K:140:LEU:HD13	1:K:210:VAL:CG1	2.09	0.83
3:A:387:ALA:HA	3:A:390:ARG:CD	2.09	0.83
1:K:168:LEU:HD13	1:K:182:LEU:HG	1.60	0.82
2:B:10:GLY:H	2:B:147:MET:HE1	1.43	0.82
1:K:322:ASP:O	1:K:326:GLY:HA3	1.79	0.82
2:B:325:GLU:O	2:B:328:GLU:HG3	1.80	0.82
3:A:256:GLN:HA	3:A:259:LEU:CD1	2.08	0.82
3:A:385:ALA:HB1	3:A:429:GLU:OE1	1.79	0.82
1:K:72:PHE:CD1	1:K:76:THR:HG21	2.14	0.82
2:B:273:LEU:HD22	2:B:274:THR:N	1.93	0.82
2:B:327:ASP:HA	2:B:330:MET:SD	2.18	0.82
3:A:19:ALA:HB1	3:A:229:ARG:HH22	1.43	0.82
3:A:273:ALA:HB3	3:A:375:VAL:CG2	2.09	0.82
3:A:286:LEU:CD1	3:A:373:ARG:HG3	2.07	0.82
3:A:317:LEU:HB2	3:A:353:VAL:CB	2.09	0.82
1:K:266:LEU:HD22	1:K:267:ALA:H	1.44	0.82
2:B:139:LEU:HD11	2:B:171:PRO:HD3	1.59	0.82
3:A:23:LEU:HA	3:A:364:PRO:CG	2.08	0.82
3:A:117:LEU:O	3:A:121:ARG:HG3	1.78	0.82
1:K:55:GLY:CA	1:K:60:LYS:HA	2.10	0.82
2:B:139:LEU:CD1	2:B:185:ALA:HB1	2.10	0.82
2:B:379:LYS:HD3	2:B:419:VAL:HB	1.60	0.82
3:A:28:HIS:CE1	3:A:49:PHE:HA	2.15	0.82
3:A:70:LEU:CD1	3:A:145:THR:HG23	2.08	0.82
1:K:55:GLY:HA3	1:K:60:LYS:CE	2.05	0.82
2:B:23:VAL:HA	2:B:26:ASP:OD2	1.79	0.82
2:B:51:TYR:CE1	2:B:61:PRO:HA	2.14	0.82
2:B:222:TYR:O	2:B:225:LEU:HG	1.79	0.82
3:A:286:LEU:HB2	3:A:291:ILE:CG1	2.08	0.82
3:A:320:ARG:CD	3:A:360:PRO:HA	2.10	0.82
3:A:383:ALA:CA	3:A:386:GLU:HG2	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:153:LEU:HD12	3:A:156:ARG:NH1	1.95	0.82
3:A:277:SER:CB	3:A:280:LYS:HG3	2.10	0.82
1:K:41:VAL:CG2	1:K:338:PRO:HA	2.10	0.82
2:B:97:ALA:HB2	2:B:143:THR:HG23	1.61	0.82
2:B:100:ASN:HB3	2:B:401:GLU:OE2	1.79	0.82
2:B:204:ASN:O	2:B:207:LEU:HG	1.80	0.82
2:B:318:ARG:HB3	2:B:358:PRO:HD3	1.60	0.82
3:A:189:LEU:HD22	3:A:418:PHE:HE2	1.42	0.82
3:A:247:ALA:HB3	3:A:355:ILE:CB	2.05	0.82
3:A:251:ASP:CB	3:A:254:GLU:HB3	2.09	0.82
1:K:82:TYR:CE2	1:K:86:VAL:HG11	2.15	0.82
1:K:171:LEU:HB3	1:K:220:LYS:HB3	1.60	0.82
3:A:64:ARG:HH21	3:A:64:ARG:HA	1.45	0.82
2:B:152:ILE:HG13	2:B:192:LEU:CD2	2.09	0.82
2:B:389:PHE:O	2:B:392:LYS:HG3	1.79	0.82
2:B:392:LYS:HB3	2:B:395:LEU:CD1	2.08	0.82
3:A:275:VAL:HB	3:A:300:ASN:HA	1.62	0.82
2:B:67:ASP:OD2	2:B:73:MET:HB3	1.79	0.81
2:B:422:TYR:HA	2:B:425:TYR:CD2	2.15	0.81
3:A:232:SER:HB3	3:A:363:VAL:CG1	2.09	0.81
1:K:329:ARG:CB	1:K:363:PRO:HB3	2.09	0.81
2:B:314:ALA:HB3	2:B:368:ILE:CG1	2.09	0.81
3:A:75:ILE:HG23	3:A:92:LEU:HD11	1.60	0.81
3:A:195:LEU:HD13	3:A:201:ALA:CB	2.10	0.81
2:B:101:TRP:CZ2	2:B:403:MET:HG3	2.15	0.81
2:B:415:MET:O	2:B:419:VAL:HG13	1.79	0.81
3:A:117:LEU:HD22	3:A:117:LEU:H	1.44	0.81
3:A:255:PHE:CZ	3:A:352:LYS:HB3	2.15	0.81
3:A:307:PRO:HD2	3:A:308:ARG:CZ	2.10	0.81
2:B:323:MET:HE1	2:B:326:VAL:HG21	1.63	0.81
3:A:50:ASN:O	3:A:64:ARG:HD3	1.80	0.81
3:A:153:LEU:HD11	3:A:157:LEU:HD11	1.62	0.81
1:K:157:LYS:HB3	1:K:201:GLU:CB	2.09	0.81
1:K:227:LEU:HG	1:K:228:MET:HE3	1.60	0.81
3:A:3:GLU:HA	3:A:51:THR:HA	1.61	0.81
3:A:107:HIS:HB2	3:A:148:GLY:CA	2.09	0.81
3:A:135:PHE:CE1	3:A:166:LYS:HA	2.16	0.81
3:A:154:MET:HE1	3:A:166:LYS:CE	2.09	0.81
3:A:242:LEU:HD23	3:A:252:LEU:CG	2.10	0.81
3:A:319:TYR:HB3	3:A:355:ILE:HG23	1.61	0.81
2:B:65:LEU:HD13	2:B:90:PHE:HB3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:LYS:NZ	3:A:222:PRO:N	2.29	0.81
3:A:41:THR:CG2	3:A:49:PHE:HB2	2.11	0.81
3:A:310:GLY:HA3	3:A:381:THR:CG2	2.11	0.81
1:K:246:LYS:CE	1:K:254:GLU:OE2	2.27	0.81
2:B:260:PHE:CZ	3:A:404:PHE:HA	2.15	0.81
3:A:279:GLU:HB3	3:A:283:HIS:CE1	2.15	0.81
1:K:181:ARG:NH2	1:K:197:LYS:CD	2.43	0.81
3:A:204:VAL:CG2	3:A:209:ILE:HD12	2.11	0.81
3:A:256:GLN:HA	3:A:259:LEU:HG	1.61	0.81
3:A:320:ARG:HG3	3:A:374:ALA:CB	2.09	0.81
1:K:47:ARG:NH1	1:K:47:ARG:HA	1.96	0.81
1:K:68:PHE:HB2	1:K:71:VAL:CG2	2.11	0.81
2:B:362:LYS:HA	2:B:362:LYS:HE3	1.61	0.81
3:A:45:GLY:HA2	3:A:49:PHE:CD2	2.15	0.81
3:A:84:ARG:HH11	3:A:85:GLN:HB3	1.45	0.81
3:A:205:ASP:CB	3:A:208:ALA:HB3	2.10	0.81
3:A:268:PRO:CB	3:A:378:LEU:HB3	2.09	0.81
3:A:318:LEU:HD11	3:A:320:ARG:HG2	1.62	0.81
1:K:77:LYS:NZ	1:K:78:GLN:HG3	1.95	0.81
1:K:304:GLU:CG	1:K:306:THR:HB	2.10	0.81
2:B:154:LYS:CE	2:B:157:GLU:HB3	2.11	0.81
2:B:262:ARG:HD3	2:B:262:ARG:H	1.45	0.81
3:A:48:SER:CB	3:A:243:ARG:HD3	2.08	0.81
3:A:81:GLY:O	3:A:84:ARG:HB3	1.81	0.81
3:A:212:ILE:O	3:A:215:ARG:HG3	1.81	0.81
3:A:344:VAL:HG23	3:A:347:CYS:H	1.46	0.81
1:K:144:PHE:CD2	1:K:207:LYS:HA	2.16	0.80
1:K:199:LEU:HD12	1:K:200:GLU:H	1.44	0.80
2:B:140:GLY:HA2	2:B:185:ALA:HB2	1.63	0.80
2:B:326:VAL:CG1	2:B:330:MET:HE1	2.07	0.80
2:B:421:GLU:HG3	2:B:425:TYR:CE1	2.14	0.80
3:A:5:ILE:HG23	3:A:65:ALA:HA	1.62	0.80
1:K:258:ILE:O	1:K:368:LYS:HE2	1.81	0.80
2:B:278:SER:HA	2:B:282:ARG:HH11	1.45	0.80
3:A:392:ASP:OD2	3:A:422:ARG:HD3	1.80	0.80
1:K:212:GLN:O	1:K:216:LYS:HG2	1.82	0.80
2:B:350:LYS:HE3	3:A:179:THR:CG2	2.10	0.80
2:B:280:GLN:HG3	2:B:281:TYR:CD1	2.16	0.80
2:B:285:THR:CG2	2:B:288:GLU:HB2	2.11	0.80
2:B:372:THR:HA	2:B:375:GLN:OE1	1.80	0.80
1:K:171:LEU:HD13	1:K:221:ARG:CA	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:TRP:HA	2:B:146:GLY:CA	2.11	0.80
2:B:144:GLY:HA2	2:B:147:MET:SD	2.22	0.80
2:B:152:ILE:HA	2:B:155:ILE:HD11	1.63	0.80
2:B:214:THR:HB	2:B:276:ARG:N	1.96	0.80
2:B:269:GLY:CA	2:B:367:PHE:HB3	2.10	0.80
2:B:342:VAL:HA	2:B:429:THR:C	2.02	0.80
3:A:313:MET:HA	3:A:344:VAL:CG2	2.11	0.80
1:K:177:ASP:HB2	1:K:179:SER:O	1.81	0.80
1:K:180:GLU:O	1:K:182:LEU:HD22	1.81	0.80
2:B:258:VAL:HG12	2:B:263:LEU:CD1	2.11	0.80
3:A:7:ILE:CG2	3:A:137:VAL:HA	2.12	0.80
3:A:277:SER:HB3	3:A:280:LYS:HG3	1.62	0.80
1:K:29:ASN:CB	1:K:32:GLU:HG2	2.12	0.80
3:A:156:ARG:NH1	3:A:156:ARG:HB3	1.96	0.80
3:A:237:SER:HA	3:A:320:ARG:NH1	1.96	0.80
2:B:242:PHE:CE2	2:B:356:ILE:HD11	2.16	0.80
2:B:322:SER:HB3	2:B:325:GLU:HG3	1.63	0.80
3:A:229:ARG:HA	3:A:229:ARG:CZ	2.12	0.80
2:B:51:TYR:CD2	2:B:59:TYR:HB3	2.16	0.80
2:B:272:PRO:HB2	2:B:279:GLN:HE22	1.44	0.80
2:B:276:ARG:HG3	2:B:277:GLY:N	1.95	0.80
3:A:35:GLN:HB2	3:A:60:LYS:HE2	1.63	0.80
3:A:269:LEU:HD23	3:A:384:ILE:CD1	2.12	0.80
1:K:140:LEU:HD13	1:K:210:VAL:HG12	1.61	0.79
1:K:320:LEU:CD1	1:K:323:SER:HB2	2.12	0.79
3:A:215:ARG:HH11	3:A:216:ASN:HD22	1.27	0.79
3:A:46:ASP:OD1	3:A:48:SER:HB3	1.83	0.79
3:A:63:PRO:HG3	3:A:86:LEU:HD21	1.64	0.79
3:A:431:ASP:HA	3:A:434:GLU:OE2	1.81	0.79
2:B:276:ARG:HD2	2:B:280:GLN:NE2	1.98	0.79
3:A:231:ILE:O	3:A:234:ILE:HG13	1.81	0.79
3:A:242:LEU:CD2	3:A:252:LEU:HG	2.09	0.79
1:K:266:LEU:HD22	1:K:267:ALA:N	1.98	0.79
1:K:274:ARG:NH1	1:K:274:ARG:HA	1.96	0.79
1:K:281:ARG:O	1:K:284:GLU:HG2	1.82	0.79
3:A:121:ARG:O	3:A:124:LYS:HG3	1.83	0.79
2:B:45:GLU:HB2	2:B:46:ARG:HH21	1.46	0.79
2:B:102:ALA:HB3	2:B:401:GLU:CD	2.03	0.79
3:A:192:HIS:CE1	3:A:421:ALA:HB2	2.17	0.79
3:A:217:LEU:HB3	3:A:219:ILE:CG1	2.12	0.79
3:A:278:ALA:HB1	3:A:282:TYR:OH	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:288:VAL:HG21	3:A:327:ASP:HB3	1.64	0.79
1:K:28:PHE:HB3	1:K:33:ARG:NE	1.98	0.79
1:K:31:ALA:HB1	1:K:34:LYS:HE2	1.65	0.79
2:B:178:THR:HG23	2:B:181:GLU:N	1.98	0.79
2:B:318:ARG:HG2	2:B:354:CYS:HB2	1.65	0.79
3:A:8:HIS:CD2	3:A:17:GLY:HA3	2.18	0.79
1:K:40:ILE:HG12	1:K:338:PRO:O	1.80	0.79
2:B:46:ARG:O	2:B:49:VAL:HG22	1.83	0.79
2:B:151:LEU:HD12	2:B:152:ILE:N	1.98	0.79
3:A:31:GLN:HB3	3:A:33:ASP:OD2	1.83	0.79
3:A:45:GLY:HA2	3:A:49:PHE:HD2	1.48	0.79
3:A:79:ARG:CZ	3:A:92:LEU:HG	2.13	0.79
3:A:311:LYS:HA	3:A:342:GLN:CG	2.11	0.79
1:K:95:MET:HE1	1:K:97:TYR:HB2	1.62	0.79
2:B:321:MET:HG2	2:B:322:SER:O	1.83	0.79
2:B:321:MET:CG	2:B:325:GLU:HB2	2.13	0.79
3:A:140:SER:HA	3:A:171:ILE:HG22	1.63	0.79
3:A:240:ALA:HA	3:A:243:ARG:HG2	1.62	0.79
2:B:117:LEU:O	2:B:121:ARG:HG2	1.82	0.79
2:B:309:ARG:CB	2:B:426:GLN:HA	2.10	0.79
2:B:316:VAL:N	2:B:366:THR:HG22	1.97	0.79
2:B:350:LYS:NZ	3:A:179:THR:HA	1.97	0.79
2:B:416:ASN:O	2:B:419:VAL:HG22	1.83	0.79
3:A:246:GLY:CA	3:A:356:ASN:HA	2.10	0.79
3:A:287:SER:CB	3:A:290:GLU:HG3	2.13	0.79
1:K:233:SER:OG	1:K:267:ALA:HA	1.82	0.79
2:B:215:LEU:O	2:B:276:ARG:HG2	1.83	0.79
3:A:8:HIS:NE2	3:A:17:GLY:HA3	1.98	0.79
1:K:95:MET:HE2	1:K:97:TYR:CD2	2.18	0.78
3:A:30:ILE:CA	3:A:36:MET:HB3	2.07	0.78
3:A:213:CYS:O	3:A:217:LEU:HG	1.83	0.78
3:A:216:ASN:CG	3:A:280:LYS:HD2	2.04	0.78
1:K:158:VAL:C	1:K:201:GLU:HG2	2.03	0.78
1:K:173:ASN:HB3	1:K:175:SER:OG	1.82	0.78
2:B:156:ARG:HH21	2:B:157:GLU:HA	1.47	0.78
2:B:341:PHE:CE2	2:B:346:PRO:HA	2.17	0.78
2:B:376:GLU:O	2:B:379:LYS:HG2	1.82	0.78
3:A:344:VAL:HB	3:A:346:TRP:HD1	1.43	0.78
1:K:339:ALA:HB1	1:K:341:LEU:HD13	1.62	0.78
2:B:103:LYS:NZ	2:B:103:LYS:HA	1.98	0.78
2:B:139:LEU:HD21	2:B:170:VAL:HG12	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:88:HIS:HB2	3:A:91:GLN:HE22	1.48	0.78
3:A:320:ARG:NE	3:A:360:PRO:HA	1.99	0.78
3:A:431:ASP:HA	3:A:434:GLU:CD	2.04	0.78
1:K:155:SER:CB	1:K:203:THR:HG21	2.05	0.78
2:B:293:MET:HA	2:B:298:ASN:CG	2.03	0.78
3:A:184:PRO:O	3:A:188:ILE:HD13	1.82	0.78
1:K:190:ASN:HB3	1:K:193:GLY:CA	2.13	0.78
2:B:33:THR:HG23	2:B:35:SER:N	1.97	0.78
2:B:103:LYS:HD2	2:B:401:GLU:HG2	1.65	0.78
2:B:246:LEU:HD12	2:B:352:ALA:CA	2.12	0.78
2:B:293:MET:HE3	2:B:367:PHE:HB2	1.64	0.78
3:A:30:ILE:HD11	3:A:34:GLY:O	1.83	0.78
3:A:56:THR:HG22	3:A:57:GLY:H	1.46	0.78
3:A:243:ARG:HD2	3:A:244:PHE:CD2	2.18	0.78
3:A:388:TRP:HB2	3:A:425:MET:CE	2.14	0.78
1:K:311:TYR:HE1	1:K:324:LEU:HG	1.47	0.78
2:B:120:VAL:HG23	2:B:121:ARG:NE	1.97	0.78
3:A:320:ARG:NH1	3:A:361:THR:HG23	1.99	0.78
3:A:383:ALA:HA	3:A:386:GLU:CG	2.13	0.78
1:K:144:PHE:HB2	1:K:207:LYS:HZ3	1.49	0.78
1:K:257:LYS:HA	1:K:368:LYS:HD3	1.65	0.78
2:B:103:LYS:HG2	2:B:401:GLU:OE2	1.84	0.78
2:B:172:SER:CB	2:B:205:GLU:HB3	2.13	0.78
3:A:320:ARG:HH12	3:A:361:THR:HG23	1.48	0.78
2:B:324:LYS:HE3	3:A:222:PRO:HD2	1.64	0.78
3:A:70:LEU:HG	3:A:110:ILE:CG2	2.13	0.78
3:A:320:ARG:HB2	3:A:360:PRO:HG3	1.64	0.78
3:A:320:ARG:HD3	3:A:360:PRO:HA	1.66	0.78
1:K:227:LEU:HD23	1:K:227:LEU:H	1.48	0.78
2:B:211:CYS:SG	2:B:220:PRO:HB3	2.24	0.78
2:B:376:GLU:HB3	2:B:380:ARG:NH1	1.98	0.78
3:A:8:HIS:HB3	3:A:13:GLY:C	2.03	0.78
3:A:328:VAL:O	3:A:332:ILE:HG12	1.82	0.78
3:A:339:ARG:HG3	3:A:340:SER:N	1.97	0.78
1:K:347:LEU:HD23	1:K:351:GLU:HG2	1.66	0.78
2:B:139:LEU:HD23	2:B:168:SER:HB2	1.65	0.78
2:B:316:VAL:O	2:B:365:ALA:HA	1.82	0.78
2:B:324:LYS:N	3:A:221:ARG:HG2	1.99	0.78
3:A:84:ARG:NH1	3:A:85:GLN:HB3	1.99	0.78
1:K:55:GLY:HA2	1:K:59:ASP:O	1.83	0.77
3:A:9:VAL:HG11	3:A:146:GLY:HA2	1.63	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:171:ILE:HA	3:A:204:VAL:CG1	2.14	0.77
3:A:185:TYR:CZ	3:A:398:MET:HB3	2.18	0.77
3:A:288:VAL:HG21	3:A:327:ASP:CB	2.14	0.77
3:A:208:ALA:O	3:A:212:ILE:HG12	1.84	0.77
3:A:286:LEU:HB2	3:A:291:ILE:HG12	1.65	0.77
3:A:287:SER:OG	3:A:290:GLU:HG3	1.82	0.77
3:A:306:ASP:HB2	3:A:309:HIS:CG	2.19	0.77
3:A:310:GLY:HA3	3:A:381:THR:CB	2.13	0.77
1:K:192:ARG:HB2	1:K:322:ASP:OD1	1.84	0.77
1:K:354:HIS:O	1:K:357:LYS:HG2	1.84	0.77
2:B:43:GLN:O	2:B:47:ILE:HG12	1.82	0.77
2:B:154:LYS:HE2	2:B:154:LYS:HA	1.67	0.77
2:B:208:TYR:CE2	2:B:220:PRO:HB2	2.19	0.77
3:A:56:THR:C	3:A:58:ALA:HA	2.03	0.77
1:K:246:LYS:HE3	1:K:254:GLU:OE1	1.83	0.77
2:B:12:CYS:SG	2:B:16:ILE:HD11	2.24	0.77
2:B:46:ARG:HA	2:B:46:ARG:CZ	2.15	0.77
2:B:148:GLY:HA2	2:B:151:LEU:CD2	2.14	0.77
3:A:176:GLN:HE21	3:A:207:GLU:HA	1.48	0.77
3:A:247:ALA:HA	3:A:357:TYR:CE1	2.20	0.77
3:A:402:ARG:HD2	3:A:415:GLU:OE1	1.84	0.77
1:K:274:ARG:HA	1:K:274:ARG:CZ	2.14	0.77
2:B:15:GLN:O	2:B:19:LYS:HG2	1.85	0.77
2:B:70:PRO:HB3	2:B:92:PHE:HE2	1.50	0.77
2:B:314:ALA:O	2:B:368:ILE:HG12	1.84	0.77
3:A:69:ASP:OD2	3:A:71:GLU:HG2	1.84	0.77
3:A:256:GLN:HA	3:A:259:LEU:CG	2.15	0.77
3:A:313:MET:HE2	3:A:344:VAL:CG1	2.13	0.77
2:B:41:ASP:CA	2:B:44:LEU:HD23	2.07	0.77
2:B:159:TYR:HB2	2:B:162:ARG:HG2	1.66	0.77
2:B:375:GLN:OE1	2:B:422:TYR:HB3	1.83	0.77
3:A:278:ALA:HA	3:A:368:LEU:CA	2.11	0.77
2:B:139:LEU:HD12	2:B:185:ALA:HB1	1.65	0.77
2:B:190:HIS:CE1	2:B:411:ALA:HA	2.20	0.77
2:B:213:ARG:NH1	2:B:213:ARG:HB2	2.00	0.77
2:B:277:GLY:HA2	2:B:280:GLN:NE2	1.99	0.77
2:B:303:CYS:SG	2:B:371:SER:HB3	2.25	0.77
3:A:6:SER:HB3	3:A:138:PHE:CZ	2.19	0.77
3:A:84:ARG:HD2	3:A:85:GLN:N	1.99	0.77
3:A:119:LEU:HD12	3:A:120:ASP:N	1.98	0.77
3:A:384:ILE:HD11	3:A:432:TYR:CE2	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:TYR:CZ	2:B:61:PRO:HA	2.20	0.77
2:B:65:LEU:H	2:B:90:PHE:HB2	1.47	0.77
2:B:381:ILE:HA	2:B:384:GLN:CD	2.04	0.77
3:A:31:GLN:HB2	3:A:37:PRO:CD	2.14	0.77
3:A:166:LYS:HG2	3:A:199:ASP:OD2	1.85	0.77
3:A:281:ALA:CB	3:A:369:ALA:HB3	2.15	0.77
3:A:286:LEU:HD12	3:A:286:LEU:O	1.84	0.77
2:B:159:TYR:CD2	2:B:162:ARG:HG2	2.20	0.77
2:B:214:THR:O	2:B:216:LYS:HD2	1.85	0.77
2:B:376:GLU:HG3	2:B:379:LYS:NZ	2.00	0.77
3:A:30:ILE:HA	3:A:36:MET:CB	2.09	0.77
3:A:154:MET:CG	3:A:197:HIS:HB2	2.15	0.77
2:B:263:LEU:HD11	2:B:265:PHE:O	1.86	0.77
2:B:342:VAL:HB	2:B:348:ASN:HD21	1.50	0.77
2:B:414:ASN:O	2:B:418:LEU:HD23	1.84	0.77
3:A:64:ARG:N	3:A:64:ARG:HD2	2.00	0.77
3:A:103:TYR:HE2	3:A:151:SER:HB3	1.50	0.77
1:K:257:LYS:HD3	1:K:367:GLN:HE22	1.50	0.76
1:K:290:GLN:NE2	3:A:410:GLY:HA3	1.98	0.76
3:A:152:LEU:HA	3:A:155:GLU:OE1	1.85	0.76
3:A:273:ALA:CB	3:A:295:CYS:HB2	2.15	0.76
1:K:135:ILE:HD12	1:K:136:ILE:N	2.00	0.76
1:K:155:SER:HB3	1:K:203:THR:CG2	2.05	0.76
1:K:256:VAL:O	1:K:368:LYS:HB2	1.85	0.76
2:B:5:VAL:HA	2:B:62:ARG:HG3	1.66	0.76
2:B:6:HIS:O	2:B:63:ALA:HA	1.84	0.76
2:B:105:HIS:CE1	2:B:150:LEU:HD23	2.20	0.76
2:B:413:SER:HA	2:B:416:ASN:ND2	2.00	0.76
3:A:78:VAL:HA	3:A:83:TYR:HE1	1.49	0.76
3:A:189:LEU:HD13	3:A:418:PHE:HD2	1.46	0.76
3:A:320:ARG:HB2	3:A:374:ALA:N	2.00	0.76
3:A:360:PRO:HB3	3:A:374:ALA:HB2	1.67	0.76
1:K:26:ARG:CG	1:K:109:THR:HA	2.15	0.76
1:K:345:GLU:O	1:K:349:THR:HG23	1.86	0.76
2:B:145:SER:OG	2:B:185:ALA:HA	1.85	0.76
2:B:183:TYR:HA	2:B:385:PHE:CE1	2.20	0.76
2:B:331:LEU:HA	2:B:334:GLN:NE2	2.00	0.76
3:A:214:ARG:CZ	3:A:215:ARG:HA	2.16	0.76
1:K:15:LYS:HE2	1:K:362:LYS:HE2	1.68	0.76
1:K:96:GLY:O	1:K:366:ASN:HB2	1.86	0.76
2:B:324:LYS:CG	3:A:221:ARG:HG2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:LYS:CA	3:A:221:ARG:HG2	2.16	0.76
3:A:23:LEU:CD1	3:A:363:VAL:HA	2.11	0.76
3:A:26:LEU:CD2	3:A:364:PRO:HB3	2.15	0.76
3:A:306:ASP:HA	3:A:308:ARG:HH21	1.51	0.76
3:A:315:CYS:HA	3:A:378:LEU:O	1.84	0.76
3:A:317:LEU:HD23	3:A:377:MET:HG3	1.66	0.76
1:K:312:ARG:CA	1:K:318:ARG:HD2	2.16	0.76
1:K:365:VAL:CG1	1:K:367:GLN:HG2	2.14	0.76
2:B:212:PHE:HB2	2:B:220:PRO:CD	2.15	0.76
3:A:262:TYR:HE2	3:A:435:VAL:HG23	1.50	0.76
1:K:289:ASN:ND2	3:A:409:VAL:HG13	1.99	0.76
2:B:3:GLU:CD	2:B:50:TYR:HA	2.06	0.76
2:B:20:PHE:CE1	2:B:24:ILE:HD11	2.20	0.76
2:B:97:ALA:HB3	2:B:143:THR:CA	2.16	0.76
2:B:251:ARG:NE	3:A:100:ALA:HB3	1.99	0.76
2:B:327:ASP:O	2:B:330:MET:HG2	1.86	0.76
3:A:103:TYR:HB2	3:A:147:SER:CB	2.16	0.76
3:A:326:LYS:HA	3:A:329:ASN:ND2	2.00	0.76
1:K:31:ALA:HB1	1:K:34:LYS:CE	2.16	0.76
1:K:92:GLU:O	1:K:97:TYR:HB2	1.84	0.76
2:B:308:GLY:HA2	2:B:372:THR:H	1.51	0.76
2:B:377:LEU:HD12	2:B:377:LEU:O	1.86	0.76
3:A:386:GLU:O	3:A:390:ARG:HG3	1.86	0.76
1:K:32:GLU:HB3	1:K:33:ARG:HH21	1.50	0.76
1:K:156:VAL:N	1:K:203:THR:HG23	2.01	0.76
2:B:140:GLY:CA	2:B:171:PRO:HG3	2.15	0.76
3:A:273:ALA:HB2	3:A:295:CYS:HB2	1.68	0.76
1:K:114:THR:O	1:K:135:ILE:HG23	1.86	0.76
2:B:147:MET:HG2	2:B:148:GLY:N	2.00	0.76
3:A:17:GLY:HA2	3:A:20:CYS:SG	2.25	0.76
3:A:174:ALA:HB2	3:A:207:GLU:H	1.50	0.76
3:A:214:ARG:HG2	3:A:221:ARG:HH12	1.49	0.76
3:A:370:LYS:NZ	3:A:372:GLN:HA	2.01	0.76
2:B:217:LEU:HD12	2:B:219:THR:O	1.85	0.76
2:B:253:LEU:HD12	2:B:254:ALA:N	2.01	0.76
3:A:154:MET:HE2	3:A:154:MET:O	1.86	0.76
3:A:174:ALA:HB1	3:A:207:GLU:CB	2.16	0.76
3:A:396:ASP:HA	3:A:422:ARG:NH2	2.00	0.76
1:K:159:SER:HA	1:K:172:LEU:CD1	2.08	0.75
2:B:210:ILE:O	2:B:213:ARG:HG3	1.85	0.75
2:B:324:LYS:N	3:A:221:ARG:CG	2.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:31:GLN:HG2	3:A:32:PRO:CD	2.14	0.75
3:A:53:PHE:HB3	3:A:62:VAL:C	2.07	0.75
3:A:319:TYR:CB	3:A:355:ILE:HG23	2.15	0.75
3:A:321:GLY:HA3	3:A:372:GLN:HE21	1.50	0.75
1:K:289:ASN:HD22	3:A:409:VAL:CG1	2.00	0.75
2:B:137:HIS:O	2:B:168:SER:HA	1.85	0.75
2:B:323:MET:HB2	3:A:221:ARG:CG	2.15	0.75
3:A:163:LYS:HE3	3:A:164:LYS:N	2.01	0.75
3:A:391:LEU:HA	3:A:394:LYS:HE2	1.68	0.75
2:B:149:THR:CG2	2:B:188:SER:HA	2.17	0.75
2:B:183:TYR:O	2:B:186:THR:HG22	1.86	0.75
3:A:9:VAL:HB	3:A:139:HIS:HB2	1.68	0.75
2:B:122:LYS:HA	2:B:125:GLU:OE1	1.86	0.75
2:B:203:ASP:OD2	2:B:301:ALA:HA	1.87	0.75
3:A:176:GLN:CG	3:A:207:GLU:HB2	2.14	0.75
3:A:282:TYR:HE1	3:A:369:ALA:HB2	1.49	0.75
3:A:390:ARG:HA	3:A:393:HIS:CD2	2.21	0.75
2:B:101:TRP:CD1	2:B:149:THR:HG21	2.21	0.75
3:A:35:GLN:CB	3:A:60:LYS:HE2	2.17	0.75
3:A:119:LEU:O	3:A:122:ILE:HG13	1.85	0.75
3:A:189:LEU:HD22	3:A:418:PHE:CE2	2.21	0.75
2:B:46:ARG:CB	2:B:241:ARG:HD3	2.16	0.75
2:B:103:LYS:NZ	2:B:401:GLU:HA	2.01	0.75
2:B:156:ARG:HH12	2:B:160:PRO:HA	1.50	0.75
3:A:396:ASP:HA	3:A:422:ARG:CZ	2.17	0.75
2:B:178:THR:OG1	2:B:180:VAL:HG22	1.87	0.75
2:B:217:LEU:HD13	2:B:218:THR:N	2.01	0.75
3:A:55:GLU:HG2	3:A:61:HIS:CD2	2.21	0.75
1:K:168:LEU:HB3	1:K:182:LEU:HD23	1.69	0.75
3:A:96:LYS:O	3:A:96:LYS:HD3	1.86	0.75
3:A:381:THR:O	3:A:384:ILE:HG12	1.86	0.75
3:A:211:ASP:O	3:A:214:ARG:HG3	1.87	0.74
1:K:15:LYS:CE	1:K:362:LYS:HE2	2.17	0.74
2:B:2:ARG:HG3	2:B:131:GLN:N	2.02	0.74
2:B:81:PHE:O	2:B:84:ILE:HG22	1.86	0.74
2:B:345:ILE:HD12	3:A:181:VAL:HG13	1.69	0.74
2:B:367:PHE:O	2:B:368:ILE:HD13	1.86	0.74
3:A:331:ALA:O	3:A:335:ILE:HG12	1.87	0.74
1:K:34:LYS:HG2	1:K:35:ALA:N	2.01	0.74
1:K:171:LEU:HA	1:K:220:LYS:HD3	1.69	0.74
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:LEU:HD11	2:B:151:LEU:CB	2.17	0.74
2:B:112:LEU:CD1	2:B:151:LEU:HB3	2.18	0.74
2:B:272:PRO:HG3	2:B:284:LEU:HD11	1.69	0.74
2:B:308:GLY:CA	2:B:372:THR:H	1.99	0.74
1:K:187:ASP:HB2	1:K:189:ARG:HD3	1.69	0.74
3:A:30:ILE:CD1	3:A:61:HIS:HB2	2.17	0.74
3:A:214:ARG:NH1	3:A:215:ARG:HA	2.02	0.74
3:A:256:GLN:HA	3:A:259:LEU:HD12	1.67	0.74
3:A:288:VAL:O	3:A:292:THR:HG23	1.87	0.74
3:A:324:VAL:HG21	3:A:326:LYS:HZ1	1.51	0.74
3:A:326:LYS:HA	3:A:329:ASN:HD22	1.53	0.74
1:K:77:LYS:HG3	1:K:79:ILE:HG22	1.69	0.74
1:K:191:LYS:H	1:K:191:LYS:HZ2	1.36	0.74
2:B:20:PHE:HA	2:B:230:SER:CB	2.16	0.74
2:B:186:THR:CG2	2:B:187:LEU:HD22	2.18	0.74
2:B:381:ILE:HA	2:B:384:GLN:NE2	2.01	0.74
3:A:171:ILE:CA	3:A:204:VAL:HG12	2.15	0.74
1:K:95:MET:HE2	1:K:97:TYR:HB2	0.76	0.74
1:K:95:MET:HG2	1:K:97:TYR:H	1.52	0.74
1:K:97:TYR:CE1	1:K:329:ARG:HB2	2.22	0.74
2:B:2:ARG:HA	2:B:129:CYS:O	1.87	0.74
2:B:71:GLY:HA2	2:B:74:ASP:OD1	1.86	0.74
2:B:181:GLU:HB3	2:B:182:PRO:HD3	1.69	0.74
2:B:259:PRO:O	3:A:403:ALA:HB1	1.87	0.74
2:B:337:ASN:HB3	2:B:340:TYR:HB2	1.68	0.74
3:A:174:ALA:HB1	3:A:207:GLU:HB2	1.70	0.74
3:A:321:GLY:CA	3:A:359:PRO:HA	2.18	0.74
1:K:157:LYS:HG2	1:K:203:THR:CA	2.18	0.74
3:A:175:PRO:HG2	3:A:304:LYS:CE	2.18	0.74
3:A:245:ASP:HA	3:A:249:ASN:HB2	1.70	0.74
3:A:381:THR:OG1	3:A:384:ILE:HG23	1.87	0.74
1:K:68:PHE:HB2	1:K:71:VAL:HG22	1.68	0.74
3:A:90:GLU:HA	3:A:121:ARG:HH21	1.51	0.74
3:A:276:ILE:CG2	3:A:281:ALA:HB2	2.18	0.74
1:K:54:THR:C	1:K:60:LYS:HG3	2.08	0.74
2:B:3:GLU:HG3	2:B:50:TYR:HA	1.69	0.74
2:B:121:ARG:HB2	2:B:122:LYS:HZ3	1.52	0.74
3:A:116:ASP:HA	3:A:119:LEU:CD2	2.16	0.74
3:A:181:VAL:HG11	3:A:404:PHE:CD1	2.23	0.74
1:K:160:LEU:H	1:K:172:LEU:HB3	1.51	0.74
2:B:336:LYS:HA	2:B:336:LYS:HE3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:78:VAL:HA	3:A:83:TYR:CE1	2.21	0.74
1:K:16:GLY:CA	1:K:362:LYS:HA	2.15	0.73
2:B:43:GLN:HA	2:B:242:PHE:HZ	1.52	0.73
2:B:284:LEU:HD13	2:B:289:LEU:CG	2.18	0.73
1:K:95:MET:O	1:K:367:GLN:HA	1.88	0.73
2:B:330:MET:CG	2:B:331:LEU:HD13	2.17	0.73
3:A:86:LEU:HD12	3:A:86:LEU:O	1.88	0.73
3:A:210:TYR:CE1	3:A:227:LEU:HB2	2.23	0.73
1:K:146:LYS:HA	1:K:149:ASP:OD2	1.88	0.73
1:K:173:ASN:HB2	1:K:176:SER:CB	2.18	0.73
1:K:312:ARG:HA	1:K:318:ARG:HG2	1.68	0.73
2:B:112:LEU:HD13	2:B:150:LEU:HD12	1.70	0.73
2:B:46:ARG:HH12	2:B:49:VAL:HG11	1.51	0.73
2:B:424:GLN:NE2	2:B:427:ASP:HB2	2.03	0.73
3:A:430:LYS:HZ2	3:A:433:GLU:HB3	1.51	0.73
1:K:17:LYS:N	1:K:363:PRO:HD2	2.03	0.73
1:K:95:MET:CE	1:K:97:TYR:CB	2.31	0.73
2:B:100:ASN:CB	2:B:103:LYS:HB2	2.17	0.73
3:A:185:TYR:HA	3:A:395:PHE:CE2	2.22	0.73
1:K:181:ARG:HH21	1:K:197:LYS:HG2	1.48	0.73
2:B:375:GLN:CD	2:B:422:TYR:HB3	2.08	0.73
3:A:67:PHE:HB2	3:A:92:LEU:CD1	2.19	0.73
3:A:210:TYR:CD1	3:A:227:LEU:HD13	2.24	0.73
3:A:276:ILE:CG1	3:A:371:VAL:HG11	2.17	0.73
2:B:21:TRP:HA	2:B:21:TRP:HE3	1.53	0.73
2:B:215:LEU:HD22	2:B:217:LEU:CB	2.18	0.73
2:B:215:LEU:HD13	2:B:217:LEU:CB	2.18	0.73
1:K:181:ARG:HH22	1:K:197:LYS:HE2	1.54	0.73
2:B:5:VAL:HA	2:B:62:ARG:CG	2.18	0.73
2:B:23:VAL:HG11	2:B:230:SER:OG	1.88	0.73
2:B:65:LEU:HB2	2:B:90:PHE:CD1	2.24	0.73
2:B:288:GLU:HG2	2:B:291:GLN:OE1	1.88	0.73
2:B:308:GLY:HA2	2:B:372:THR:HB	1.69	0.73
3:A:8:HIS:CB	3:A:14:VAL:HA	2.19	0.73
3:A:20:CYS:HB3	3:A:24:TYR:OH	1.88	0.73
3:A:60:LYS:HD3	3:A:61:HIS:H	1.52	0.73
3:A:226:ASN:HA	3:A:229:ARG:CG	2.17	0.73
3:A:313:MET:HA	3:A:344:VAL:CG1	2.19	0.73
3:A:316:CYS:O	3:A:377:MET:HA	1.89	0.73
1:K:258:ILE:H	1:K:368:LYS:CE	2.02	0.73
2:B:122:LYS:HA	2:B:125:GLU:CD	2.08	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:THR:O	2:B:375:GLN:HG2	1.89	0.73
2:B:392:LYS:HA	2:B:395:LEU:HD21	1.71	0.73
3:A:263:PRO:HD2	3:A:264:ARG:HD3	1.70	0.73
1:K:78:GLN:NE2	1:K:113:PHE:CD2	2.57	0.73
1:K:162:GLU:HG3	1:K:235:SER:HB2	1.66	0.73
2:B:324:LYS:NZ	3:A:221:ARG:CD	2.50	0.73
3:A:35:GLN:N	3:A:60:LYS:HE2	2.04	0.73
3:A:243:ARG:HG3	3:A:244:PHE:N	2.04	0.73
2:B:41:ASP:CG	2:B:42:LEU:HD22	2.10	0.72
2:B:190:HIS:NE2	2:B:411:ALA:HA	2.04	0.72
3:A:205:ASP:OD2	3:A:303:VAL:HG23	1.89	0.72
3:A:277:SER:H	3:A:280:LYS:CB	1.99	0.72
1:K:26:ARG:HB3	1:K:109:THR:HA	1.70	0.72
2:B:250:LEU:HD12	2:B:253:LEU:CD1	2.05	0.72
3:A:5:ILE:H	3:A:132:LEU:CD2	2.02	0.72
3:A:8:HIS:HB3	3:A:14:VAL:N	2.03	0.72
3:A:200:CYS:HA	3:A:266:HIS:CB	1.99	0.72
3:A:306:ASP:HA	3:A:308:ARG:NH2	2.04	0.72
3:A:387:ALA:HA	3:A:390:ARG:NE	2.05	0.72
1:K:147:LEU:O	1:K:150:ASN:HB2	1.89	0.72
1:K:162:GLU:CD	1:K:223:THR:HG22	2.10	0.72
2:B:141:GLY:HA3	5:B:501:G2P:O5'	1.89	0.72
3:A:21:TRP:CZ2	3:A:65:ALA:HB2	2.24	0.72
3:A:132:LEU:HB3	3:A:134:GLY:O	1.89	0.72
2:B:103:LYS:O	2:B:107:THR:HG22	1.88	0.72
2:B:363:MET:H	2:B:363:MET:HE3	1.54	0.72
3:A:188:ILE:HB	3:A:395:PHE:CD1	2.24	0.72
1:K:105:GLY:HA3	1:K:335:THR:OG1	1.89	0.72
1:K:311:TYR:CD2	1:K:321:GLN:HG3	2.24	0.72
2:B:12:CYS:CB	2:B:138:SER:HB3	2.19	0.72
1:K:344:GLU:CB	3:A:414:GLU:HG2	2.12	0.72
2:B:97:ALA:HA	2:B:104:GLY:HA3	1.70	0.72
3:A:164:LYS:HA	3:A:164:LYS:CE	2.19	0.72
1:K:15:LYS:CD	1:K:362:LYS:HB3	2.19	0.72
3:A:205:ASP:HB3	3:A:208:ALA:HB3	1.71	0.72
1:K:23:VAL:HG21	1:K:68:PHE:CE1	2.24	0.72
1:K:171:LEU:HA	1:K:220:LYS:CD	2.20	0.72
1:K:181:ARG:HH22	1:K:197:LYS:CE	2.00	0.72
2:B:190:HIS:O	2:B:193:VAL:HG12	1.90	0.72
2:B:285:THR:H	2:B:288:GLU:HB2	1.55	0.72
3:A:388:TRP:HB2	3:A:425:MET:HE1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:LYS:O	2:B:395:LEU:HG	1.90	0.72
3:A:33:ASP:O	3:A:86:LEU:HA	1.90	0.72
3:A:215:ARG:HD3	3:A:216:ASN:ND2	2.04	0.72
1:K:172:LEU:HG	1:K:173:ASN:N	2.05	0.72
1:K:269:SER:HB3	1:K:288:ILE:HG13	1.71	0.72
2:B:3:GLU:CG	2:B:50:TYR:HA	2.20	0.72
2:B:43:GLN:HA	2:B:242:PHE:CZ	2.25	0.72
2:B:179:VAL:O	2:B:182:PRO:HD2	1.90	0.72
2:B:215:LEU:HA	2:B:276:ARG:CG	2.19	0.72
2:B:267:MET:HG3	2:B:369:GLY:O	1.90	0.72
2:B:285:THR:HG23	2:B:288:GLU:H	1.55	0.72
3:A:265:ILE:HD12	3:A:432:TYR:CE1	2.25	0.72
1:K:144:PHE:HB2	1:K:207:LYS:HG3	1.71	0.71
2:B:15:GLN:O	2:B:19:LYS:HE2	1.89	0.71
2:B:350:LYS:CE	3:A:179:THR:C	2.58	0.71
3:A:90:GLU:HA	3:A:121:ARG:NH2	2.05	0.71
2:B:159:TYR:CB	2:B:162:ARG:HG2	2.20	0.71
2:B:167:PHE:CD1	2:B:200:TYR:HB2	2.25	0.71
2:B:313:VAL:O	2:B:349:VAL:HA	1.91	0.71
2:B:405:GLU:HA	2:B:408:PHE:HD1	1.54	0.71
3:A:346:TRP:O	3:A:348:PRO:HD3	1.89	0.71
1:K:97:TYR:CE2	1:K:365:VAL:HG22	2.25	0.71
1:K:226:THR:HG23	1:K:232:SER:OG	1.89	0.71
1:K:255:LEU:HA	1:K:369:LEU:OXT	1.90	0.71
2:B:140:GLY:HA2	2:B:171:PRO:HG3	1.71	0.71
2:B:322:SER:O	2:B:326:VAL:HG23	1.90	0.71
3:A:233:GLN:HE21	3:A:234:ILE:CG2	2.02	0.71
3:A:288:VAL:CG1	3:A:331:ALA:HB2	2.19	0.71
1:K:181:ARG:HH21	1:K:197:LYS:HG3	0.55	0.71
3:A:274:PRO:HG3	3:A:291:ILE:CG1	2.17	0.71
1:K:156:VAL:O	1:K:203:THR:HA	1.91	0.71
1:K:311:TYR:HE1	1:K:324:LEU:CG	2.04	0.71
2:B:97:ALA:CB	2:B:143:THR:HG23	2.20	0.71
3:A:70:LEU:HB3	3:A:97:GLU:O	1.91	0.71
3:A:276:ILE:CD1	3:A:371:VAL:HG11	2.20	0.71
1:K:162:GLU:CG	1:K:235:SER:HB3	2.01	0.71
1:K:355:ARG:CG	4:K:501:MZK:F3	2.28	0.71
2:B:64:ILE:CD1	2:B:119:VAL:HG21	2.21	0.71
1:K:159:SER:OG	1:K:240:SER:OG	2.08	0.71
2:B:339:SER:HA	2:B:429:THR:HB	1.73	0.71
2:B:375:GLN:CG	2:B:422:TYR:HB3	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:VAL:HA	2:B:422:TYR:CE2	2.25	0.71
3:A:185:TYR:OH	3:A:398:MET:HB3	1.90	0.71
3:A:225:THR:O	3:A:229:ARG:HG2	1.90	0.71
3:A:262:TYR:HE2	3:A:435:VAL:CG2	2.03	0.71
3:A:275:VAL:CB	3:A:300:ASN:HD22	2.02	0.71
1:K:37:ALA:HB1	1:K:339:ALA:CB	2.21	0.71
1:K:52:VAL:HG11	1:K:346:THR:HG21	1.71	0.71
2:B:11:GLN:H	5:B:501:G2P:PB	2.14	0.71
2:B:67:ASP:HB3	2:B:69:GLU:O	1.90	0.71
2:B:86:ARG:HB3	2:B:88:ASP:OD1	1.89	0.71
2:B:102:ALA:HB1	2:B:403:MET:SD	2.31	0.71
2:B:350:LYS:HE3	3:A:179:THR:HG22	1.71	0.71
2:B:375:GLN:HG3	2:B:422:TYR:HB3	1.71	0.71
3:A:3:GLU:CA	3:A:51:THR:HA	2.20	0.71
3:A:317:LEU:HG	3:A:353:VAL:HG11	1.72	0.71
1:K:48:LYS:CE	1:K:71:VAL:H	2.04	0.71
1:K:304:GLU:HG2	1:K:306:THR:HB	1.72	0.71
1:K:320:LEU:CD2	1:K:324:LEU:HD11	2.21	0.71
2:B:20:PHE:CD1	2:B:230:SER:HB2	2.22	0.71
2:B:198:GLU:OE1	2:B:265:PHE:HB2	1.90	0.71
2:B:350:LYS:CE	3:A:179:THR:HA	2.21	0.71
3:A:115:ILE:HD12	3:A:152:LEU:HD21	1.72	0.71
3:A:206:ASN:O	3:A:210:TYR:HB2	1.91	0.71
3:A:242:LEU:HB2	3:A:252:LEU:HD11	1.73	0.71
3:A:275:VAL:HG13	3:A:280:LYS:HE3	1.73	0.71
1:K:136:ILE:HG21	1:K:214:LEU:HD11	1.72	0.71
1:K:212:GLN:HA	1:K:215:GLU:OE2	1.91	0.71
1:K:272:ILE:H	1:K:272:ILE:HD13	1.55	0.71
1:K:311:TYR:CG	1:K:321:GLN:HG3	2.25	0.71
2:B:6:HIS:HB3	2:B:62:ARG:O	1.90	0.71
2:B:161:ASP:OD1	2:B:162:ARG:HD2	1.91	0.71
2:B:190:HIS:CD2	2:B:411:ALA:HA	2.24	0.71
2:B:273:LEU:CB	2:B:298:ASN:HA	2.21	0.71
2:B:274:THR:CG2	2:B:278:SER:HB2	2.18	0.71
2:B:304:ASP:OD1	2:B:306:ARG:HB3	1.90	0.71
2:B:324:LYS:HG2	3:A:221:ARG:CB	2.21	0.71
2:B:215:LEU:HA	2:B:276:ARG:HG2	1.70	0.70
2:B:275:SER:HB3	2:B:278:SER:OG	1.91	0.70
3:A:176:GLN:HE21	3:A:207:GLU:CA	2.03	0.70
1:K:246:LYS:HE2	1:K:254:GLU:OE2	1.90	0.70
2:B:16:ILE:HG12	2:B:226:ASN:ND2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:ILE:HA	2:B:155:ILE:CD1	2.20	0.70
2:B:250:LEU:HA	2:B:253:LEU:CD2	2.20	0.70
3:A:5:ILE:HG23	3:A:65:ALA:CA	2.21	0.70
3:A:132:LEU:CD2	3:A:135:PHE:HB3	2.20	0.70
3:A:277:SER:N	3:A:280:LYS:HB2	2.05	0.70
1:K:157:LYS:HG2	1:K:203:THR:N	2.06	0.70
1:K:227:LEU:HD21	1:K:270:GLU:OE2	1.90	0.70
2:B:42:LEU:HD22	2:B:42:LEU:H	1.55	0.70
2:B:105:HIS:HD1	2:B:106:TYR:HD2	1.36	0.70
3:A:4:CYS:N	3:A:51:THR:HA	2.06	0.70
3:A:8:HIS:CE1	3:A:21:TRP:HE1	2.09	0.70
3:A:23:LEU:HD12	3:A:363:VAL:HG12	1.71	0.70
3:A:217:LEU:CB	3:A:219:ILE:HG12	2.20	0.70
3:A:240:ALA:HA	3:A:243:ARG:CG	2.20	0.70
1:K:187:ASP:CG	1:K:195:ILE:HG13	2.09	0.70
2:B:101:TRP:CH2	2:B:187:LEU:HG	2.26	0.70
3:A:8:HIS:HE1	3:A:21:TRP:HE1	1.38	0.70
3:A:64:ARG:HH21	3:A:64:ARG:CA	2.03	0.70
3:A:66:VAL:HG21	3:A:122:ILE:HG22	1.74	0.70
3:A:212:ILE:HG22	3:A:216:ASN:OD1	1.91	0.70
1:K:170:ASP:H	1:K:180:GLU:H	1.39	0.70
2:B:8:GLN:NE2	2:B:14:ASN:HA	2.05	0.70
2:B:421:GLU:OE1	2:B:424:GLN:HB3	1.92	0.70
3:A:255:PHE:O	3:A:259:LEU:HG	1.91	0.70
3:A:268:PRO:HG2	3:A:378:LEU:CD1	2.14	0.70
3:A:318:LEU:HD13	3:A:319:TYR:N	2.06	0.70
1:K:170:ASP:HB2	1:K:180:GLU:CA	2.22	0.70
3:A:332:ILE:O	3:A:336:LYS:HG2	1.91	0.70
2:B:1:MET:SD	2:B:3:GLU:HG2	2.32	0.70
2:B:143:THR:HG22	2:B:147:MET:CE	2.22	0.70
2:B:350:LYS:HE2	3:A:179:THR:C	2.11	0.70
2:B:350:LYS:HZ1	3:A:179:THR:HA	1.55	0.70
3:A:7:ILE:HG23	3:A:137:VAL:HA	1.73	0.70
3:A:204:VAL:HG23	3:A:209:ILE:CD1	2.20	0.70
2:B:47:ILE:HG22	2:B:59:TYR:CD1	2.27	0.70
2:B:135:LEU:HB2	2:B:166:THR:HG23	1.73	0.70
2:B:266:PHE:CZ	2:B:369:GLY:HA2	2.26	0.70
2:B:279:GLN:NE2	2:B:284:LEU:HD21	2.06	0.70
3:A:24:TYR:O	3:A:27:GLU:HG3	1.91	0.70
3:A:269:LEU:CD2	3:A:384:ILE:HD12	2.21	0.70
1:K:221:ARG:HH22	1:K:233:SER:HB2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:MET:HG3	2:B:301:ALA:O	1.92	0.70
3:A:351:PHE:HB2	3:A:352:LYS:NZ	2.07	0.70
1:K:40:ILE:HD13	1:K:340:SER:HA	1.73	0.70
1:K:57:LEU:HD21	3:A:427:ALA:CB	2.21	0.70
2:B:145:SER:HG	2:B:185:ALA:HA	1.57	0.70
2:B:215:LEU:CA	2:B:276:ARG:HG2	2.22	0.70
3:A:36:MET:CE	3:A:38:SER:HB3	2.22	0.70
3:A:269:LEU:O	3:A:378:LEU:HA	1.92	0.70
1:K:47:ARG:HB3	1:K:49:GLU:CG	2.22	0.69
1:K:257:LYS:HD3	1:K:367:GLN:NE2	2.06	0.69
1:K:283:ARG:HH22	2:B:160:PRO:HB2	1.56	0.69
2:B:46:ARG:HG3	2:B:242:PHE:CD1	2.27	0.69
2:B:51:TYR:HB2	2:B:59:TYR:CD1	2.26	0.69
2:B:65:LEU:HD13	2:B:90:PHE:CB	2.21	0.69
3:A:210:TYR:CE1	3:A:227:LEU:HD13	2.26	0.69
1:K:66:TYR:HE2	1:K:68:PHE:HA	1.57	0.69
1:K:157:LYS:HG2	1:K:203:THR:OG1	1.88	0.69
2:B:34:GLY:HA3	2:B:58:LYS:HG3	1.74	0.69
2:B:113:VAL:O	2:B:117:LEU:HD23	1.92	0.69
2:B:323:MET:HA	2:B:323:MET:CE	2.21	0.69
2:B:323:MET:HA	2:B:326:VAL:HG23	1.72	0.69
3:A:60:LYS:HD3	3:A:61:HIS:N	2.07	0.69
3:A:286:LEU:HD13	3:A:291:ILE:CD1	2.16	0.69
1:K:172:LEU:O	1:K:174:PRO:HD3	1.91	0.69
2:B:342:VAL:HA	2:B:429:THR:OXT	1.91	0.69
2:B:375:GLN:HG3	2:B:422:TYR:CB	2.22	0.69
3:A:41:THR:HG21	3:A:49:PHE:CB	2.22	0.69
3:A:103:TYR:CD1	3:A:189:LEU:HD23	2.27	0.69
3:A:221:ARG:CB	3:A:221:ARG:N	2.55	0.69
3:A:346:TRP:NE1	3:A:438:ASP:HA	2.07	0.69
1:K:32:GLU:O	1:K:35:ALA:HB3	1.93	0.69
1:K:221:ARG:HD3	1:K:237:SER:HB3	1.72	0.69
2:B:81:PHE:HA	2:B:83:GLN:OE1	1.92	0.69
2:B:324:LYS:CE	3:A:222:PRO:HD3	2.19	0.69
3:A:259:LEU:O	3:A:261:PRO:HD3	1.93	0.69
1:K:171:LEU:CA	1:K:220:LYS:HD3	2.23	0.69
1:K:221:ARG:CD	1:K:237:SER:HB3	2.20	0.69
2:B:19:LYS:HA	2:B:22:GLU:OE2	1.92	0.69
2:B:20:PHE:CZ	2:B:24:ILE:HD11	2.26	0.69
2:B:23:VAL:HG22	2:B:27:GLU:OE1	1.93	0.69
2:B:148:GLY:O	2:B:152:ILE:HG12	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:MET:CG	2:B:370:ASN:HA	2.22	0.69
2:B:289:LEU:H	2:B:289:LEU:HD12	1.56	0.69
2:B:293:MET:HE1	2:B:366:THR:O	1.93	0.69
2:B:375:GLN:HG3	2:B:422:TYR:CD2	2.28	0.69
1:K:169:PHE:CA	1:K:179:SER:HA	2.17	0.69
3:A:243:ARG:HG3	3:A:244:PHE:H	1.55	0.69
3:A:301:GLN:OE1	3:A:307:PRO:HG3	1.92	0.69
3:A:318:LEU:O	3:A:375:VAL:HA	1.93	0.69
1:K:17:LYS:HD3	1:K:363:PRO:CB	2.22	0.69
2:B:30:ILE:HD12	2:B:59:TYR:HB2	1.73	0.69
2:B:181:GLU:OE2	5:B:501:G2P:H3'	1.93	0.69
2:B:251:ARG:CZ	3:A:100:ALA:HB3	2.23	0.69
3:A:1:MET:HG2	3:A:47:ASP:CA	2.22	0.69
3:A:52:PHE:HB3	3:A:53:PHE:CE1	2.28	0.69
3:A:286:LEU:HD22	3:A:291:ILE:CD1	2.23	0.69
1:K:48:LYS:O	1:K:71:VAL:HG21	1.91	0.69
1:K:144:PHE:CB	1:K:207:LYS:HZ3	2.06	0.69
1:K:237:SER:OG	1:K:265:ASP:HB3	1.91	0.69
2:B:65:LEU:HD23	2:B:73:MET:SD	2.33	0.69
2:B:99:ASN:N	5:B:501:G2P:O3G	2.25	0.69
2:B:270:PHE:HB3	2:B:300:MET:SD	2.32	0.69
3:A:4:CYS:H	3:A:51:THR:CA	2.05	0.69
3:A:172:TYR:H	3:A:204:VAL:HG12	1.56	0.69
3:A:272:TYR:CE1	3:A:374:ALA:HB1	2.26	0.69
3:A:311:LYS:HG3	3:A:342:GLN:NE2	2.08	0.69
1:K:321:GLN:HA	1:K:324:LEU:CD2	2.23	0.69
2:B:148:GLY:HA2	2:B:151:LEU:CG	2.22	0.69
2:B:296:ALA:HA	2:B:305:PRO:HG3	1.73	0.69
2:B:334:GLN:HG2	2:B:335:ASN:N	2.08	0.69
3:A:318:LEU:HD22	3:A:319:TYR:N	2.06	0.69
1:K:355:ARG:HG2	4:K:501:MZK:F3	1.82	0.69
2:B:112:LEU:HD21	2:B:116:VAL:HG11	1.74	0.69
2:B:273:LEU:HD11	2:B:297:LYS:CD	2.07	0.69
2:B:288:GLU:HA	2:B:291:GLN:CD	2.13	0.69
3:A:170:SER:HB3	3:A:202:PHE:O	1.93	0.69
1:K:25:CYS:O	1:K:74:ALA:HA	1.93	0.68
1:K:157:LYS:CD	1:K:203:THR:OG1	2.40	0.68
1:K:174:PRO:HA	1:K:220:LYS:HZ2	1.57	0.68
2:B:205:GLU:HG3	2:B:206:ALA:N	2.08	0.68
2:B:206:ALA:O	2:B:210:ILE:HG13	1.93	0.68
2:B:330:MET:HG3	2:B:331:LEU:CD1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:PHE:CE1	2:B:348:ASN:HB2	2.28	0.68
3:A:247:ALA:CB	3:A:355:ILE:HB	2.13	0.68
3:A:302:MET:H	3:A:302:MET:CE	2.07	0.68
1:K:246:LYS:HE2	1:K:254:GLU:CD	2.14	0.68
2:B:59:TYR:O	2:B:61:PRO:HD3	1.94	0.68
2:B:139:LEU:CD1	2:B:171:PRO:HD3	2.24	0.68
2:B:278:SER:HA	2:B:282:ARG:NH1	2.06	0.68
3:A:5:ILE:N	3:A:132:LEU:HD21	2.05	0.68
3:A:85:GLN:HG3	3:A:86:LEU:N	2.07	0.68
3:A:298:PRO:HA	3:A:301:GLN:HG3	1.75	0.68
3:A:302:MET:H	3:A:302:MET:HE3	1.58	0.68
1:K:26:ARG:HD3	1:K:109:THR:N	2.08	0.68
1:K:77:LYS:CE	1:K:78:GLN:H	2.05	0.68
2:B:214:THR:HB	2:B:276:ARG:H	1.58	0.68
2:B:245:GLN:HE21	2:B:353:VAL:HG23	1.57	0.68
2:B:371:SER:O	2:B:374:ILE:HG22	1.93	0.68
3:A:3:GLU:HA	3:A:51:THR:CA	2.22	0.68
1:K:66:TYR:HD2	1:K:68:PHE:CE2	2.12	0.68
1:K:160:LEU:HD21	1:K:221:ARG:HB2	1.75	0.68
2:B:7:ILE:H	2:B:134:GLN:HE22	1.42	0.68
2:B:187:LEU:HD11	2:B:408:PHE:CD2	2.28	0.68
2:B:250:LEU:O	2:B:253:LEU:HG	1.93	0.68
3:A:41:THR:HG22	3:A:42:ILE:H	1.57	0.68
3:A:155:GLU:O	3:A:159:VAL:HG23	1.93	0.68
3:A:273:ALA:O	3:A:375:VAL:HG22	1.93	0.68
1:K:17:LYS:CE	1:K:329:ARG:HD3	2.21	0.68
1:K:78:GLN:NE2	1:K:113:PHE:CE2	2.62	0.68
1:K:290:GLN:HA	3:A:409:VAL:HG11	1.75	0.68
2:B:313:VAL:HA	2:B:368:ILE:O	1.93	0.68
3:A:8:HIS:HA	3:A:138:PHE:HB2	1.75	0.68
3:A:265:ILE:HD11	3:A:435:VAL:HG11	1.73	0.68
3:A:384:ILE:CD1	3:A:432:TYR:HE2	2.04	0.68
3:A:402:ARG:CZ	3:A:402:ARG:HB2	2.23	0.68
1:K:48:LYS:HD2	1:K:71:VAL:H	1.59	0.68
1:K:327:ARG:O	1:K:363:PRO:HA	1.93	0.68
2:B:4:ILE:HG23	2:B:133:PHE:CA	2.21	0.68
2:B:339:SER:HA	2:B:429:THR:CB	2.23	0.68
3:A:9:VAL:HG22	3:A:149:PHE:CD1	2.29	0.68
3:A:217:LEU:HD12	3:A:222:PRO:HG3	1.75	0.68
1:K:226:THR:HG23	1:K:232:SER:CB	2.24	0.68
1:K:312:ARG:HD3	2:B:414:ASN:HD21	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:329:ARG:CA	1:K:363:PRO:HB3	2.24	0.68
3:A:270:ALA:HB2	3:A:378:LEU:CD2	2.24	0.68
3:A:294:ALA:HA	3:A:297:GLU:OE2	1.94	0.68
1:K:192:ARG:CD	1:K:327:ARG:HH12	2.07	0.68
1:K:192:ARG:NE	1:K:322:ASP:HA	2.09	0.68
2:B:315:ALA:HA	2:B:366:THR:O	1.94	0.68
3:A:1:MET:HB2	3:A:47:ASP:HA	1.74	0.68
3:A:46:ASP:N	3:A:49:PHE:HB3	2.09	0.68
3:A:126:ALA:HA	3:A:129:CYS:SG	2.33	0.68
3:A:430:LYS:NZ	3:A:433:GLU:HB3	2.09	0.68
1:K:169:PHE:HB3	1:K:178:VAL:O	1.93	0.68
2:B:186:THR:HG21	2:B:385:PHE:CD1	2.28	0.68
2:B:289:LEU:HA	2:B:292:GLN:NE2	2.09	0.68
3:A:301:GLN:CD	3:A:307:PRO:HG3	2.14	0.68
3:A:358:GLN:HG2	3:A:359:PRO:HD2	1.76	0.68
2:B:30:ILE:HG22	2:B:36:TYR:CD1	2.29	0.68
3:A:96:LYS:HA	3:A:96:LYS:HZ2	1.58	0.68
3:A:260:VAL:CG1	3:A:268:PRO:HD3	2.24	0.68
3:A:287:SER:H	3:A:290:GLU:HB2	1.59	0.68
2:B:322:SER:OG	3:A:221:ARG:CB	2.42	0.67
3:A:8:HIS:HB3	3:A:14:VAL:HA	1.75	0.67
3:A:156:ARG:HB3	3:A:156:ARG:CZ	2.25	0.67
3:A:409:VAL:O	3:A:409:VAL:HG12	1.94	0.67
2:B:245:GLN:HB2	2:B:353:VAL:CG2	2.24	0.67
2:B:259:PRO:HA	3:A:404:PHE:CZ	2.29	0.67
3:A:26:LEU:HD23	3:A:364:PRO:HB3	1.75	0.67
3:A:205:ASP:CG	3:A:303:VAL:HA	2.14	0.67
3:A:390:ARG:HA	3:A:393:HIS:NE2	2.09	0.67
1:K:41:VAL:HG23	1:K:338:PRO:HA	1.74	0.67
1:K:199:LEU:HD12	1:K:200:GLU:N	2.09	0.67
1:K:312:ARG:NH1	1:K:318:ARG:NH2	2.42	0.67
2:B:103:LYS:CD	2:B:401:GLU:HG2	2.23	0.67
2:B:143:THR:HB	5:B:501:G2P:PB	2.34	0.67
3:A:5:ILE:HD13	3:A:125:LEU:HD23	1.77	0.67
3:A:9:VAL:HG12	3:A:146:GLY:HA2	1.76	0.67
1:K:167:GLU:HA	1:K:167:GLU:OE1	1.94	0.67
1:K:312:ARG:NH1	1:K:318:ARG:HH21	1.92	0.67
2:B:293:MET:HA	2:B:298:ASN:OD1	1.95	0.67
3:A:6:SER:HB2	3:A:21:TRP:CZ2	2.29	0.67
3:A:36:MET:HG3	3:A:38:SER:O	1.94	0.67
3:A:133:GLN:OE1	3:A:242:LEU:HG	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:164:LYS:HA	3:A:164:LYS:NZ	2.09	0.67
3:A:176:GLN:HE21	3:A:207:GLU:CB	2.07	0.67
1:K:171:LEU:CB	1:K:220:LYS:HB3	2.25	0.67
2:B:3:GLU:HA	2:B:3:GLU:OE2	1.95	0.67
2:B:58:LYS:HG2	2:B:59:TYR:N	2.10	0.67
2:B:121:ARG:HB2	2:B:122:LYS:NZ	2.08	0.67
2:B:183:TYR:HB3	2:B:398:TYR:OH	1.95	0.67
2:B:200:TYR:CG	2:B:268:PRO:HG3	2.30	0.67
2:B:323:MET:CB	3:A:221:ARG:HG3	2.24	0.67
2:B:379:LYS:HD3	2:B:419:VAL:CB	2.24	0.67
3:A:21:TRP:CE2	3:A:65:ALA:HB2	2.30	0.67
3:A:147:SER:HB3	3:A:190:THR:OG1	1.95	0.67
3:A:256:GLN:CA	3:A:259:LEU:HG	2.23	0.67
1:K:104:TYR:CE2	1:K:266:LEU:HG	2.29	0.67
1:K:227:LEU:HG	1:K:228:MET:CE	2.23	0.67
2:B:97:ALA:HB3	2:B:143:THR:OG1	1.94	0.67
2:B:103:LYS:HA	2:B:103:LYS:HZ2	1.56	0.67
3:A:79:ARG:CD	3:A:92:LEU:HD23	2.24	0.67
3:A:210:TYR:CE1	3:A:227:LEU:HD22	2.29	0.67
3:A:271:THR:HG21	3:A:295:CYS:SG	2.35	0.67
2:B:132:GLY:HA3	2:B:163:ILE:O	1.95	0.67
1:K:95:MET:HB2	1:K:365:VAL:HG11	1.76	0.67
1:K:170:ASP:H	1:K:180:GLU:N	1.92	0.67
2:B:7:ILE:H	2:B:134:GLN:NE2	1.92	0.67
2:B:170:VAL:HG23	2:B:203:ASP:HA	1.75	0.67
3:A:200:CYS:HB3	3:A:266:HIS:O	1.95	0.67
2:B:187:LEU:HD11	2:B:408:PHE:HD2	1.60	0.67
2:B:204:ASN:HA	2:B:207:LEU:HD23	1.77	0.67
2:B:285:THR:HG23	2:B:288:GLU:N	2.08	0.67
2:B:324:LYS:CD	3:A:220:GLU:O	2.43	0.67
3:A:152:LEU:HD23	3:A:152:LEU:O	1.95	0.67
3:A:223:THR:HB	3:A:226:ASN:CG	2.15	0.67
1:K:77:LYS:NZ	1:K:78:GLN:CG	2.57	0.67
2:B:4:ILE:HG13	2:B:132:GLY:O	1.95	0.67
2:B:11:GLN:N	5:B:501:G2P:O1B	2.28	0.67
2:B:24:ILE:HG22	2:B:28:HIS:NE2	2.10	0.67
2:B:142:GLY:HA2	2:B:184:ASN:ND2	2.10	0.67
1:K:29:ASN:O	1:K:32:GLU:HB2	1.96	0.66
2:B:44:LEU:HG	2:B:45:GLU:N	2.10	0.66
2:B:101:TRP:HA	2:B:146:GLY:HA2	1.77	0.66
2:B:110:ALA:O	2:B:113:VAL:HG22	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:210:TYR:HE1	3:A:227:LEU:HB2	1.60	0.66
3:A:262:TYR:HB3	3:A:264:ARG:NE	2.10	0.66
3:A:294:ALA:HA	3:A:297:GLU:CD	2.14	0.66
1:K:171:LEU:HA	1:K:220:LYS:HG2	1.77	0.66
1:K:171:LEU:HA	1:K:220:LYS:CB	2.24	0.66
1:K:289:ASN:HD22	3:A:409:VAL:HG11	1.60	0.66
2:B:156:ARG:NH1	2:B:160:PRO:HA	2.10	0.66
2:B:341:PHE:HE2	2:B:346:PRO:HA	1.56	0.66
3:A:23:LEU:CD1	3:A:363:VAL:HG12	2.25	0.66
3:A:263:PRO:HD2	3:A:264:ARG:HH11	1.58	0.66
3:A:273:ALA:HB1	3:A:274:PRO:HA	1.77	0.66
3:A:281:ALA:HB1	3:A:369:ALA:HB3	1.76	0.66
3:A:313:MET:HA	3:A:344:VAL:HG22	1.77	0.66
3:A:321:GLY:N	3:A:359:PRO:HA	2.10	0.66
3:A:334:THR:O	3:A:338:LYS:HG2	1.95	0.66
1:K:172:LEU:HG	1:K:173:ASN:H	1.61	0.66
3:A:96:LYS:HA	3:A:96:LYS:NZ	2.10	0.66
1:K:15:LYS:HD3	1:K:362:LYS:HD2	1.77	0.66
1:K:135:ILE:CD1	1:K:136:ILE:HG13	2.26	0.66
1:K:271:ASN:HD22	1:K:274:ARG:H	1.44	0.66
1:K:365:VAL:HG12	1:K:367:GLN:HG2	1.78	0.66
2:B:336:LYS:HA	2:B:336:LYS:CE	2.25	0.66
2:B:404:ASP:O	2:B:407:GLU:HG3	1.95	0.66
3:A:2:ARG:O	3:A:51:THR:HG23	1.95	0.66
3:A:270:ALA:HA	3:A:378:LEU:HD23	1.76	0.66
3:A:320:ARG:O	3:A:373:ARG:HA	1.96	0.66
1:K:298:VAL:HG23	1:K:310:PRO:CD	2.26	0.66
1:K:302:LEU:O	1:K:305:ARG:HD2	1.95	0.66
2:B:322:SER:H	2:B:325:GLU:CD	1.99	0.66
3:A:79:ARG:HD3	3:A:92:LEU:CD2	2.24	0.66
3:A:133:GLN:HE21	3:A:253:THR:HG23	1.61	0.66
1:K:192:ARG:HE	1:K:327:ARG:HH22	1.42	0.66
1:K:342:ASN:ND2	1:K:345:GLU:H	1.92	0.66
1:K:352:TYR:CB	4:K:501:MZK:C15	2.73	0.66
2:B:70:PRO:HG3	2:B:94:GLN:HA	1.78	0.66
2:B:179:VAL:CG2	2:B:388:MET:HG3	2.26	0.66
2:B:245:GLN:HB2	2:B:353:VAL:HG21	1.77	0.66
3:A:9:VAL:HB	3:A:139:HIS:HB3	1.76	0.66
3:A:104:ALA:HB2	3:A:413:MET:HG3	1.78	0.66
3:A:276:ILE:HG13	3:A:371:VAL:CG1	2.24	0.66
1:K:168:LEU:CD1	1:K:182:LEU:HG	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:327:ARG:HA	1:K:364:GLU:OE1	1.95	0.66
2:B:276:ARG:HD2	2:B:280:GLN:HE22	1.61	0.66
2:B:313:VAL:HB	2:B:349:VAL:HG22	1.77	0.66
2:B:323:MET:HB2	3:A:221:ARG:HD2	1.77	0.66
2:B:342:VAL:HA	2:B:429:THR:O	1.94	0.66
3:A:69:ASP:OD2	3:A:74:VAL:HG22	1.95	0.66
3:A:318:LEU:O	3:A:375:VAL:HG12	1.95	0.66
1:K:31:ALA:HB1	1:K:34:LYS:NZ	2.10	0.66
1:K:168:LEU:HB3	1:K:182:LEU:CD2	2.26	0.66
1:K:169:PHE:HD1	1:K:179:SER:HB2	1.59	0.66
1:K:303:VAL:CG1	1:K:358:ASN:HD22	2.09	0.66
2:B:17:GLY:CA	2:B:136:THR:HG21	2.26	0.66
2:B:47:ILE:HG22	2:B:59:TYR:CE1	2.31	0.66
2:B:200:TYR:HB3	2:B:268:PRO:HG3	1.76	0.66
2:B:203:ASP:OD2	2:B:206:ALA:HB3	1.95	0.66
3:A:424:ASP:O	3:A:427:ALA:HB3	1.96	0.66
1:K:26:ARG:CD	1:K:109:THR:HA	2.25	0.66
2:B:200:TYR:CB	2:B:268:PRO:HG3	2.26	0.66
2:B:210:ILE:O	2:B:214:THR:HG23	1.95	0.66
2:B:323:MET:HA	2:B:326:VAL:CG2	2.25	0.66
2:B:390:ARG:HA	2:B:390:ARG:CZ	2.25	0.66
2:B:286:VAL:HG11	2:B:325:GLU:CG	2.26	0.66
3:A:33:ASP:HA	3:A:85:GLN:CD	2.17	0.66
3:A:54:SER:CB	3:A:64:ARG:HH11	2.08	0.66
3:A:171:ILE:HD13	5:A:501:G2P:H1'	1.77	0.66
3:A:270:ALA:HA	3:A:377:MET:O	1.96	0.66
3:A:320:ARG:CB	3:A:374:ALA:H	2.09	0.66
3:A:333:ALA:O	3:A:337:THR:HG22	1.95	0.66
3:A:428:LEU:HA	3:A:431:ASP:OD1	1.95	0.66
1:K:15:LYS:HD3	1:K:362:LYS:HB3	1.78	0.65
1:K:27:PRO:CA	1:K:74:ALA:HB1	2.26	0.65
1:K:160:LEU:H	1:K:172:LEU:CD2	2.08	0.65
3:A:8:HIS:CD2	3:A:14:VAL:HA	2.32	0.65
3:A:243:ARG:HD2	3:A:244:PHE:CE2	2.31	0.65
1:K:26:ARG:CB	1:K:109:THR:HA	2.25	0.65
1:K:256:VAL:H	1:K:369:LEU:C	1.99	0.65
2:B:34:GLY:C	2:B:58:LYS:HA	2.16	0.65
2:B:215:LEU:C	2:B:276:ARG:HG2	2.16	0.65
2:B:382:SER:O	2:B:385:PHE:HB2	1.96	0.65
3:A:5:ILE:CD1	3:A:125:LEU:HD23	2.27	0.65
3:A:56:THR:HG22	3:A:57:GLY:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:288:VAL:HG12	3:A:331:ALA:CB	2.24	0.65
3:A:430:LYS:O	3:A:430:LYS:HD3	1.95	0.65
1:K:297:ARG:NH1	2:B:262:ARG:NE	2.45	0.65
2:B:6:HIS:O	2:B:7:ILE:HD13	1.95	0.65
2:B:156:ARG:NH2	2:B:157:GLU:HA	2.11	0.65
2:B:289:LEU:HD21	2:B:363:MET:HB2	1.78	0.65
2:B:376:GLU:CB	2:B:379:LYS:HE2	2.25	0.65
3:A:308:ARG:H	3:A:308:ARG:NE	1.94	0.65
3:A:321:GLY:HA2	3:A:359:PRO:HA	1.79	0.65
3:A:401:LYS:HA	3:A:401:LYS:NZ	2.12	0.65
1:K:356:ALA:O	1:K:359:ILE:HG22	1.95	0.65
3:A:57:GLY:N	3:A:58:ALA:HA	2.09	0.65
1:K:95:MET:CE	1:K:97:TYR:CD2	2.80	0.65
1:K:301:ALA:HB1	1:K:306:THR:HG21	1.79	0.65
2:B:103:LYS:HG2	2:B:401:GLU:HG2	1.78	0.65
2:B:167:PHE:CE1	2:B:200:TYR:HD2	2.15	0.65
2:B:324:LYS:HZ2	3:A:221:ARG:CD	2.09	0.65
1:K:136:ILE:O	1:K:139:THR:HG22	1.96	0.65
2:B:67:ASP:OD2	2:B:70:PRO:HA	1.97	0.65
3:A:25:CYS:HA	3:A:30:ILE:CG2	2.27	0.65
3:A:75:ILE:HD12	3:A:92:LEU:HD11	1.78	0.65
3:A:75:ILE:HG22	3:A:79:ARG:HE	1.62	0.65
3:A:189:LEU:HD13	3:A:418:PHE:CE2	2.31	0.65
3:A:251:ASP:HB3	3:A:254:GLU:OE1	1.97	0.65
3:A:288:VAL:CG2	3:A:327:ASP:HB3	2.26	0.65
1:K:50:VAL:HB	1:K:68:PHE:CZ	2.32	0.65
1:K:225:ALA:HB1	1:K:230:ALA:O	1.97	0.65
2:B:5:VAL:HG22	2:B:133:PHE:CD1	2.31	0.65
2:B:46:ARG:HA	2:B:46:ARG:NH1	2.12	0.65
2:B:323:MET:CA	3:A:221:ARG:HG3	2.27	0.65
3:A:32:PRO:O	3:A:86:LEU:HB2	1.97	0.65
1:K:104:TYR:CE2	4:K:501:MZK:C2	2.80	0.65
1:K:144:PHE:HE2	1:K:210:VAL:HG21	1.61	0.65
1:K:172:LEU:H	1:K:172:LEU:HD23	1.61	0.65
2:B:52:ASN:H	2:B:62:ARG:HH22	1.44	0.65
2:B:97:ALA:HA	2:B:104:GLY:CA	2.26	0.65
2:B:143:THR:HG22	2:B:147:MET:HE3	1.79	0.65
2:B:215:LEU:HD13	2:B:217:LEU:HB2	1.76	0.65
2:B:274:THR:HG22	2:B:275:SER:H	1.61	0.65
2:B:288:GLU:HA	2:B:291:GLN:OE1	1.97	0.65
2:B:361:LEU:HD23	2:B:361:LEU:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:LYS:HA	2:B:415:MET:SD	2.36	0.65
3:A:46:ASP:H	3:A:49:PHE:HB3	1.62	0.65
3:A:188:ILE:HG12	3:A:395:PHE:HD1	1.62	0.65
3:A:242:LEU:HD23	3:A:252:LEU:H	1.61	0.65
1:K:31:ALA:CA	1:K:34:LYS:HD3	2.22	0.65
1:K:82:TYR:OH	1:K:86:VAL:CG1	2.44	0.65
1:K:301:ALA:HB1	1:K:306:THR:CG2	2.27	0.65
2:B:1:MET:HE2	2:B:1:MET:HA	1.76	0.65
2:B:238:THR:O	2:B:241:ARG:HG3	1.97	0.65
2:B:271:ALA:HB3	2:B:365:ALA:O	1.97	0.65
3:A:132:LEU:HD22	3:A:135:PHE:HB3	1.78	0.65
2:B:9:ALA:O	2:B:137:HIS:HA	1.97	0.65
2:B:25:SER:O	2:B:28:HIS:HB2	1.97	0.65
2:B:139:LEU:HD12	2:B:140:GLY:N	2.12	0.65
2:B:320:ARG:HB3	2:B:320:ARG:NH1	2.11	0.65
2:B:321:MET:HG3	2:B:325:GLU:OE1	1.97	0.65
2:B:324:LYS:CD	3:A:221:ARG:HG2	2.27	0.65
3:A:7:ILE:HG22	3:A:136:LEU:O	1.97	0.65
3:A:70:LEU:CD2	3:A:99:ALA:HA	2.27	0.65
3:A:147:SER:O	3:A:150:THR:HG22	1.97	0.65
3:A:231:ILE:O	3:A:235:VAL:HG23	1.97	0.65
3:A:324:VAL:HG21	3:A:326:LYS:NZ	2.12	0.65
1:K:189:ARG:CD	1:K:189:ARG:H	2.09	0.64
1:K:329:ARG:HD2	1:K:363:PRO:CG	2.27	0.64
1:K:341:LEU:H	1:K:341:LEU:HD12	1.62	0.64
2:B:327:ASP:O	2:B:331:LEU:HD22	1.97	0.64
3:A:3:GLU:O	3:A:132:LEU:HA	1.97	0.64
3:A:78:VAL:CG1	3:A:92:LEU:HD22	2.27	0.64
3:A:105:ARG:HB2	3:A:411:GLU:CD	2.17	0.64
3:A:311:LYS:HA	3:A:342:GLN:CD	2.17	0.64
3:A:375:VAL:HG21	3:A:377:MET:HE1	1.79	0.64
1:K:66:TYR:HD2	1:K:68:PHE:CD2	2.14	0.64
1:K:192:ARG:HB3	1:K:322:ASP:HA	1.79	0.64
2:B:377:LEU:HA	2:B:380:ARG:CZ	2.27	0.64
3:A:174:ALA:HB1	3:A:176:GLN:HG2	1.77	0.64
1:K:168:LEU:CB	1:K:182:LEU:HD23	2.26	0.64
1:K:221:ARG:NE	1:K:237:SER:HB3	2.12	0.64
2:B:116:VAL:O	2:B:120:VAL:HG13	1.97	0.64
2:B:159:TYR:HD2	2:B:162:ARG:HG2	1.60	0.64
3:A:103:TYR:CE2	3:A:151:SER:HB3	2.32	0.64
3:A:209:ILE:CG1	3:A:302:MET:HB2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:318:LEU:CD1	3:A:320:ARG:HG2	2.27	0.64
3:A:388:TRP:HZ3	3:A:428:LEU:HG	1.61	0.64
1:K:173:ASN:CB	1:K:176:SER:H	2.11	0.64
2:B:11:GLN:HA	2:B:14:ASN:HB2	1.79	0.64
2:B:317:PHE:HA	2:B:364:SER:O	1.97	0.64
3:A:49:PHE:CE1	3:A:53:PHE:HD1	2.16	0.64
3:A:214:ARG:HG3	3:A:215:ARG:N	2.12	0.64
1:K:17:LYS:HD3	1:K:363:PRO:HG2	1.77	0.64
1:K:109:THR:CB	1:K:335:THR:HB	2.27	0.64
1:K:144:PHE:CG	1:K:207:LYS:HG3	2.32	0.64
1:K:156:VAL:H	1:K:203:THR:HG23	1.60	0.64
1:K:164:TYR:HB2	1:K:235:SER:OG	1.97	0.64
2:B:214:THR:CG2	2:B:275:SER:HA	2.27	0.64
3:A:28:HIS:HE1	3:A:49:PHE:HA	1.58	0.64
1:K:48:LYS:HD2	1:K:71:VAL:N	2.12	0.64
1:K:94:ILE:HD13	1:K:150:ASN:HD21	1.63	0.64
1:K:289:ASN:ND2	3:A:409:VAL:CG1	2.60	0.64
2:B:21:TRP:HD1	2:B:85:PHE:HE2	1.44	0.64
2:B:27:GLU:HA	2:B:359:ARG:NH1	2.12	0.64
2:B:45:GLU:HB2	2:B:46:ARG:NH2	2.12	0.64
2:B:183:TYR:CZ	2:B:385:PHE:HB3	2.31	0.64
2:B:244:GLY:HA2	2:B:355:ASP:H	1.63	0.64
2:B:258:VAL:HG11	2:B:263:LEU:O	1.98	0.64
3:A:1:MET:CB	3:A:47:ASP:HA	2.28	0.64
3:A:123:ARG:CZ	3:A:123:ARG:HB2	2.27	0.64
3:A:236:SER:HB2	3:A:361:THR:OG1	1.98	0.64
3:A:240:ALA:CA	3:A:243:ARG:HG2	2.27	0.64
3:A:287:SER:O	3:A:291:ILE:HG13	1.97	0.64
3:A:312:TYR:CE2	3:A:341:ILE:HD12	2.31	0.64
1:K:33:ARG:CZ	1:K:33:ARG:HA	2.28	0.64
1:K:171:LEU:HA	1:K:220:LYS:HB3	1.79	0.64
1:K:174:PRO:HA	1:K:220:LYS:NZ	2.12	0.64
1:K:227:LEU:HG	1:K:228:MET:SD	2.37	0.64
1:K:234:ARG:HE	1:K:281:ARG:HH21	1.44	0.64
1:K:312:ARG:HA	1:K:318:ARG:HG3	1.77	0.64
2:B:4:ILE:HG23	2:B:132:GLY:O	1.98	0.64
2:B:244:GLY:HA2	2:B:355:ASP:CA	2.27	0.64
2:B:245:GLN:OE1	2:B:355:ASP:HA	1.98	0.64
2:B:269:GLY:HA3	2:B:367:PHE:CB	2.23	0.64
2:B:329:GLN:OE1	2:B:330:MET:HE3	1.98	0.64
2:B:379:LYS:CB	2:B:419:VAL:HG11	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:45:GLY:CA	3:A:49:PHE:HD2	2.11	0.64
3:A:53:PHE:HA	3:A:64:ARG:HD2	1.80	0.64
2:B:291:GLN:HG2	2:B:292:GLN:N	2.13	0.64
2:B:324:LYS:NZ	3:A:221:ARG:HD2	2.12	0.64
3:A:274:PRO:O	3:A:276:ILE:HG12	1.98	0.64
3:A:311:LYS:HG3	3:A:342:GLN:CD	2.18	0.64
3:A:339:ARG:HH22	3:A:342:GLN:HB3	1.62	0.64
3:A:397:LEU:O	3:A:397:LEU:HD23	1.98	0.64
1:K:55:GLY:C	1:K:62:SER:HB2	2.18	0.64
1:K:366:ASN:O	1:K:368:LYS:HD2	1.97	0.64
2:B:28:HIS:HA	2:B:43:GLN:OE1	1.98	0.64
2:B:63:ALA:O	2:B:64:ILE:HD13	1.97	0.64
2:B:67:ASP:HB3	2:B:69:GLU:C	2.18	0.64
2:B:245:GLN:NE2	2:B:245:GLN:H	1.95	0.64
3:A:78:VAL:HG11	3:A:92:LEU:HD22	1.80	0.64
1:K:26:ARG:HD3	1:K:109:THR:CA	2.28	0.64
1:K:258:ILE:H	1:K:368:LYS:HE2	1.62	0.64
2:B:135:LEU:HD22	2:B:135:LEU:N	2.13	0.64
3:A:189:LEU:CD2	3:A:418:PHE:HE2	2.11	0.64
3:A:281:ALA:HB3	3:A:369:ALA:HB3	1.80	0.64
1:K:57:LEU:HD22	3:A:427:ALA:HA	1.80	0.63
1:K:157:LYS:HG3	1:K:203:THR:HG1	1.59	0.63
1:K:192:ARG:HB3	1:K:322:ASP:CA	2.28	0.63
1:K:192:ARG:O	1:K:194:VAL:HG13	1.98	0.63
1:K:271:ASN:OD1	3:A:412:GLY:HA3	1.98	0.63
2:B:261:PRO:HD2	3:A:406:HIS:CD2	2.32	0.63
2:B:271:ALA:HB2	2:B:293:MET:SD	2.38	0.63
2:B:274:THR:HG22	2:B:275:SER:N	2.13	0.63
3:A:35:GLN:HB2	3:A:60:LYS:CE	2.28	0.63
3:A:154:MET:SD	3:A:197:HIS:HB2	2.38	0.63
2:B:66:VAL:HG11	2:B:147:MET:HE2	1.79	0.63
2:B:178:THR:CG2	2:B:181:GLU:HB2	2.28	0.63
3:A:116:ASP:O	3:A:119:LEU:HG	1.98	0.63
3:A:253:THR:O	3:A:257:THR:HG23	1.99	0.63
3:A:317:LEU:CG	3:A:353:VAL:HG11	2.28	0.63
1:K:94:ILE:O	1:K:245:MET:CE	2.45	0.63
1:K:158:VAL:HG12	1:K:241:VAL:HG22	1.79	0.63
1:K:171:LEU:CA	1:K:220:LYS:HB3	2.28	0.63
1:K:285:ALA:O	1:K:288:ILE:HG12	1.99	0.63
1:K:293:LEU:CD2	3:A:409:VAL:CG2	2.76	0.63
1:K:298:VAL:O	1:K:302:LEU:HD13	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ALA:HB3	2:B:143:THR:CB	2.28	0.63
2:B:149:THR:CA	2:B:191:GLN:HE22	2.05	0.63
2:B:320:ARG:NH1	2:B:320:ARG:H	1.95	0.63
2:B:324:LYS:CD	3:A:221:ARG:HD3	2.28	0.63
2:B:342:VAL:HB	2:B:348:ASN:ND2	2.13	0.63
3:A:164:LYS:HA	3:A:164:LYS:HE2	1.80	0.63
3:A:205:ASP:CG	3:A:303:VAL:HG23	2.19	0.63
1:K:25:CYS:SG	1:K:41:VAL:HG11	2.38	0.63
1:K:212:GLN:HA	1:K:215:GLU:CD	2.18	0.63
2:B:272:PRO:HG3	2:B:284:LEU:CD1	2.27	0.63
2:B:318:ARG:CB	2:B:358:PRO:HD3	2.29	0.63
3:A:8:HIS:CG	3:A:14:VAL:HA	2.33	0.63
1:K:227:LEU:HG	1:K:228:MET:N	2.13	0.63
1:K:258:ILE:H	1:K:368:LYS:HD3	1.64	0.63
2:B:101:TRP:H	2:B:184:ASN:HB2	1.64	0.63
2:B:127:CYS:SG	2:B:130:LEU:HG	2.38	0.63
2:B:253:LEU:HB2	2:B:257:MET:HE2	1.77	0.63
2:B:286:VAL:CG1	2:B:325:GLU:HB3	2.19	0.63
2:B:303:CYS:CB	2:B:371:SER:HB3	2.29	0.63
2:B:309:ARG:HD2	2:B:429:THR:HA	1.79	0.63
2:B:70:PRO:HB3	2:B:92:PHE:CE2	2.33	0.63
2:B:167:PHE:CE1	2:B:200:TYR:HB2	2.34	0.63
1:K:57:LEU:CD2	3:A:427:ALA:CB	2.77	0.63
1:K:92:GLU:HB3	1:K:97:TYR:CD2	2.34	0.63
1:K:144:PHE:CE2	1:K:210:VAL:HG21	2.34	0.63
1:K:365:VAL:HG11	1:K:367:GLN:HG2	1.78	0.63
2:B:48:ASN:HA	2:B:59:TYR:CE1	2.33	0.63
2:B:77:ARG:HH11	2:B:82:GLY:CA	2.09	0.63
2:B:245:GLN:HE21	2:B:353:VAL:CG2	2.11	0.63
2:B:251:ARG:HH21	3:A:99:ALA:C	2.02	0.63
2:B:357:PRO:HB3	2:B:362:LYS:O	1.98	0.63
1:K:47:ARG:HA	1:K:47:ARG:CZ	2.29	0.63
2:B:103:LYS:CD	2:B:401:GLU:HA	2.25	0.63
2:B:103:LYS:HZ2	2:B:401:GLU:HA	1.61	0.63
2:B:193:VAL:HG13	2:B:194:GLU:N	2.14	0.63
2:B:199:THR:HG23	2:B:265:PHE:CD2	2.34	0.63
2:B:215:LEU:CD1	2:B:217:LEU:HB2	2.28	0.63
2:B:323:MET:C	3:A:221:ARG:HG3	2.19	0.63
3:A:124:LYS:HD2	3:A:125:LEU:N	2.14	0.63
3:A:143:GLY:HA2	5:A:501:G2P:H3A1	1.80	0.63
3:A:188:ILE:HB	3:A:395:PHE:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:247:ALA:HA	3:A:357:TYR:HE1	1.62	0.63
3:A:286:LEU:HD21	3:A:373:ARG:H	1.64	0.63
3:A:305:CYS:O	3:A:307:PRO:HD3	1.98	0.63
1:K:299:ILE:HG22	1:K:355:ARG:HB3	1.81	0.63
2:B:46:ARG:HG3	2:B:241:ARG:HD2	1.80	0.63
2:B:98:GLY:C	5:B:501:G2P:O3G	2.37	0.63
2:B:324:LYS:CB	3:A:221:ARG:HG2	2.29	0.63
2:B:404:ASP:HB3	2:B:406:MET:HG2	1.81	0.63
3:A:9:VAL:O	3:A:139:HIS:HA	1.98	0.63
3:A:242:LEU:O	3:A:242:LEU:HD13	1.98	0.63
3:A:261:PRO:HB2	3:A:262:TYR:CE1	2.34	0.63
3:A:430:LYS:NZ	3:A:430:LYS:HA	2.13	0.63
1:K:25:CYS:SG	1:K:338:PRO:HG3	2.38	0.62
1:K:191:LYS:HD3	1:K:191:LYS:N	2.13	0.62
1:K:204:VAL:HG11	1:K:209:GLU:CB	2.29	0.62
2:B:324:LYS:CE	3:A:222:PRO:HD2	2.24	0.62
3:A:385:ALA:HA	3:A:388:TRP:CZ2	2.33	0.62
1:K:55:GLY:HA2	1:K:59:ASP:C	2.20	0.62
1:K:320:LEU:HG	1:K:324:LEU:HD22	1.80	0.62
2:B:4:ILE:HD11	2:B:131:GLN:CB	2.23	0.62
2:B:159:TYR:HB3	2:B:161:ASP:CG	2.19	0.62
2:B:210:ILE:HG23	2:B:297:LYS:HE3	1.81	0.62
2:B:275:SER:HG	2:B:276:ARG:N	1.97	0.62
2:B:102:ALA:HB1	2:B:401:GLU:HB3	1.82	0.62
2:B:309:ARG:NH2	2:B:309:ARG:HA	2.15	0.62
2:B:324:LYS:N	3:A:221:ARG:HG3	2.14	0.62
3:A:8:HIS:HB3	3:A:14:VAL:CA	2.28	0.62
3:A:214:ARG:O	3:A:217:LEU:HB2	1.98	0.62
3:A:430:LYS:HD3	3:A:430:LYS:C	2.19	0.62
2:B:65:LEU:HD22	2:B:90:PHE:CG	2.35	0.62
2:B:103:LYS:HA	2:B:103:LYS:CE	2.29	0.62
2:B:215:LEU:CA	2:B:276:ARG:HB3	2.25	0.62
2:B:324:LYS:HZ2	3:A:221:ARG:HG3	1.64	0.62
3:A:7:ILE:HD12	3:A:8:HIS:H	1.63	0.62
3:A:30:ILE:HD11	3:A:61:HIS:HB2	1.80	0.62
3:A:214:ARG:HA	3:A:222:PRO:HG3	1.80	0.62
1:K:144:PHE:CB	1:K:207:LYS:HG3	2.29	0.62
1:K:227:LEU:HD23	1:K:227:LEU:N	2.15	0.62
1:K:327:ARG:HD3	1:K:327:ARG:N	2.13	0.62
2:B:12:CYS:C	2:B:16:ILE:HG13	2.19	0.62
2:B:271:ALA:HB3	2:B:365:ALA:C	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ARG:HB3	2:B:320:ARG:HH11	1.63	0.62
3:A:31:GLN:CB	3:A:37:PRO:HD3	2.26	0.62
3:A:104:ALA:HB1	3:A:413:MET:SD	2.39	0.62
3:A:139:HIS:HE1	3:A:141:PHE:CD2	2.17	0.62
3:A:191:THR:HG23	3:A:192:HIS:N	2.15	0.62
3:A:368:LEU:HD12	3:A:368:LEU:O	1.98	0.62
1:K:96:GLY:HA3	1:K:366:ASN:O	1.98	0.62
1:K:181:ARG:HG3	1:K:181:ARG:O	1.98	0.62
2:B:112:LEU:CD2	2:B:116:VAL:HG11	2.29	0.62
3:A:217:LEU:HD11	3:A:222:PRO:HB3	1.81	0.62
3:A:275:VAL:CG1	3:A:280:LYS:HE3	2.28	0.62
3:A:286:LEU:HD21	3:A:371:VAL:HB	1.78	0.62
1:K:94:ILE:HG12	1:K:147:LEU:CD2	2.28	0.62
1:K:109:THR:HB	1:K:335:THR:HB	1.81	0.62
2:B:10:GLY:N	2:B:147:MET:HE1	2.15	0.62
2:B:191:GLN:HG2	2:B:195:ASN:ND2	2.14	0.62
2:B:289:LEU:HD12	2:B:289:LEU:N	2.15	0.62
3:A:117:LEU:HD22	3:A:117:LEU:N	2.14	0.62
2:B:97:ALA:CA	2:B:104:GLY:HA3	2.30	0.62
2:B:138:SER:CB	2:B:169:VAL:HG22	2.29	0.62
2:B:155:ILE:O	2:B:158:GLU:HG3	1.99	0.62
2:B:258:VAL:O	3:A:404:PHE:CE2	2.52	0.62
2:B:304:ASP:HB3	2:B:307:HIS:CD2	2.33	0.62
3:A:72:PRO:HA	3:A:94:THR:OG1	2.00	0.62
1:K:17:LYS:CD	1:K:363:PRO:HG2	2.28	0.62
1:K:160:LEU:N	1:K:172:LEU:HD22	2.12	0.62
1:K:227:LEU:CG	1:K:228:MET:HE3	2.30	0.62
2:B:361:LEU:HG	2:B:363:MET:O	2.00	0.62
3:A:19:ALA:HA	3:A:22:GLU:OE1	2.00	0.62
3:A:31:GLN:NE2	3:A:33:ASP:HB3	2.15	0.62
3:A:240:ALA:O	3:A:243:ARG:HG3	2.00	0.62
2:B:240:LEU:HD12	2:B:247:ASN:OD1	2.00	0.62
2:B:323:MET:HB2	2:B:324:LYS:HZ2	1.65	0.62
3:A:101:ASN:O	3:A:182:VAL:HG11	2.00	0.62
3:A:234:ILE:HD12	3:A:235:VAL:N	2.15	0.62
3:A:274:PRO:N	3:A:291:ILE:HG23	2.15	0.62
3:A:402:ARG:O	3:A:405:VAL:HG23	2.00	0.62
1:K:115:MET:HE1	1:K:135:ILE:HD11	1.80	0.61
1:K:173:ASN:HB2	1:K:176:SER:HB2	1.81	0.61
2:B:70:PRO:CD	2:B:94:GLN:HG2	2.30	0.61
2:B:260:PHE:CZ	3:A:404:PHE:CA	2.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:MET:H	2:B:363:MET:CE	2.12	0.61
2:B:421:GLU:O	2:B:424:GLN:HB3	1.99	0.61
3:A:103:TYR:HE2	3:A:151:SER:CB	2.12	0.61
1:K:200:GLU:O	1:K:200:GLU:HG2	1.98	0.61
1:K:202:ILE:HD12	1:K:203:THR:N	2.15	0.61
2:B:323:MET:CE	2:B:326:VAL:HG21	2.29	0.61
2:B:404:ASP:OD1	2:B:406:MET:HE2	2.00	0.61
3:A:176:GLN:HE21	3:A:207:GLU:HB2	1.64	0.61
1:K:78:GLN:CD	1:K:113:PHE:CE2	2.74	0.61
2:B:116:VAL:O	2:B:120:VAL:HG22	2.00	0.61
2:B:200:TYR:CD1	2:B:268:PRO:HG3	2.36	0.61
2:B:214:THR:HG22	2:B:275:SER:HA	1.82	0.61
2:B:285:THR:HG22	2:B:288:GLU:CB	2.17	0.61
2:B:305:PRO:HB3	2:B:310:TYR:OH	1.99	0.61
3:A:9:VAL:HG13	3:A:149:PHE:HD1	1.65	0.61
3:A:310:GLY:CA	3:A:381:THR:HB	2.28	0.61
1:K:93:VAL:O	1:K:259:GLY:HA3	2.00	0.61
1:K:269:SER:CB	1:K:288:ILE:HD11	2.29	0.61
2:B:101:TRP:HB2	2:B:145:SER:HB3	1.81	0.61
2:B:170:VAL:HG13	2:B:201:CYS:HB2	1.80	0.61
2:B:258:VAL:HG21	2:B:261:PRO:HA	1.81	0.61
2:B:318:ARG:NH2	2:B:356:ILE:HG13	2.14	0.61
2:B:321:MET:HG3	2:B:325:GLU:HB2	1.82	0.61
3:A:143:GLY:CA	5:A:501:G2P:H3A1	2.30	0.61
3:A:324:VAL:HG23	3:A:327:ASP:H	1.65	0.61
3:A:406:HIS:HA	3:A:409:VAL:HB	1.82	0.61
1:K:48:LYS:CD	1:K:71:VAL:H	2.13	0.61
1:K:329:ARG:HA	1:K:363:PRO:HB3	1.83	0.61
2:B:1:MET:HA	2:B:49:VAL:HB	1.82	0.61
2:B:30:ILE:HA	2:B:36:TYR:HD1	1.65	0.61
2:B:234:SER:O	2:B:238:THR:HG23	1.99	0.61
2:B:273:LEU:O	2:B:292:GLN:HB3	1.99	0.61
2:B:288:GLU:HA	2:B:291:GLN:NE2	2.16	0.61
2:B:362:LYS:HA	2:B:362:LYS:CE	2.30	0.61
3:A:22:GLU:HA	3:A:25:CYS:SG	2.40	0.61
3:A:46:ASP:OD2	3:A:49:PHE:HB2	2.00	0.61
3:A:75:ILE:HG22	3:A:79:ARG:NE	2.15	0.61
3:A:312:TYR:CD2	3:A:341:ILE:HG23	2.35	0.61
3:A:430:LYS:O	3:A:434:GLU:HG3	1.99	0.61
1:K:361:ASN:CG	1:K:363:PRO:HD3	2.20	0.61
2:B:20:PHE:HD1	2:B:230:SER:CB	2.10	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:GLY:HA3	2:B:171:PRO:HG3	1.80	0.61
2:B:273:LEU:HG	2:B:298:ASN:CA	2.23	0.61
3:A:163:LYS:HB2	3:A:163:LYS:NZ	2.16	0.61
1:K:115:MET:CE	1:K:135:ILE:HD11	2.31	0.61
1:K:181:ARG:HB2	1:K:181:ARG:NH1	2.12	0.61
2:B:107:THR:HG23	2:B:108:GLU:N	2.15	0.61
2:B:186:THR:HG21	2:B:385:PHE:HD1	1.64	0.61
2:B:204:ASN:HA	2:B:207:LEU:CD2	2.31	0.61
3:A:122:ILE:HD12	3:A:123:ARG:N	2.15	0.61
1:K:159:SER:CB	1:K:199:LEU:HD21	2.22	0.61
1:K:270:GLU:CD	1:K:275:SER:HB2	2.20	0.61
1:K:311:TYR:O	1:K:318:ARG:HG3	2.00	0.61
2:B:42:LEU:HD22	2:B:42:LEU:N	2.16	0.61
2:B:143:THR:CG2	2:B:147:MET:HE3	2.31	0.61
2:B:314:ALA:H	2:B:368:ILE:CB	2.06	0.61
2:B:318:ARG:CD	2:B:358:PRO:HG3	2.31	0.61
3:A:63:PRO:CG	3:A:86:LEU:HD21	2.31	0.61
3:A:307:PRO:HD2	3:A:308:ARG:NH2	2.15	0.61
3:A:431:ASP:O	3:A:435:VAL:HG12	2.00	0.61
1:K:54:THR:HG23	1:K:55:GLY:N	2.16	0.61
1:K:68:PHE:CG	1:K:71:VAL:HG22	2.36	0.61
2:B:260:PHE:CZ	3:A:407:TRP:N	2.64	0.61
2:B:260:PHE:CD1	3:A:404:PHE:HD2	2.19	0.61
2:B:381:ILE:HA	2:B:384:GLN:CG	2.29	0.61
3:A:248:LEU:HD23	3:A:249:ASN:N	2.16	0.61
3:A:277:SER:H	3:A:280:LYS:CG	2.14	0.61
1:K:26:ARG:HD3	1:K:109:THR:HA	1.81	0.61
1:K:303:VAL:HG13	1:K:358:ASN:HD22	1.66	0.61
1:K:320:LEU:HD21	1:K:324:LEU:HD11	1.83	0.61
2:B:45:GLU:HG3	2:B:46:ARG:NE	2.13	0.61
2:B:108:GLU:HA	2:B:111:GLU:OE2	2.01	0.61
2:B:162:ARG:HA	2:B:162:ARG:NE	2.16	0.61
2:B:421:GLU:CD	2:B:424:GLN:HB3	2.21	0.61
3:A:130:THR:HG23	3:A:131:GLY:N	2.15	0.61
3:A:140:SER:HA	3:A:171:ILE:CG2	2.31	0.61
3:A:172:TYR:HE2	3:A:391:LEU:HD23	1.66	0.61
3:A:344:VAL:HA	3:A:438:ASP:CG	2.21	0.61
1:K:28:PHE:CD2	1:K:32:GLU:HB3	2.36	0.60
1:K:77:LYS:HB3	1:K:80:ASP:OD2	2.00	0.60
2:B:140:GLY:HA2	2:B:185:ALA:CB	2.31	0.60
2:B:208:TYR:CD2	2:B:220:PRO:HG2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:23:LEU:HD12	3:A:363:VAL:CG1	2.30	0.60
3:A:78:VAL:HG13	3:A:83:TYR:CE1	2.36	0.60
3:A:183:GLU:HB2	3:A:184:PRO:HD3	1.83	0.60
1:K:17:LYS:HD3	1:K:363:PRO:CG	2.30	0.60
1:K:189:ARG:NH1	1:K:193:GLY:HA3	2.15	0.60
2:B:215:LEU:O	2:B:215:LEU:HD23	2.01	0.60
1:K:272:ILE:HB	1:K:282:ALA:HB1	1.83	0.60
2:B:108:GLU:OE1	2:B:147:MET:HA	2.01	0.60
2:B:151:LEU:O	2:B:155:ILE:HG12	2.01	0.60
2:B:244:GLY:HA2	2:B:355:ASP:HB2	1.81	0.60
2:B:246:LEU:H	2:B:353:VAL:CG2	2.14	0.60
3:A:78:VAL:HB	3:A:92:LEU:HD21	1.82	0.60
3:A:229:ARG:O	3:A:363:VAL:HG11	2.00	0.60
3:A:274:PRO:HB2	3:A:276:ILE:HD11	1.83	0.60
1:K:15:LYS:HE2	1:K:362:LYS:CE	2.31	0.60
1:K:55:GLY:N	1:K:60:LYS:HA	2.15	0.60
2:B:46:ARG:HH12	2:B:49:VAL:CG1	2.14	0.60
2:B:139:LEU:HD13	2:B:185:ALA:HB1	1.81	0.60
2:B:271:ALA:HB3	2:B:365:ALA:HB3	1.82	0.60
2:B:382:SER:HB3	2:B:415:MET:HE1	1.84	0.60
1:K:228:MET:HA	1:K:228:MET:HE2	1.83	0.60
2:B:347:ASN:ND2	2:B:350:LYS:HZ3	2.00	0.60
3:A:26:LEU:HD22	3:A:364:PRO:HB3	1.81	0.60
3:A:155:GLU:HG2	3:A:156:ARG:N	2.16	0.60
3:A:317:LEU:HD22	3:A:377:MET:CE	2.31	0.60
3:A:321:GLY:HA3	3:A:372:GLN:O	2.01	0.60
1:K:190:ASN:HD22	1:K:191:LYS:N	1.99	0.60
2:B:1:MET:HA	2:B:1:MET:CE	2.30	0.60
2:B:151:LEU:HD12	2:B:152:ILE:CA	2.32	0.60
2:B:337:ASN:OD1	2:B:339:SER:HB3	2.02	0.60
3:A:70:LEU:CG	3:A:110:ILE:HG21	2.19	0.60
3:A:216:ASN:HB3	3:A:280:LYS:CD	2.31	0.60
3:A:407:TRP:HA	3:A:407:TRP:HE3	1.66	0.60
1:K:215:GLU:OE2	1:K:216:LYS:HE3	2.01	0.60
1:K:246:LYS:NZ	1:K:254:GLU:OE2	2.35	0.60
2:B:101:TRP:CH2	2:B:403:MET:HG3	2.36	0.60
2:B:262:ARG:CD	2:B:262:ARG:H	2.14	0.60
2:B:324:LYS:NZ	3:A:221:ARG:CA	2.64	0.60
3:A:115:ILE:HG23	3:A:116:ASP:N	2.17	0.60
3:A:154:MET:HE2	3:A:154:MET:CA	2.31	0.60
3:A:179:THR:HB	3:A:183:GLU:OE2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:271:THR:O	3:A:376:CYS:HA	2.02	0.60
3:A:287:SER:HB3	3:A:290:GLU:HG3	1.83	0.60
1:K:77:LYS:HE3	1:K:78:GLN:HB2	1.83	0.60
1:K:145:GLU:HG2	1:K:207:LYS:NZ	2.17	0.60
1:K:170:ASP:OD2	1:K:180:GLU:HG2	2.02	0.60
1:K:297:ARG:HH12	2:B:262:ARG:NE	1.98	0.60
2:B:67:ASP:CG	2:B:73:MET:HB3	2.22	0.60
2:B:225:LEU:HD12	2:B:226:ASN:N	2.17	0.60
2:B:293:MET:CE	2:B:367:PHE:HA	2.31	0.60
2:B:318:ARG:NH2	2:B:358:PRO:HA	2.16	0.60
3:A:31:GLN:HE22	3:A:33:ASP:HB3	1.65	0.60
1:K:48:LYS:NZ	1:K:70:MET:HG3	2.16	0.60
1:K:152:THR:O	1:K:154:PHE:HD2	1.85	0.60
1:K:215:GLU:HG2	1:K:216:LYS:N	2.17	0.60
2:B:36:TYR:CD2	2:B:44:LEU:HB2	2.37	0.60
2:B:90:PHE:HE1	2:B:92:PHE:CE1	2.19	0.60
2:B:241:ARG:HD2	2:B:242:PHE:N	2.17	0.60
3:A:16:ILE:HG23	3:A:17:GLY:N	2.16	0.60
3:A:101:ASN:CA	3:A:144:GLY:HA3	2.30	0.60
3:A:135:PHE:HE1	3:A:166:LYS:HA	1.66	0.60
3:A:317:LEU:HD22	3:A:377:MET:HE3	1.84	0.60
2:B:260:PHE:CG	3:A:406:HIS:NE2	2.69	0.60
2:B:381:ILE:HA	2:B:384:GLN:HG3	1.82	0.60
3:A:171:ILE:HG13	3:A:204:VAL:CG1	2.32	0.60
3:A:204:VAL:HG13	3:A:206:ASN:OD1	2.01	0.60
3:A:255:PHE:HZ	3:A:352:LYS:H	1.50	0.60
3:A:259:LEU:CD1	3:A:378:LEU:HD12	2.30	0.60
3:A:326:LYS:NZ	3:A:326:LYS:HB3	2.17	0.60
1:K:16:GLY:CA	1:K:363:PRO:HD2	2.31	0.59
1:K:102:PHE:HD1	1:K:264:VAL:CG1	2.15	0.59
1:K:293:LEU:HD21	3:A:409:VAL:CG2	2.32	0.59
2:B:154:LYS:HE2	2:B:157:GLU:CB	2.26	0.59
2:B:272:PRO:HB3	2:B:292:GLN:HE22	1.67	0.59
2:B:318:ARG:CZ	2:B:358:PRO:HA	2.31	0.59
3:A:78:VAL:O	3:A:84:ARG:HB2	2.02	0.59
3:A:103:TYR:HD2	3:A:147:SER:C	2.05	0.59
3:A:174:ALA:HB2	3:A:207:GLU:N	2.15	0.59
3:A:349:THR:HG1	3:A:351:PHE:HD1	1.50	0.59
1:K:77:LYS:CD	1:K:78:GLN:H	2.15	0.59
1:K:226:THR:HG23	1:K:232:SER:HB3	1.84	0.59
1:K:297:ARG:HH22	2:B:260:PHE:HD2	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:329:ARG:HA	1:K:363:PRO:HG3	1.84	0.59
2:B:84:ILE:HG23	2:B:85:PHE:CD1	2.37	0.59
2:B:217:LEU:HD13	2:B:218:THR:H	1.65	0.59
2:B:323:MET:CA	2:B:326:VAL:HG23	2.33	0.59
1:K:59:ASP:HA	1:K:60:LYS:NZ	2.17	0.59
1:K:204:VAL:HG11	1:K:209:GLU:HB3	1.84	0.59
2:B:113:VAL:HG23	2:B:114:ASP:N	2.17	0.59
2:B:137:HIS:HE1	2:B:166:THR:CG2	2.15	0.59
2:B:404:ASP:OD1	2:B:406:MET:HG2	2.02	0.59
3:A:189:LEU:HD12	3:A:192:HIS:HE1	1.66	0.59
3:A:294:ALA:HA	3:A:297:GLU:OE1	2.02	0.59
1:K:60:LYS:H	1:K:60:LYS:HD2	1.67	0.59
1:K:192:ARG:CB	1:K:322:ASP:HA	2.32	0.59
1:K:344:GLU:HB3	3:A:414:GLU:CG	2.15	0.59
2:B:9:ALA:HB1	2:B:147:MET:SD	2.42	0.59
2:B:118:ASP:O	2:B:122:LYS:HD2	2.03	0.59
2:B:141:GLY:HA3	5:B:501:G2P:C5'	2.32	0.59
2:B:167:PHE:HE1	2:B:200:TYR:CD2	2.20	0.59
2:B:170:VAL:HG22	2:B:203:ASP:HA	1.83	0.59
2:B:178:THR:CG2	2:B:180:VAL:HG22	2.32	0.59
3:A:6:SER:HB2	3:A:21:TRP:HZ2	1.68	0.59
3:A:274:PRO:CD	3:A:291:ILE:HG23	2.32	0.59
3:A:276:ILE:HG22	3:A:277:SER:O	2.02	0.59
1:K:41:VAL:HB	1:K:338:PRO:HA	1.85	0.59
1:K:184:MET:SD	1:K:194:VAL:HG21	2.42	0.59
1:K:258:ILE:H	1:K:368:LYS:CD	2.16	0.59
1:K:266:LEU:HD13	1:K:267:ALA:C	2.23	0.59
1:K:283:ARG:HH22	2:B:160:PRO:CB	2.14	0.59
1:K:293:LEU:HD23	3:A:409:VAL:HG11	1.83	0.59
2:B:131:GLN:NE2	2:B:131:GLN:HA	2.17	0.59
2:B:276:ARG:O	2:B:280:GLN:HG2	2.03	0.59
2:B:350:LYS:HE3	3:A:179:THR:HA	1.83	0.59
1:K:82:TYR:CZ	1:K:86:VAL:CB	2.85	0.59
1:K:272:ILE:HD11	3:A:411:GLU:O	2.03	0.59
2:B:272:PRO:CG	2:B:284:LEU:HD11	2.33	0.59
2:B:375:GLN:HG3	2:B:376:GLU:OE2	2.03	0.59
3:A:4:CYS:SG	3:A:135:PHE:HA	2.42	0.59
3:A:188:ILE:CG2	3:A:421:ALA:HB1	2.31	0.59
3:A:242:LEU:HB2	3:A:252:LEU:CD1	2.31	0.59
3:A:280:LYS:HA	3:A:283:HIS:HD2	1.66	0.59
1:K:23:VAL:HG21	1:K:68:PHE:HE1	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:66:TYR:HB3	1:K:68:PHE:CZ	2.37	0.59
2:B:145:SER:HB3	2:B:188:SER:OG	2.02	0.59
2:B:167:PHE:HE1	2:B:200:TYR:HD2	1.49	0.59
2:B:221:THR:HG22	2:B:223:GLY:H	1.66	0.59
2:B:243:PRO:C	2:B:355:ASP:HB2	2.23	0.59
2:B:306:ARG:HH21	2:B:309:ARG:NH2	2.00	0.59
3:A:277:SER:HB3	3:A:280:LYS:H	1.67	0.59
1:K:15:LYS:O	1:K:362:LYS:HA	2.02	0.59
2:B:324:LYS:CD	3:A:221:ARG:CD	2.81	0.59
3:A:78:VAL:HB	3:A:92:LEU:CD2	2.32	0.59
3:A:214:ARG:HH21	3:A:219:ILE:N	2.00	0.59
1:K:48:LYS:HA	1:K:71:VAL:HB	1.85	0.59
1:K:157:LYS:CB	1:K:201:GLU:HB3	2.21	0.59
1:K:181:ARG:HH22	1:K:183:GLN:HB2	1.68	0.59
1:K:228:MET:CE	1:K:228:MET:HA	2.33	0.59
1:K:284:GLU:HA	1:K:287:ASN:HD22	1.67	0.59
2:B:53:GLU:HA	2:B:58:LYS:O	2.03	0.59
2:B:303:CYS:HB2	2:B:371:SER:HB3	1.83	0.59
2:B:324:LYS:HD3	3:A:221:ARG:CD	2.33	0.59
3:A:295:CYS:HA	3:A:300:ASN:CG	2.22	0.59
1:K:171:LEU:N	1:K:171:LEU:HD23	2.18	0.59
1:K:272:ILE:HD13	1:K:272:ILE:N	2.17	0.59
2:B:34:GLY:HA2	2:B:84:ILE:HD13	1.84	0.59
2:B:215:LEU:HD23	2:B:276:ARG:NE	2.17	0.59
3:A:146:GLY:O	3:A:150:THR:HG22	2.03	0.59
3:A:229:ARG:HH21	3:A:363:VAL:HB	1.68	0.59
3:A:351:PHE:HB2	3:A:352:LYS:HZ3	1.68	0.59
1:K:321:GLN:CA	1:K:324:LEU:HD23	2.31	0.58
2:B:20:PHE:CE1	2:B:233:MET:HB2	2.37	0.58
2:B:139:LEU:HD11	2:B:171:PRO:CD	2.32	0.58
2:B:251:ARG:NH2	3:A:99:ALA:O	2.36	0.58
2:B:260:PHE:CE2	3:A:406:HIS:N	2.71	0.58
2:B:272:PRO:HA	2:B:292:GLN:HE22	1.67	0.58
2:B:309:ARG:HB2	2:B:426:GLN:CA	2.19	0.58
3:A:171:ILE:HG13	3:A:204:VAL:HG11	1.84	0.58
1:K:57:LEU:CD2	3:A:427:ALA:HA	2.33	0.58
1:K:191:LYS:H	1:K:191:LYS:NZ	2.01	0.58
2:B:20:PHE:O	2:B:23:VAL:HG12	2.04	0.58
2:B:140:GLY:CA	2:B:185:ALA:HB2	2.32	0.58
2:B:277:GLY:CA	2:B:280:GLN:HE21	2.08	0.58
2:B:376:GLU:HB2	2:B:380:ARG:HH22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:VAL:HG23	2:B:420:SER:N	2.18	0.58
3:A:141:PHE:HB2	3:A:171:ILE:O	2.03	0.58
3:A:239:THR:O	3:A:243:ARG:HG2	2.03	0.58
3:A:428:LEU:HD12	3:A:428:LEU:O	2.03	0.58
1:K:26:ARG:HH21	1:K:337:SER:HB2	1.67	0.58
1:K:95:MET:HB2	1:K:365:VAL:CG1	2.32	0.58
1:K:109:THR:HG21	1:K:336:ILE:H	1.65	0.58
2:B:156:ARG:HE	2:B:157:GLU:HA	1.67	0.58
2:B:174:LYS:HD2	2:B:175:VAL:HG23	1.86	0.58
2:B:339:SER:HA	2:B:429:THR:HG22	1.84	0.58
2:B:392:LYS:CA	2:B:395:LEU:HD21	2.33	0.58
3:A:93:ILE:CD1	3:A:118:VAL:HG12	2.33	0.58
3:A:185:TYR:CE1	3:A:404:PHE:HB2	2.38	0.58
3:A:287:SER:HB3	3:A:290:GLU:OE2	2.02	0.58
3:A:420:GLU:OE1	3:A:420:GLU:HA	2.02	0.58
1:K:48:LYS:C	1:K:71:VAL:HG21	2.23	0.58
1:K:92:GLU:HB3	1:K:97:TYR:CG	2.38	0.58
2:B:228:LEU:HD21	2:B:300:MET:HE1	1.85	0.58
2:B:260:PHE:CE2	3:A:405:VAL:N	2.71	0.58
2:B:318:ARG:HD3	2:B:358:PRO:HG3	1.85	0.58
3:A:78:VAL:CA	3:A:83:TYR:HE1	2.15	0.58
3:A:217:LEU:HD23	3:A:277:SER:OG	2.03	0.58
1:K:84:SER:CB	1:K:84:SER:HG	1.24	0.58
1:K:109:THR:HB	1:K:335:THR:CB	2.34	0.58
1:K:170:ASP:HB3	1:K:177:ASP:O	2.03	0.58
1:K:202:ILE:HD12	1:K:203:THR:H	1.68	0.58
1:K:275:SER:OG	1:K:277:ALA:HB2	2.03	0.58
1:K:311:TYR:CE1	1:K:324:LEU:HD23	2.39	0.58
2:B:190:HIS:CG	2:B:411:ALA:HB1	2.38	0.58
2:B:246:LEU:O	2:B:352:ALA:HB1	2.04	0.58
2:B:260:PHE:CZ	3:A:404:PHE:C	2.77	0.58
2:B:347:ASN:CG	2:B:350:LYS:HZ3	2.06	0.58
3:A:99:ALA:HB2	3:A:145:THR:CA	2.34	0.58
3:A:114:ILE:HG23	3:A:115:ILE:N	2.18	0.58
1:K:48:LYS:HE3	1:K:70:MET:CA	2.25	0.58
1:K:191:LYS:HZ2	1:K:191:LYS:N	2.01	0.58
1:K:293:LEU:HD21	3:A:409:VAL:HG21	1.84	0.58
2:B:119:VAL:HG12	2:B:123:GLU:HG2	1.85	0.58
2:B:296:ALA:HB2	2:B:305:PRO:CD	2.33	0.58
2:B:324:LYS:HD2	3:A:220:GLU:O	2.04	0.58
3:A:156:ARG:NH1	3:A:157:LEU:HG	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:215:ARG:HH11	3:A:216:ASN:HA	1.69	0.58
3:A:216:ASN:ND2	3:A:280:LYS:HD2	2.18	0.58
1:K:15:LYS:HD3	1:K:362:LYS:CD	2.33	0.58
1:K:180:GLU:CD	1:K:199:LEU:HA	2.24	0.58
1:K:190:ASN:HB3	1:K:193:GLY:H	1.69	0.58
1:K:355:ARG:HG3	4:K:501:MZK:F3	1.94	0.58
2:B:309:ARG:HD2	2:B:429:THR:CA	2.33	0.58
3:A:102:ASN:HB2	3:A:407:TRP:HE1	1.69	0.58
3:A:360:PRO:HG3	3:A:374:ALA:N	2.18	0.58
1:K:68:PHE:CB	1:K:71:VAL:HG22	2.33	0.58
2:B:21:TRP:HH2	2:B:50:TYR:CZ	2.22	0.58
2:B:54:ALA:CB	2:B:58:LYS:HB3	2.24	0.58
2:B:323:MET:HA	2:B:323:MET:HE3	1.86	0.58
2:B:324:LYS:CG	3:A:221:ARG:CG	2.81	0.58
2:B:362:LYS:HD2	2:B:362:LYS:N	2.17	0.58
3:A:78:VAL:HG13	3:A:83:TYR:HE1	1.69	0.58
3:A:174:ALA:CB	3:A:176:GLN:HG2	2.33	0.58
3:A:217:LEU:HA	3:A:277:SER:OG	2.03	0.58
3:A:339:ARG:HH22	3:A:342:GLN:CB	2.17	0.58
1:K:236:HIS:N	1:K:267:ALA:HB2	2.19	0.58
2:B:111:GLU:HA	2:B:114:ASP:OD2	2.04	0.58
3:A:8:HIS:O	3:A:68:VAL:HG22	2.04	0.58
3:A:67:PHE:HB2	3:A:92:LEU:HD12	1.85	0.58
3:A:67:PHE:HB2	3:A:92:LEU:HD13	1.85	0.58
1:K:44:ASP:OD2	1:K:47:ARG:HG2	2.04	0.58
1:K:190:ASN:HB3	1:K:193:GLY:N	2.19	0.58
1:K:235:SER:C	1:K:267:ALA:HB2	2.24	0.58
2:B:45:GLU:HG2	2:B:46:ARG:N	2.18	0.58
2:B:138:SER:O	2:B:144:GLY:HA3	2.04	0.58
2:B:258:VAL:O	3:A:404:PHE:HE2	1.87	0.58
3:A:430:LYS:HD3	3:A:434:GLU:HG3	1.84	0.58
1:K:222:THR:HG23	1:K:231:TYR:CE2	2.39	0.57
2:B:44:LEU:O	2:B:48:ASN:HB2	2.03	0.57
2:B:191:GLN:HG2	2:B:195:ASN:HD21	1.69	0.57
2:B:213:ARG:HE	2:B:214:THR:HG22	1.68	0.57
2:B:410:GLU:HA	2:B:410:GLU:OE2	2.03	0.57
3:A:2:ARG:HG3	3:A:131:GLY:O	2.04	0.57
3:A:272:TYR:HE1	3:A:374:ALA:CB	2.15	0.57
1:K:136:ILE:CG2	1:K:214:LEU:HD11	2.34	0.57
2:B:139:LEU:HD12	2:B:185:ALA:CB	2.34	0.57
2:B:145:SER:OG	2:B:188:SER:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:LEU:CD1	2:B:152:ILE:HG12	2.34	0.57
3:A:9:VAL:HG23	3:A:138:PHE:O	2.04	0.57
3:A:156:ARG:HH12	3:A:157:LEU:HG	1.68	0.57
3:A:409:VAL:C	3:A:412:GLY:H	2.07	0.57
3:A:429:GLU:OE1	3:A:429:GLU:HA	2.04	0.57
1:K:272:ILE:HG12	1:K:273:GLY:N	2.19	0.57
2:B:67:ASP:H	2:B:92:PHE:HB2	1.68	0.57
2:B:288:GLU:O	2:B:292:GLN:HG3	2.04	0.57
3:A:5:ILE:CG2	3:A:65:ALA:HA	2.34	0.57
3:A:185:TYR:HB3	3:A:408:TYR:HE1	1.68	0.57
3:A:260:VAL:HG23	3:A:260:VAL:O	2.04	0.57
3:A:268:PRO:HB3	3:A:380:ASN:OD1	2.05	0.57
3:A:388:TRP:CZ3	3:A:428:LEU:HD21	2.39	0.57
1:K:92:GLU:HB3	1:K:97:TYR:CB	2.34	0.57
1:K:189:ARG:HH11	1:K:193:GLY:HA3	1.70	0.57
1:K:227:LEU:H	1:K:227:LEU:CD2	2.16	0.57
2:B:108:GLU:OE2	2:B:147:MET:HB3	2.04	0.57
2:B:260:PHE:CD2	3:A:406:HIS:NE2	2.73	0.57
2:B:324:LYS:HD3	3:A:221:ARG:HD3	1.87	0.57
2:B:337:ASN:HB3	2:B:340:TYR:CB	2.32	0.57
3:A:12:ALA:HA	3:A:15:GLN:HE22	1.70	0.57
3:A:67:PHE:O	3:A:93:ILE:HG12	2.03	0.57
3:A:273:ALA:HB3	3:A:375:VAL:HG21	1.86	0.57
3:A:319:TYR:CB	3:A:355:ILE:HA	2.08	0.57
1:K:110:GLY:HA3	1:K:113:PHE:HB3	1.87	0.57
1:K:215:GLU:HG3	1:K:216:LYS:HE3	1.85	0.57
1:K:293:LEU:HD12	3:A:405:VAL:CG1	2.33	0.57
1:K:327:ARG:H	1:K:327:ARG:NH2	1.99	0.57
2:B:32:PRO:HG3	2:B:81:PHE:CE1	2.40	0.57
2:B:112:LEU:O	2:B:116:VAL:HG13	2.03	0.57
2:B:252:LYS:HG2	3:A:100:ALA:HB1	1.87	0.57
2:B:284:LEU:HD22	2:B:288:GLU:OE1	2.04	0.57
2:B:309:ARG:HD2	2:B:429:THR:O	2.04	0.57
2:B:326:VAL:O	2:B:329:GLN:HG3	2.04	0.57
3:A:176:GLN:NE2	3:A:207:GLU:HA	2.18	0.57
3:A:246:GLY:HA3	3:A:355:ILE:O	2.03	0.57
1:K:223:THR:HG21	1:K:235:SER:N	2.11	0.57
1:K:327:ARG:HA	1:K:362:LYS:O	2.05	0.57
1:K:104:TYR:HD2	1:K:105:GLY:H	1.52	0.57
2:B:186:THR:HG23	2:B:187:LEU:N	2.19	0.57
2:B:271:ALA:CB	2:B:365:ALA:HB3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:97:GLU:OE2	3:A:110:ILE:HD11	2.03	0.57
1:K:54:THR:HG23	1:K:56:GLY:N	2.19	0.57
1:K:109:THR:HG21	1:K:335:THR:HB	1.83	0.57
1:K:162:GLU:OE2	1:K:235:SER:HB2	2.05	0.57
2:B:1:MET:SD	2:B:127:CYS:HB3	2.44	0.57
2:B:20:PHE:O	2:B:24:ILE:HG12	2.04	0.57
2:B:62:ARG:NH1	2:B:62:ARG:HA	2.19	0.57
2:B:217:LEU:HD13	2:B:219:THR:H	1.69	0.57
2:B:240:LEU:HD13	2:B:248:ALA:O	2.05	0.57
2:B:244:GLY:CA	2:B:355:ASP:HB2	2.34	0.57
3:A:35:GLN:OE1	3:A:35:GLN:HA	2.03	0.57
3:A:248:LEU:HB3	3:A:354:GLY:HA2	1.87	0.57
3:A:282:TYR:CD1	3:A:369:ALA:HB2	2.39	0.57
3:A:319:TYR:CD2	3:A:375:VAL:HG12	2.40	0.57
2:B:99:ASN:CA	2:B:142:GLY:HA3	2.35	0.57
2:B:103:LYS:CG	2:B:401:GLU:HG2	2.34	0.57
3:A:30:ILE:HD12	3:A:61:HIS:CG	2.40	0.57
3:A:33:ASP:CG	3:A:35:GLN:H	2.08	0.57
3:A:41:THR:HG22	3:A:46:ASP:OD2	2.05	0.57
3:A:187:SER:O	3:A:191:THR:HG22	2.05	0.57
3:A:246:GLY:HA2	3:A:357:TYR:N	2.17	0.57
3:A:275:VAL:HG13	3:A:275:VAL:O	2.05	0.57
3:A:388:TRP:HB2	3:A:425:MET:HE2	1.87	0.57
1:K:26:ARG:HE	1:K:337:SER:CB	2.17	0.57
1:K:43:CYS:C	1:K:45:PRO:HD3	2.26	0.57
1:K:290:GLN:NE2	3:A:410:GLY:CA	2.58	0.57
2:B:245:GLN:NE2	2:B:355:ASP:HA	2.20	0.57
3:A:4:CYS:N	3:A:51:THR:HG22	2.19	0.57
3:A:153:LEU:HD11	3:A:157:LEU:CD1	2.33	0.57
3:A:176:GLN:HG3	3:A:177:VAL:H	1.69	0.57
3:A:278:ALA:HB1	3:A:282:TYR:CZ	2.40	0.57
1:K:181:ARG:HH22	1:K:197:LYS:NZ	2.03	0.56
1:K:303:VAL:HG22	1:K:358:ASN:HB2	1.87	0.56
1:K:343:LEU:H	1:K:343:LEU:CD2	2.10	0.56
1:K:347:LEU:HD23	1:K:347:LEU:O	2.04	0.56
1:K:361:ASN:OD1	1:K:363:PRO:HG3	2.05	0.56
2:B:19:LYS:HZ3	2:B:19:LYS:N	2.02	0.56
2:B:187:LEU:HG	2:B:408:PHE:CE2	2.40	0.56
2:B:266:PHE:CE2	2:B:311:LEU:HG	2.40	0.56
3:A:108:TYR:O	3:A:112:LYS:HG2	2.05	0.56
3:A:112:LYS:O	3:A:115:ILE:HG22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:122:ILE:HD12	3:A:123:ARG:HA	1.86	0.56
3:A:311:LYS:HA	3:A:342:GLN:NE2	2.20	0.56
3:A:395:PHE:HA	3:A:398:MET:HG2	1.87	0.56
3:A:401:LYS:HA	3:A:401:LYS:HZ3	1.69	0.56
1:K:41:VAL:CB	1:K:338:PRO:HA	2.34	0.56
1:K:221:ARG:HD2	1:K:221:ARG:O	2.05	0.56
1:K:361:ASN:C	1:K:363:PRO:HD3	2.25	0.56
2:B:81:PHE:HA	2:B:83:GLN:HE22	1.70	0.56
2:B:116:VAL:HG23	2:B:117:LEU:N	2.20	0.56
2:B:183:TYR:CE1	2:B:385:PHE:HB3	2.40	0.56
2:B:216:LYS:HE2	2:B:277:GLY:CA	2.31	0.56
3:A:9:VAL:HG11	3:A:149:PHE:HB3	1.87	0.56
3:A:317:LEU:HG	3:A:353:VAL:CG1	2.34	0.56
3:A:358:GLN:HG2	3:A:359:PRO:CD	2.35	0.56
1:K:26:ARG:NH1	1:K:338:PRO:HD2	2.20	0.56
1:K:68:PHE:HB2	1:K:71:VAL:HG23	1.85	0.56
1:K:106:GLN:HB2	1:K:109:THR:OG1	2.05	0.56
1:K:290:GLN:HA	1:K:293:LEU:HD23	1.86	0.56
1:K:341:LEU:HD12	1:K:341:LEU:N	2.19	0.56
2:B:4:ILE:CG2	2:B:133:PHE:HA	2.24	0.56
2:B:102:ALA:HB3	2:B:401:GLU:OE1	2.03	0.56
2:B:149:THR:HG21	2:B:188:SER:HA	1.87	0.56
2:B:216:LYS:HD3	2:B:276:ARG:NH1	2.20	0.56
2:B:251:ARG:HD3	3:A:105:ARG:HH21	1.68	0.56
2:B:284:LEU:HD13	2:B:289:LEU:CD2	2.36	0.56
2:B:308:GLY:HA2	2:B:372:THR:N	2.20	0.56
2:B:327:ASP:O	2:B:331:LEU:HD13	2.05	0.56
2:B:350:LYS:HE3	3:A:179:THR:CA	2.36	0.56
2:B:350:LYS:CE	3:A:179:THR:CA	2.83	0.56
2:B:374:ILE:HG13	2:B:378:PHE:CZ	2.40	0.56
3:A:5:ILE:HD11	3:A:125:LEU:HG	1.87	0.56
3:A:70:LEU:HD22	3:A:99:ALA:HA	1.87	0.56
3:A:172:TYR:N	3:A:204:VAL:HG12	2.18	0.56
3:A:188:ILE:CG1	3:A:395:PHE:HD1	2.18	0.56
3:A:246:GLY:HA3	3:A:356:ASN:CA	2.18	0.56
3:A:263:PRO:HD2	3:A:264:ARG:CD	2.33	0.56
3:A:275:VAL:HB	3:A:300:ASN:ND2	2.18	0.56
3:A:387:ALA:HA	3:A:390:ARG:HD2	1.85	0.56
1:K:32:GLU:CB	1:K:33:ARG:HH21	2.18	0.56
2:B:322:SER:HB3	2:B:325:GLU:CG	2.34	0.56
3:A:262:TYR:HD2	3:A:265:ILE:HG12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:275:VAL:HG13	3:A:280:LYS:CE	2.35	0.56
3:A:390:ARG:O	3:A:394:LYS:HD2	2.04	0.56
1:K:43:CYS:O	1:K:45:PRO:HD3	2.06	0.56
2:B:83:GLN:NE2	2:B:83:GLN:H	2.04	0.56
3:A:1:MET:HB2	3:A:47:ASP:CB	2.35	0.56
3:A:4:CYS:CA	3:A:132:LEU:HG	2.04	0.56
3:A:205:ASP:HB3	3:A:208:ALA:CB	2.36	0.56
1:K:135:ILE:HD11	1:K:136:ILE:HG13	1.88	0.56
1:K:272:ILE:H	1:K:272:ILE:CD1	2.18	0.56
2:B:42:LEU:O	2:B:45:GLU:HG2	2.05	0.56
2:B:84:ILE:HG23	2:B:85:PHE:N	2.19	0.56
2:B:266:PHE:CE1	2:B:369:GLY:HA2	2.40	0.56
2:B:320:ARG:H	2:B:320:ARG:CZ	2.19	0.56
2:B:377:LEU:HA	2:B:380:ARG:HG3	1.88	0.56
2:B:384:GLN:O	2:B:388:MET:HG2	2.05	0.56
3:A:63:PRO:CD	3:A:86:LEU:HD11	2.30	0.56
3:A:117:LEU:H	3:A:117:LEU:CD2	2.17	0.56
3:A:240:ALA:HA	3:A:243:ARG:NE	2.20	0.56
1:K:48:LYS:NZ	1:K:71:VAL:H	2.03	0.56
2:B:2:ARG:HG3	2:B:131:GLN:H	1.70	0.56
2:B:208:TYR:HE2	2:B:225:LEU:HD23	1.69	0.56
3:A:71:GLU:HB3	3:A:98:ASP:CB	2.36	0.56
3:A:150:THR:HG23	3:A:151:SER:N	2.21	0.56
3:A:191:THR:O	3:A:194:THR:HG22	2.06	0.56
3:A:235:VAL:HA	3:A:238:ILE:HD12	1.87	0.56
3:A:313:MET:HA	3:A:344:VAL:HG13	1.87	0.56
1:K:57:LEU:CD2	3:A:427:ALA:HB2	2.36	0.56
1:K:321:GLN:O	1:K:324:LEU:HD23	2.06	0.56
2:B:15:GLN:OE1	2:B:19:LYS:HE3	2.05	0.56
2:B:31:ASP:HB2	2:B:33:THR:HG22	1.88	0.56
2:B:130:LEU:HD12	2:B:130:LEU:N	2.20	0.56
2:B:213:ARG:HG3	2:B:214:THR:H	1.70	0.56
3:A:125:LEU:HD12	3:A:128:GLN:CG	2.36	0.56
3:A:172:TYR:H	3:A:204:VAL:CG1	2.19	0.56
3:A:288:VAL:HG21	3:A:327:ASP:HB2	1.88	0.56
3:A:305:CYS:SG	3:A:383:ALA:HB3	2.45	0.56
3:A:323:VAL:HB	3:A:355:ILE:HG21	1.86	0.56
1:K:26:ARG:NH2	1:K:32:GLU:HG3	2.20	0.56
1:K:97:TYR:HA	1:K:366:ASN:H	1.70	0.56
2:B:3:GLU:OE1	2:B:49:VAL:HG23	2.05	0.56
2:B:284:LEU:CD1	2:B:361:LEU:HD12	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:53:PHE:CD2	3:A:63:PRO:HA	2.41	0.56
3:A:163:LYS:HB2	3:A:163:LYS:HZ1	1.69	0.56
1:K:82:TYR:CE2	1:K:86:VAL:CB	2.88	0.56
1:K:95:MET:CG	1:K:365:VAL:CG1	2.79	0.56
1:K:172:LEU:HD21	1:K:199:LEU:CD1	2.35	0.56
2:B:192:LEU:HD13	2:B:192:LEU:C	2.26	0.56
2:B:214:THR:HB	2:B:275:SER:HA	1.87	0.56
2:B:260:PHE:H	2:B:262:ARG:NH2	2.04	0.56
2:B:379:LYS:HB3	2:B:419:VAL:HG11	1.88	0.56
2:B:382:SER:HB3	2:B:415:MET:CE	2.36	0.56
3:A:154:MET:HA	3:A:154:MET:CE	2.36	0.56
3:A:233:GLN:HB3	3:A:363:VAL:HG13	1.88	0.56
1:K:15:LYS:HG2	1:K:16:GLY:N	2.20	0.55
1:K:94:ILE:HA	1:K:245:MET:HE1	1.87	0.55
2:B:11:GLN:N	5:B:501:G2P:O2A	2.39	0.55
2:B:28:HIS:HB3	2:B:30:ILE:HG23	1.86	0.55
2:B:139:LEU:HG	2:B:169:VAL:O	2.06	0.55
2:B:215:LEU:CG	2:B:217:LEU:HB2	2.36	0.55
3:A:75:ILE:HG23	3:A:92:LEU:CD1	2.35	0.55
3:A:182:VAL:HG12	3:A:186:ASN:OD1	2.06	0.55
1:K:226:THR:CG2	1:K:232:SER:HB3	2.37	0.55
1:K:303:VAL:CG2	1:K:358:ASN:HD22	2.19	0.55
2:B:35:SER:HA	2:B:57:ASN:O	2.05	0.55
2:B:175:VAL:HG12	2:B:176:SER:N	2.21	0.55
2:B:345:ILE:HD11	3:A:181:VAL:HA	1.88	0.55
3:A:52:PHE:O	3:A:63:PRO:HA	2.06	0.55
3:A:137:VAL:HB	3:A:168:GLU:HA	1.88	0.55
3:A:233:GLN:NE2	3:A:234:ILE:HA	2.20	0.55
3:A:271:THR:CG2	3:A:377:MET:HB2	2.36	0.55
1:K:15:LYS:HD3	1:K:362:LYS:CG	2.36	0.55
1:K:15:LYS:HE3	1:K:364:GLU:CD	2.26	0.55
1:K:172:LEU:CD1	1:K:199:LEU:HD11	2.28	0.55
1:K:187:ASP:OD1	1:K:195:ILE:HG12	1.99	0.55
1:K:312:ARG:CA	1:K:318:ARG:CG	2.71	0.55
1:K:360:LEU:HD12	1:K:360:LEU:N	2.20	0.55
2:B:42:LEU:HA	2:B:45:GLU:CD	2.27	0.55
2:B:62:ARG:HA	2:B:62:ARG:HH11	1.71	0.55
2:B:112:LEU:HD23	2:B:112:LEU:C	2.27	0.55
2:B:113:VAL:HG23	2:B:114:ASP:OD1	2.07	0.55
2:B:245:GLN:CD	2:B:355:ASP:HA	2.26	0.55
2:B:260:PHE:CZ	3:A:405:VAL:N	2.73	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:31:GLN:H	3:A:36:MET:HA	1.71	0.55
3:A:118:VAL:HG23	3:A:119:LEU:N	2.21	0.55
3:A:171:ILE:HD12	5:A:501:G2P:N3	2.22	0.55
3:A:311:LYS:HG2	3:A:438:ASP:OD2	2.05	0.55
3:A:321:GLY:HA3	3:A:372:GLN:NE2	2.20	0.55
1:K:26:ARG:NH1	1:K:28:PHE:HA	2.18	0.55
2:B:3:GLU:HG3	2:B:50:TYR:CA	2.37	0.55
2:B:11:GLN:CA	2:B:14:ASN:HB2	2.37	0.55
2:B:43:GLN:CA	2:B:242:PHE:HZ	2.19	0.55
2:B:142:GLY:HA2	2:B:184:ASN:OD1	2.06	0.55
2:B:199:THR:O	2:B:265:PHE:HD2	1.90	0.55
3:A:121:ARG:NH1	3:A:121:ARG:HG2	2.22	0.55
3:A:189:LEU:CD1	3:A:417:GLU:HG3	2.37	0.55
1:K:29:ASN:H	1:K:32:GLU:HG3	1.71	0.55
1:K:134:GLY:CA	1:K:138:ARG:HG2	2.37	0.55
1:K:140:LEU:HD22	1:K:210:VAL:HG11	1.89	0.55
2:B:1:MET:HG3	2:B:2:ARG:H	1.72	0.55
2:B:81:PHE:HA	2:B:83:GLN:NE2	2.22	0.55
2:B:263:LEU:HD22	2:B:264:HIS:N	2.21	0.55
2:B:347:ASN:HD22	3:A:177:VAL:CG2	2.20	0.55
3:A:4:CYS:O	3:A:64:ARG:HB2	2.07	0.55
3:A:52:PHE:HB3	3:A:53:PHE:CZ	2.40	0.55
3:A:230:LEU:HD23	3:A:230:LEU:C	2.27	0.55
1:K:16:GLY:HA3	1:K:363:PRO:HD2	1.87	0.55
1:K:136:ILE:HG21	1:K:214:LEU:CD1	2.37	0.55
1:K:145:GLU:HG2	1:K:207:LYS:HZ1	1.70	0.55
2:B:225:LEU:O	2:B:229:VAL:HG23	2.06	0.55
2:B:306:ARG:HA	2:B:340:TYR:HE1	1.70	0.55
2:B:375:GLN:HG2	2:B:376:GLU:N	2.21	0.55
2:B:398:TYR:O	2:B:401:GLU:HB2	2.07	0.55
3:A:259:LEU:HD13	3:A:378:LEU:CD1	2.31	0.55
1:K:82:TYR:CE2	1:K:86:VAL:CG1	2.87	0.55
1:K:102:PHE:CD1	1:K:264:VAL:CG1	2.90	0.55
1:K:115:MET:SD	1:K:135:ILE:HG12	2.46	0.55
1:K:223:THR:OG1	1:K:233:SER:HA	2.06	0.55
2:B:3:GLU:C	2:B:4:ILE:HD12	2.27	0.55
2:B:23:VAL:HG11	2:B:230:SER:CB	2.37	0.55
2:B:46:ARG:HG3	2:B:241:ARG:CD	2.35	0.55
2:B:246:LEU:H	2:B:353:VAL:HG22	1.70	0.55
2:B:307:HIS:O	2:B:426:GLN:HG3	2.07	0.55
2:B:308:GLY:HA2	2:B:372:THR:OG1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:396:HIS:O	2:B:399:THR:HB	2.06	0.55
3:A:1:MET:CG	3:A:47:ASP:HB2	2.36	0.55
3:A:210:TYR:HA	3:A:213:CYS:SG	2.46	0.55
3:A:229:ARG:HG2	3:A:229:ARG:HH11	1.72	0.55
3:A:317:LEU:HB2	3:A:353:VAL:CG1	2.36	0.55
1:K:224:ALA:HB3	1:K:234:ARG:CG	2.33	0.55
1:K:271:ASN:ND2	1:K:274:ARG:H	2.05	0.55
2:B:86:ARG:HB2	2:B:89:ASN:OD1	2.06	0.55
2:B:178:THR:HG22	2:B:181:GLU:HB2	1.89	0.55
2:B:214:THR:CB	2:B:275:SER:HA	2.37	0.55
2:B:321:MET:HG2	2:B:325:GLU:HB2	1.89	0.55
3:A:34:GLY:HA2	3:A:86:LEU:HD13	1.89	0.55
3:A:286:LEU:HD22	3:A:291:ILE:HD11	1.87	0.55
3:A:370:LYS:HE2	3:A:371:VAL:O	2.07	0.55
1:K:144:PHE:HD2	1:K:207:LYS:HG3	1.64	0.55
1:K:311:TYR:CE1	1:K:324:LEU:HG	2.36	0.55
2:B:101:TRP:HB2	2:B:188:SER:OG	2.07	0.55
3:A:205:ASP:OD1	3:A:303:VAL:HG23	2.07	0.55
3:A:262:TYR:HB2	3:A:265:ILE:H	1.72	0.55
3:A:318:LEU:HD13	3:A:318:LEU:C	2.27	0.55
1:K:144:PHE:HB2	1:K:207:LYS:CG	2.37	0.55
1:K:172:LEU:HD21	1:K:199:LEU:HD11	1.87	0.55
2:B:41:ASP:OD1	2:B:42:LEU:HD22	2.07	0.55
2:B:215:LEU:HD13	2:B:217:LEU:HB3	1.87	0.55
2:B:341:PHE:CZ	2:B:346:PRO:HA	2.41	0.55
2:B:421:GLU:HA	2:B:421:GLU:OE2	2.05	0.55
3:A:99:ALA:HB3	5:A:501:G2P:O2G	2.07	0.55
3:A:115:ILE:HD12	3:A:152:LEU:CD2	2.37	0.55
3:A:271:THR:HG22	3:A:377:MET:HB2	1.89	0.55
3:A:344:VAL:HA	3:A:438:ASP:OD1	2.06	0.55
3:A:358:GLN:CG	3:A:359:PRO:HD2	2.35	0.55
3:A:401:LYS:HG3	3:A:403:ALA:HB2	1.88	0.55
2:B:415:MET:HG2	2:B:419:VAL:HG13	1.89	0.54
3:A:274:PRO:HB2	3:A:276:ILE:CD1	2.37	0.54
2:B:8:GLN:HE22	2:B:14:ASN:HA	1.72	0.54
2:B:11:GLN:O	2:B:14:ASN:HB2	2.07	0.54
2:B:15:GLN:HG3	2:B:19:LYS:CG	2.37	0.54
2:B:36:TYR:HD2	2:B:44:LEU:HB2	1.72	0.54
2:B:228:LEU:HD21	2:B:300:MET:CE	2.37	0.54
2:B:324:LYS:HZ3	3:A:221:ARG:CA	2.19	0.54
3:A:101:ASN:HA	3:A:144:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:224:TYR:CD2	5:A:501:G2P:C6	2.91	0.54
3:A:317:LEU:N	3:A:353:VAL:HG12	2.22	0.54
3:A:388:TRP:CH2	3:A:432:TYR:CE2	2.95	0.54
3:A:405:VAL:O	3:A:409:VAL:HG23	2.06	0.54
1:K:55:GLY:HA2	1:K:60:LYS:CA	2.35	0.54
1:K:190:ASN:HD22	1:K:192:ARG:H	1.55	0.54
2:B:149:THR:HA	2:B:191:GLN:NE2	2.09	0.54
2:B:154:LYS:NZ	2:B:157:GLU:HG3	2.23	0.54
2:B:214:THR:HA	2:B:275:SER:OG	2.07	0.54
3:A:16:ILE:HD11	3:A:231:ILE:HB	1.89	0.54
3:A:172:TYR:CG	3:A:203:MET:HB2	2.43	0.54
3:A:298:PRO:HA	3:A:301:GLN:CG	2.37	0.54
3:A:311:LYS:N	3:A:311:LYS:HE3	2.22	0.54
3:A:385:ALA:HA	3:A:388:TRP:CE3	2.42	0.54
3:A:409:VAL:CG1	3:A:409:VAL:O	2.55	0.54
1:K:162:GLU:HG3	1:K:221:ARG:NH1	2.22	0.54
1:K:191:LYS:H	1:K:191:LYS:HD3	1.71	0.54
2:B:113:VAL:O	2:B:116:VAL:HG22	2.08	0.54
2:B:253:LEU:O	2:B:257:MET:HG2	2.07	0.54
2:B:258:VAL:HB	2:B:260:PHE:O	2.08	0.54
2:B:262:ARG:HD3	2:B:262:ARG:N	2.20	0.54
2:B:266:PHE:CD1	2:B:368:ILE:HG22	2.43	0.54
2:B:280:GLN:HG3	2:B:281:TYR:N	2.23	0.54
2:B:376:GLU:OE2	2:B:422:TYR:HB2	2.07	0.54
3:A:154:MET:HE2	3:A:154:MET:HA	1.90	0.54
3:A:155:GLU:HG2	3:A:156:ARG:H	1.71	0.54
3:A:189:LEU:HD13	3:A:417:GLU:HG3	1.90	0.54
3:A:250:VAL:HG22	3:A:251:ASP:N	2.23	0.54
3:A:294:ALA:O	3:A:300:ASN:HB2	2.07	0.54
3:A:349:THR:HG21	3:A:351:PHE:CD1	2.43	0.54
3:A:394:LYS:HD2	3:A:394:LYS:H	1.73	0.54
3:A:433:GLU:O	3:A:437:VAL:HG13	2.08	0.54
1:K:171:LEU:HD13	1:K:221:ARG:CB	2.37	0.54
2:B:45:GLU:HG2	2:B:46:ARG:H	1.71	0.54
2:B:214:THR:C	2:B:276:ARG:H	2.11	0.54
2:B:255:VAL:HG13	2:B:256:ASN:N	2.23	0.54
3:A:46:ASP:OD1	3:A:244:PHE:HZ	1.90	0.54
3:A:99:ALA:HB2	3:A:145:THR:N	2.23	0.54
3:A:391:LEU:HA	3:A:394:LYS:CE	2.37	0.54
1:K:158:VAL:O	1:K:201:GLU:HG2	2.07	0.54
2:B:102:ALA:HB3	2:B:401:GLU:CB	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:PRO:O	2:B:260:PHE:HB2	2.07	0.54
2:B:306:ARG:HA	2:B:340:TYR:CE1	2.43	0.54
3:A:143:GLY:HA3	5:A:501:G2P:O1B	2.07	0.54
3:A:270:ALA:HB2	3:A:378:LEU:HD21	1.88	0.54
3:A:307:PRO:HB3	3:A:312:TYR:OH	2.08	0.54
3:A:319:TYR:HB3	3:A:323:VAL:HG21	1.90	0.54
3:A:323:VAL:HG12	3:A:324:VAL:N	2.23	0.54
1:K:102:PHE:HD1	1:K:264:VAL:HB	1.72	0.54
2:B:139:LEU:H	2:B:168:SER:HB3	1.71	0.54
2:B:155:ILE:HG13	2:B:156:ARG:N	2.23	0.54
2:B:213:ARG:HE	2:B:214:THR:CG2	2.21	0.54
2:B:232:THR:HG23	2:B:270:PHE:HD1	1.72	0.54
1:K:50:VAL:HG23	1:K:71:VAL:CG1	2.38	0.54
2:B:178:THR:HG21	2:B:180:VAL:CG2	2.38	0.54
2:B:186:THR:HB	2:B:385:PHE:HE1	1.72	0.54
2:B:372:THR:HA	2:B:375:GLN:CD	2.28	0.54
3:A:24:TYR:HB3	3:A:52:PHE:CG	2.42	0.54
3:A:270:ALA:CA	3:A:378:LEU:HD23	2.38	0.54
3:A:298:PRO:HB3	3:A:301:GLN:HE21	1.72	0.54
3:A:407:TRP:HA	3:A:407:TRP:CE3	2.42	0.54
1:K:140:LEU:HD13	1:K:210:VAL:HG11	1.90	0.54
1:K:144:PHE:HB3	1:K:207:LYS:HD2	1.90	0.54
2:B:70:PRO:HA	2:B:92:PHE:CE2	2.43	0.54
2:B:154:LYS:O	2:B:158:GLU:HG3	2.08	0.54
2:B:259:PRO:HA	3:A:404:PHE:CE2	2.43	0.54
2:B:309:ARG:HD2	2:B:429:THR:C	2.28	0.54
3:A:23:LEU:HA	3:A:364:PRO:HG2	1.89	0.54
3:A:23:LEU:HD23	3:A:23:LEU:C	2.27	0.54
3:A:174:ALA:HB1	3:A:207:GLU:HB3	1.90	0.54
3:A:346:TRP:HD1	3:A:346:TRP:H	1.55	0.54
3:A:402:ARG:HG3	3:A:405:VAL:HG21	1.89	0.54
1:K:102:PHE:HZ	1:K:266:LEU:HD23	1.72	0.54
1:K:181:ARG:CG	1:K:198:GLY:HA3	2.38	0.54
2:B:41:ASP:OD2	2:B:42:LEU:HD22	2.08	0.54
2:B:70:PRO:HG3	2:B:94:GLN:CB	2.38	0.54
2:B:154:LYS:O	2:B:154:LYS:HD3	2.08	0.54
2:B:263:LEU:C	2:B:263:LEU:HD13	2.28	0.54
2:B:374:ILE:HG23	2:B:375:GLN:N	2.23	0.54
3:A:1:MET:HB2	3:A:47:ASP:CA	2.38	0.54
3:A:74:VAL:HG23	3:A:75:ILE:N	2.23	0.54
3:A:136:LEU:N	3:A:136:LEU:HD22	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:17:LYS:HE3	1:K:329:ARG:CD	2.26	0.53
1:K:134:GLY:HA2	1:K:138:ARG:HG2	1.89	0.53
1:K:290:GLN:CA	3:A:409:VAL:HG11	2.38	0.53
2:B:24:ILE:CA	2:B:27:GLU:HG2	2.36	0.53
2:B:72:THR:O	2:B:76:VAL:HG23	2.08	0.53
2:B:90:PHE:HE1	2:B:92:PHE:HE1	1.55	0.53
2:B:148:GLY:O	2:B:151:LEU:HG	2.07	0.53
2:B:221:THR:HG22	2:B:222:TYR:N	2.23	0.53
2:B:228:LEU:HD23	2:B:228:LEU:C	2.29	0.53
2:B:267:MET:HE2	2:B:370:ASN:C	2.29	0.53
2:B:278:SER:HB3	2:B:282:ARG:HD2	1.91	0.53
2:B:324:LYS:NZ	3:A:222:PRO:CD	2.70	0.53
2:B:418:LEU:HB3	2:B:422:TYR:CZ	2.43	0.53
3:A:107:HIS:HD2	3:A:152:LEU:HB2	1.63	0.53
3:A:202:PHE:HE1	3:A:267:PHE:CB	2.22	0.53
3:A:217:LEU:CD1	3:A:222:PRO:HG3	2.37	0.53
3:A:286:LEU:HB2	3:A:291:ILE:HG13	1.87	0.53
3:A:317:LEU:HD13	3:A:319:TYR:OH	2.08	0.53
1:K:284:GLU:HA	1:K:287:ASN:ND2	2.23	0.53
2:B:15:GLN:HG3	2:B:19:LYS:CD	2.38	0.53
2:B:154:LYS:HZ3	2:B:158:GLU:N	2.06	0.53
2:B:155:ILE:HA	2:B:158:GLU:OE1	2.08	0.53
2:B:159:TYR:HB3	2:B:161:ASP:OD1	2.08	0.53
2:B:238:THR:O	2:B:242:PHE:HB2	2.08	0.53
2:B:260:PHE:O	2:B:262:ARG:N	2.42	0.53
2:B:388:MET:O	2:B:391:ARG:HB2	2.09	0.53
3:A:194:THR:HG23	3:A:195:LEU:N	2.23	0.53
3:A:234:ILE:O	3:A:238:ILE:HG13	2.08	0.53
3:A:273:ALA:HA	3:A:274:PRO:C	2.29	0.53
3:A:370:LYS:CE	3:A:372:GLN:HA	2.37	0.53
1:K:48:LYS:HZ1	1:K:70:MET:HG3	1.73	0.53
1:K:66:TYR:CD2	1:K:68:PHE:CE1	2.95	0.53
1:K:215:GLU:HG2	1:K:216:LYS:HE3	1.85	0.53
1:K:312:ARG:HH11	1:K:318:ARG:NH2	2.05	0.53
2:B:32:PRO:HG3	2:B:81:PHE:HE1	1.74	0.53
2:B:215:LEU:HB3	2:B:217:LEU:H	1.73	0.53
2:B:306:ARG:NH2	2:B:339:SER:HB3	2.23	0.53
3:A:53:PHE:HA	3:A:63:PRO:HA	1.89	0.53
3:A:53:PHE:HD2	3:A:63:PRO:CA	2.20	0.53
1:K:66:TYR:CE2	1:K:68:PHE:HA	2.41	0.53
1:K:66:TYR:CD2	1:K:68:PHE:CZ	2.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:162:GLU:CD	1:K:235:SER:HG	2.11	0.53
2:B:1:MET:HA	2:B:3:GLU:OE1	2.09	0.53
2:B:246:LEU:HD12	2:B:352:ALA:CB	2.38	0.53
2:B:285:THR:H	2:B:288:GLU:CB	2.20	0.53
3:A:224:TYR:CE2	5:A:501:G2P:C6	2.91	0.53
3:A:276:ILE:HG21	3:A:281:ALA:HB2	1.90	0.53
1:K:29:ASN:H	1:K:32:GLU:CG	2.21	0.53
1:K:37:ALA:HB1	1:K:339:ALA:HB1	1.88	0.53
1:K:57:LEU:HD22	3:A:427:ALA:CA	2.38	0.53
1:K:96:GLY:HA2	1:K:258:ILE:O	2.09	0.53
1:K:221:ARG:CZ	1:K:237:SER:HB3	2.39	0.53
2:B:145:SER:HB2	2:B:184:ASN:OD1	2.09	0.53
2:B:156:ARG:NE	2:B:157:GLU:HA	2.24	0.53
2:B:260:PHE:N	2:B:262:ARG:CZ	2.71	0.53
3:A:62:VAL:HG13	3:A:62:VAL:O	2.08	0.53
3:A:93:ILE:HG21	3:A:121:ARG:CD	2.38	0.53
3:A:101:ASN:N	5:A:501:G2P:O3G	2.41	0.53
3:A:115:ILE:O	3:A:118:VAL:HG22	2.07	0.53
3:A:195:LEU:CD1	3:A:201:ALA:HB2	2.29	0.53
3:A:209:ILE:CD1	3:A:302:MET:HB2	2.39	0.53
1:K:31:ALA:O	1:K:34:LYS:HG2	2.09	0.53
1:K:43:CYS:SG	1:K:73:GLY:HA2	2.48	0.53
2:B:11:GLN:C	2:B:14:ASN:HB2	2.29	0.53
2:B:150:LEU:C	2:B:150:LEU:HD13	2.28	0.53
2:B:207:LEU:HD12	2:B:208:TYR:N	2.23	0.53
2:B:271:ALA:HB2	2:B:293:MET:HG2	1.90	0.53
2:B:289:LEU:H	2:B:289:LEU:CD1	2.22	0.53
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.23	0.53
3:A:101:ASN:HA	3:A:144:GLY:CA	2.38	0.53
3:A:242:LEU:CD2	3:A:252:LEU:H	2.21	0.53
3:A:251:ASP:CG	3:A:254:GLU:H	2.12	0.53
2:B:2:ARG:HD2	2:B:131:GLN:HA	1.91	0.53
2:B:4:ILE:HG13	2:B:132:GLY:H	1.73	0.53
2:B:225:LEU:HD11	5:B:501:G2P:H2N1	1.72	0.53
2:B:246:LEU:HD13	2:B:246:LEU:C	2.29	0.53
2:B:286:VAL:HG21	2:B:325:GLU:CD	2.29	0.53
2:B:388:MET:CE	2:B:388:MET:HA	2.39	0.53
3:A:21:TRP:HD1	3:A:67:PHE:HZ	1.56	0.53
3:A:260:VAL:HG13	3:A:268:PRO:HD3	1.91	0.53
3:A:265:ILE:HG23	3:A:432:TYR:OH	2.08	0.53
3:A:317:LEU:CD2	3:A:377:MET:HG3	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:368:LEU:HD12	3:A:368:LEU:C	2.29	0.53
1:K:357:LYS:HG3	1:K:358:ASN:OD1	2.08	0.53
2:B:68:LEU:CD1	5:B:501:G2P:O2G	2.56	0.53
2:B:73:MET:HG2	2:B:92:PHE:HE1	1.65	0.53
2:B:118:ASP:OD2	2:B:119:VAL:HG23	2.09	0.53
2:B:121:ARG:O	2:B:125:GLU:HG3	2.08	0.53
2:B:152:ILE:O	2:B:155:ILE:HG12	2.08	0.53
2:B:379:LYS:HB2	2:B:419:VAL:HG11	1.90	0.53
3:A:298:PRO:HB3	3:A:301:GLN:NE2	2.24	0.53
2:B:73:MET:HG3	2:B:74:ASP:N	2.24	0.53
2:B:207:LEU:HD12	2:B:207:LEU:C	2.29	0.53
2:B:334:GLN:HG2	2:B:335:ASN:ND2	2.24	0.53
2:B:339:SER:CA	2:B:429:THR:HB	2.38	0.53
3:A:63:PRO:HB2	3:A:87:PHE:CZ	2.44	0.53
3:A:103:TYR:HD1	3:A:189:LEU:HD23	1.72	0.53
3:A:124:LYS:HZ3	3:A:125:LEU:HB2	1.73	0.53
3:A:143:GLY:HA3	5:A:501:G2P:C3A	2.38	0.53
3:A:153:LEU:CD1	3:A:157:LEU:HG	2.39	0.53
3:A:337:THR:HG23	3:A:338:LYS:N	2.24	0.53
3:A:360:PRO:HG2	3:A:371:VAL:HG23	1.90	0.53
1:K:50:VAL:HB	1:K:68:PHE:CE2	2.44	0.53
1:K:278:VAL:HG12	1:K:279:ASP:N	2.23	0.53
2:B:5:VAL:HG12	2:B:123:GLU:HG3	1.91	0.53
2:B:6:HIS:HA	2:B:134:GLN:OE1	2.08	0.53
2:B:345:ILE:HG12	2:B:346:PRO:O	2.09	0.53
2:B:350:LYS:HE2	3:A:179:THR:O	2.09	0.53
3:A:3:GLU:HB3	3:A:64:ARG:HG2	1.91	0.53
3:A:144:GLY:HA2	3:A:186:ASN:ND2	2.25	0.53
3:A:181:VAL:CG1	3:A:404:PHE:CD1	2.92	0.53
3:A:430:LYS:HD3	3:A:434:GLU:CG	2.39	0.53
1:K:16:GLY:C	1:K:363:PRO:HD2	2.29	0.52
1:K:102:PHE:CD1	1:K:264:VAL:HG12	2.43	0.52
1:K:135:ILE:HD12	1:K:136:ILE:HG13	1.90	0.52
1:K:173:ASN:HB2	1:K:176:SER:H	1.75	0.52
1:K:326:GLY:HA2	1:K:362:LYS:NZ	2.24	0.52
2:B:172:SER:HB2	2:B:205:GLU:CB	2.24	0.52
2:B:318:ARG:HA	2:B:354:CYS:CB	2.39	0.52
2:B:376:GLU:CB	2:B:380:ARG:HH22	2.22	0.52
3:A:19:ALA:HB1	3:A:229:ARG:NH2	2.21	0.52
3:A:21:TRP:HA	3:A:24:TYR:CD2	2.44	0.52
3:A:21:TRP:CE3	3:A:24:TYR:HD2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:176:GLN:HG3	3:A:177:VAL:N	2.24	0.52
3:A:214:ARG:HB2	3:A:222:PRO:HD3	1.91	0.52
3:A:256:GLN:HE22	3:A:260:VAL:CG1	2.22	0.52
1:K:320:LEU:HD21	1:K:324:LEU:CD1	2.39	0.52
2:B:42:LEU:H	2:B:42:LEU:CD2	2.21	0.52
2:B:77:ARG:HD3	2:B:82:GLY:CA	2.39	0.52
2:B:116:VAL:HG23	2:B:117:LEU:CD2	2.36	0.52
2:B:213:ARG:HB2	2:B:213:ARG:HH11	1.70	0.52
2:B:244:GLY:HA2	2:B:355:ASP:CB	2.39	0.52
2:B:260:PHE:O	2:B:262:ARG:HD3	2.09	0.52
2:B:284:LEU:HB3	2:B:289:LEU:CD1	2.38	0.52
2:B:334:GLN:HG2	2:B:335:ASN:H	1.73	0.52
2:B:358:PRO:HG2	2:B:364:SER:OG	2.09	0.52
2:B:422:TYR:HD1	2:B:425:TYR:CZ	2.27	0.52
3:A:84:ARG:HD2	3:A:85:GLN:CA	2.38	0.52
3:A:256:GLN:HE22	3:A:260:VAL:HG13	1.73	0.52
3:A:387:ALA:HA	3:A:390:ARG:CZ	2.39	0.52
1:K:60:LYS:HD2	1:K:60:LYS:N	2.24	0.52
1:K:147:LEU:HD11	1:K:243:ILE:HD13	1.90	0.52
1:K:187:ASP:HB2	1:K:189:ARG:NE	2.25	0.52
1:K:246:LYS:CE	1:K:254:GLU:OE1	2.50	0.52
2:B:97:ALA:CB	2:B:143:THR:CA	2.75	0.52
2:B:97:ALA:H	2:B:143:THR:CG2	2.22	0.52
2:B:280:GLN:HG3	2:B:281:TYR:CE1	2.44	0.52
3:A:188:ILE:HG22	3:A:421:ALA:HB1	1.90	0.52
3:A:255:PHE:HZ	3:A:352:LYS:N	2.08	0.52
3:A:430:LYS:HZ2	3:A:430:LYS:HA	1.72	0.52
1:K:26:ARG:CZ	1:K:32:GLU:HG3	2.39	0.52
1:K:64:LYS:HD3	1:K:350:LEU:HG	1.91	0.52
1:K:172:LEU:HD11	1:K:173:ASN:HD21	1.75	0.52
1:K:206:ASN:ND2	1:K:209:GLU:H	2.08	0.52
1:K:327:ARG:NH2	1:K:327:ARG:HG2	2.24	0.52
2:B:120:VAL:CG2	2:B:121:ARG:HH21	2.22	0.52
2:B:252:LYS:CD	3:A:101:ASN:HB3	2.25	0.52
2:B:293:MET:HE1	2:B:367:PHE:CA	2.36	0.52
2:B:293:MET:HA	2:B:298:ASN:CB	2.38	0.52
2:B:308:GLY:HA3	2:B:372:THR:H	1.73	0.52
2:B:324:LYS:NZ	3:A:221:ARG:C	2.62	0.52
2:B:324:LYS:HZ1	3:A:222:PRO:CD	2.22	0.52
3:A:101:ASN:HA	3:A:144:GLY:N	2.24	0.52
3:A:122:ILE:HD12	3:A:123:ARG:CA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:306:ASP:CA	3:A:308:ARG:HH21	2.21	0.52
3:A:411:GLU:HB2	3:A:413:MET:HG2	1.90	0.52
1:K:173:ASN:HB2	1:K:176:SER:OG	2.09	0.52
1:K:192:ARG:HD3	1:K:327:ARG:HH12	1.74	0.52
2:B:65:LEU:O	2:B:92:PHE:HB3	2.10	0.52
2:B:101:TRP:CA	2:B:146:GLY:HA2	2.39	0.52
2:B:101:TRP:O	2:B:146:GLY:HA2	2.09	0.52
2:B:159:TYR:HB3	2:B:161:ASP:OD2	2.09	0.52
2:B:284:LEU:HB2	2:B:289:LEU:HD11	1.92	0.52
2:B:337:ASN:HB3	2:B:340:TYR:CG	2.45	0.52
2:B:341:PHE:HE1	2:B:348:ASN:H	1.55	0.52
2:B:375:GLN:HG2	2:B:376:GLU:H	1.75	0.52
3:A:417:GLU:HG3	3:A:418:PHE:CD2	2.44	0.52
2:B:273:LEU:C	2:B:273:LEU:HD13	2.30	0.52
2:B:285:THR:N	2:B:288:GLU:HB2	2.25	0.52
3:A:111:GLY:O	3:A:114:ILE:HG22	2.09	0.52
3:A:263:PRO:CD	3:A:264:ARG:HH11	2.22	0.52
3:A:355:ILE:HG22	3:A:356:ASN:N	2.25	0.52
1:K:68:PHE:CD2	1:K:71:VAL:HG22	2.45	0.52
1:K:236:HIS:CE1	1:K:267:ALA:HB3	2.45	0.52
2:B:277:GLY:O	2:B:280:GLN:HG2	2.08	0.52
2:B:324:LYS:HZ2	3:A:221:ARG:HD2	1.69	0.52
3:A:205:ASP:HB2	3:A:208:ALA:HB3	1.88	0.52
1:K:27:PRO:HA	1:K:74:ALA:HB1	1.91	0.52
1:K:48:LYS:CE	1:K:70:MET:HG3	2.39	0.52
1:K:144:PHE:CE1	1:K:156:VAL:HG21	2.44	0.52
1:K:181:ARG:NH2	1:K:197:LYS:NZ	2.58	0.52
2:B:203:ASP:OD1	2:B:206:ALA:HB2	2.09	0.52
2:B:240:LEU:HA	2:B:247:ASN:HD21	1.75	0.52
3:A:16:ILE:HA	3:A:228:ASN:ND2	2.17	0.52
3:A:140:SER:OG	3:A:143:GLY:HA3	2.10	0.52
3:A:174:ALA:HB2	3:A:206:ASN:HB2	1.92	0.52
3:A:233:GLN:HG3	3:A:234:ILE:N	2.25	0.52
3:A:286:LEU:CG	3:A:291:ILE:HD11	2.39	0.52
3:A:339:ARG:HG3	3:A:340:SER:CA	2.40	0.52
1:K:15:LYS:HG2	1:K:364:GLU:OE2	2.10	0.52
1:K:25:CYS:HB3	1:K:43:CYS:SG	2.50	0.52
1:K:160:LEU:H	1:K:172:LEU:CB	2.23	0.52
1:K:311:TYR:CD1	1:K:321:GLN:HG3	2.44	0.52
2:B:363:MET:HE3	2:B:363:MET:N	2.23	0.52
2:B:422:TYR:CD1	2:B:425:TYR:CE2	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:23:LEU:HA	3:A:364:PRO:HG3	1.89	0.52
3:A:276:ILE:HG23	3:A:281:ALA:CA	2.40	0.52
3:A:286:LEU:HD11	3:A:372:GLN:HB3	1.92	0.52
3:A:313:MET:O	3:A:347:CYS:HB3	2.09	0.52
1:K:212:GLN:O	1:K:215:GLU:HG2	2.10	0.52
1:K:233:SER:HG	1:K:267:ALA:HA	1.75	0.52
1:K:297:ARG:NH2	2:B:260:PHE:HD2	2.08	0.52
2:B:12:CYS:SG	5:B:501:G2P:C4	2.98	0.52
2:B:34:GLY:HA3	2:B:58:LYS:CG	2.37	0.52
2:B:34:GLY:HA2	2:B:84:ILE:CD1	2.40	0.52
2:B:208:TYR:CE2	2:B:225:LEU:HD23	2.44	0.52
3:A:41:THR:HG22	3:A:42:ILE:N	2.24	0.52
3:A:214:ARG:HG3	3:A:215:ARG:H	1.74	0.52
3:A:214:ARG:CB	3:A:222:PRO:HD3	2.40	0.52
3:A:215:ARG:HH11	3:A:216:ASN:ND2	2.04	0.52
1:K:110:GLY:HA2	1:K:113:PHE:H	1.74	0.51
1:K:289:ASN:O	1:K:292:LEU:HB2	2.10	0.51
2:B:23:VAL:HG13	2:B:24:ILE:N	2.24	0.51
2:B:167:PHE:CE1	2:B:200:TYR:CD2	2.96	0.51
2:B:174:LYS:CD	2:B:175:VAL:HG23	2.40	0.51
2:B:251:ARG:NH2	3:A:100:ALA:O	2.43	0.51
2:B:260:PHE:CD2	3:A:406:HIS:CE1	2.97	0.51
2:B:299:MET:HE2	2:B:299:MET:HA	1.92	0.51
2:B:313:VAL:O	2:B:349:VAL:HG13	2.10	0.51
3:A:30:ILE:HD12	3:A:61:HIS:HB2	1.92	0.51
3:A:189:LEU:HD11	3:A:417:GLU:OE2	2.10	0.51
3:A:399:TYR:OH	3:A:415:GLU:HB3	2.10	0.51
1:K:192:ARG:HG2	1:K:192:ARG:NH1	2.26	0.51
1:K:240:SER:HB3	1:K:262:ASN:OD1	2.10	0.51
2:B:1:MET:HE2	2:B:49:VAL:CA	2.41	0.51
2:B:14:ASN:CB	2:B:72:THR:HG21	2.40	0.51
2:B:252:LYS:CG	3:A:100:ALA:HB1	2.40	0.51
2:B:272:PRO:CB	2:B:292:GLN:HE22	2.23	0.51
3:A:3:GLU:C	3:A:51:THR:HG22	2.30	0.51
3:A:7:ILE:HD12	3:A:8:HIS:N	2.24	0.51
3:A:102:ASN:CG	3:A:105:ARG:H	2.14	0.51
1:K:57:LEU:HD21	3:A:427:ALA:HB1	1.91	0.51
1:K:93:VAL:CG1	1:K:243:ILE:HD12	2.40	0.51
2:B:1:MET:HG3	2:B:127:CYS:CB	2.34	0.51
2:B:251:ARG:NH2	3:A:102:ASN:H	2.08	0.51
2:B:361:LEU:HD21	2:B:364:SER:OG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:26:LEU:HD23	3:A:364:PRO:CB	2.40	0.51
3:A:90:GLU:CA	3:A:121:ARG:HH21	2.21	0.51
3:A:145:THR:HB	5:A:501:G2P:O1B	2.11	0.51
3:A:233:GLN:CA	3:A:363:VAL:HG13	2.40	0.51
1:K:15:LYS:HE3	1:K:364:GLU:OE2	2.09	0.51
1:K:68:PHE:CD2	1:K:71:VAL:CG2	2.94	0.51
1:K:189:ARG:CZ	1:K:189:ARG:HB2	2.39	0.51
2:B:1:MET:CG	2:B:127:CYS:HB2	2.33	0.51
2:B:179:VAL:HG13	2:B:180:VAL:N	2.24	0.51
2:B:260:PHE:C	2:B:262:ARG:HD3	2.31	0.51
3:A:317:LEU:CB	3:A:353:VAL:HB	2.25	0.51
3:A:332:ILE:HG22	3:A:336:LYS:HG2	1.93	0.51
1:K:26:ARG:NH1	1:K:26:ARG:HG3	2.25	0.51
1:K:180:GLU:HG3	1:K:199:LEU:CD1	2.36	0.51
2:B:47:ILE:HG22	2:B:59:TYR:HD1	1.76	0.51
2:B:99:ASN:HA	2:B:142:GLY:HA3	1.93	0.51
2:B:117:LEU:O	2:B:120:VAL:HG22	2.10	0.51
2:B:159:TYR:HD2	2:B:162:ARG:CG	2.23	0.51
2:B:225:LEU:HD12	2:B:225:LEU:C	2.31	0.51
2:B:252:LYS:CG	3:A:100:ALA:O	2.59	0.51
2:B:376:GLU:HG3	2:B:379:LYS:HZ3	1.75	0.51
3:A:54:SER:O	3:A:61:HIS:HA	2.11	0.51
3:A:344:VAL:HG12	3:A:438:ASP:OD2	2.10	0.51
1:K:352:TYR:HB2	4:K:501:MZK:C12	2.40	0.51
2:B:193:VAL:HG13	2:B:194:GLU:H	1.76	0.51
3:A:20:CYS:HB3	3:A:24:TYR:CZ	2.45	0.51
3:A:132:LEU:HD23	3:A:134:GLY:O	2.11	0.51
3:A:215:ARG:HD3	3:A:216:ASN:N	2.25	0.51
3:A:416:GLY:O	3:A:420:GLU:HG2	2.11	0.51
1:K:154:PHE:CE2	1:K:205:HIS:HE1	2.29	0.51
1:K:168:LEU:CD1	1:K:182:LEU:HB3	2.38	0.51
1:K:257:LYS:CA	1:K:368:LYS:HD3	2.38	0.51
2:B:189:VAL:HG13	2:B:190:HIS:N	2.26	0.51
2:B:272:PRO:CA	2:B:292:GLN:HE22	2.24	0.51
2:B:273:LEU:O	2:B:273:LEU:HD13	2.11	0.51
2:B:323:MET:HG3	3:A:210:TYR:CE2	2.46	0.51
3:A:99:ALA:CB	3:A:145:THR:N	2.74	0.51
3:A:188:ILE:O	3:A:191:THR:HG22	2.10	0.51
3:A:382:THR:HG22	3:A:433:GLU:HA	1.92	0.51
1:K:19:ILE:HB	1:K:361:ASN:HB2	1.93	0.51
1:K:312:ARG:HD3	2:B:414:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:341:LEU:H	1:K:341:LEU:CD1	2.23	0.51
2:B:33:THR:CG2	2:B:35:SER:H	2.13	0.51
2:B:210:ILE:HA	2:B:213:ARG:HG2	1.92	0.51
3:A:14:VAL:HG23	3:A:15:GLN:N	2.25	0.51
3:A:115:ILE:O	3:A:119:LEU:HG	2.11	0.51
3:A:188:ILE:HG22	3:A:421:ALA:CB	2.40	0.51
3:A:286:LEU:CD2	3:A:291:ILE:HD11	2.41	0.51
3:A:370:LYS:HZ3	3:A:372:GLN:HA	1.74	0.51
3:A:397:LEU:HD23	3:A:397:LEU:C	2.30	0.51
1:K:17:LYS:CD	1:K:17:LYS:H	2.24	0.51
1:K:97:TYR:HB3	1:K:99:CYS:SG	2.50	0.51
2:B:77:ARG:NH1	2:B:82:GLY:HA2	2.11	0.51
2:B:113:VAL:HA	2:B:116:VAL:HG22	1.93	0.51
2:B:213:ARG:HG3	2:B:214:THR:N	2.24	0.51
2:B:392:LYS:CG	2:B:395:LEU:HD11	2.41	0.51
3:A:35:GLN:CA	3:A:60:LYS:HE2	2.41	0.51
3:A:153:LEU:HD12	3:A:156:ARG:CZ	2.40	0.51
3:A:277:SER:HB2	3:A:280:LYS:HG3	1.92	0.51
1:K:31:ALA:CB	1:K:34:LYS:HE2	2.40	0.51
1:K:190:ASN:ND2	1:K:192:ARG:H	2.09	0.51
1:K:327:ARG:HD3	1:K:362:LYS:HZ1	1.76	0.51
2:B:101:TRP:HD1	2:B:149:THR:HG21	1.74	0.51
3:A:272:TYR:H	3:A:302:MET:HE1	1.76	0.51
3:A:273:ALA:HB2	3:A:295:CYS:CB	2.40	0.51
3:A:316:CYS:O	3:A:317:LEU:HD23	2.11	0.51
3:A:349:THR:HG21	3:A:351:PHE:CE1	2.46	0.51
1:K:271:ASN:HD22	1:K:274:ARG:N	2.09	0.50
2:B:117:LEU:HA	2:B:120:VAL:HG22	1.93	0.50
2:B:148:GLY:HA2	2:B:151:LEU:HG	1.92	0.50
2:B:306:ARG:HH21	2:B:309:ARG:CZ	2.24	0.50
2:B:324:LYS:HE3	3:A:221:ARG:HH11	1.74	0.50
3:A:21:TRP:CE3	3:A:24:TYR:CD2	2.99	0.50
3:A:30:ILE:N	3:A:36:MET:HE1	2.26	0.50
3:A:54:SER:HB2	3:A:64:ARG:HE	1.76	0.50
3:A:153:LEU:CD1	3:A:157:LEU:HD11	2.37	0.50
3:A:154:MET:HE2	3:A:154:MET:C	2.31	0.50
1:K:15:LYS:HD3	1:K:362:LYS:CB	2.39	0.50
1:K:192:ARG:HG2	1:K:192:ARG:HH11	1.76	0.50
1:K:215:GLU:CD	1:K:216:LYS:HE3	2.31	0.50
1:K:314:SER:HB3	1:K:317:THR:OG1	2.10	0.50
2:B:52:ASN:H	2:B:62:ARG:NH2	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:THR:HB	5:B:501:G2P:O2B	2.10	0.50
2:B:279:GLN:HE22	2:B:284:LEU:HD21	1.76	0.50
3:A:9:VAL:HG22	3:A:149:PHE:CE1	2.46	0.50
3:A:123:ARG:HG3	3:A:127:ASP:OD1	2.12	0.50
3:A:295:CYS:HA	3:A:300:ASN:OD1	2.12	0.50
3:A:395:PHE:HB3	3:A:422:ARG:HH12	1.75	0.50
3:A:401:LYS:CG	3:A:403:ALA:HB2	2.42	0.50
1:K:157:LYS:HE3	1:K:203:THR:HG1	1.73	0.50
1:K:311:TYR:CE2	1:K:321:GLN:HG3	2.46	0.50
1:K:350:LEU:HD13	1:K:350:LEU:C	2.31	0.50
2:B:28:HIS:HE1	2:B:51:TYR:CZ	2.29	0.50
2:B:143:THR:HG22	2:B:147:MET:SD	2.52	0.50
3:A:65:ALA:HB3	3:A:87:PHE:CE2	2.47	0.50
3:A:217:LEU:HD12	3:A:222:PRO:CG	2.40	0.50
3:A:417:GLU:O	3:A:420:GLU:HB2	2.11	0.50
1:K:33:ARG:HG3	1:K:33:ARG:HH11	1.76	0.50
1:K:33:ARG:HG3	1:K:33:ARG:NH1	2.26	0.50
1:K:293:LEU:CD1	3:A:405:VAL:HG11	2.35	0.50
2:B:47:ILE:HD13	2:B:241:ARG:HH12	1.75	0.50
2:B:309:ARG:HG2	2:B:428:ALA:O	2.11	0.50
3:A:24:TYR:HB3	3:A:52:PHE:CE1	2.46	0.50
3:A:316:CYS:SG	3:A:377:MET:HA	2.52	0.50
1:K:221:ARG:NH2	1:K:233:SER:HB2	2.25	0.50
2:B:48:ASN:HB2	2:B:59:TYR:OH	2.12	0.50
2:B:260:PHE:CD2	3:A:404:PHE:N	2.80	0.50
2:B:286:VAL:CB	2:B:287:PRO:HD3	2.38	0.50
2:B:321:MET:HG2	2:B:322:SER:N	2.26	0.50
2:B:350:LYS:HE2	3:A:180:ALA:N	2.26	0.50
3:A:47:ASP:OD2	3:A:243:ARG:HA	2.10	0.50
3:A:90:GLU:OE1	3:A:121:ARG:HB3	2.11	0.50
3:A:96:LYS:HD3	3:A:96:LYS:C	2.30	0.50
3:A:237:SER:HB3	3:A:320:ARG:HD2	1.93	0.50
3:A:385:ALA:HB2	3:A:432:TYR:CD2	2.45	0.50
1:K:32:GLU:HA	1:K:32:GLU:OE2	2.11	0.50
1:K:301:ALA:O	1:K:304:GLU:HB3	2.12	0.50
1:K:320:LEU:O	1:K:324:LEU:HD22	2.12	0.50
1:K:344:GLU:HG2	3:A:414:GLU:HB2	1.94	0.50
1:K:344:GLU:HG2	3:A:414:GLU:CB	2.42	0.50
2:B:151:LEU:O	2:B:155:ILE:HG23	2.12	0.50
2:B:205:GLU:HG3	2:B:206:ALA:H	1.76	0.50
3:A:118:VAL:O	3:A:122:ILE:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:312:TYR:CD2	3:A:341:ILE:CG2	2.95	0.50
1:K:54:THR:HG23	1:K:56:GLY:H	1.77	0.50
1:K:170:ASP:HB2	1:K:180:GLU:N	2.27	0.50
1:K:170:ASP:N	1:K:180:GLU:H	2.06	0.50
1:K:171:LEU:HD13	1:K:221:ARG:HB2	1.93	0.50
2:B:4:ILE:HD12	2:B:4:ILE:N	2.26	0.50
2:B:97:ALA:HB2	2:B:143:THR:HA	1.84	0.50
2:B:214:THR:HB	2:B:275:SER:CA	2.42	0.50
2:B:252:LYS:HG3	3:A:100:ALA:C	2.32	0.50
2:B:273:LEU:HD22	2:B:274:THR:H	1.73	0.50
2:B:311:LEU:O	2:B:342:VAL:HG21	2.12	0.50
3:A:9:VAL:HG13	3:A:149:PHE:CD1	2.47	0.50
3:A:76:ASP:HA	3:A:79:ARG:HG2	1.94	0.50
3:A:275:VAL:CA	3:A:300:ASN:HD22	2.23	0.50
1:K:16:GLY:HA3	1:K:363:PRO:CD	2.41	0.50
1:K:66:TYR:HD2	1:K:68:PHE:CZ	2.30	0.50
2:B:51:TYR:CD1	2:B:61:PRO:HA	2.46	0.50
2:B:98:GLY:O	2:B:99:ASN:HB2	2.11	0.50
2:B:271:ALA:HB2	2:B:293:MET:CG	2.41	0.50
2:B:323:MET:HG3	3:A:210:TYR:HE2	1.76	0.50
3:A:9:VAL:HG22	3:A:149:PHE:HD1	1.75	0.50
3:A:70:LEU:HD23	3:A:99:ALA:HA	1.94	0.50
3:A:99:ALA:HB2	3:A:145:THR:HA	1.94	0.50
3:A:101:ASN:HA	3:A:144:GLY:H	1.76	0.50
3:A:319:TYR:HB2	3:A:355:ILE:HG23	1.94	0.50
1:K:23:VAL:CG2	1:K:68:PHE:CD1	2.95	0.50
2:B:13:GLY:HA2	2:B:16:ILE:HB	1.93	0.50
2:B:59:TYR:O	2:B:84:ILE:HD11	2.10	0.50
2:B:101:TRP:CG	2:B:102:ALA:N	2.78	0.50
2:B:342:VAL:HG12	2:B:344:TRP:H	1.76	0.50
2:B:353:VAL:HG23	2:B:353:VAL:O	2.12	0.50
3:A:164:LYS:HA	3:A:164:LYS:HZ1	1.76	0.50
3:A:188:ILE:HD12	3:A:188:ILE:N	2.27	0.50
3:A:223:THR:HB	3:A:226:ASN:H	1.77	0.50
1:K:48:LYS:HZ1	1:K:70:MET:CG	2.25	0.49
2:B:2:ARG:CG	2:B:131:GLN:HB2	2.42	0.49
2:B:14:ASN:CG	2:B:72:THR:HG21	2.32	0.49
2:B:379:LYS:HB2	2:B:415:MET:SD	2.52	0.49
3:A:72:PRO:HG3	3:A:96:LYS:HZ2	1.77	0.49
1:K:44:ASP:HB3	1:K:47:ARG:HB2	1.94	0.49
2:B:148:GLY:CA	2:B:151:LEU:HD21	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:PHE:CZ	3:A:405:VAL:C	2.86	0.49
2:B:350:LYS:HZ1	3:A:179:THR:CA	2.22	0.49
3:A:4:CYS:H	3:A:51:THR:CB	2.25	0.49
3:A:240:ALA:HA	3:A:243:ARG:HE	1.77	0.49
3:A:310:GLY:HA3	3:A:381:THR:HG22	1.91	0.49
1:K:369:LEU:HD22	1:K:369:LEU:N	2.27	0.49
2:B:6:HIS:HB3	2:B:21:TRP:CE2	2.46	0.49
2:B:45:GLU:CG	2:B:46:ARG:HE	2.16	0.49
2:B:156:ARG:HA	2:B:164:MET:CE	2.43	0.49
2:B:186:THR:HB	2:B:385:PHE:CE1	2.47	0.49
2:B:272:PRO:CB	2:B:279:GLN:HE22	2.19	0.49
2:B:396:HIS:H	2:B:396:HIS:CD2	2.28	0.49
2:B:405:GLU:HA	2:B:408:PHE:CD1	2.43	0.49
2:B:418:LEU:HB3	2:B:422:TYR:OH	2.12	0.49
3:A:3:GLU:HA	3:A:51:THR:N	2.26	0.49
3:A:150:THR:CG2	3:A:190:THR:HG21	2.42	0.49
3:A:166:LYS:HD2	3:A:198:SER:CA	2.21	0.49
3:A:232:SER:HB3	3:A:363:VAL:HG12	1.90	0.49
3:A:404:PHE:N	3:A:404:PHE:CD2	2.79	0.49
3:A:430:LYS:HD3	3:A:434:GLU:OE1	2.13	0.49
1:K:29:ASN:HB2	1:K:32:GLU:H	1.78	0.49
1:K:181:ARG:HG3	1:K:198:GLY:HA3	1.95	0.49
2:B:137:HIS:HB2	2:B:144:GLY:CA	2.42	0.49
2:B:251:ARG:HH22	3:A:102:ASN:H	1.59	0.49
2:B:266:PHE:CE2	2:B:370:ASN:HB3	2.48	0.49
2:B:313:VAL:HG13	2:B:367:PHE:CE2	2.48	0.49
2:B:339:SER:O	2:B:429:THR:HB	2.12	0.49
2:B:422:TYR:HD1	2:B:425:TYR:CE2	2.31	0.49
3:A:8:HIS:HB2	3:A:14:VAL:HG12	1.94	0.49
3:A:153:LEU:HG	3:A:157:LEU:CD1	2.42	0.49
3:A:171:ILE:O	3:A:171:ILE:HG23	2.11	0.49
3:A:256:GLN:OE1	3:A:259:LEU:HD12	2.12	0.49
1:K:82:TYR:CE1	1:K:86:VAL:HB	2.47	0.49
1:K:168:LEU:HB2	1:K:182:LEU:CB	2.42	0.49
1:K:329:ARG:HA	1:K:363:PRO:CB	2.42	0.49
2:B:46:ARG:CG	2:B:242:PHE:CE1	2.95	0.49
2:B:148:GLY:CA	2:B:151:LEU:HG	2.42	0.49
2:B:157:GLU:HA	2:B:157:GLU:OE1	2.12	0.49
2:B:375:GLN:HG3	2:B:422:TYR:CG	2.47	0.49
3:A:6:SER:CB	3:A:21:TRP:CZ2	2.95	0.49
3:A:265:ILE:CD1	3:A:432:TYR:CE1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:181:ARG:NE	1:K:197:LYS:HG3	2.27	0.49
1:K:292:LEU:HD23	4:K:501:MZK:N1	2.27	0.49
2:B:260:PHE:HB3	2:B:262:ARG:CD	2.41	0.49
2:B:318:ARG:CB	2:B:358:PRO:HG3	2.43	0.49
2:B:320:ARG:HG2	2:B:321:MET:N	2.21	0.49
3:A:181:VAL:CG1	3:A:404:PHE:CE1	2.79	0.49
3:A:388:TRP:CZ3	3:A:428:LEU:CD2	2.95	0.49
1:K:39:SER:HA	1:K:338:PRO:HB2	1.93	0.49
1:K:66:TYR:HD2	1:K:68:PHE:CG	2.31	0.49
1:K:157:LYS:HE2	1:K:203:THR:OG1	2.07	0.49
1:K:283:ARG:HG2	1:K:287:ASN:HD21	1.78	0.49
2:B:137:HIS:HB2	2:B:144:GLY:HA2	1.94	0.49
2:B:149:THR:HG23	2:B:188:SER:CB	2.43	0.49
2:B:154:LYS:HE2	2:B:154:LYS:CA	2.39	0.49
2:B:419:VAL:HA	2:B:422:TYR:CG	2.45	0.49
3:A:9:VAL:CG1	3:A:149:PHE:HD1	2.25	0.49
3:A:23:LEU:HA	3:A:364:PRO:CD	2.42	0.49
3:A:124:LYS:NZ	3:A:125:LEU:HB2	2.28	0.49
3:A:255:PHE:HZ	3:A:352:LYS:CA	2.26	0.49
1:K:50:VAL:H	1:K:68:PHE:HE2	1.59	0.49
1:K:104:TYR:HD2	1:K:105:GLY:N	2.11	0.49
2:B:151:LEU:HD12	2:B:152:ILE:HG12	1.95	0.49
2:B:180:VAL:HG23	2:B:181:GLU:N	2.28	0.49
2:B:208:TYR:CE2	2:B:225:LEU:CD2	2.95	0.49
2:B:306:ARG:HH22	2:B:339:SER:HB3	1.77	0.49
2:B:331:LEU:HA	2:B:334:GLN:HE22	1.74	0.49
2:B:342:VAL:HG12	2:B:344:TRP:N	2.28	0.49
3:A:23:LEU:HD22	3:A:24:TYR:CD1	2.47	0.49
3:A:286:LEU:HD12	3:A:286:LEU:C	2.32	0.49
3:A:430:LYS:CD	3:A:434:GLU:HG3	2.43	0.49
1:K:28:PHE:CD2	1:K:32:GLU:CB	2.96	0.49
1:K:59:ASP:HA	1:K:60:LYS:HZ2	1.76	0.49
1:K:192:ARG:HH21	1:K:326:GLY:HA3	1.77	0.49
2:B:27:GLU:HA	2:B:27:GLU:OE2	2.12	0.49
2:B:390:ARG:HA	2:B:390:ARG:NH1	2.27	0.49
3:A:35:GLN:HG2	3:A:59:GLY:O	2.13	0.49
3:A:72:PRO:HG3	3:A:96:LYS:HA	1.95	0.49
3:A:220:GLU:CD	3:A:221:ARG:H	2.16	0.49
1:K:66:TYR:CD2	1:K:68:PHE:CG	3.01	0.49
2:B:120:VAL:HG23	2:B:121:ARG:N	2.28	0.49
2:B:156:ARG:HH21	2:B:157:GLU:CA	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:THR:CG2	2:B:385:PHE:CE1	2.96	0.49
2:B:249:ASP:O	2:B:253:LEU:HD23	2.13	0.49
2:B:418:LEU:HB3	2:B:422:TYR:CE1	2.48	0.49
3:A:7:ILE:HG22	3:A:137:VAL:HA	1.95	0.49
3:A:12:ALA:O	3:A:16:ILE:HG22	2.13	0.49
3:A:177:VAL:HG22	3:A:178:SER:O	2.12	0.49
3:A:388:TRP:CH2	3:A:432:TYR:CD2	3.01	0.49
3:A:401:LYS:O	3:A:401:LYS:HE3	2.13	0.49
1:K:320:LEU:HD23	1:K:324:LEU:HD11	1.95	0.48
2:B:24:ILE:O	2:B:27:GLU:HB2	2.13	0.48
2:B:47:ILE:CG2	2:B:59:TYR:CE1	2.96	0.48
2:B:156:ARG:HA	2:B:164:MET:SD	2.53	0.48
3:A:111:GLY:HA3	3:A:152:LEU:CD1	2.42	0.48
3:A:130:THR:HG23	3:A:131:GLY:H	1.78	0.48
3:A:226:ASN:O	3:A:229:ARG:HB2	2.12	0.48
3:A:311:LYS:HG3	3:A:342:GLN:OE1	2.13	0.48
3:A:358:GLN:HG2	3:A:359:PRO:N	2.28	0.48
3:A:407:TRP:CE3	3:A:407:TRP:CA	2.96	0.48
1:K:277:ALA:HB1	1:K:281:ARG:HB2	1.93	0.48
2:B:36:TYR:CD2	2:B:44:LEU:CB	2.95	0.48
2:B:46:ARG:HG2	2:B:242:PHE:CE1	2.48	0.48
2:B:156:ARG:HB2	2:B:164:MET:HE3	1.95	0.48
2:B:322:SER:HG	3:A:221:ARG:CB	2.26	0.48
2:B:390:ARG:O	2:B:392:LYS:HE2	2.13	0.48
3:A:113:GLU:CD	3:A:113:GLU:H	2.16	0.48
3:A:154:MET:HG2	3:A:197:HIS:HB2	1.93	0.48
3:A:200:CYS:CB	3:A:267:PHE:HB3	2.33	0.48
3:A:267:PHE:N	3:A:267:PHE:CD2	2.81	0.48
3:A:349:THR:CG2	3:A:351:PHE:HD1	2.25	0.48
3:A:385:ALA:HB1	3:A:429:GLU:CD	2.32	0.48
3:A:387:ALA:HB2	3:A:390:ARG:NH1	2.28	0.48
1:K:170:ASP:OD2	1:K:176:SER:HB2	2.12	0.48
2:B:156:ARG:HA	2:B:164:MET:HE1	1.95	0.48
3:A:214:ARG:HH22	3:A:218:ASP:HA	1.78	0.48
3:A:243:ARG:HD3	3:A:244:PHE:CZ	2.49	0.48
3:A:338:LYS:HZ3	3:A:338:LYS:HA	1.78	0.48
1:K:78:GLN:CG	1:K:113:PHE:HE2	2.27	0.48
2:B:33:THR:HG23	2:B:34:GLY:N	2.29	0.48
2:B:208:TYR:CG	2:B:220:PRO:HG2	2.47	0.48
2:B:258:VAL:O	2:B:258:VAL:HG23	2.13	0.48
2:B:318:ARG:HG2	2:B:354:CYS:CB	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:42:ILE:O	3:A:46:ASP:HB3	2.13	0.48
3:A:179:THR:N	3:A:183:GLU:OE1	2.46	0.48
3:A:420:GLU:O	3:A:424:ASP:HB3	2.13	0.48
1:K:77:LYS:HE3	1:K:78:GLN:H	1.75	0.48
1:K:78:GLN:CG	1:K:113:PHE:CE2	2.96	0.48
1:K:293:LEU:CD1	3:A:405:VAL:CG1	2.91	0.48
1:K:347:LEU:HD23	1:K:347:LEU:C	2.34	0.48
2:B:31:ASP:OD1	2:B:37:HIS:HB2	2.13	0.48
2:B:81:PHE:HA	2:B:83:GLN:CD	2.33	0.48
2:B:242:PHE:HD1	2:B:242:PHE:HA	1.51	0.48
2:B:376:GLU:HG3	2:B:379:LYS:HZ1	1.75	0.48
3:A:141:PHE:HD2	3:A:141:PHE:HA	1.57	0.48
3:A:174:ALA:CB	3:A:207:GLU:H	2.22	0.48
3:A:181:VAL:O	3:A:184:PRO:HD2	2.14	0.48
3:A:243:ARG:CD	3:A:244:PHE:CE2	2.95	0.48
2:B:111:GLU:H	2:B:111:GLU:CD	2.16	0.48
2:B:117:LEU:CA	2:B:120:VAL:HG22	2.44	0.48
2:B:166:THR:O	2:B:167:PHE:HD1	1.96	0.48
2:B:225:LEU:HD11	2:B:226:ASN:ND2	2.28	0.48
2:B:228:LEU:HD23	2:B:229:VAL:N	2.29	0.48
2:B:371:SER:CB	2:B:374:ILE:HG22	2.34	0.48
2:B:394:PHE:HD1	2:B:396:HIS:NE2	2.10	0.48
3:A:2:ARG:HE	3:A:132:LEU:C	2.17	0.48
3:A:52:PHE:CB	3:A:53:PHE:CE1	2.96	0.48
3:A:339:ARG:HG3	3:A:340:SER:HA	1.95	0.48
3:A:368:LEU:HD13	3:A:369:ALA:O	2.13	0.48
3:A:408:TYR:CD1	3:A:418:PHE:CZ	3.01	0.48
1:K:117:GLY:HA2	1:K:134:GLY:O	2.14	0.48
1:K:181:ARG:HH22	1:K:183:GLN:N	2.12	0.48
1:K:243:ILE:HG22	1:K:245:MET:HG3	1.95	0.48
1:K:295:LEU:O	1:K:298:VAL:HG12	2.12	0.48
1:K:320:LEU:HD12	1:K:320:LEU:O	2.13	0.48
2:B:252:LYS:CG	3:A:100:ALA:C	2.82	0.48
2:B:343:GLU:HG2	2:B:344:TRP:N	2.29	0.48
2:B:377:LEU:CA	2:B:380:ARG:HG3	2.43	0.48
2:B:394:PHE:HA	2:B:396:HIS:NE2	2.29	0.48
3:A:91:GLN:NE2	3:A:91:GLN:H	2.10	0.48
3:A:174:ALA:HB3	3:A:176:GLN:CG	2.43	0.48
3:A:210:TYR:HD1	3:A:213:CYS:SG	2.36	0.48
3:A:360:PRO:HB3	3:A:374:ALA:CB	2.40	0.48
3:A:391:LEU:O	3:A:394:LYS:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:399:TYR:HB2	3:A:422:ARG:NH2	2.29	0.48
1:K:27:PRO:HA	1:K:74:ALA:CB	2.44	0.48
1:K:94:ILE:HD13	1:K:150:ASN:ND2	2.27	0.48
1:K:168:LEU:HB3	1:K:182:LEU:HG	1.96	0.48
1:K:206:ASN:CG	1:K:209:GLU:HG3	2.33	0.48
1:K:323:SER:HA	1:K:328:THR:HB	1.95	0.48
2:B:167:PHE:CE2	2:B:233:MET:SD	3.07	0.48
2:B:169:VAL:O	2:B:169:VAL:HG23	2.14	0.48
2:B:183:TYR:CD1	2:B:385:PHE:CD1	3.02	0.48
2:B:252:LYS:HG2	3:A:100:ALA:O	2.13	0.48
1:K:66:TYR:CD2	1:K:68:PHE:CD1	3.01	0.48
1:K:190:ASN:HD22	1:K:192:ARG:N	2.12	0.48
1:K:234:ARG:CZ	1:K:284:GLU:HG3	2.44	0.48
1:K:288:ILE:O	1:K:291:SER:HB3	2.14	0.48
2:B:45:GLU:O	2:B:49:VAL:HG13	2.14	0.48
2:B:148:GLY:C	2:B:151:LEU:HG	2.34	0.48
2:B:150:LEU:HD13	2:B:150:LEU:O	2.13	0.48
2:B:260:PHE:C	2:B:262:ARG:N	2.68	0.48
2:B:380:ARG:O	2:B:383:GLU:HB3	2.14	0.48
3:A:21:TRP:HE3	3:A:24:TYR:HD2	1.62	0.48
3:A:274:PRO:HG2	3:A:286:LEU:HD23	1.95	0.48
1:K:28:PHE:CE2	1:K:37:ALA:HB3	2.49	0.48
1:K:57:LEU:CD1	3:A:427:ALA:HB2	2.43	0.48
1:K:159:SER:HB2	1:K:199:LEU:CD2	2.26	0.48
1:K:297:ARG:NH1	2:B:262:ARG:HE	2.12	0.48
1:K:312:ARG:HH12	1:K:318:ARG:HH21	1.60	0.48
2:B:276:ARG:HG3	2:B:276:ARG:HH11	1.79	0.48
2:B:337:ASN:HB3	2:B:340:TYR:CD2	2.49	0.48
2:B:413:SER:HA	2:B:416:ASN:HD22	1.77	0.48
3:A:188:ILE:CB	3:A:395:PHE:HD1	2.27	0.48
1:K:25:CYS:CB	1:K:43:CYS:SG	3.02	0.47
1:K:139:THR:HG23	1:K:140:LEU:N	2.28	0.47
1:K:170:ASP:OD1	1:K:172:LEU:HD23	2.14	0.47
1:K:178:VAL:HA	1:K:220:LYS:CE	2.33	0.47
2:B:152:ILE:HA	2:B:155:ILE:CG1	2.43	0.47
2:B:258:VAL:HG12	2:B:263:LEU:HB3	1.96	0.47
2:B:267:MET:SD	2:B:299:MET:HE1	2.53	0.47
2:B:313:VAL:HG22	2:B:368:ILE:O	2.14	0.47
2:B:415:MET:HG2	2:B:419:VAL:CG1	2.44	0.47
3:A:49:PHE:CE1	3:A:53:PHE:CD1	3.00	0.47
3:A:176:GLN:NE2	3:A:207:GLU:HB2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:188:ILE:CB	3:A:395:PHE:CD1	2.95	0.47
3:A:286:LEU:CB	3:A:291:ILE:HG12	2.40	0.47
1:K:157:LYS:HG2	1:K:203:THR:HA	1.92	0.47
1:K:181:ARG:CD	1:K:198:GLY:HA3	2.45	0.47
1:K:311:TYR:CG	1:K:321:GLN:CG	2.95	0.47
2:B:149:THR:HB	2:B:191:GLN:OE1	2.14	0.47
2:B:217:LEU:CD1	2:B:219:THR:H	2.27	0.47
2:B:219:THR:HB	2:B:220:PRO:HD2	1.95	0.47
2:B:271:ALA:HA	2:B:272:PRO:C	2.34	0.47
2:B:307:HIS:O	2:B:372:THR:HB	2.14	0.47
3:A:262:TYR:CD1	3:A:264:ARG:CZ	2.97	0.47
3:A:317:LEU:H	3:A:353:VAL:HG12	1.79	0.47
3:A:343:PHE:HD2	3:A:343:PHE:HA	1.49	0.47
3:A:387:ALA:HA	3:A:390:ARG:CG	2.44	0.47
1:K:97:TYR:CD2	1:K:365:VAL:HA	2.50	0.47
1:K:222:THR:CG2	1:K:231:TYR:HE2	2.28	0.47
2:B:2:ARG:HG2	2:B:131:GLN:HB2	1.95	0.47
2:B:18:ALA:C	2:B:19:LYS:HZ3	2.18	0.47
2:B:30:ILE:CD1	2:B:59:TYR:HB2	2.43	0.47
2:B:51:TYR:CB	2:B:59:TYR:HB3	2.45	0.47
2:B:105:HIS:HD2	2:B:149:THR:CB	2.26	0.47
3:A:1:MET:CE	3:A:1:MET:HA	2.45	0.47
3:A:275:VAL:CB	3:A:300:ASN:HA	2.38	0.47
3:A:303:VAL:HG22	3:A:304:LYS:N	2.28	0.47
3:A:435:VAL:HG13	3:A:436:GLY:N	2.30	0.47
1:K:24:ARG:NH1	1:K:109:THR:O	2.48	0.47
1:K:47:ARG:CD	1:K:49:GLU:OE2	2.62	0.47
1:K:95:MET:CE	1:K:97:TYR:HD2	2.27	0.47
1:K:103:ALA:O	1:K:266:LEU:HB2	2.14	0.47
1:K:160:LEU:O	1:K:172:LEU:HD23	2.14	0.47
2:B:266:PHE:CZ	2:B:311:LEU:HG	2.49	0.47
3:A:4:CYS:SG	3:A:136:LEU:HD22	2.55	0.47
3:A:63:PRO:HD2	3:A:87:PHE:CD1	2.50	0.47
3:A:115:ILE:HA	3:A:118:VAL:HG22	1.96	0.47
3:A:122:ILE:HD12	3:A:122:ILE:C	2.35	0.47
3:A:234:ILE:HD12	3:A:234:ILE:C	2.35	0.47
1:K:26:ARG:HE	1:K:337:SER:HB3	1.79	0.47
1:K:297:ARG:NH1	2:B:262:ARG:CG	2.77	0.47
1:K:299:ILE:HG21	4:K:501:MZK:F2	2.04	0.47
1:K:329:ARG:HD2	1:K:363:PRO:HG2	1.97	0.47
1:K:343:LEU:HG	1:K:344:GLU:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:VAL:CG2	2:B:133:PHE:HB3	2.44	0.47
2:B:21:TRP:NE1	2:B:63:ALA:HB2	2.30	0.47
2:B:69:GLU:OE2	2:B:94:GLN:HG2	2.15	0.47
2:B:102:ALA:HB2	2:B:403:MET:CG	2.45	0.47
2:B:191:GLN:CG	2:B:195:ASN:HD21	2.27	0.47
3:A:233:GLN:N	3:A:363:VAL:HG13	2.29	0.47
3:A:338:LYS:HZ2	3:A:338:LYS:HB3	1.78	0.47
3:A:351:PHE:CB	3:A:352:LYS:HA	2.41	0.47
3:A:370:LYS:HE2	3:A:372:GLN:HA	1.95	0.47
1:K:290:GLN:N	3:A:409:VAL:HG11	2.29	0.47
1:K:290:GLN:HG2	3:A:410:GLY:N	2.30	0.47
2:B:192:LEU:HD21	2:B:196:THR:OG1	2.14	0.47
2:B:269:GLY:C	2:B:367:PHE:HB3	2.35	0.47
3:A:64:ARG:HA	3:A:64:ARG:NH2	2.20	0.47
3:A:90:GLU:CD	3:A:124:LYS:HE3	2.35	0.47
3:A:189:LEU:HD21	3:A:417:GLU:OE2	2.15	0.47
1:K:104:TYR:CD2	1:K:266:LEU:HG	2.49	0.47
1:K:180:GLU:C	1:K:182:LEU:HD22	2.34	0.47
1:K:204:VAL:HG11	1:K:209:GLU:HB2	1.97	0.47
1:K:293:LEU:CD2	3:A:409:VAL:HG11	2.44	0.47
2:B:65:LEU:HD22	2:B:90:PHE:CD1	2.50	0.47
2:B:70:PRO:HG3	2:B:94:GLN:HB2	1.96	0.47
2:B:70:PRO:HG3	2:B:94:GLN:CA	2.42	0.47
2:B:101:TRP:O	2:B:105:HIS:HB2	2.15	0.47
2:B:139:LEU:HD12	2:B:140:GLY:CA	2.45	0.47
2:B:139:LEU:O	2:B:185:ALA:HB2	2.14	0.47
2:B:212:PHE:CB	2:B:220:PRO:HG3	2.44	0.47
2:B:270:PHE:CG	2:B:271:ALA:N	2.83	0.47
2:B:380:ARG:HG2	2:B:380:ARG:HH11	1.80	0.47
3:A:9:VAL:CG2	3:A:149:PHE:CD1	2.97	0.47
3:A:11:GLN:O	3:A:15:GLN:CD	2.53	0.47
3:A:53:PHE:HB3	3:A:62:VAL:O	2.14	0.47
3:A:53:PHE:HD2	3:A:63:PRO:CG	2.28	0.47
3:A:75:ILE:HG21	3:A:79:ARG:NH2	2.30	0.47
3:A:103:TYR:CD2	3:A:148:GLY:HA2	2.49	0.47
3:A:111:GLY:HA3	3:A:152:LEU:HD12	1.96	0.47
3:A:205:ASP:O	3:A:209:ILE:HB	2.15	0.47
3:A:245:ASP:OD1	3:A:249:ASN:HB2	2.15	0.47
3:A:270:ALA:CB	3:A:378:LEU:HD23	2.45	0.47
1:K:17:LYS:O	1:K:361:ASN:HB3	2.15	0.47
2:B:143:THR:CG2	2:B:147:MET:CE	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:TYR:CG	2:B:162:ARG:HG2	2.49	0.47
2:B:217:LEU:HD13	2:B:218:THR:OG1	2.14	0.47
2:B:249:ASP:HB3	3:A:100:ALA:CB	2.45	0.47
2:B:284:LEU:CB	2:B:289:LEU:HD11	2.45	0.47
2:B:318:ARG:HB3	2:B:358:PRO:CD	2.39	0.47
3:A:1:MET:HG2	3:A:47:ASP:H	1.74	0.47
3:A:30:ILE:HG23	3:A:30:ILE:O	2.15	0.47
3:A:93:ILE:HD13	3:A:118:VAL:HG12	1.96	0.47
3:A:192:HIS:NE2	3:A:193:THR:HG23	2.29	0.47
1:K:37:ALA:HB1	1:K:339:ALA:HB2	1.95	0.47
1:K:168:LEU:HB3	1:K:182:LEU:CG	2.45	0.47
1:K:311:TYR:HE1	1:K:324:LEU:CD2	2.26	0.47
2:B:28:HIS:CE1	2:B:47:ILE:HG23	2.49	0.47
2:B:67:ASP:N	2:B:92:PHE:HB2	2.29	0.47
2:B:324:LYS:HD3	3:A:221:ARG:NH1	2.30	0.47
2:B:377:LEU:O	2:B:380:ARG:HG3	2.15	0.47
2:B:394:PHE:HD1	2:B:396:HIS:CE1	2.33	0.47
2:B:419:VAL:O	2:B:422:TYR:HB2	2.14	0.47
3:A:88:HIS:H	3:A:88:HIS:CD2	2.33	0.47
3:A:360:PRO:HG2	3:A:371:VAL:O	2.14	0.47
1:K:72:PHE:HB3	1:K:76:THR:OG1	2.14	0.47
1:K:311:TYR:CE1	1:K:324:LEU:CD2	2.98	0.47
2:B:46:ARG:CG	2:B:242:PHE:CD1	2.98	0.47
2:B:149:THR:HG23	2:B:188:SER:OG	2.14	0.47
2:B:151:LEU:HD12	2:B:152:ILE:CG1	2.45	0.47
2:B:162:ARG:HA	2:B:162:ARG:NH1	2.29	0.47
3:A:1:MET:HA	3:A:1:MET:HE3	1.97	0.47
3:A:104:ALA:HB3	3:A:411:GLU:HG3	1.97	0.47
3:A:141:PHE:H	3:A:171:ILE:CG2	2.28	0.47
1:K:26:ARG:NH2	1:K:337:SER:HB2	2.30	0.46
1:K:47:ARG:O	1:K:48:LYS:HB2	2.16	0.46
1:K:57:LEU:CD2	3:A:427:ALA:CA	2.92	0.46
1:K:102:PHE:CE1	1:K:264:VAL:HG12	2.50	0.46
2:B:49:VAL:HG23	2:B:50:TYR:N	2.30	0.46
2:B:214:THR:CB	2:B:276:ARG:H	2.26	0.46
2:B:371:SER:HB2	2:B:374:ILE:HG21	1.91	0.46
3:A:83:TYR:O	3:A:86:LEU:HB3	2.15	0.46
1:K:288:ILE:HG13	1:K:289:ASN:N	2.31	0.46
2:B:3:GLU:HG3	2:B:50:TYR:O	2.15	0.46
2:B:3:GLU:OE2	2:B:50:TYR:HA	2.15	0.46
2:B:103:LYS:HG2	2:B:401:GLU:CG	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:GLN:NE2	2:B:353:VAL:HG23	2.28	0.46
2:B:291:GLN:HE21	2:B:291:GLN:HB3	1.38	0.46
2:B:321:MET:HG3	2:B:325:GLU:CB	2.45	0.46
2:B:331:LEU:HD12	2:B:334:GLN:HE22	1.80	0.46
2:B:377:LEU:HD12	2:B:377:LEU:C	2.34	0.46
2:B:394:PHE:CZ	2:B:397:TRP:CH2	3.03	0.46
3:A:9:VAL:CG1	3:A:149:PHE:HB3	2.46	0.46
3:A:53:PHE:HD2	3:A:63:PRO:CB	2.27	0.46
3:A:233:GLN:NE2	3:A:234:ILE:HG22	2.20	0.46
1:K:68:PHE:CD2	1:K:68:PHE:N	2.83	0.46
1:K:171:LEU:C	1:K:220:LYS:HD3	2.36	0.46
1:K:204:VAL:HG12	1:K:209:GLU:OE1	2.16	0.46
1:K:286:GLY:O	1:K:290:GLN:HG3	2.14	0.46
1:K:365:VAL:HG11	1:K:367:GLN:CG	2.44	0.46
2:B:97:ALA:H	2:B:143:THR:HG23	1.80	0.46
2:B:102:ALA:O	2:B:105:HIS:HB3	2.16	0.46
2:B:152:ILE:C	2:B:155:ILE:HG12	2.36	0.46
2:B:343:GLU:HG2	2:B:344:TRP:CD1	2.50	0.46
3:A:78:VAL:CG1	3:A:83:TYR:HE1	2.28	0.46
3:A:121:ARG:HG2	3:A:121:ARG:HH11	1.80	0.46
3:A:321:GLY:HA2	3:A:359:PRO:CA	2.46	0.46
1:K:41:VAL:HB	1:K:338:PRO:HB3	1.97	0.46
1:K:204:VAL:CG2	1:K:210:VAL:HG22	2.45	0.46
2:B:103:LYS:HD2	2:B:401:GLU:CG	2.40	0.46
2:B:260:PHE:C	2:B:262:ARG:H	2.18	0.46
2:B:284:LEU:HB3	2:B:289:LEU:HD12	1.96	0.46
2:B:341:PHE:HZ	2:B:346:PRO:C	2.19	0.46
3:A:1:MET:HB2	3:A:47:ASP:HB2	1.97	0.46
3:A:48:SER:HB3	3:A:244:PHE:CZ	2.51	0.46
3:A:214:ARG:HG2	3:A:221:ARG:NH1	2.24	0.46
1:K:50:VAL:HG23	1:K:71:VAL:HG13	1.97	0.46
2:B:186:THR:O	2:B:189:VAL:HG12	2.16	0.46
2:B:273:LEU:HD22	2:B:273:LEU:C	2.34	0.46
3:A:30:ILE:HD12	3:A:61:HIS:CB	2.45	0.46
3:A:192:HIS:ND1	3:A:421:ALA:HB2	2.30	0.46
3:A:324:VAL:HG22	3:A:327:ASP:CG	2.36	0.46
3:A:389:ALA:O	3:A:392:ASP:HB3	2.16	0.46
1:K:112:THR:O	1:K:116:GLU:HG3	2.16	0.46
1:K:161:LEU:HA	1:K:171:LEU:HG	1.98	0.46
1:K:211:TYR:O	1:K:214:LEU:HB3	2.16	0.46
1:K:255:LEU:HD22	1:K:369:LEU:HA	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:LEU:HD23	2:B:276:ARG:HE	1.81	0.46
2:B:251:ARG:CZ	3:A:105:ARG:NE	2.78	0.46
2:B:321:MET:SD	2:B:326:VAL:HA	2.55	0.46
3:A:349:THR:CG2	3:A:351:PHE:CD1	2.99	0.46
1:K:55:GLY:N	1:K:60:LYS:HG3	2.30	0.46
1:K:97:TYR:CD2	1:K:365:VAL:HG22	2.51	0.46
1:K:317:THR:HA	1:K:320:LEU:HB3	1.98	0.46
1:K:327:ARG:HH21	1:K:327:ARG:N	2.01	0.46
1:K:357:LYS:HG3	1:K:358:ASN:N	2.31	0.46
2:B:7:ILE:N	2:B:134:GLN:HE22	2.12	0.46
2:B:45:GLU:CB	2:B:46:ARG:HH21	2.23	0.46
2:B:99:ASN:C	2:B:142:GLY:HA3	2.36	0.46
2:B:152:ILE:CA	2:B:155:ILE:HG12	2.46	0.46
2:B:324:LYS:CD	3:A:221:ARG:HH11	2.29	0.46
3:A:97:GLU:OE2	3:A:105:ARG:NH1	2.48	0.46
3:A:108:TYR:CE2	3:A:413:MET:SD	3.09	0.46
3:A:143:GLY:HA3	5:A:501:G2P:H3A1	1.98	0.46
3:A:223:THR:HB	3:A:226:ASN:OD1	2.14	0.46
3:A:224:TYR:HE2	3:A:227:LEU:HD23	1.80	0.46
3:A:298:PRO:HA	3:A:301:GLN:NE2	2.31	0.46
1:K:77:LYS:HA	1:K:77:LYS:HD2	1.76	0.46
1:K:308:HIS:CE1	2:B:420:SER:HB2	2.51	0.46
1:K:350:LEU:HD13	1:K:354:HIS:CD2	2.51	0.46
2:B:34:GLY:CA	2:B:84:ILE:HD13	2.46	0.46
2:B:242:PHE:HD1	2:B:243:PRO:HD3	1.81	0.46
2:B:331:LEU:HD13	2:B:331:LEU:N	2.31	0.46
2:B:381:ILE:HG23	2:B:384:GLN:OE1	2.15	0.46
3:A:2:ARG:NH1	3:A:131:GLY:HA3	2.31	0.46
3:A:7:ILE:HD11	3:A:68:VAL:HG22	1.95	0.46
3:A:63:PRO:HB2	3:A:87:PHE:CE1	2.50	0.46
3:A:104:ALA:CB	3:A:413:MET:HG3	2.43	0.46
3:A:308:ARG:H	3:A:308:ARG:HE	1.63	0.46
3:A:318:LEU:HD11	3:A:320:ARG:CG	2.41	0.46
1:K:144:PHE:CB	1:K:207:LYS:HD2	2.46	0.46
2:B:3:GLU:HG3	2:B:50:TYR:HD1	1.81	0.46
2:B:154:LYS:NZ	2:B:157:GLU:HB3	2.31	0.46
2:B:154:LYS:HZ3	2:B:157:GLU:C	2.18	0.46
3:A:75:ILE:HG21	3:A:79:ARG:HH21	1.80	0.46
3:A:209:ILE:HG22	3:A:227:LEU:HD11	1.98	0.46
3:A:288:VAL:HG11	3:A:328:VAL:HA	1.97	0.46
3:A:334:THR:O	3:A:337:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:384:ILE:HG13	3:A:385:ALA:N	2.30	0.46
1:K:352:TYR:CD2	1:K:352:TYR:O	2.69	0.46
2:B:5:VAL:HA	2:B:62:ARG:HG2	1.97	0.46
2:B:200:TYR:HD1	2:B:268:PRO:HD3	1.81	0.46
2:B:253:LEU:HD12	2:B:254:ALA:CA	2.46	0.46
3:A:351:PHE:HB2	3:A:352:LYS:HZ2	1.80	0.46
3:A:388:TRP:HH2	3:A:432:TYR:CE2	2.31	0.46
1:K:102:PHE:HD1	1:K:264:VAL:CB	2.29	0.45
1:K:109:THR:HG23	1:K:336:ILE:O	2.16	0.45
1:K:221:ARG:HD3	1:K:237:SER:CB	2.42	0.45
1:K:293:LEU:HD22	1:K:293:LEU:N	2.32	0.45
2:B:28:HIS:CG	2:B:47:ILE:CG2	2.99	0.45
2:B:44:LEU:C	2:B:44:LEU:HD12	2.36	0.45
2:B:138:SER:HA	2:B:169:VAL:HG22	1.97	0.45
2:B:323:MET:O	2:B:326:VAL:HB	2.16	0.45
3:A:2:ARG:CZ	3:A:131:GLY:HA3	2.46	0.45
3:A:86:LEU:HD12	3:A:86:LEU:C	2.37	0.45
3:A:214:ARG:CG	3:A:221:ARG:HH12	2.22	0.45
3:A:248:LEU:HD23	3:A:248:LEU:C	2.36	0.45
3:A:264:ARG:HD3	3:A:264:ARG:N	2.18	0.45
3:A:291:ILE:CD1	3:A:373:ARG:HB2	2.46	0.45
3:A:351:PHE:HD2	3:A:352:LYS:HZ3	1.63	0.45
1:K:189:ARG:HD3	1:K:189:ARG:H	1.80	0.45
1:K:191:LYS:HZ2	1:K:191:LYS:HB2	1.81	0.45
1:K:236:HIS:ND1	1:K:267:ALA:HB3	2.31	0.45
2:B:12:CYS:O	2:B:15:GLN:HB3	2.17	0.45
2:B:77:ARG:HD3	2:B:82:GLY:HA3	1.98	0.45
2:B:102:ALA:CB	2:B:403:MET:CG	2.94	0.45
2:B:159:TYR:CD2	2:B:162:ARG:CG	2.98	0.45
2:B:214:THR:CG2	2:B:297:LYS:CE	2.95	0.45
2:B:222:TYR:CG	5:B:501:G2P:C6	2.98	0.45
2:B:262:ARG:HH21	2:B:263:LEU:H	1.64	0.45
2:B:266:PHE:HD2	2:B:266:PHE:HA	1.40	0.45
2:B:318:ARG:HA	2:B:354:CYS:HB3	1.97	0.45
2:B:350:LYS:HE3	3:A:179:THR:CB	2.46	0.45
2:B:358:PRO:HD2	2:B:362:LYS:O	2.15	0.45
2:B:422:TYR:HA	2:B:425:TYR:CZ	2.49	0.45
3:A:49:PHE:CD1	3:A:53:PHE:HD1	2.34	0.45
3:A:273:ALA:C	3:A:375:VAL:HG22	2.36	0.45
3:A:306:ASP:HB2	3:A:309:HIS:CD2	2.51	0.45
1:K:29:ASN:CG	1:K:32:GLU:HG2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:181:ARG:HH22	1:K:183:GLN:CB	2.28	0.45
2:B:70:PRO:HD3	2:B:94:GLN:HA	1.98	0.45
2:B:106:TYR:N	2:B:106:TYR:CD2	2.82	0.45
2:B:211:CYS:O	2:B:215:LEU:HB2	2.16	0.45
2:B:299:MET:CE	2:B:367:PHE:HD1	2.30	0.45
2:B:325:GLU:O	2:B:329:GLN:HG3	2.16	0.45
3:A:49:PHE:CZ	3:A:61:HIS:HD2	2.33	0.45
3:A:53:PHE:CD2	3:A:63:PRO:CA	2.99	0.45
3:A:101:ASN:ND2	3:A:142:GLY:O	2.50	0.45
3:A:175:PRO:HG2	3:A:304:LYS:NZ	2.31	0.45
3:A:281:ALA:HB3	3:A:369:ALA:H	1.81	0.45
3:A:375:VAL:CG2	3:A:377:MET:CE	2.95	0.45
1:K:50:VAL:CG2	1:K:71:VAL:HG13	2.46	0.45
1:K:57:LEU:HA	3:A:423:GLU:OE1	2.16	0.45
1:K:204:VAL:HG23	1:K:204:VAL:O	2.17	0.45
2:B:5:VAL:HG23	2:B:5:VAL:O	2.15	0.45
2:B:12:CYS:CB	2:B:138:SER:CB	2.93	0.45
2:B:68:LEU:HD12	5:B:501:G2P:O2G	2.17	0.45
2:B:299:MET:CE	2:B:367:PHE:CD1	3.00	0.45
2:B:342:VAL:CB	2:B:348:ASN:HD21	2.23	0.45
3:A:21:TRP:CZ2	3:A:65:ALA:CB	2.97	0.45
3:A:152:LEU:HD23	3:A:152:LEU:C	2.36	0.45
3:A:279:GLU:HB3	3:A:283:HIS:NE2	2.31	0.45
3:A:298:PRO:HA	3:A:301:GLN:HE21	1.81	0.45
2:B:123:GLU:HA	2:B:123:GLU:OE2	2.16	0.45
2:B:186:THR:HA	2:B:189:VAL:HG12	1.99	0.45
2:B:266:PHE:HE1	2:B:312:THR:CG2	2.29	0.45
2:B:326:VAL:O	2:B:330:MET:HE3	2.16	0.45
2:B:341:PHE:CE1	2:B:348:ASN:CB	2.98	0.45
2:B:419:VAL:CG2	2:B:420:SER:N	2.78	0.45
3:A:97:GLU:CD	3:A:105:ARG:HH22	2.19	0.45
3:A:172:TYR:HB3	3:A:204:VAL:O	2.16	0.45
3:A:317:LEU:CB	3:A:353:VAL:CG1	2.95	0.45
3:A:391:LEU:N	3:A:391:LEU:HD22	2.32	0.45
1:K:15:LYS:CD	1:K:362:LYS:HD2	2.46	0.45
1:K:15:LYS:HG2	1:K:362:LYS:HB3	1.99	0.45
1:K:37:ALA:CB	1:K:341:LEU:HD13	2.47	0.45
1:K:191:LYS:H	1:K:191:LYS:CD	2.29	0.45
1:K:303:VAL:HG13	1:K:358:ASN:ND2	2.31	0.45
1:K:311:TYR:CD2	1:K:321:GLN:CG	2.98	0.45
2:B:70:PRO:CG	2:B:94:GLN:HA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ALA:CB	2:B:143:THR:CG2	2.94	0.45
2:B:213:ARG:HH21	2:B:214:THR:HA	1.81	0.45
3:A:25:CYS:O	3:A:30:ILE:HG22	2.17	0.45
3:A:28:HIS:CE1	3:A:52:PHE:HD1	2.35	0.45
3:A:71:GLU:HB3	3:A:98:ASP:OD2	2.17	0.45
3:A:147:SER:HA	3:A:190:THR:HG21	1.98	0.45
3:A:150:THR:CG2	3:A:190:THR:CG2	2.95	0.45
3:A:172:TYR:H	3:A:204:VAL:H	1.65	0.45
3:A:202:PHE:HE1	3:A:267:PHE:HB2	1.80	0.45
3:A:212:ILE:HG21	3:A:299:ALA:O	2.16	0.45
3:A:233:GLN:CB	3:A:363:VAL:HG13	2.47	0.45
1:K:209:GLU:O	1:K:213:ILE:HG12	2.17	0.45
2:B:105:HIS:HD2	2:B:149:THR:HB	1.82	0.45
2:B:154:LYS:HD3	2:B:154:LYS:C	2.37	0.45
2:B:271:ALA:HB1	2:B:272:PRO:HA	1.99	0.45
3:A:5:ILE:HG22	3:A:6:SER:N	2.31	0.45
3:A:62:VAL:CG2	3:A:88:HIS:HD2	2.30	0.45
3:A:104:ALA:CB	3:A:413:MET:CG	2.94	0.45
1:K:15:LYS:HE3	1:K:362:LYS:HE2	1.94	0.45
1:K:109:THR:HB	1:K:335:THR:OG1	2.17	0.45
1:K:145:GLU:CG	1:K:207:LYS:HZ1	2.30	0.45
1:K:203:THR:HG22	1:K:204:VAL:N	2.32	0.45
2:B:1:MET:CG	2:B:2:ARG:H	2.27	0.45
2:B:81:PHE:CA	2:B:83:GLN:HE22	2.29	0.45
2:B:108:GLU:OE2	2:B:143:THR:HG23	2.17	0.45
2:B:266:PHE:HE2	2:B:370:ASN:HB3	1.81	0.45
2:B:267:MET:CE	2:B:367:PHE:HE1	2.30	0.45
2:B:288:GLU:O	2:B:291:GLN:HG2	2.17	0.45
2:B:323:MET:C	3:A:221:ARG:CG	2.83	0.45
3:A:54:SER:HB3	3:A:64:ARG:NH1	2.20	0.45
3:A:132:LEU:HD23	3:A:135:PHE:HA	1.99	0.45
3:A:136:LEU:HD12	3:A:169:PHE:HE1	1.82	0.45
3:A:188:ILE:CG2	3:A:421:ALA:CB	2.95	0.45
3:A:223:THR:HG22	3:A:225:THR:N	2.22	0.45
3:A:255:PHE:O	3:A:258:ASN:HB3	2.16	0.45
1:K:144:PHE:CD1	1:K:154:PHE:HE1	2.34	0.45
2:B:112:LEU:CD2	2:B:116:VAL:CG1	2.95	0.45
2:B:180:VAL:O	2:B:183:TYR:HB2	2.17	0.45
2:B:242:PHE:CE2	2:B:356:ILE:CD1	2.96	0.45
2:B:260:PHE:HE2	3:A:406:HIS:N	2.15	0.45
2:B:324:LYS:HE2	3:A:221:ARG:CB	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LEU:HA	2:B:334:GLN:CD	2.37	0.45
2:B:331:LEU:O	2:B:334:GLN:HG2	2.16	0.45
2:B:376:GLU:CD	2:B:422:TYR:HB2	2.37	0.45
3:A:4:CYS:HG	3:A:135:PHE:HA	1.82	0.45
3:A:24:TYR:HA	3:A:27:GLU:CG	2.47	0.45
3:A:50:ASN:HA	3:A:53:PHE:O	2.17	0.45
3:A:62:VAL:CG2	3:A:88:HIS:CD2	3.00	0.45
3:A:316:CYS:O	3:A:377:MET:HG3	2.17	0.45
1:K:23:VAL:CG2	1:K:68:PHE:CE1	2.98	0.45
1:K:72:PHE:HB3	1:K:76:THR:CB	2.47	0.45
2:B:138:SER:HB2	2:B:169:VAL:CG2	2.47	0.45
2:B:151:LEU:HD11	2:B:152:ILE:HG12	1.98	0.45
2:B:207:LEU:HG	2:B:208:TYR:N	2.32	0.45
2:B:310:TYR:N	2:B:310:TYR:CD2	2.82	0.45
3:A:26:LEU:O	3:A:26:LEU:HD12	2.17	0.45
3:A:70:LEU:N	3:A:70:LEU:HD12	2.31	0.45
3:A:153:LEU:HD12	3:A:156:ARG:NH2	2.32	0.45
3:A:224:TYR:CD2	5:A:501:G2P:O6	2.70	0.45
3:A:383:ALA:C	3:A:386:GLU:HG2	2.37	0.45
2:B:422:TYR:CD1	2:B:422:TYR:N	2.82	0.44
3:A:153:LEU:CG	3:A:157:LEU:CD1	2.95	0.44
3:A:352:LYS:HG3	3:A:353:VAL:H	1.82	0.44
3:A:414:GLU:CG	3:A:415:GLU:N	2.80	0.44
1:K:28:PHE:CG	1:K:33:ARG:NH2	2.85	0.44
1:K:246:LYS:NZ	1:K:254:GLU:CD	2.69	0.44
2:B:58:LYS:HZ2	2:B:86:ARG:HE	1.65	0.44
2:B:121:ARG:HE	2:B:121:ARG:N	2.15	0.44
3:A:154:MET:CA	3:A:154:MET:CE	2.95	0.44
3:A:174:ALA:CB	3:A:176:GLN:CG	2.95	0.44
3:A:174:ALA:CB	3:A:207:GLU:HB2	2.42	0.44
3:A:176:GLN:OE1	3:A:177:VAL:HG12	2.18	0.44
3:A:256:GLN:OE1	3:A:259:LEU:HB2	2.18	0.44
3:A:287:SER:HB3	3:A:290:GLU:CG	2.47	0.44
3:A:311:LYS:O	3:A:312:TYR:HD1	2.00	0.44
3:A:405:VAL:O	3:A:408:TYR:N	2.51	0.44
2:B:21:TRP:HH2	2:B:50:TYR:OH	1.98	0.44
2:B:166:THR:HG22	2:B:167:PHE:N	2.32	0.44
2:B:260:PHE:CE2	3:A:405:VAL:CA	3.00	0.44
3:A:204:VAL:HG22	3:A:205:ASP:N	2.32	0.44
3:A:211:ASP:HA	3:A:214:ARG:HG2	1.99	0.44
3:A:274:PRO:HD3	3:A:291:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:66:TYR:CD2	1:K:68:PHE:CE2	3.00	0.44
1:K:298:VAL:HG13	1:K:299:ILE:N	2.32	0.44
1:K:303:VAL:HG22	1:K:358:ASN:ND2	2.32	0.44
2:B:61:PRO:HB2	2:B:85:PHE:CE2	2.53	0.44
2:B:202:ILE:O	2:B:202:ILE:HG13	2.17	0.44
2:B:260:PHE:CE2	3:A:405:VAL:C	2.91	0.44
2:B:291:GLN:HG2	2:B:292:GLN:H	1.80	0.44
2:B:330:MET:HG2	2:B:331:LEU:HD13	1.98	0.44
2:B:345:ILE:CD1	3:A:181:VAL:CG2	2.88	0.44
3:A:46:ASP:H	3:A:49:PHE:CB	2.27	0.44
3:A:210:TYR:HB3	3:A:221:ARG:NH2	2.32	0.44
3:A:211:ASP:OD1	3:A:212:ILE:HD13	2.17	0.44
3:A:267:PHE:H	3:A:267:PHE:HD2	1.64	0.44
3:A:360:PRO:HG3	3:A:373:ARG:C	2.38	0.44
1:K:15:LYS:CE	1:K:362:LYS:HB3	2.46	0.44
1:K:82:TYR:CZ	1:K:86:VAL:HB	2.51	0.44
1:K:135:ILE:HD12	1:K:136:ILE:CA	2.48	0.44
1:K:191:LYS:HZ2	1:K:191:LYS:CB	2.31	0.44
1:K:228:MET:CE	1:K:228:MET:CA	2.96	0.44
1:K:258:ILE:N	1:K:368:LYS:HD3	2.32	0.44
2:B:20:PHE:CE1	2:B:24:ILE:CD1	2.97	0.44
2:B:24:ILE:HD11	2:B:234:SER:HA	1.98	0.44
2:B:154:LYS:HZ3	2:B:157:GLU:HB3	1.82	0.44
2:B:194:GLU:H	2:B:194:GLU:CD	2.21	0.44
2:B:199:THR:CG2	2:B:265:PHE:CD2	3.00	0.44
2:B:200:TYR:HB3	2:B:268:PRO:CG	2.45	0.44
2:B:225:LEU:CD1	5:B:501:G2P:H2N1	2.30	0.44
2:B:381:ILE:CA	2:B:384:GLN:HG3	2.46	0.44
3:A:28:HIS:CD2	3:A:41:THR:CG2	3.00	0.44
3:A:103:TYR:CD1	3:A:104:ALA:N	2.86	0.44
3:A:107:HIS:CE1	3:A:108:TYR:HE1	2.34	0.44
3:A:141:PHE:H	3:A:171:ILE:HG23	1.81	0.44
3:A:312:TYR:HB2	3:A:342:GLN:O	2.18	0.44
3:A:370:LYS:HD3	3:A:371:VAL:C	2.38	0.44
1:K:87:CYS:HB2	1:K:88:PRO:HD3	2.00	0.44
1:K:115:MET:SD	1:K:135:ILE:CG1	3.05	0.44
1:K:211:TYR:HD2	1:K:211:TYR:HA	1.41	0.44
1:K:255:LEU:HB3	1:K:369:LEU:HD13	1.94	0.44
1:K:304:GLU:HG3	1:K:306:THR:CA	2.48	0.44
2:B:65:LEU:HD22	2:B:90:PHE:CD2	2.52	0.44
2:B:112:LEU:O	2:B:116:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:LYS:CE	3:A:179:THR:O	2.65	0.44
2:B:383:GLU:O	2:B:386:THR:HB	2.17	0.44
2:B:396:HIS:CE1	2:B:397:TRP:CD1	3.05	0.44
2:B:398:TYR:HA	2:B:398:TYR:HD1	1.41	0.44
3:A:24:TYR:C	3:A:27:GLU:HG3	2.38	0.44
3:A:98:ASP:C	3:A:100:ALA:H	2.21	0.44
3:A:175:PRO:HG2	3:A:304:LYS:HE2	1.96	0.44
3:A:414:GLU:HG3	3:A:415:GLU:N	2.32	0.44
1:K:15:LYS:HE3	1:K:362:LYS:HB3	1.99	0.44
1:K:329:ARG:HA	1:K:363:PRO:CG	2.46	0.44
2:B:67:ASP:OD1	2:B:73:MET:HB3	2.18	0.44
2:B:139:LEU:HD23	2:B:168:SER:CB	2.43	0.44
2:B:187:LEU:HD22	2:B:187:LEU:H	1.83	0.44
2:B:246:LEU:CD1	2:B:352:ALA:CB	2.95	0.44
2:B:263:LEU:HD22	2:B:264:HIS:H	1.82	0.44
2:B:345:ILE:HD12	3:A:181:VAL:CG1	2.45	0.44
3:A:23:LEU:HG	3:A:364:PRO:HD3	2.00	0.44
3:A:123:ARG:HH11	3:A:123:ARG:HG2	1.82	0.44
3:A:176:GLN:HG2	3:A:207:GLU:CB	2.22	0.44
3:A:319:TYR:HD2	3:A:375:VAL:HG12	1.83	0.44
3:A:375:VAL:HB	3:A:377:MET:HE3	1.99	0.44
1:K:15:LYS:HD3	1:K:15:LYS:N	2.32	0.44
1:K:15:LYS:CG	1:K:362:LYS:HB3	2.48	0.44
1:K:19:ILE:N	1:K:361:ASN:HB3	2.33	0.44
1:K:26:ARG:NE	1:K:337:SER:HA	2.33	0.44
1:K:50:VAL:HG23	1:K:71:VAL:HG11	2.00	0.44
1:K:157:LYS:HG2	1:K:203:THR:CB	2.47	0.44
1:K:168:LEU:CB	1:K:182:LEU:HG	2.48	0.44
2:B:33:THR:HG21	2:B:35:SER:HB2	1.99	0.44
2:B:190:HIS:CD2	2:B:411:ALA:CA	2.99	0.44
2:B:252:LYS:HE2	3:A:101:ASN:O	2.16	0.44
2:B:323:MET:N	3:A:221:ARG:HG3	2.32	0.44
2:B:341:PHE:CZ	2:B:348:ASN:N	2.85	0.44
2:B:347:ASN:ND2	2:B:350:LYS:NZ	2.65	0.44
3:A:21:TRP:CD1	3:A:67:PHE:CZ	3.06	0.44
3:A:153:LEU:CD1	3:A:157:LEU:CD1	2.96	0.44
3:A:345:ASP:H	3:A:438:ASP:HB3	1.83	0.44
3:A:387:ALA:HA	3:A:390:ARG:HG3	2.00	0.44
1:K:26:ARG:CG	1:K:26:ARG:HH11	2.29	0.44
1:K:54:THR:CG2	1:K:56:GLY:H	2.31	0.44
1:K:222:THR:CG2	1:K:231:TYR:CE2	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:327:ARG:HH21	1:K:327:ARG:HG2	1.82	0.44
2:B:2:ARG:HE	2:B:2:ARG:HB2	1.68	0.44
2:B:30:ILE:HB	2:B:35:SER:O	2.18	0.44
2:B:117:LEU:C	2:B:120:VAL:HG22	2.39	0.44
2:B:244:GLY:N	2:B:355:ASP:HB2	2.32	0.44
3:A:24:TYR:HA	3:A:27:GLU:HG3	1.99	0.44
3:A:234:ILE:HD12	3:A:235:VAL:CA	2.48	0.44
3:A:301:GLN:HE22	3:A:307:PRO:HD3	1.83	0.44
3:A:311:LYS:HD3	3:A:436:GLY:O	2.18	0.44
3:A:407:TRP:CZ3	3:A:411:GLU:OE2	2.71	0.44
3:A:409:VAL:O	3:A:410:GLY:C	2.53	0.44
1:K:109:THR:HG21	1:K:335:THR:C	2.38	0.43
1:K:324:LEU:HD22	1:K:324:LEU:N	2.33	0.43
1:K:347:LEU:CD2	1:K:351:GLU:HG2	2.44	0.43
2:B:2:ARG:O	2:B:4:ILE:HD12	2.18	0.43
2:B:113:VAL:CA	2:B:116:VAL:HG22	2.47	0.43
2:B:324:LYS:NZ	3:A:222:PRO:HD2	2.33	0.43
2:B:324:LYS:HD3	3:A:221:ARG:HH11	1.82	0.43
2:B:339:SER:HA	2:B:429:THR:HG21	1.97	0.43
3:A:1:MET:HG2	3:A:47:ASP:CB	2.48	0.43
3:A:5:ILE:CD1	3:A:125:LEU:CD2	2.96	0.43
3:A:103:TYR:CE2	3:A:151:SER:CB	2.95	0.43
3:A:185:TYR:H	3:A:185:TYR:HD2	1.66	0.43
3:A:391:LEU:HA	3:A:394:LYS:CD	2.48	0.43
3:A:399:TYR:CE1	3:A:402:ARG:NE	2.86	0.43
1:K:168:LEU:CB	1:K:182:LEU:CG	2.95	0.43
1:K:358:ASN:O	1:K:360:LEU:HD12	2.18	0.43
2:B:15:GLN:HG3	2:B:19:LYS:HD2	1.99	0.43
2:B:40:SER:O	2:B:44:LEU:HB3	2.18	0.43
2:B:105:HIS:HD2	2:B:149:THR:OG1	2.01	0.43
2:B:106:TYR:CZ	2:B:403:MET:SD	3.11	0.43
2:B:151:LEU:CD1	2:B:152:ILE:CD1	2.96	0.43
2:B:178:THR:HG21	2:B:180:VAL:HG22	1.96	0.43
2:B:222:TYR:CD1	5:B:501:G2P:C6	3.01	0.43
2:B:249:ASP:HB3	3:A:100:ALA:HB2	2.00	0.43
2:B:263:LEU:HG	2:B:311:LEU:CD1	2.47	0.43
2:B:275:SER:HG	2:B:276:ARG:H	1.66	0.43
2:B:390:ARG:HA	2:B:392:LYS:NZ	2.33	0.43
3:A:276:ILE:HG23	3:A:281:ALA:HA	2.00	0.43
1:K:40:ILE:HG23	1:K:340:SER:HB2	2.01	0.43
1:K:136:ILE:CG2	1:K:214:LEU:CD1	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:303:VAL:HG22	1:K:358:ASN:HD22	1.81	0.43
2:B:12:CYS:HB2	2:B:138:SER:OG	2.17	0.43
2:B:58:LYS:HG2	2:B:59:TYR:H	1.80	0.43
2:B:70:PRO:HD3	2:B:94:GLN:HG2	1.98	0.43
2:B:216:LYS:HD3	2:B:276:ARG:CZ	2.48	0.43
2:B:269:GLY:HA3	2:B:367:PHE:CD1	2.52	0.43
2:B:319:GLY:H	2:B:354:CYS:HB3	1.83	0.43
3:A:8:HIS:CE1	3:A:67:PHE:CE1	3.06	0.43
3:A:98:ASP:OD1	5:A:501:G2P:O2G	2.36	0.43
1:K:48:LYS:HE3	1:K:70:MET:HG3	2.00	0.43
1:K:144:PHE:CB	1:K:207:LYS:CD	2.96	0.43
2:B:85:PHE:CD1	2:B:85:PHE:N	2.86	0.43
2:B:199:THR:HG22	2:B:265:PHE:CB	2.48	0.43
2:B:222:TYR:HB3	5:B:501:G2P:O6	2.18	0.43
2:B:299:MET:HE1	2:B:367:PHE:HD1	1.83	0.43
2:B:324:LYS:CE	3:A:221:ARG:HH11	2.31	0.43
3:A:11:GLN:CB	3:A:74:VAL:HG11	2.48	0.43
3:A:25:CYS:HB3	3:A:30:ILE:HG23	2.00	0.43
3:A:240:ALA:HA	3:A:243:ARG:CD	2.49	0.43
3:A:375:VAL:HG21	3:A:377:MET:CE	2.46	0.43
1:K:169:PHE:HA	1:K:179:SER:CA	2.24	0.43
2:B:48:ASN:HD21	2:B:53:GLU:CG	2.31	0.43
2:B:288:GLU:OE2	2:B:292:GLN:HG2	2.18	0.43
2:B:309:ARG:HG3	2:B:310:TYR:N	2.33	0.43
2:B:309:ARG:NH1	2:B:426:GLN:HG2	2.34	0.43
2:B:310:TYR:CD1	2:B:313:VAL:CG2	3.01	0.43
2:B:385:PHE:HA	2:B:388:MET:HG2	2.01	0.43
2:B:405:GLU:O	2:B:408:PHE:HB2	2.18	0.43
3:A:21:TRP:HA	3:A:21:TRP:CE3	2.54	0.43
3:A:70:LEU:CG	3:A:110:ILE:HG13	2.47	0.43
3:A:185:TYR:CD2	3:A:185:TYR:N	2.87	0.43
3:A:278:ALA:HB2	3:A:367:ASP:O	2.18	0.43
3:A:296:PHE:CE1	3:A:335:ILE:HG23	2.54	0.43
3:A:318:LEU:HD13	3:A:374:ALA:O	2.18	0.43
3:A:320:ARG:HB2	3:A:360:PRO:CG	2.41	0.43
1:K:40:ILE:HG13	1:K:41:VAL:N	2.34	0.43
1:K:47:ARG:CZ	1:K:47:ARG:CA	2.95	0.43
2:B:21:TRP:HD1	2:B:85:PHE:CE2	2.29	0.43
2:B:117:LEU:HA	2:B:120:VAL:CG2	2.48	0.43
2:B:156:ARG:CZ	2:B:157:GLU:HA	2.48	0.43
2:B:251:ARG:NH2	3:A:99:ALA:C	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:CYS:HB2	2:B:371:SER:CB	2.48	0.43
3:A:430:LYS:CD	3:A:434:GLU:CG	2.96	0.43
1:K:93:VAL:HG12	1:K:243:ILE:HD12	2.00	0.43
1:K:215:GLU:HG2	1:K:216:LYS:H	1.81	0.43
1:K:295:LEU:O	1:K:299:ILE:HG12	2.18	0.43
1:K:350:LEU:HD13	1:K:350:LEU:O	2.19	0.43
1:K:361:ASN:ND2	1:K:363:PRO:HD3	2.33	0.43
1:K:367:GLN:HE21	1:K:367:GLN:HB3	1.44	0.43
2:B:34:GLY:CA	2:B:84:ILE:CD1	2.96	0.43
2:B:143:THR:HG22	2:B:143:THR:O	2.18	0.43
2:B:147:MET:O	2:B:151:LEU:HG	2.18	0.43
2:B:258:VAL:HG21	2:B:261:PRO:CA	2.49	0.43
3:A:26:LEU:HB3	3:A:364:PRO:HG3	2.00	0.43
3:A:185:TYR:HB3	3:A:408:TYR:CE1	2.50	0.43
3:A:218:ASP:OD2	3:A:279:GLU:HG2	2.19	0.43
3:A:234:ILE:CG1	3:A:235:VAL:N	2.82	0.43
3:A:246:GLY:CA	3:A:356:ASN:HD22	2.32	0.43
3:A:312:TYR:C	3:A:344:VAL:HG13	2.39	0.43
3:A:375:VAL:CG2	3:A:377:MET:HE1	2.47	0.43
1:K:54:THR:CG2	1:K:55:GLY:N	2.82	0.43
1:K:78:GLN:NE2	1:K:113:PHE:O	2.45	0.43
2:B:266:PHE:CD1	2:B:368:ILE:CG2	3.02	0.43
2:B:284:LEU:CB	2:B:289:LEU:CD1	2.96	0.43
2:B:313:VAL:CG1	2:B:367:PHE:CE2	3.01	0.43
2:B:327:ASP:C	2:B:331:LEU:HD22	2.39	0.43
1:K:72:PHE:CD1	1:K:76:THR:CG2	2.97	0.43
1:K:95:MET:HG3	1:K:365:VAL:CG1	2.28	0.43
1:K:95:MET:CB	1:K:365:VAL:CG1	2.95	0.43
1:K:290:GLN:HA	3:A:409:VAL:CG1	2.44	0.43
1:K:304:GLU:HG3	1:K:306:THR:HB	1.98	0.43
2:B:49:VAL:CG2	2:B:50:TYR:N	2.82	0.43
2:B:198:GLU:OE1	2:B:198:GLU:HA	2.19	0.43
3:A:21:TRP:CD1	3:A:67:PHE:HZ	2.35	0.43
3:A:123:ARG:HD3	3:A:127:ASP:OD2	2.18	0.43
3:A:262:TYR:CD1	3:A:264:ARG:NH2	2.87	0.43
1:K:172:LEU:HG	1:K:173:ASN:ND2	2.34	0.43
2:B:9:ALA:CB	2:B:147:MET:SD	3.07	0.43
2:B:178:THR:CG2	2:B:180:VAL:CG2	2.95	0.43
2:B:315:ALA:HB1	2:B:365:ALA:HB1	2.01	0.43
3:A:31:GLN:NE2	3:A:33:ASP:H	2.16	0.43
3:A:49:PHE:HE1	3:A:53:PHE:CD1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:153:LEU:HG	3:A:157:LEU:HD12	2.00	0.43
3:A:172:TYR:CE2	3:A:391:LEU:HD23	2.51	0.43
3:A:280:LYS:NZ	3:A:280:LYS:HB3	2.34	0.43
3:A:388:TRP:CZ3	3:A:428:LEU:HG	2.48	0.43
1:K:26:ARG:HG3	1:K:26:ARG:HH11	1.83	0.42
1:K:28:PHE:CE1	1:K:39:SER:N	2.86	0.42
1:K:292:LEU:CD2	4:K:501:MZK:N1	2.82	0.42
1:K:314:SER:O	1:K:318:ARG:HG3	2.19	0.42
2:B:21:TRP:HE1	2:B:62:ARG:N	2.16	0.42
2:B:48:ASN:HD21	2:B:53:GLU:HG3	1.84	0.42
2:B:70:PRO:CB	2:B:92:PHE:HE2	2.24	0.42
2:B:103:LYS:HD2	2:B:401:GLU:N	2.30	0.42
2:B:398:TYR:CA	2:B:401:GLU:HG3	2.40	0.42
3:A:174:ALA:HB3	3:A:176:GLN:HG3	2.01	0.42
3:A:233:GLN:N	3:A:363:VAL:CG1	2.82	0.42
1:K:139:THR:CG2	1:K:140:LEU:N	2.82	0.42
1:K:191:LYS:N	1:K:191:LYS:CD	2.82	0.42
1:K:202:ILE:HG23	1:K:202:ILE:O	2.18	0.42
1:K:204:VAL:HG21	1:K:209:GLU:HB2	2.00	0.42
1:K:255:LEU:CD2	1:K:369:LEU:CA	2.77	0.42
1:K:347:LEU:HD23	1:K:351:GLU:CG	2.42	0.42
2:B:1:MET:CG	2:B:127:CYS:CB	2.95	0.42
2:B:107:THR:CG2	2:B:108:GLU:N	2.82	0.42
2:B:212:PHE:HB2	2:B:220:PRO:CG	2.48	0.42
2:B:241:ARG:NE	2:B:242:PHE:CG	2.86	0.42
2:B:274:THR:CG2	2:B:279:GLN:N	2.83	0.42
2:B:280:GLN:CG	2:B:281:TYR:N	2.81	0.42
2:B:293:MET:CE	2:B:367:PHE:CA	2.96	0.42
2:B:394:PHE:CZ	2:B:397:TRP:CZ3	3.07	0.42
3:A:3:GLU:OE1	3:A:54:SER:HB2	2.19	0.42
3:A:139:HIS:HE1	3:A:141:PHE:CE2	2.37	0.42
3:A:163:LYS:HE3	3:A:163:LYS:N	2.33	0.42
3:A:233:GLN:CG	3:A:234:ILE:N	2.83	0.42
3:A:248:LEU:HD13	3:A:353:VAL:O	2.19	0.42
3:A:302:MET:HG2	3:A:303:VAL:H	1.84	0.42
3:A:313:MET:CA	3:A:344:VAL:HG13	2.48	0.42
3:A:387:ALA:O	3:A:391:LEU:HD23	2.19	0.42
1:K:135:ILE:HD12	1:K:136:ILE:CG1	2.49	0.42
1:K:226:THR:CG2	1:K:232:SER:CB	2.95	0.42
1:K:320:LEU:CD2	1:K:324:LEU:CD1	2.95	0.42
2:B:30:ILE:HA	2:B:36:TYR:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:THR:CG2	2:B:188:SER:CA	2.95	0.42
2:B:273:LEU:HD21	2:B:297:LYS:CD	2.49	0.42
3:A:71:GLU:HA	3:A:72:PRO:HD3	1.82	0.42
3:A:111:GLY:HA2	3:A:114:ILE:HG22	2.01	0.42
3:A:135:PHE:O	3:A:135:PHE:HD1	2.02	0.42
3:A:185:TYR:HB2	3:A:408:TYR:OH	2.19	0.42
3:A:229:ARG:HE	3:A:363:VAL:HB	1.85	0.42
3:A:286:LEU:HD22	3:A:291:ILE:HD13	2.00	0.42
3:A:310:GLY:C	3:A:311:LYS:HE3	2.40	0.42
3:A:342:GLN:O	3:A:342:GLN:HG3	2.19	0.42
3:A:347:CYS:SG	3:A:349:THR:CG2	3.07	0.42
3:A:413:MET:HB3	3:A:413:MET:HE2	1.95	0.42
1:K:16:GLY:HA3	1:K:362:LYS:C	2.37	0.42
1:K:33:ARG:CZ	1:K:33:ARG:CA	2.97	0.42
1:K:255:LEU:HD23	1:K:369:LEU:HB3	1.06	0.42
2:B:9:ALA:HA	2:B:66:VAL:HB	2.02	0.42
2:B:15:GLN:OE1	2:B:15:GLN:HA	2.19	0.42
2:B:29:GLY:O	2:B:37:HIS:HB3	2.19	0.42
2:B:97:ALA:CB	2:B:143:THR:CB	2.95	0.42
2:B:151:LEU:CD1	2:B:152:ILE:HD13	2.49	0.42
2:B:154:LYS:CE	2:B:154:LYS:HA	2.44	0.42
2:B:267:MET:SD	2:B:299:MET:CE	3.07	0.42
2:B:292:GLN:HA	2:B:295:ASP:OD1	2.19	0.42
3:A:11:GLN:O	3:A:14:VAL:HG22	2.20	0.42
3:A:226:ASN:HB3	3:A:367:ASP:OD2	2.20	0.42
3:A:312:TYR:CD2	3:A:315:CYS:SG	3.12	0.42
1:K:272:ILE:CB	1:K:282:ALA:HB1	2.48	0.42
1:K:327:ARG:HH21	1:K:327:ARG:CG	2.33	0.42
2:B:36:TYR:CE1	2:B:38:GLY:N	2.84	0.42
2:B:58:LYS:HZ2	2:B:86:ARG:HG2	1.84	0.42
2:B:101:TRP:HB3	2:B:184:ASN:O	2.19	0.42
2:B:113:VAL:CG2	2:B:114:ASP:N	2.82	0.42
2:B:155:ILE:CG1	2:B:156:ARG:N	2.83	0.42
2:B:187:LEU:CD1	2:B:408:PHE:CD2	3.00	0.42
2:B:241:ARG:CD	2:B:242:PHE:N	2.82	0.42
2:B:276:ARG:HH11	2:B:280:GLN:NE2	2.18	0.42
2:B:314:ALA:HB3	2:B:368:ILE:HG12	1.99	0.42
2:B:374:ILE:CG2	2:B:375:GLN:N	2.81	0.42
2:B:381:ILE:HG12	2:B:384:GLN:NE2	2.33	0.42
2:B:382:SER:CB	2:B:415:MET:CE	2.98	0.42
3:A:4:CYS:SG	3:A:132:LEU:HD23	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:5:ILE:CG1	3:A:64:ARG:HB3	2.32	0.42
3:A:161:TYR:O	3:A:163:LYS:HD3	2.19	0.42
3:A:229:ARG:HG2	3:A:229:ARG:NH1	2.34	0.42
3:A:274:PRO:CB	3:A:276:ILE:HD11	2.49	0.42
1:K:27:PRO:CA	1:K:74:ALA:CB	2.97	0.42
1:K:60:LYS:N	1:K:60:LYS:CD	2.83	0.42
1:K:102:PHE:CZ	1:K:266:LEU:HB2	2.54	0.42
1:K:312:ARG:CA	1:K:318:ARG:HG2	2.43	0.42
2:B:1:MET:CG	2:B:2:ARG:N	2.83	0.42
2:B:116:VAL:CG2	2:B:117:LEU:N	2.82	0.42
2:B:154:LYS:HZ3	2:B:157:GLU:CB	2.32	0.42
2:B:210:ILE:HG23	2:B:297:LYS:CE	2.45	0.42
2:B:258:VAL:O	3:A:404:PHE:CZ	2.72	0.42
2:B:267:MET:HA	2:B:268:PRO:HD3	1.76	0.42
2:B:347:ASN:OD1	2:B:350:LYS:NZ	2.50	0.42
2:B:362:LYS:CE	2:B:362:LYS:CA	2.96	0.42
3:A:14:VAL:CG2	3:A:15:GLN:N	2.82	0.42
3:A:135:PHE:HE1	3:A:166:LYS:CB	2.33	0.42
3:A:138:PHE:O	3:A:139:HIS:HB3	2.20	0.42
3:A:202:PHE:CD1	3:A:267:PHE:CD1	3.07	0.42
3:A:234:ILE:HD12	3:A:235:VAL:HA	2.02	0.42
3:A:255:PHE:HZ	3:A:352:LYS:HB3	1.78	0.42
3:A:351:PHE:HA	3:A:352:LYS:HA	1.67	0.42
1:K:40:ILE:CG1	1:K:41:VAL:N	2.83	0.42
1:K:293:LEU:HG	3:A:405:VAL:HG12	2.01	0.42
2:B:181:GLU:OE2	5:B:501:G2P:H5'1	2.20	0.42
2:B:187:LEU:HD22	2:B:187:LEU:N	2.34	0.42
2:B:207:LEU:CG	2:B:208:TYR:N	2.83	0.42
2:B:294:PHE:N	2:B:294:PHE:CD2	2.87	0.42
2:B:306:ARG:NH2	2:B:340:TYR:CD1	2.88	0.42
2:B:324:LYS:CD	3:A:221:ARG:CB	2.98	0.42
2:B:386:THR:O	2:B:389:PHE:HB3	2.19	0.42
3:A:11:GLN:HB3	3:A:74:VAL:HG11	2.02	0.42
3:A:53:PHE:CA	3:A:63:PRO:HA	2.49	0.42
3:A:62:VAL:HB	3:A:88:HIS:NE2	2.35	0.42
3:A:70:LEU:HD22	3:A:99:ALA:CA	2.49	0.42
3:A:153:LEU:CD1	3:A:157:LEU:CG	2.97	0.42
3:A:305:CYS:SG	3:A:383:ALA:CB	3.08	0.42
3:A:314:ALA:HA	3:A:343:PHE:CE2	2.55	0.42
3:A:387:ALA:CA	3:A:390:ARG:CZ	2.97	0.42
3:A:402:ARG:HH11	3:A:402:ARG:HG2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:ILE:HB	1:K:53:ARG:HB2	2.01	0.42
1:K:136:ILE:HB	1:K:137:PRO:CD	2.50	0.42
1:K:321:GLN:C	1:K:324:LEU:HD23	2.40	0.42
2:B:65:LEU:N	2:B:65:LEU:CD1	2.83	0.42
2:B:138:SER:HB2	2:B:169:VAL:HG22	1.99	0.42
2:B:164:MET:HB2	2:B:164:MET:HE2	1.84	0.42
2:B:207:LEU:HD11	2:B:225:LEU:HD22	2.00	0.42
2:B:217:LEU:HD22	2:B:218:THR:H	1.85	0.42
2:B:258:VAL:CG1	2:B:263:LEU:HB3	2.49	0.42
3:A:114:ILE:CG2	3:A:115:ILE:N	2.83	0.42
3:A:203:MET:SD	3:A:267:PHE:HZ	2.43	0.42
3:A:254:GLU:OE2	3:A:255:PHE:HA	2.19	0.42
3:A:274:PRO:HG2	3:A:286:LEU:CD2	2.50	0.42
3:A:384:ILE:CG1	3:A:385:ALA:N	2.83	0.42
3:A:390:ARG:CA	3:A:393:HIS:CD2	2.99	0.42
3:A:413:MET:HB3	3:A:417:GLU:OE2	2.20	0.42
1:K:28:PHE:HE1	1:K:39:SER:N	2.18	0.42
1:K:109:THR:HG22	1:K:335:THR:HB	1.93	0.42
1:K:295:LEU:HD23	1:K:295:LEU:C	2.39	0.42
1:K:352:TYR:O	1:K:352:TYR:HD2	2.03	0.42
2:B:2:ARG:HG3	2:B:2:ARG:O	2.20	0.42
2:B:14:ASN:HB3	2:B:72:THR:HG21	2.01	0.42
2:B:28:HIS:CG	2:B:47:ILE:HG23	2.55	0.42
2:B:105:HIS:NE2	2:B:150:LEU:HA	2.35	0.42
2:B:285:THR:N	2:B:288:GLU:CB	2.83	0.42
2:B:321:MET:CG	2:B:322:SER:N	2.83	0.42
2:B:343:GLU:H	2:B:343:GLU:CD	2.23	0.42
2:B:407:GLU:HG3	2:B:408:PHE:N	2.35	0.42
3:A:125:LEU:HD12	3:A:128:GLN:HG3	2.01	0.42
3:A:135:PHE:HE1	3:A:166:LYS:CA	2.33	0.42
3:A:244:PHE:N	3:A:244:PHE:CD1	2.85	0.42
1:K:30:LEU:HD12	1:K:33:ARG:HB2	2.01	0.42
2:B:4:ILE:N	2:B:4:ILE:CD1	2.83	0.42
2:B:36:TYR:CE1	2:B:38:GLY:HA3	2.53	0.42
2:B:152:ILE:HA	2:B:155:ILE:HG12	2.01	0.42
2:B:190:HIS:CG	2:B:411:ALA:CB	3.02	0.42
2:B:260:PHE:CG	3:A:404:PHE:N	2.84	0.42
2:B:315:ALA:HA	2:B:366:THR:HG23	2.02	0.42
2:B:368:ILE:HG22	2:B:369:GLY:N	2.35	0.42
3:A:107:HIS:ND1	3:A:108:TYR:CE1	2.88	0.42
1:K:234:ARG:HD3	1:K:234:ARG:HA	1.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:298:VAL:HB	1:K:310:PRO:HG2	2.01	0.41
2:B:23:VAL:HG11	2:B:230:SER:HB2	2.01	0.41
2:B:250:LEU:C	2:B:253:LEU:HG	2.40	0.41
2:B:260:PHE:CD1	2:B:261:PRO:HD2	2.55	0.41
2:B:293:MET:HE3	2:B:367:PHE:CB	2.42	0.41
2:B:296:ALA:CB	2:B:305:PRO:HD3	2.50	0.41
2:B:313:VAL:HG13	2:B:367:PHE:CD2	2.55	0.41
3:A:122:ILE:CG1	3:A:123:ARG:N	2.83	0.41
3:A:188:ILE:CG1	3:A:395:PHE:CD1	3.02	0.41
3:A:306:ASP:CB	3:A:309:HIS:CE1	3.03	0.41
3:A:311:LYS:H	3:A:311:LYS:HD2	1.84	0.41
3:A:318:LEU:HD13	3:A:319:TYR:C	2.40	0.41
3:A:425:MET:SD	3:A:429:GLU:HG2	2.59	0.41
3:A:432:TYR:O	3:A:435:VAL:HG13	2.20	0.41
1:K:22:VAL:HG11	1:K:70:MET:HE2	2.01	0.41
1:K:92:GLU:CB	1:K:97:TYR:CD2	3.01	0.41
1:K:347:LEU:O	1:K:351:GLU:HG2	2.20	0.41
1:K:365:VAL:CG1	1:K:367:GLN:CG	2.95	0.41
2:B:4:ILE:HG22	2:B:5:VAL:O	2.19	0.41
2:B:68:LEU:CD2	2:B:68:LEU:C	2.89	0.41
2:B:138:SER:OG	5:B:501:G2P:O2A	2.37	0.41
2:B:151:LEU:HD12	2:B:152:ILE:HA	2.02	0.41
2:B:172:SER:HB3	2:B:205:GLU:N	2.35	0.41
2:B:251:ARG:HH22	3:A:102:ASN:N	2.18	0.41
3:A:21:TRP:CE2	3:A:65:ALA:CB	3.00	0.41
3:A:188:ILE:N	3:A:188:ILE:CD1	2.83	0.41
3:A:318:LEU:CD1	3:A:320:ARG:CG	2.96	0.41
3:A:325:PRO:O	3:A:328:VAL:HB	2.20	0.41
1:K:94:ILE:HA	1:K:245:MET:CE	2.50	0.41
1:K:159:SER:CB	1:K:172:LEU:HD13	2.47	0.41
1:K:173:ASN:HB3	1:K:176:SER:H	1.83	0.41
1:K:295:LEU:O	1:K:296:GLY:C	2.55	0.41
2:B:23:VAL:CG1	2:B:24:ILE:N	2.83	0.41
2:B:165:ASN:ND2	2:B:167:PHE:CZ	2.89	0.41
2:B:260:PHE:N	2:B:262:ARG:NH2	2.68	0.41
2:B:260:PHE:HB3	3:A:406:HIS:NE2	2.36	0.41
2:B:263:LEU:O	2:B:263:LEU:HD13	2.20	0.41
3:A:102:ASN:ND2	3:A:407:TRP:CE2	2.86	0.41
3:A:171:ILE:HD12	5:A:501:G2P:H1'	1.94	0.41
3:A:224:TYR:CE2	3:A:227:LEU:HD23	2.55	0.41
3:A:250:VAL:HG22	3:A:254:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:255:PHE:C	3:A:259:LEU:HG	2.40	0.41
3:A:296:PHE:N	3:A:296:PHE:CD2	2.85	0.41
3:A:370:LYS:HD3	3:A:370:LYS:C	2.40	0.41
3:A:389:ALA:N	3:A:425:MET:CE	2.83	0.41
1:K:97:TYR:OH	1:K:363:PRO:HB2	2.20	0.41
1:K:272:ILE:HD11	3:A:411:GLU:C	2.40	0.41
1:K:272:ILE:CG2	1:K:282:ALA:HB1	2.50	0.41
1:K:342:ASN:C	1:K:342:ASN:HD22	2.23	0.41
2:B:112:LEU:HD11	2:B:151:LEU:CA	2.49	0.41
2:B:251:ARG:HG3	3:A:100:ALA:CB	2.51	0.41
2:B:345:ILE:HG23	2:B:348:ASN:ND2	2.35	0.41
3:A:9:VAL:CG2	3:A:149:PHE:HD1	2.32	0.41
3:A:122:ILE:CD1	3:A:123:ARG:N	2.82	0.41
3:A:192:HIS:CD2	3:A:193:THR:HG23	2.55	0.41
3:A:210:TYR:CZ	3:A:227:LEU:HD22	2.55	0.41
3:A:275:VAL:HG13	3:A:280:LYS:NZ	2.34	0.41
3:A:311:LYS:N	3:A:311:LYS:CD	2.83	0.41
3:A:393:HIS:O	3:A:396:ASP:HB3	2.19	0.41
1:K:162:GLU:HG3	1:K:235:SER:CB	2.29	0.41
1:K:272:ILE:HB	1:K:282:ALA:CB	2.50	0.41
1:K:355:ARG:HG3	4:K:501:MZK:C16	2.51	0.41
2:B:99:ASN:O	2:B:142:GLY:HA3	2.20	0.41
2:B:186:THR:CG2	2:B:187:LEU:N	2.82	0.41
2:B:304:ASP:CB	2:B:307:HIS:CE1	3.04	0.41
3:A:36:MET:HB2	3:A:38:SER:HB3	2.03	0.41
3:A:79:ARG:NH1	3:A:92:LEU:HG	2.36	0.41
3:A:118:VAL:CG2	3:A:119:LEU:N	2.82	0.41
3:A:143:GLY:HA3	5:A:501:G2P:PB	2.60	0.41
3:A:262:TYR:CB	3:A:264:ARG:HD3	2.35	0.41
3:A:270:ALA:HB2	3:A:378:LEU:HD23	2.01	0.41
3:A:352:LYS:CG	3:A:353:VAL:N	2.83	0.41
1:K:28:PHE:CZ	1:K:37:ALA:C	2.93	0.41
1:K:227:LEU:CD1	1:K:228:MET:CE	2.98	0.41
1:K:258:ILE:N	1:K:368:LYS:HE2	2.33	0.41
2:B:192:LEU:HD13	2:B:192:LEU:O	2.21	0.41
2:B:350:LYS:NZ	3:A:179:THR:O	2.54	0.41
3:A:1:MET:N	3:A:47:ASP:HA	2.36	0.41
3:A:13:GLY:O	3:A:16:ILE:HG22	2.20	0.41
3:A:242:LEU:HB2	3:A:252:LEU:CG	2.50	0.41
3:A:253:THR:O	3:A:256:GLN:HB3	2.21	0.41
3:A:308:ARG:CD	3:A:308:ARG:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:321:GLY:CA	3:A:372:GLN:HE21	2.25	0.41
3:A:336:LYS:HD2	3:A:336:LYS:HA	1.76	0.41
1:K:272:ILE:HG22	1:K:282:ALA:HA	2.01	0.41
1:K:312:ARG:CD	2:B:414:ASN:HD21	2.31	0.41
1:K:343:LEU:HD23	1:K:343:LEU:N	2.12	0.41
2:B:47:ILE:CD1	2:B:241:ARG:HH12	2.33	0.41
2:B:106:TYR:HD2	2:B:106:TYR:N	2.18	0.41
2:B:137:HIS:HD2	2:B:144:GLY:O	2.04	0.41
2:B:183:TYR:CE1	2:B:385:PHE:CD1	3.09	0.41
2:B:190:HIS:CG	2:B:411:ALA:HA	2.56	0.41
2:B:271:ALA:CB	2:B:293:MET:SD	3.07	0.41
2:B:303:CYS:CB	2:B:371:SER:CB	2.99	0.41
2:B:410:GLU:CD	2:B:413:SER:HB2	2.41	0.41
3:A:36:MET:HA	3:A:37:PRO:HD3	1.88	0.41
3:A:74:VAL:CG2	3:A:75:ILE:N	2.83	0.41
3:A:87:PHE:CE1	3:A:91:GLN:HG2	2.55	0.41
3:A:214:ARG:CG	3:A:215:ARG:N	2.82	0.41
3:A:219:ILE:HG22	3:A:221:ARG:N	2.36	0.41
3:A:219:ILE:O	3:A:220:GLU:O	2.39	0.41
3:A:272:TYR:CG	3:A:273:ALA:N	2.86	0.41
1:K:17:LYS:HG3	1:K:329:ARG:NE	2.35	0.41
1:K:97:TYR:HA	1:K:366:ASN:OD1	2.21	0.41
1:K:145:GLU:OE2	1:K:207:LYS:NZ	2.49	0.41
1:K:168:LEU:HB2	1:K:182:LEU:HB2	2.02	0.41
1:K:352:TYR:CG	4:K:501:MZK:C15	3.04	0.41
2:B:154:LYS:O	2:B:157:GLU:HB3	2.21	0.41
2:B:221:THR:HG22	2:B:223:GLY:N	2.35	0.41
3:A:20:CYS:HA	3:A:232:SER:OG	2.21	0.41
3:A:108:TYR:C	3:A:112:LYS:HZ2	2.24	0.41
3:A:224:TYR:CZ	5:A:501:G2P:C5	3.04	0.41
1:K:26:ARG:HG2	1:K:109:THR:HA	2.01	0.41
1:K:77:LYS:CE	1:K:78:GLN:HB2	2.51	0.41
1:K:134:GLY:CA	1:K:138:ARG:CG	2.99	0.41
1:K:139:THR:O	1:K:143:ILE:HG13	2.21	0.41
1:K:190:ASN:CB	1:K:193:GLY:H	2.32	0.41
2:B:19:LYS:HA	2:B:19:LYS:NZ	2.36	0.41
2:B:31:ASP:OD1	2:B:37:HIS:HA	2.21	0.41
2:B:32:PRO:HB3	2:B:81:PHE:CE1	2.56	0.41
2:B:34:GLY:O	2:B:58:LYS:HA	2.20	0.41
2:B:94:GLN:HE21	2:B:94:GLN:HB3	1.52	0.41
2:B:127:CYS:SG	2:B:130:LEU:CD1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:LEU:CD2	2:B:133:PHE:HE1	2.10	0.41
2:B:186:THR:HG21	2:B:385:PHE:CE1	2.56	0.41
2:B:196:THR:HG22	2:B:198:GLU:N	2.36	0.41
2:B:199:THR:HG23	2:B:199:THR:O	2.21	0.41
2:B:213:ARG:HB2	2:B:213:ARG:CZ	2.51	0.41
2:B:252:LYS:HG2	3:A:100:ALA:CB	2.51	0.41
2:B:255:VAL:CG1	2:B:256:ASN:N	2.83	0.41
2:B:266:PHE:HE1	2:B:312:THR:HG23	1.85	0.41
2:B:323:MET:HE1	2:B:326:VAL:CG2	2.44	0.41
2:B:324:LYS:CG	3:A:221:ARG:CB	2.95	0.41
2:B:337:ASN:CB	2:B:340:TYR:CD2	3.03	0.41
2:B:347:ASN:CG	2:B:350:LYS:NZ	2.74	0.41
2:B:347:ASN:HD21	2:B:350:LYS:HZ3	1.66	0.41
3:A:24:TYR:CA	3:A:27:GLU:HG3	2.51	0.41
3:A:35:GLN:NE2	3:A:40:LYS:HE3	2.36	0.41
3:A:99:ALA:CB	3:A:101:ASN:H	2.34	0.41
3:A:108:TYR:O	3:A:112:LYS:HD3	2.21	0.41
3:A:130:THR:CG2	3:A:131:GLY:N	2.82	0.41
3:A:150:THR:CG2	3:A:151:SER:N	2.82	0.41
3:A:234:ILE:CD1	3:A:235:VAL:N	2.82	0.41
3:A:245:ASP:CA	3:A:249:ASN:HB2	2.45	0.41
3:A:251:ASP:CG	3:A:254:GLU:HB3	2.40	0.41
3:A:262:TYR:CD2	3:A:265:ILE:HG12	2.54	0.41
3:A:298:PRO:CG	3:A:308:ARG:HH12	2.34	0.41
3:A:320:ARG:HD3	3:A:360:PRO:CA	2.43	0.41
3:A:347:CYS:SG	3:A:349:THR:HG23	2.61	0.41
3:A:351:PHE:HB2	3:A:352:LYS:HA	2.03	0.41
1:K:54:THR:HG23	1:K:62:SER:HB2	2.02	0.41
1:K:54:THR:CB	1:K:56:GLY:H	2.34	0.41
1:K:59:ASP:C	1:K:61:SER:H	2.24	0.41
1:K:272:ILE:CG1	1:K:273:GLY:N	2.82	0.41
2:B:24:ILE:CG2	2:B:28:HIS:NE2	2.82	0.41
2:B:259:PRO:CA	3:A:404:PHE:CE2	3.03	0.41
2:B:260:PHE:HD1	2:B:260:PHE:HA	1.72	0.41
2:B:269:GLY:HA3	2:B:367:PHE:HD1	1.86	0.41
3:A:7:ILE:O	3:A:138:PHE:CD1	2.74	0.41
3:A:28:HIS:CD2	3:A:41:THR:HG23	2.56	0.41
3:A:242:LEU:HD23	3:A:252:LEU:N	2.33	0.41
3:A:261:PRO:C	3:A:262:TYR:CD1	2.95	0.41
3:A:276:ILE:HB	3:A:368:LEU:HD22	2.03	0.41
3:A:278:ALA:O	3:A:282:TYR:CD1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:306:ASP:CB	3:A:308:ARG:HH21	2.34	0.41
3:A:311:LYS:N	3:A:311:LYS:CE	2.83	0.41
3:A:318:LEU:O	3:A:319:TYR:CD2	2.74	0.41
1:K:16:GLY:HA3	1:K:363:PRO:N	2.35	0.40
1:K:141:HIS:HB2	1:K:211:TYR:OH	2.21	0.40
2:B:6:HIS:C	2:B:7:ILE:HD13	2.41	0.40
2:B:21:TRP:CZ2	2:B:62:ARG:O	2.74	0.40
2:B:152:ILE:HG21	2:B:192:LEU:CD2	2.51	0.40
2:B:175:VAL:CG1	2:B:176:SER:N	2.84	0.40
2:B:214:THR:HB	2:B:275:SER:C	2.40	0.40
2:B:245:GLN:HE22	2:B:355:ASP:HA	1.85	0.40
2:B:320:ARG:CZ	2:B:320:ARG:N	2.83	0.40
2:B:390:ARG:CZ	2:B:390:ARG:CA	2.96	0.40
3:A:11:GLN:HA	3:A:74:VAL:HG11	2.03	0.40
3:A:111:GLY:HA2	3:A:114:ILE:CG2	2.51	0.40
3:A:243:ARG:C	3:A:244:PHE:CD1	2.94	0.40
3:A:255:PHE:CD1	3:A:259:LEU:HD21	2.56	0.40
3:A:311:LYS:HA	3:A:342:GLN:HG2	1.99	0.40
1:K:19:ILE:HD11	1:K:332:ILE:HG13	2.03	0.40
2:B:10:GLY:N	2:B:147:MET:SD	2.94	0.40
2:B:20:PHE:CZ	2:B:24:ILE:CD1	3.01	0.40
2:B:193:VAL:HG13	2:B:194:GLU:CD	2.41	0.40
2:B:250:LEU:HA	2:B:253:LEU:CG	2.51	0.40
2:B:251:ARG:NE	3:A:105:ARG:NE	2.70	0.40
2:B:309:ARG:HG2	2:B:425:TYR:O	2.22	0.40
2:B:378:PHE:O	2:B:381:ILE:HB	2.20	0.40
2:B:396:HIS:ND1	2:B:397:TRP:CD1	2.89	0.40
3:A:16:ILE:CG2	3:A:17:GLY:N	2.82	0.40
3:A:68:VAL:O	3:A:68:VAL:HG23	2.21	0.40
3:A:308:ARG:H	3:A:308:ARG:CD	2.34	0.40
1:K:50:VAL:CG2	1:K:71:VAL:CG1	2.99	0.40
1:K:144:PHE:CB	1:K:207:LYS:CG	2.97	0.40
2:B:200:TYR:CD1	2:B:268:PRO:HD3	2.56	0.40
2:B:253:LEU:CB	2:B:257:MET:HE1	2.40	0.40
3:A:63:PRO:O	3:A:87:PHE:CE1	2.75	0.40
3:A:179:THR:C	3:A:183:GLU:OE1	2.59	0.40
3:A:304:LYS:HG3	3:A:304:LYS:O	2.22	0.40
3:A:318:LEU:H	3:A:376:CYS:H	1.69	0.40
1:K:15:LYS:HE3	1:K:362:LYS:CB	2.50	0.40
1:K:27:PRO:N	1:K:74:ALA:HB1	2.37	0.40
1:K:162:GLU:CD	1:K:235:SER:OG	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:255:LEU:CD2	1:K:369:LEU:HA	2.50	0.40
1:K:368:LYS:HD2	1:K:368:LYS:N	2.37	0.40
2:B:51:TYR:CE2	2:B:61:PRO:HA	2.56	0.40
2:B:108:GLU:CD	2:B:147:MET:HA	2.41	0.40
2:B:186:THR:CG2	2:B:385:PHE:HE1	2.33	0.40
2:B:274:THR:CG2	2:B:275:SER:N	2.83	0.40
2:B:404:ASP:O	2:B:408:PHE:CD1	2.75	0.40
3:A:1:MET:CB	3:A:47:ASP:CA	2.96	0.40
3:A:3:GLU:HG2	3:A:50:ASN:C	2.41	0.40
3:A:5:ILE:HG23	3:A:65:ALA:N	2.36	0.40
3:A:10:GLY:HA2	3:A:145:THR:HB	2.03	0.40
3:A:11:GLN:HG3	3:A:71:GLU:OE1	2.22	0.40
3:A:153:LEU:HD11	3:A:157:LEU:CG	2.52	0.40
3:A:156:ARG:HB3	3:A:156:ARG:HH11	1.84	0.40
3:A:346:TRP:HZ2	3:A:437:VAL:O	2.04	0.40
3:A:349:THR:OG1	3:A:351:PHE:HD1	2.01	0.40
3:A:407:TRP:CE3	3:A:407:TRP:O	2.75	0.40
1:K:204:VAL:HG23	1:K:206:ASN:O	2.22	0.40
1:K:288:ILE:O	1:K:292:LEU:HD13	2.21	0.40
1:K:311:TYR:CD2	1:K:321:GLN:CD	2.95	0.40
1:K:369:LEU:N	1:K:369:LEU:CD2	2.84	0.40
2:B:43:GLN:OE1	2:B:47:ILE:HD11	2.21	0.40
2:B:70:PRO:HD3	2:B:94:GLN:O	2.21	0.40
2:B:81:PHE:N	2:B:81:PHE:CD1	2.88	0.40
2:B:196:THR:HG22	2:B:198:GLU:H	1.86	0.40
3:A:36:MET:HB2	3:A:38:SER:H	1.85	0.40
3:A:56:THR:CG2	3:A:57:GLY:N	2.82	0.40
3:A:63:PRO:CB	3:A:87:PHE:CE1	3.04	0.40
3:A:70:LEU:HD22	3:A:99:ALA:HB2	2.04	0.40
3:A:215:ARG:CD	3:A:216:ASN:N	2.84	0.40
3:A:377:MET:N	3:A:377:MET:SD	2.95	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 PDB entries followed by that with respect to all EM entries.

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	K	328/391 (84%)	322 (98%)	6 (2%)	0	100	100
2	B	427/429 (100%)	421 (99%)	4 (1%)	2 (0%)	25	58
3	A	436/438 (100%)	422 (97%)	10 (2%)	4 (1%)	14	45
All	All	1191/1258 (95%)	1165 (98%)	20 (2%)	6 (0%)	27	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	261	PRO
3	A	179	THR
3	A	100	ALA
3	A	405	VAL
3	A	406	HIS
2	B	347	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	K	292/343 (85%)	255 (87%)	37 (13%)	3	19
2	B	369/369 (100%)	299 (81%)	70 (19%)	1	8
3	A	369/369 (100%)	306 (83%)	63 (17%)	1	11
All	All	1030/1081 (95%)	860 (84%)	170 (16%)	4	12

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	15	LYS
1	K	17	LYS
1	K	28	PHE
1	K	33	ARG

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Mol	Chain	Res	Type
1	K	34	LYS
1	K	38	HIS
1	K	54	THR
1	K	60	LYS
1	K	77	LYS
1	K	84	SER
1	K	95	MET
1	K	97	TYR
1	K	104	TYR
1	K	171	LEU
1	K	172	LEU
1	K	181	ARG
1	K	182	LEU
1	K	187	ASP
1	K	189	ARG
1	K	190	ASN
1	K	191	LYS
1	K	202	ILE
1	K	207	LYS
1	K	208	ASP
1	K	228	MET
1	K	247	GLU
1	K	257	LYS
1	K	266	LEU
1	K	272	ILE
1	K	289	ASN
1	K	327	ARG
1	K	342	ASN
1	K	343	LEU
1	K	345	GLU
1	K	352	TYR
1	K	367	GLN
1	K	368	LYS
2	B	3	GLU
2	B	6	HIS
2	B	8	GLN
2	B	19	LYS
2	B	21	TRP
2	B	22	GLU
2	B	31	ASP
2	B	37	HIS
2	B	43	GLN

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Mol	Chain	Res	Type
2	B	44	LEU
2	B	50	TYR
2	B	68	LEU
2	B	73	MET
2	B	83	GLN
2	B	88	ASP
2	B	94	GLN
2	B	101	TRP
2	B	103	LYS
2	B	114	ASP
2	B	122	LYS
2	B	134	GLN
2	B	145	SER
2	B	147	MET
2	B	154	LYS
2	B	156	ARG
2	B	158	GLU
2	B	161	ASP
2	B	183	TYR
2	B	184	ASN
2	B	190	HIS
2	B	197	ASP
2	B	208	TYR
2	B	212	PHE
2	B	213	ARG
2	B	216	LYS
2	B	217	LEU
2	B	222	TYR
2	B	227	HIS
2	B	241	ARG
2	B	242	PHE
2	B	251	ARG
2	B	252	LYS
2	B	260	PHE
2	B	262	ARG
2	B	265	PHE
2	B	266	PHE
2	B	267	MET
2	B	273	LEU
2	B	276	ARG
2	B	291	GLN
2	B	292	GLN

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Mol	Chain	Res	Type
2	B	297	LYS
2	B	306	ARG
2	B	307	HIS
2	B	320	ARG
2	B	324	LYS
2	B	329	GLN
2	B	330	MET
2	B	331	LEU
2	B	336	LYS
2	B	343	GLU
2	B	350	LYS
2	B	361	LEU
2	B	363	MET
2	B	375	GLN
2	B	376	GLU
2	B	383	GLU
2	B	414	ASN
2	B	420	SER
2	B	423	GLN
3	A	15	GLN
3	A	18	ASN
3	A	22	GLU
3	A	31	GLN
3	A	46	ASP
3	A	53	PHE
3	A	60	LYS
3	A	64	ARG
3	A	84	ARG
3	A	85	GLN
3	A	87	PHE
3	A	91	GLN
3	A	96	LYS
3	A	101	ASN
3	A	103	TYR
3	A	105	ARG
3	A	120	ASP
3	A	128	GLN
3	A	135	PHE
3	A	154	MET
3	A	156	ARG
3	A	163	LYS
3	A	164	LYS

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Mol	Chain	Res	Type
3	A	179	THR
3	A	203	MET
3	A	210	TYR
3	A	211	ASP
3	A	214	ARG
3	A	215	ARG
3	A	218	ASP
3	A	220	GLU
3	A	221	ARG
3	A	224	TYR
3	A	229	ARG
3	A	242	LEU
3	A	243	ARG
3	A	254	GLU
3	A	255	PHE
3	A	264	ARG
3	A	267	PHE
3	A	285	GLN
3	A	302	MET
3	A	308	ARG
3	A	309	HIS
3	A	311	LYS
3	A	313	MET
3	A	320	ARG
3	A	326	LYS
3	A	339	ARG
3	A	343	PHE
3	A	346	TRP
3	A	351	PHE
3	A	352	LYS
3	A	392	ASP
3	A	394	LYS
3	A	396	ASP
3	A	401	LYS
3	A	405	VAL
3	A	407	TRP
3	A	423	GLU
3	A	424	ASP
3	A	430	LYS
3	A	432	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	98	ASN
1	K	150	ASN
1	K	173	ASN
1	K	190	ASN
1	K	205	HIS
1	K	271	ASN
1	K	287	ASN
1	K	289	ASN
1	K	290	GLN
1	K	308	HIS
1	K	342	ASN
1	K	367	GLN
2	B	11	GLN
2	B	28	HIS
2	B	94	GLN
2	B	105	HIS
2	B	131	GLN
2	B	226	ASN
2	B	245	GLN
2	B	279	GLN
2	B	280	GLN
2	B	291	GLN
2	B	292	GLN
2	B	334	GLN
2	B	335	ASN
2	B	347	ASN
2	B	348	ASN
2	B	375	GLN
2	B	414	ASN
2	B	424	GLN
2	B	426	GLN
3	A	8	HIS
3	A	15	GLN
3	A	31	GLN
3	A	61	HIS
3	A	88	HIS
3	A	91	GLN
3	A	101	ASN
3	A	139	HIS
3	A	176	GLN
3	A	186	ASN
3	A	216	ASN
3	A	228	ASN

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Mol	Chain	Res	Type
3	A	233	GLN
3	A	283	HIS
3	A	285	GLN
3	A	300	ASN
3	A	301	GLN
3	A	329	ASN
3	A	342	GLN
3	A	358	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
5	G2P	B	501	6	25,34,34	1.24	3 (12%)	32,54,54	2.24	6 (18%)
4	MZK	K	501	-	23,23,23	0.93	1 (4%)	34,34,34	0.76	0
5	G2P	A	501	6	25,34,34	1.10	1 (4%)	32,54,54	2.10	4 (12%)

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
5	G2P	B	501	6	-	4/15/38/38	0/3/3/3
4	MZK	K	501	-	-	0/10/19/19	0/3/3/3
5	G2P	A	501	6	-	7/15/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	501	MZK	C7-N1	3.11	1.38	1.35
5	B	501	G2P	C6-N1	3.08	1.38	1.33
5	A	501	G2P	C6-N1	3.05	1.38	1.33
5	B	501	G2P	PA-O1A	-2.37	1.50	1.56
5	B	501	G2P	PB-O1B	-2.31	1.50	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	G2P	C5-C6-N1	-8.31	112.31	123.42
5	B	501	G2P	C5-C6-N1	-8.20	112.46	123.42
5	B	501	G2P	C2-N1-C6	6.53	125.04	115.96
5	A	501	G2P	C2-N1-C6	6.49	124.99	115.96
5	B	501	G2P	N3-C2-N1	-3.19	123.15	127.21
5	B	501	G2P	O1B-PB-C3A	3.10	119.55	106.73
5	A	501	G2P	N3-C2-N1	-3.05	123.33	127.21
5	B	501	G2P	O1A-PA-C3A	2.86	118.59	106.73
5	B	501	G2P	C2-N3-C4	-2.52	112.77	115.48
5	A	501	G2P	C2-N3-C4	-2.41	112.88	115.48

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	G2P	PB-C3A-PA-O1A
5	B	501	G2P	PB-C3A-PA-O2A
5	B	501	G2P	PB-C3A-PA-O5'
5	A	501	G2P	PB-O3B-PG-O1G
5	A	501	G2P	PB-C3A-PA-O1A
5	A	501	G2P	PB-C3A-PA-O2A
5	A	501	G2P	PB-C3A-PA-O5'

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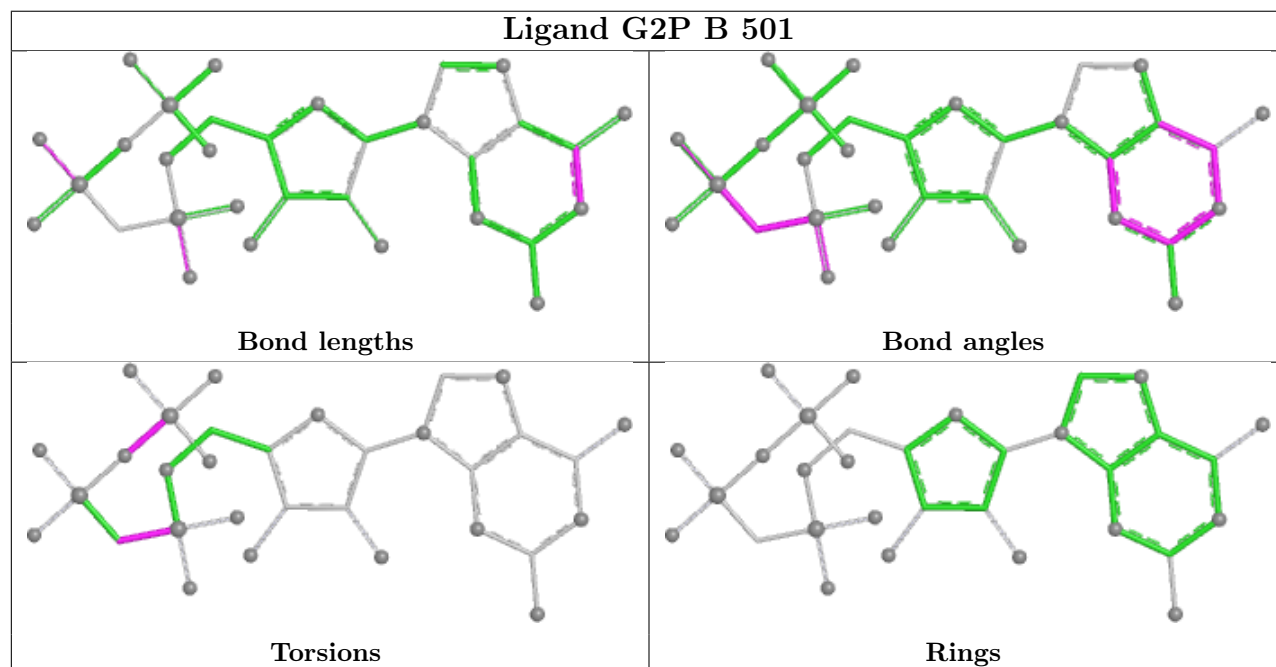
Mol	Chain	Res	Type	Atoms
5	A	501	G2P	C5'-O5'-PA-O1A
5	B	501	G2P	PB-O3B-PG-O3G
5	A	501	G2P	PB-O3B-PG-O3G
5	A	501	G2P	PB-O3B-PG-O2G

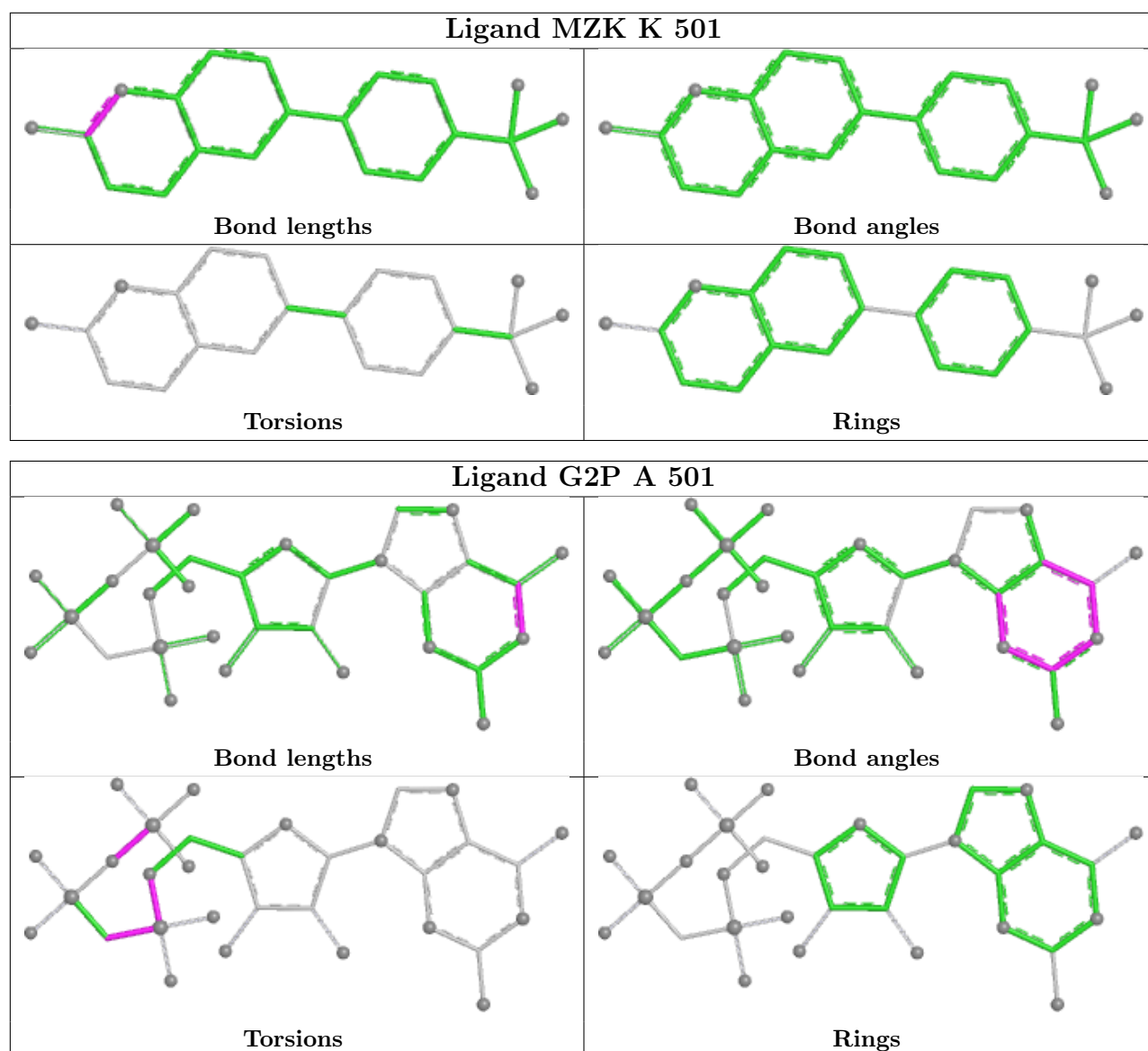
There are no ring outliers.

3 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	G2P	20	0
4	K	501	MZK	14	0
5	A	501	G2P	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10421. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.