Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 09:59 pm BST

PDB ID	:	6TA3 / pdb_00006ta3
EMDB ID	:	EMD-10421
Title	:	Human kinesin-5 motor domain in the GSK-1 state bound to microtubules (Conformation 1)
Authors	:	Pena, A.; Sweeney, A.; Cook, A.D.; Moores, C.A.; Topf, M.
Deposited on	:	2019-10-29
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:

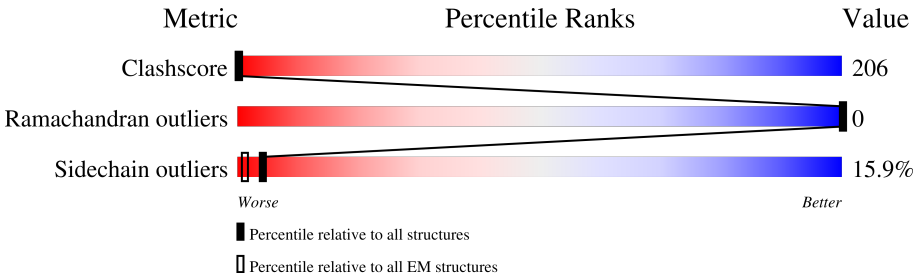
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	B	429	10% 75% 15%
2	A	438	8% 78% 15%
3	K	391	17% 58% 9% • 15%

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	G2P	A	501	-	-	X	-
4	G2P	B	501	-	-	X	-

2 Entry composition (i)

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 Tubulin beta chain.

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

- Molecule 2 is a protein called Tubulin alpha-1B chain.

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

- Molecule 3 is a protein called Kinesin-like protein KIF11.

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

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

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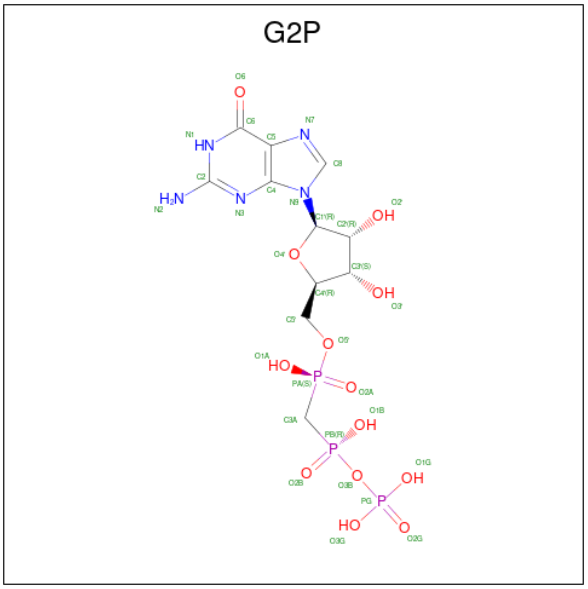
Chain	Residue	Modelled	Actual	Comment	Reference
K	-6	GLU	-	expression tag	UNP P52732
K	-5	ASN	-	expression tag	UNP P52732
K	-4	LEU	-	expression tag	UNP P52732
K	-3	TYR	-	expression tag	UNP P52732
K	-2	PHE	-	expression tag	UNP P52732
K	-1	GLN	-	expression tag	UNP P52732
K	0	SER	-	expression tag	UNP P52732

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



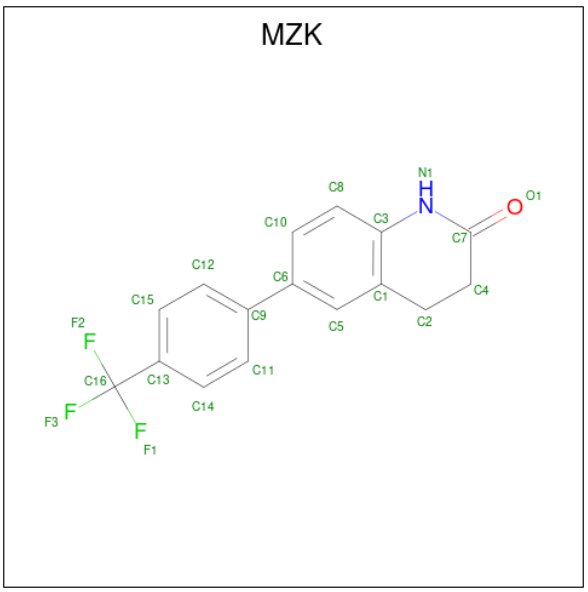
Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			32	11	5	13	3	
4	A	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is 6-[4-(trifluoromethyl)phenyl]-3,4-dihydro-1 {H}-quinolin-2-one (CCD ID:

MZK) (formula: $C_{16}H_{12}F_3NO$) (labeled as "Ligand of Interest" by depositor).



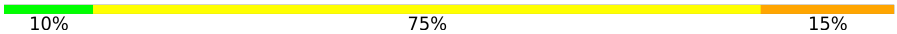
Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
6	K	1	21	16	3	1	1	0

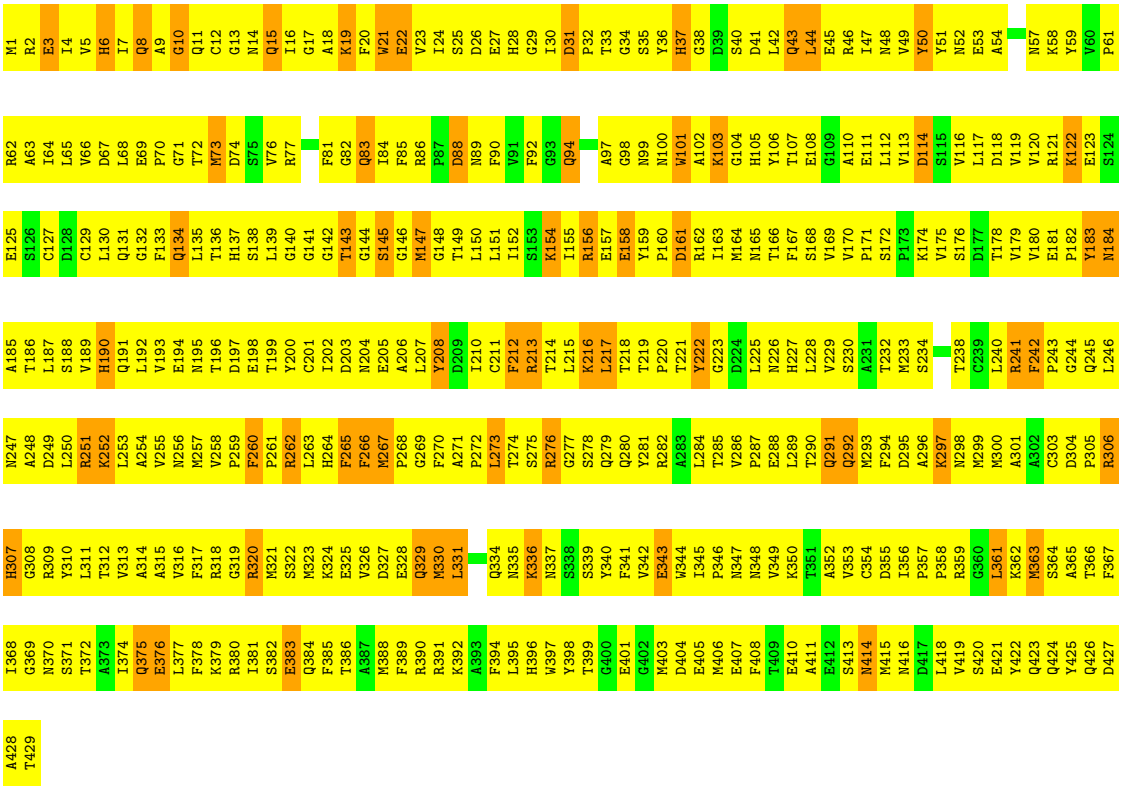
3 Residue-property plots (i)

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

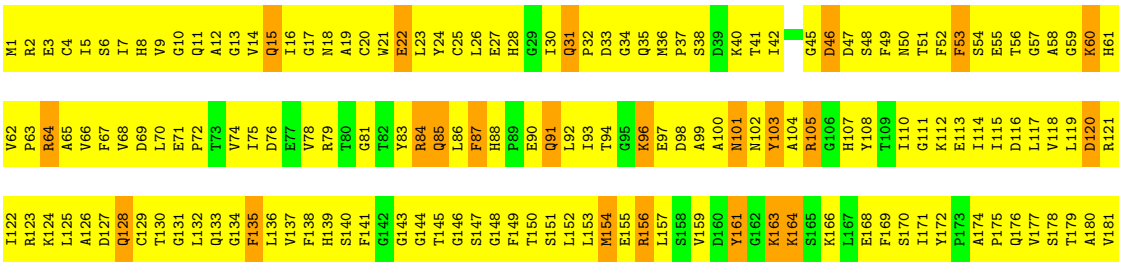
Chain B:





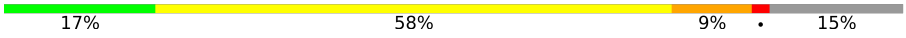
- Molecule 2: Tubulin alpha-1B chain

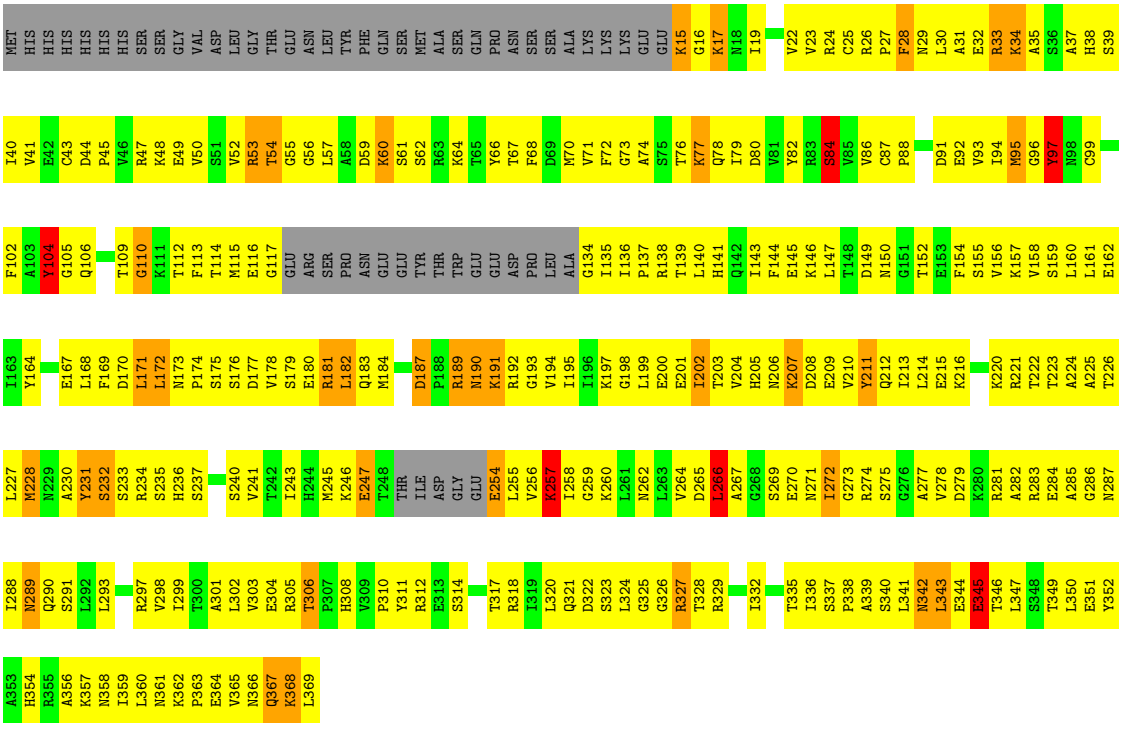
Chain A:



• Molecule 3: Kinesin-like protein KIF11

Chain K:





4 Experimental information (i)

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 ($e^-/Å^2$)	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: MZK, MG, G2P

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	B	1.06	0/3447	1.21	3/4669 (0.1%)
2	A	1.04	0/3503	1.14	1/4754 (0.0%)
3	K	1.67	11/2640 (0.4%)	1.26	18/3557 (0.5%)
All	All	1.25	11/9590 (0.1%)	1.20	22/12980 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	A	0	3
3	K	0	6
All	All	0	10

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	84	SER	CB-OG	-56.93	0.68	1.42
3	K	254	GLU	CB-CG	-24.02	1.06	1.52
3	K	247	GLU	CB-CG	-13.94	1.25	1.52
3	K	247	GLU	CD-OE1	-11.45	1.13	1.25
3	K	257	LYS	CB-CG	-10.64	1.23	1.52
3	K	260	LYS	CG-CD	-9.29	1.20	1.52
3	K	306	THR	C-O	-7.66	1.08	1.23
3	K	97	TYR	CE1-CZ	-7.65	1.28	1.38
3	K	97	TYR	CE2-CZ	-6.52	1.30	1.38
3	K	97	TYR	CG-CD2	5.89	1.46	1.39
3	K	254	GLU	CD-OE2	-5.46	1.19	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	10	GLY	O-C-N	-19.90	90.86	122.70
1	B	10	GLY	CA-C-N	14.42	148.93	117.20
3	K	254	GLU	CA-CB-CG	11.92	139.62	113.40
3	K	84	SER	CA-CB-OG	10.40	139.29	111.20
3	K	257	LYS	CA-CB-CG	9.90	135.18	113.40
3	K	231	TYR	CZ-CE2-CD2	-9.46	111.28	119.80
3	K	97	TYR	CG-CD2-CE2	-8.82	114.25	121.30
3	K	257	LYS	CB-CG-CD	8.78	134.43	111.60
3	K	231	TYR	CG-CD2-CE2	8.33	127.97	121.30
3	K	266	LEU	CB-CG-CD2	7.86	124.36	111.00
3	K	104	TYR	CB-CG-CD2	7.51	125.51	121.00
2	A	161	TYR	CA-CB-CG	-7.43	99.28	113.40
3	K	104	TYR	CB-CG-CD1	-6.30	117.22	121.00
3	K	260	LYS	CG-CD-CE	6.25	130.64	111.90
3	K	211	TYR	CA-CB-CG	-6.12	101.77	113.40
3	K	232	SER	N-CA-CB	6.10	119.65	110.50
3	K	260	LYS	CB-CG-CD	5.96	127.11	111.60
1	B	143	THR	N-CA-CB	5.56	120.87	110.30
3	K	247	GLU	CA-CB-CG	5.50	125.51	113.40
3	K	254	GLU	CB-CG-CD	5.49	129.03	114.20
3	K	211	TYR	CG-CD2-CE2	-5.49	116.91	121.30
3	K	352	TYR	CB-CG-CD1	-5.03	117.98	121.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	399	TYR	Sidechain
2	A	402	ARG	Mainchain
2	A	415	GLU	Sidechain
1	B	15	GLN	Peptide
3	K	104	TYR	Sidechain
3	K	106	GLN	Sidechain
3	K	110	GLY	Peptide
3	K	266	LEU	Mainchain
3	K	345	GLU	Sidechain
3	K	53	ARG	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3372	0	3243	1485	0
2	A	3425	0	3330	1589	0
3	K	2607	0	2670	964	0
4	A	32	0	14	31	0
4	B	32	0	14	19	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	K	21	0	0	0	0
All	All	9491	0	9271	3868	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 206.

All (3868) 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:A:427:ALA:HB2	3:K:57:LEU:CD2	1.27	1.56
2:A:427:ALA:CB	3:K:57:LEU:CD2	1.84	1.55
3:K:181:ARG:HH21	3:K:197:LYS:CG	1.19	1.51
2:A:409:VAL:HG21	3:K:293:LEU:CG	1.46	1.44
3:K:95:MET:CE	3:K:97:TYR:HB2	1.45	1.43
3:K:181:ARG:NH2	3:K:197:LYS:HG3	1.27	1.42
1:B:420:SER:OG	3:K:308:HIS:CE1	1.74	1.39
1:B:260:PHE:CE2	2:A:406:HIS:N	1.68	1.38
3:K:95:MET:HE2	3:K:97:TYR:CB	1.53	1.38
2:A:427:ALA:CB	3:K:57:LEU:HD21	1.44	1.38
1:B:323:MET:HB2	2:A:221:ARG:CD	1.55	1.36
2:A:409:VAL:CG2	3:K:293:LEU:HG	1.56	1.34
2:A:409:VAL:CG2	3:K:293:LEU:CD2	2.06	1.33
2:A:409:VAL:HG21	3:K:293:LEU:CD2	1.58	1.32
2:A:423:GLU:OE1	3:K:57:LEU:CD1	1.77	1.31
1:B:252:LYS:HD3	2:A:101:ASN:CB	1.36	1.30
2:A:224:TYR:CZ	4:A:501:G2P:C5	2.15	1.29
2:A:405:VAL:HG11	3:K:293:LEU:CD1	1.63	1.29
2:A:411:GLU:O	3:K:272:ILE:HD11	1.24	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:224:TYR:CE2	4:A:501:G2P:C6	2.16	1.27
3:K:82:TYR:CE2	3:K:86:VAL:HG21	1.69	1.26
1:B:252:LYS:CD	2:A:101:ASN:CB	1.96	1.25
1:B:323:MET:HB2	2:A:221:ARG:CG	1.66	1.24
3:K:162:GLU:CG	3:K:235:SER:HB2	1.68	1.24
1:B:262:ARG:CD	3:K:297:ARG:HH12	1.50	1.23
3:K:82:TYR:CD2	3:K:86:VAL:HG21	1.73	1.23
2:A:409:VAL:HG11	3:K:290:GLN:CA	1.68	1.21
3:K:162:GLU:HG2	3:K:235:SER:CB	1.70	1.21
1:B:64:ILE:HD11	1:B:119:VAL:HG11	1.23	1.20
2:A:411:GLU:O	3:K:272:ILE:CD1	1.89	1.20
3:K:162:GLU:OE2	3:K:223:THR:CG2	1.89	1.20
3:K:187:ASP:OD1	3:K:195:ILE:HG13	1.33	1.20
3:K:157:LYS:CG	3:K:203:THR:OG1	1.89	1.19
2:A:319:TYR:HD1	2:A:355:ILE:HG12	1.08	1.19
3:K:162:GLU:CG	3:K:235:SER:CB	2.19	1.19
2:A:278:ALA:HA	2:A:368:LEU:HA	1.24	1.19
2:A:23:LEU:HD12	2:A:363:VAL:HA	1.24	1.18
2:A:268:PRO:HG2	2:A:378:LEU:HD13	1.26	1.17
2:A:409:VAL:CG1	3:K:290:GLN:HA	1.73	1.17
1:B:260:PHE:CZ	2:A:406:HIS:N	2.11	1.17
1:B:420:SER:OG	3:K:308:HIS:HE1	0.84	1.17
3:K:162:GLU:HG2	3:K:235:SER:HB3	1.26	1.17
2:A:247:ALA:HB3	2:A:355:ILE:HB	1.20	1.16
3:K:82:TYR:CZ	3:K:86:VAL:HG11	1.80	1.16
3:K:157:LYS:HG3	3:K:203:THR:OG1	1.45	1.15
2:A:48:SER:HB2	2:A:243:ARG:HD3	1.20	1.15
2:A:176:GLN:HG2	2:A:207:GLU:HB2	1.29	1.15
1:B:326:VAL:HG12	1:B:330:MET:HE1	1.15	1.14
2:A:172:TYR:HB2	2:A:203:MET:HB2	1.25	1.14
2:A:286:LEU:HD13	2:A:291:ILE:HD11	1.30	1.14
3:K:162:GLU:OE2	3:K:223:THR:HG22	1.47	1.14
1:B:285:THR:HG22	1:B:288:GLU:HB2	1.28	1.13
2:A:427:ALA:CB	3:K:57:LEU:HD22	1.57	1.13
1:B:41:ASP:HA	1:B:44:LEU:HD23	1.15	1.12
2:A:274:PRO:HG3	2:A:291:ILE:HG12	1.32	1.12
2:A:166:LYS:HD2	2:A:198:SER:HA	1.28	1.12
3:K:312:ARG:HA	3:K:318:ARG:CG	1.79	1.12
2:A:409:VAL:CG2	3:K:293:LEU:CG	2.15	1.11
3:K:181:ARG:NH2	3:K:197:LYS:HE2	1.63	1.11
2:A:216:ASN:HB3	2:A:277:SER:HB2	1.29	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:405:VAL:HG12	3:K:293:LEU:HG	1.12	1.10
3:K:84:SER:OG	3:K:84:SER:HB2	1.29	1.10
3:K:55:GLY:HA3	3:K:60:LYS:HE3	1.11	1.10
2:A:251:ASP:HB3	2:A:254:GLU:HB3	1.33	1.10
3:K:157:LYS:HB3	3:K:201:GLU:HB3	1.33	1.10
2:A:319:TYR:HB2	2:A:355:ILE:HA	1.12	1.09
3:K:162:GLU:CD	3:K:235:SER:HB2	1.73	1.09
3:K:181:ARG:NH2	3:K:197:LYS:CE	2.15	1.09
2:A:3:GLU:HG2	2:A:50:ASN:HB3	1.16	1.09
2:A:30:ILE:HA	2:A:36:MET:HB3	1.15	1.09
2:A:70:LEU:HD13	2:A:145:THR:HG23	1.25	1.09
2:A:246:GLY:HA3	2:A:356:ASN:HA	1.25	1.09
1:B:250:LEU:HD12	1:B:253:LEU:HD11	1.10	1.09
2:A:70:LEU:HG	2:A:110:ILE:HG21	1.28	1.09
2:A:242:LEU:HD23	2:A:252:LEU:HG	1.24	1.09
1:B:274:THR:HB	1:B:279:GLN:HB2	1.15	1.09
1:B:309:ARG:HB2	1:B:426:GLN:HA	1.30	1.09
2:A:405:VAL:CG1	3:K:293:LEU:HD12	1.82	1.09
3:K:53:ARG:HB3	3:K:60:LYS:HB3	1.14	1.09
2:A:34:GLY:HA3	2:A:86:LEU:HD13	1.35	1.08
3:K:16:GLY:HA3	3:K:362:LYS:HA	1.33	1.08
3:K:181:ARG:NH2	3:K:197:LYS:CG	1.95	1.08
2:A:423:GLU:OE1	3:K:57:LEU:HD13	1.35	1.08
3:K:169:PHE:HA	3:K:179:SER:HA	1.32	1.08
2:A:268:PRO:HB2	2:A:378:LEU:HB3	1.35	1.08
2:A:320:ARG:HG3	2:A:374:ALA:HB3	1.25	1.08
3:K:160:LEU:HG	3:K:171:LEU:HD12	1.20	1.08
2:A:414:GLU:HG2	3:K:344:GLU:HB3	1.11	1.07
1:B:1:MET:HE2	1:B:49:VAL:HB	1.26	1.07
1:B:350:LYS:CG	2:A:179:THR:HG22	1.81	1.07
2:A:317:LEU:HB2	2:A:353:VAL:HB	1.36	1.07
1:B:172:SER:HB2	1:B:205:GLU:HB3	1.34	1.07
1:B:323:MET:HB2	2:A:221:ARG:HG3	1.32	1.07
1:B:273:LEU:HD11	1:B:297:LYS:HD2	1.11	1.07
1:B:392:LYS:HB3	1:B:395:LEU:HD11	1.24	1.07
2:A:405:VAL:CG1	3:K:293:LEU:CD1	2.32	1.07
3:K:155:SER:HB3	3:K:203:THR:HG21	1.13	1.07
3:K:171:LEU:HD13	3:K:221:ARG:HA	1.36	1.07
1:B:54:ALA:HB3	1:B:58:LYS:HB3	1.37	1.07
1:B:212:PHE:HB2	1:B:220:PRO:HD3	1.37	1.06
3:K:159:SER:HA	3:K:172:LEU:HD13	1.18	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:187:ASP:OD1	3:K:195:ILE:CG1	2.02	1.06
2:A:31:GLN:HG2	2:A:32:PRO:HD2	1.32	1.06
2:A:410:GLY:HA3	3:K:290:GLN:HE21	1.16	1.06
3:K:84:SER:OG	3:K:84:SER:HB3	1.29	1.06
1:B:269:GLY:HA3	1:B:367:PHE:HB3	1.38	1.05
2:A:68:VAL:HG12	2:A:93:ILE:HD11	1.38	1.05
3:K:159:SER:HB2	3:K:199:LEU:HD21	1.35	1.05
3:K:246:LYS:CE	3:K:254:GLU:CD	2.24	1.05
1:B:260:PHE:CD1	2:A:406:HIS:NE2	1.89	1.05
2:A:313:MET:HE2	2:A:344:VAL:HG11	1.31	1.05
2:A:104:ALA:HB3	2:A:411:GLU:HG3	1.36	1.04
1:B:99:ASN:N	4:B:501:G2P:O3G	1.89	1.04
2:A:4:CYS:HA	2:A:132:LEU:HG	1.08	1.04
3:K:47:ARG:NE	3:K:49:GLU:OE2	1.89	1.04
1:B:323:MET:CG	2:A:221:ARG:HD2	1.86	1.04
2:A:423:GLU:OE1	3:K:57:LEU:HD12	1.54	1.04
1:B:258:VAL:HG12	1:B:263:LEU:HD12	1.37	1.04
1:B:262:ARG:HD2	3:K:297:ARG:HH12	0.90	1.04
1:B:286:VAL:HG11	1:B:325:GLU:HB3	1.37	1.04
2:A:409:VAL:HG21	3:K:293:LEU:HG	1.08	1.04
2:A:409:VAL:HG11	3:K:290:GLN:HA	1.04	1.04
2:A:224:TYR:CE1	4:A:501:G2P:N7	2.25	1.03
1:B:130:LEU:HD22	1:B:133:PHE:HE1	1.24	1.03
3:K:17:LYS:HG2	3:K:363:PRO:HG2	1.35	1.03
1:B:154:LYS:HE2	1:B:157:GLU:HB3	1.39	1.03
1:B:97:ALA:CB	1:B:143:THR:HA	1.88	1.03
1:B:274:THR:HG22	1:B:278:SER:HB2	1.39	1.03
2:A:171:ILE:HA	2:A:204:VAL:HG12	1.36	1.02
2:A:409:VAL:HG13	3:K:289:ASN:HD22	1.18	1.02
3:K:246:LYS:HE3	3:K:254:GLU:CD	1.79	1.02
1:B:246:LEU:HD12	1:B:352:ALA:HA	1.35	1.02
2:A:200:CYS:HA	2:A:266:HIS:HB3	1.02	1.02
1:B:215:LEU:HD22	1:B:217:LEU:HB2	1.38	1.02
2:A:101:ASN:HA	2:A:144:GLY:HA3	1.41	1.02
3:K:84:SER:OG	3:K:84:SER:CA	2.08	1.02
1:B:314:ALA:H	1:B:368:ILE:HB	1.22	1.01
3:K:95:MET:HG3	3:K:365:VAL:HG13	1.40	1.01
3:K:157:LYS:CE	3:K:203:THR:OG1	2.08	1.01
1:B:323:MET:CB	2:A:221:ARG:HD2	1.91	1.01
1:B:262:ARG:HD2	3:K:297:ARG:NH1	1.74	1.01
2:A:217:LEU:HB3	2:A:219:ILE:HG12	1.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:405:VAL:CG1	3:K:293:LEU:HG	1.89	1.01
1:B:149:THR:HA	1:B:191:GLN:HE22	1.25	1.01
1:B:323:MET:CB	2:A:221:ARG:CD	2.38	1.01
2:A:409:VAL:HG22	3:K:293:LEU:HD21	1.39	1.01
2:A:115:ILE:HG12	2:A:119:LEU:HD23	1.41	1.00
2:A:410:GLY:CA	3:K:290:GLN:HE21	1.74	1.00
3:K:31:ALA:HA	3:K:34:LYS:HD3	1.38	1.00
1:B:100:ASN:HB2	1:B:103:LYS:HB2	1.43	1.00
3:K:48:LYS:HE3	3:K:70:MET:HA	1.42	1.00
1:B:4:ILE:HG23	1:B:133:PHE:HA	1.39	1.00
3:K:312:ARG:HA	3:K:318:ARG:CD	1.90	1.00
1:B:273:LEU:HG	1:B:298:ASN:HA	1.39	1.00
2:A:226:ASN:HA	2:A:229:ARG:HG3	1.41	0.99
1:B:120:VAL:HG23	1:B:121:ARG:HE	1.26	0.99
3:K:17:LYS:HE3	3:K:329:ARG:HD3	1.43	0.99
1:B:97:ALA:HB3	1:B:143:THR:HA	1.43	0.99
1:B:178:THR:HG23	1:B:181:GLU:H	1.25	0.99
2:A:70:LEU:HD23	2:A:110:ILE:HG13	1.45	0.99
3:K:187:ASP:HB3	3:K:195:ILE:HD11	1.44	0.99
3:K:26:ARG:HD2	3:K:29:ASN:HD21	1.28	0.99
3:K:320:LEU:HD12	3:K:323:SER:HB2	1.44	0.99
1:B:103:LYS:HD2	1:B:401:GLU:HA	1.44	0.99
1:B:321:MET:HE3	1:B:326:VAL:HG22	1.44	0.99
2:A:319:TYR:CD1	2:A:355:ILE:HG12	1.98	0.99
2:A:5:ILE:HG12	2:A:64:ARG:HB3	1.45	0.98
3:K:77:LYS:HZ2	3:K:78:GLN:HG3	1.21	0.98
1:B:323:MET:HB2	2:A:221:ARG:HD2	1.42	0.98
1:B:323:MET:HG2	2:A:221:ARG:HD2	1.45	0.98
1:B:324:LYS:CD	2:A:220:GLU:O	2.11	0.98
1:B:316:VAL:H	1:B:366:THR:HG22	1.28	0.98
1:B:422:TYR:HA	1:B:425:TYR:CE2	1.99	0.98
2:A:383:ALA:HA	2:A:386:GLU:HG2	1.44	0.98
1:B:376:GLU:HB3	1:B:380:ARG:HH12	1.27	0.97
2:A:405:VAL:HG12	3:K:293:LEU:CG	1.94	0.97
1:B:252:LYS:CD	2:A:101:ASN:HB3	1.65	0.97
2:A:195:LEU:HD13	2:A:201:ALA:HB2	1.45	0.97
3:K:84:SER:OG	3:K:84:SER:CB	0.68	0.97
3:K:82:TYR:OH	3:K:86:VAL:HG11	1.63	0.97
1:B:262:ARG:CD	3:K:297:ARG:NH1	2.27	0.97
2:A:5:ILE:H	2:A:132:LEU:HD21	1.27	0.97
2:A:221:ARG:HD3	2:A:222:PRO:HD2	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:223:THR:HG21	3:K:235:SER:H	1.29	0.97
1:B:4:ILE:HD11	1:B:131:GLN:HB3	1.44	0.96
2:A:409:VAL:HG21	3:K:293:LEU:HD23	1.46	0.96
3:K:343:LEU:HD23	3:K:343:LEU:H	1.29	0.96
1:B:182:PRO:HB2	1:B:385:PHE:HZ	1.26	0.96
2:A:262:TYR:HB3	2:A:264:ARG:HD3	1.47	0.96
1:B:160:PRO:HB2	3:K:283:ARG:NH2	1.81	0.96
3:K:312:ARG:HA	3:K:318:ARG:HD2	1.46	0.96
2:A:224:TYR:CD2	4:A:501:G2P:O6	2.19	0.96
1:B:324:LYS:HD2	2:A:220:GLU:O	1.66	0.96
3:K:95:MET:CG	3:K:365:VAL:HG13	1.96	0.96
3:K:329:ARG:HB2	3:K:363:PRO:HB3	1.48	0.95
2:A:185:TYR:HA	2:A:395:PHE:CZ	2.01	0.95
3:K:172:LEU:HD11	3:K:199:LEU:HD11	1.46	0.95
1:B:77:ARG:HH11	1:B:82:GLY:HA2	1.29	0.95
1:B:324:LYS:N	2:A:221:ARG:HG3	1.81	0.95
2:A:154:MET:HE1	2:A:166:LYS:HE2	1.46	0.95
1:B:419:VAL:HA	1:B:422:TYR:CD2	2.00	0.95
2:A:409:VAL:HG22	3:K:293:LEU:CD2	1.92	0.95
1:B:277:GLY:HA2	1:B:280:GLN:HE21	1.28	0.95
2:A:81:GLY:HA3	2:A:83:TYR:CE2	2.01	0.95
2:A:204:VAL:HG23	2:A:209:ILE:HD12	1.48	0.95
2:A:405:VAL:CG1	3:K:293:LEU:CG	2.44	0.95
1:B:46:ARG:HB3	1:B:241:ARG:HD3	1.46	0.95
2:A:296:PHE:CE1	2:A:335:ILE:HD12	2.01	0.95
3:K:29:ASN:HB2	3:K:32:GLU:HG2	1.47	0.95
2:A:427:ALA:HB1	3:K:57:LEU:HD21	0.96	0.95
1:B:152:ILE:HG13	1:B:192:LEU:HD23	1.47	0.94
1:B:376:GLU:HA	1:B:379:LYS:HE2	1.49	0.94
2:A:288:VAL:HG12	2:A:331:ALA:HB2	1.48	0.94
2:A:296:PHE:HE1	2:A:335:ILE:HD12	1.31	0.94
1:B:33:THR:HG23	1:B:35:SER:H	1.28	0.94
3:K:26:ARG:HG2	3:K:109:THR:HG23	1.49	0.94
2:A:63:PRO:HD3	2:A:86:LEU:HD11	1.49	0.94
2:A:200:CYS:HB2	2:A:267:PHE:HB3	1.49	0.94
3:K:190:ASN:HB3	3:K:193:GLY:HA3	1.50	0.94
1:B:20:PHE:HD1	1:B:230:SER:HB2	1.32	0.94
3:K:178:VAL:HA	3:K:220:LYS:HE2	1.48	0.94
2:A:409:VAL:HG13	3:K:289:ASN:ND2	1.83	0.93
1:B:250:LEU:CD1	1:B:253:LEU:HD11	1.99	0.93
1:B:267:MET:HG3	1:B:370:ASN:HA	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:313:MET:HG3	2:A:344:VAL:HG21	1.48	0.93
1:B:215:LEU:HA	1:B:276:ARG:HB3	1.49	0.93
2:A:116:ASP:HA	2:A:119:LEU:HD21	1.49	0.93
2:A:216:ASN:CB	2:A:277:SER:HB2	1.99	0.93
2:A:277:SER:H	2:A:280:LYS:HB2	1.33	0.93
2:A:414:GLU:HG3	2:A:416:GLY:H	1.33	0.93
1:B:73:MET:HG2	1:B:92:PHE:CE1	2.04	0.93
2:A:224:TYR:CD2	4:A:501:G2P:C6	2.52	0.93
2:A:34:GLY:CA	2:A:86:LEU:HD13	1.98	0.93
1:B:252:LYS:HD3	2:A:101:ASN:HB3	0.93	0.93
1:B:284:LEU:HD13	1:B:289:LEU:HG	1.51	0.93
1:B:314:ALA:HB3	1:B:368:ILE:HG13	1.51	0.93
1:B:326:VAL:HG12	1:B:330:MET:CE	1.99	0.93
2:A:409:VAL:CG2	3:K:293:LEU:HD21	1.93	0.93
2:A:79:ARG:HD3	2:A:92:LEU:HD23	1.51	0.92
1:B:112:LEU:HD11	1:B:151:LEU:HB3	1.50	0.92
1:B:252:LYS:HD3	2:A:101:ASN:HB2	1.48	0.92
2:A:31:GLN:HB2	2:A:37:PRO:HD3	1.51	0.92
2:A:351:PHE:HD2	2:A:352:LYS:HB2	1.34	0.92
1:B:64:ILE:HD11	1:B:119:VAL:CG1	2.00	0.92
2:A:224:TYR:OH	4:A:501:G2P:C4	2.18	0.92
2:A:229:ARG:HB3	2:A:363:VAL:HG21	1.51	0.92
1:B:290:THR:HB	1:B:294:PHE:CZ	2.05	0.92
2:A:9:VAL:HB	2:A:139:HIS:CB	1.99	0.92
1:B:304:ASP:HB3	1:B:307:HIS:CG	2.05	0.92
2:A:409:VAL:HG11	3:K:293:LEU:HD23	1.49	0.92
3:K:187:ASP:HB2	3:K:189:ARG:CD	2.00	0.91
2:A:286:LEU:HD11	2:A:373:ARG:HG3	1.49	0.91
1:B:273:LEU:CD1	1:B:297:LYS:HD2	1.99	0.91
3:K:320:LEU:HG	3:K:324:LEU:CD2	2.00	0.91
1:B:321:MET:CE	1:B:326:VAL:HG22	2.01	0.91
1:B:323:MET:CB	2:A:221:ARG:HG3	1.99	0.91
1:B:186:THR:HG23	1:B:187:LEU:HD22	1.51	0.91
3:K:171:LEU:HA	3:K:220:LYS:CG	2.01	0.91
1:B:273:LEU:CG	1:B:298:ASN:HA	2.00	0.91
1:B:284:LEU:HD11	1:B:361:LEU:HD12	1.53	0.91
2:A:385:ALA:HA	2:A:388:TRP:CE2	2.06	0.91
3:K:47:ARG:HB3	3:K:49:GLU:HG3	1.51	0.91
3:K:320:LEU:HG	3:K:324:LEU:HD21	1.52	0.91
2:A:171:ILE:CD1	4:A:501:G2P:H1'	1.99	0.90
3:K:144:PHE:CD2	3:K:207:LYS:HG3	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ALA:CB	1:B:401:GLU:HB3	2.02	0.90
1:B:421:GLU:HG3	1:B:425:TYR:HE1	1.36	0.90
2:A:287:SER:HA	2:A:373:ARG:HH21	1.36	0.90
1:B:215:LEU:CD2	1:B:217:LEU:HB2	2.01	0.90
2:A:319:TYR:HB2	2:A:355:ILE:CA	1.99	0.90
2:A:153:LEU:HD12	2:A:156:ARG:HH12	1.37	0.90
3:K:82:TYR:CD2	3:K:86:VAL:CG2	2.54	0.90
3:K:157:LYS:HE3	3:K:203:THR:OG1	1.69	0.90
3:K:325:GLY:HA2	3:K:361:ASN:HA	1.54	0.90
1:B:324:LYS:HE3	2:A:221:ARG:HH11	1.35	0.90
2:A:3:GLU:HG2	2:A:50:ASN:CB	2.00	0.90
2:A:346:TRP:HE1	2:A:438:ASP:HA	1.34	0.90
2:A:409:VAL:CG1	3:K:293:LEU:HD23	2.01	0.90
3:K:159:SER:CA	3:K:172:LEU:HD13	2.02	0.90
1:B:250:LEU:HA	1:B:253:LEU:HD21	1.53	0.90
3:K:82:TYR:CE2	3:K:86:VAL:CG2	2.54	0.90
1:B:28:HIS:CD2	1:B:47:ILE:HD12	2.07	0.90
3:K:206:ASN:HD21	3:K:209:GLU:HG3	1.37	0.90
3:K:66:TYR:CE2	3:K:67:THR:O	2.25	0.89
3:K:144:PHE:CE2	3:K:207:LYS:HA	2.06	0.89
1:B:148:GLY:HA2	1:B:151:LEU:HD21	1.54	0.89
2:A:286:LEU:CD1	2:A:291:ILE:HD11	2.02	0.89
3:K:160:LEU:CG	3:K:171:LEU:HD12	2.01	0.89
2:A:9:VAL:CG1	2:A:146:GLY:HA2	2.03	0.89
2:A:41:THR:HG21	2:A:49:PHE:HB2	1.54	0.89
2:A:262:TYR:HB3	2:A:264:ARG:CD	2.01	0.89
3:K:215:GLU:CG	3:K:216:LYS:HE3	2.03	0.89
1:B:9:ALA:HB1	1:B:147:MET:CE	2.02	0.89
1:B:102:ALA:HB3	1:B:401:GLU:HB3	1.51	0.89
2:A:200:CYS:CA	2:A:266:HIS:HB3	1.98	0.89
2:A:286:LEU:CD2	2:A:371:VAL:HB	2.02	0.89
2:A:344:VAL:HB	2:A:346:TRP:CD1	2.08	0.89
3:K:55:GLY:CA	3:K:60:LYS:HE3	2.00	0.89
1:B:103:LYS:HD2	1:B:401:GLU:CA	2.02	0.89
2:A:278:ALA:CA	2:A:368:LEU:HA	2.01	0.89
2:A:318:LEU:HD22	2:A:319:TYR:H	1.37	0.89
2:A:351:PHE:CD2	2:A:352:LYS:HB2	2.08	0.89
3:K:82:TYR:CZ	3:K:86:VAL:CG1	2.55	0.89
3:K:53:ARG:CB	3:K:60:LYS:HB3	2.02	0.89
3:K:223:THR:HB	3:K:234:ARG:HB2	1.53	0.89
1:B:253:LEU:HB2	1:B:257:MET:CE	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:384:ILE:HD11	2:A:432:TYR:HE2	1.36	0.88
2:A:405:VAL:HG11	3:K:293:LEU:HD12	0.91	0.88
2:A:189:LEU:HD13	2:A:418:PHE:CD2	2.07	0.88
3:K:109:THR:CG2	3:K:335:THR:HB	2.03	0.88
3:K:170:ASP:HB2	3:K:180:GLU:HB2	1.54	0.88
3:K:181:ARG:CZ	3:K:197:LYS:HG3	2.02	0.88
1:B:392:LYS:CB	1:B:395:LEU:HD11	2.03	0.88
2:A:259:LEU:HD13	2:A:378:LEU:HD12	1.53	0.88
3:K:187:ASP:HB3	3:K:195:ILE:CD1	2.04	0.88
1:B:9:ALA:HB1	1:B:147:MET:HE2	1.54	0.88
1:B:51:TYR:HD2	1:B:59:TYR:HB3	1.38	0.88
2:A:276:ILE:HG13	2:A:371:VAL:HG11	1.53	0.88
1:B:324:LYS:HE3	2:A:222:PRO:CD	2.02	0.88
2:A:16:ILE:HA	2:A:228:ASN:HD22	1.39	0.88
3:K:181:ARG:CZ	3:K:197:LYS:HE2	2.02	0.88
1:B:20:PHE:HA	1:B:230:SER:HB2	1.53	0.88
2:A:4:CYS:HA	2:A:132:LEU:CG	2.01	0.88
2:A:107:HIS:HB2	2:A:148:GLY:HA2	1.56	0.88
3:K:53:ARG:HB3	3:K:60:LYS:CB	2.01	0.88
1:B:162:ARG:CZ	1:B:162:ARG:HA	2.03	0.88
2:A:216:ASN:HB3	2:A:280:LYS:HD2	1.55	0.88
1:B:324:LYS:HG3	2:A:220:GLU:O	1.73	0.88
1:B:371:SER:HB2	1:B:374:ILE:HG22	1.55	0.88
2:A:3:GLU:CG	2:A:50:ASN:HB3	2.04	0.88
3:K:169:PHE:CD1	3:K:179:SER:HB2	2.09	0.88
1:B:324:LYS:HG3	2:A:220:GLU:C	1.93	0.88
2:A:286:LEU:HD23	2:A:371:VAL:HB	1.56	0.88
2:A:409:VAL:CG1	3:K:290:GLN:CA	2.40	0.88
2:A:237:SER:HA	2:A:320:ARG:HH11	1.37	0.87
3:K:91:ASP:O	3:K:95:MET:SD	2.32	0.87
2:A:269:LEU:HD23	2:A:384:ILE:HD12	1.56	0.87
3:K:95:MET:HE2	3:K:97:TYR:CG	2.08	0.87
2:A:1:MET:HG2	2:A:47:ASP:N	1.89	0.87
3:K:327:ARG:H	3:K:327:ARG:HH21	1.21	0.87
2:A:232:SER:HB3	2:A:363:VAL:HG11	1.56	0.87
2:A:272:TYR:HE1	2:A:374:ALA:HB1	1.37	0.87
1:B:339:SER:HA	1:B:429:THR:CG2	2.04	0.87
2:A:102:ASN:HB2	2:A:407:TRP:HE1	1.39	0.87
3:K:94:ILE:O	3:K:245:MET:HE3	1.73	0.87
1:B:371:SER:HB2	1:B:374:ILE:CG2	2.04	0.87
2:A:103:TYR:HB2	2:A:147:SER:HB3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:181:VAL:HG11	2:A:404:PHE:HE1	1.38	0.87
1:B:216:LYS:HE2	1:B:277:GLY:HA3	1.57	0.87
2:A:68:VAL:HG21	2:A:149:PHE:CE1	2.08	0.87
2:A:70:LEU:CD2	2:A:110:ILE:HG13	2.04	0.87
3:K:160:LEU:H	3:K:172:LEU:HD22	1.39	0.87
3:K:269:SER:HB3	3:K:288:ILE:HD11	1.56	0.87
3:K:298:VAL:HG23	3:K:310:PRO:HD2	1.54	0.87
2:A:275:VAL:HB	2:A:300:ASN:HD22	1.40	0.87
1:B:244:GLY:HA2	1:B:355:ASP:N	1.90	0.86
3:K:16:GLY:HA3	3:K:362:LYS:CA	2.05	0.86
2:A:282:TYR:CE1	2:A:369:ALA:HB2	2.10	0.86
2:A:414:GLU:HG2	3:K:344:GLU:CB	2.01	0.86
1:B:1:MET:HE2	1:B:49:VAL:CB	2.04	0.86
1:B:45:GLU:HG3	1:B:46:ARG:HE	1.37	0.86
1:B:253:LEU:HB2	1:B:257:MET:HE1	1.57	0.86
1:B:142:GLY:HA2	1:B:184:ASN:CG	1.96	0.86
1:B:286:VAL:HB	1:B:287:PRO:HD3	1.58	0.86
2:A:209:ILE:HG12	2:A:302:MET:HB2	1.57	0.86
2:A:246:GLY:HA2	2:A:357:TYR:H	1.41	0.86
1:B:376:GLU:CA	1:B:379:LYS:HE2	2.05	0.86
2:A:107:HIS:CD2	2:A:152:LEU:HB2	2.10	0.86
2:A:172:TYR:CB	2:A:203:MET:HB2	2.05	0.86
3:K:181:ARG:HB2	3:K:181:ARG:HH11	1.40	0.86
2:A:264:ARG:HD3	2:A:264:ARG:H	1.39	0.86
2:A:54:SER:HB3	2:A:64:ARG:HH11	1.40	0.86
2:A:233:GLN:HE21	2:A:234:ILE:HG22	1.41	0.86
3:K:206:ASN:ND2	3:K:209:GLU:HG3	1.91	0.86
2:A:320:ARG:HB2	2:A:374:ALA:H	1.37	0.85
2:A:409:VAL:HG11	3:K:290:GLN:N	1.91	0.85
1:B:24:ILE:HA	1:B:27:GLU:HG2	1.58	0.85
1:B:130:LEU:HD22	1:B:133:PHE:CE1	2.10	0.85
1:B:242:PHE:CD2	1:B:356:ILE:HD11	2.10	0.85
1:B:314:ALA:N	1:B:368:ILE:HB	1.92	0.85
2:A:166:LYS:CD	2:A:198:SER:HA	2.04	0.85
1:B:116:VAL:HG23	1:B:117:LEU:HD22	1.58	0.85
2:A:280:LYS:HA	2:A:283:HIS:CD2	2.11	0.85
3:K:26:ARG:HH12	3:K:28:PHE:HA	1.41	0.85
3:K:109:THR:HG21	3:K:336:ILE:N	1.92	0.85
3:K:162:GLU:OE2	3:K:221:ARG:NH1	2.10	0.85
1:B:1:MET:HG3	1:B:127:CYS:HB2	1.56	0.85
2:A:279:GLU:HA	2:A:282:TYR:CD2	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:385:ALA:HA	2:A:388:TRP:CD2	2.11	0.85
3:K:26:ARG:CZ	3:K:338:PRO:HD2	2.06	0.85
3:K:37:ALA:HA	3:K:341:LEU:HD11	1.57	0.85
3:K:55:GLY:HA2	3:K:60:LYS:HA	1.58	0.85
3:K:160:LEU:N	3:K:172:LEU:HB3	1.92	0.85
1:B:260:PHE:CD1	2:A:404:PHE:HD2	1.90	0.85
2:A:6:SER:HB3	2:A:138:PHE:CE1	2.11	0.85
3:K:17:LYS:HD3	3:K:363:PRO:HB2	1.58	0.85
1:B:152:ILE:HD13	1:B:155:ILE:HD11	1.58	0.85
1:B:170:VAL:CG2	1:B:203:ASP:HA	2.05	0.85
1:B:215:LEU:HA	1:B:276:ARG:CB	2.06	0.85
2:A:4:CYS:H	2:A:51:THR:HA	1.42	0.85
2:A:313:MET:CE	2:A:344:VAL:HG11	2.06	0.85
1:B:179:VAL:HG21	1:B:388:MET:HG3	1.56	0.84
1:B:377:LEU:HA	1:B:380:ARG:NE	1.92	0.84
1:B:398:TYR:HA	1:B:401:GLU:HG3	1.59	0.84
2:A:101:ASN:HA	2:A:144:GLY:CA	2.07	0.84
3:K:92:GLU:OE1	3:K:329:ARG:HG2	1.76	0.84
1:B:182:PRO:HB2	1:B:385:PHE:CZ	2.12	0.84
1:B:324:LYS:CE	2:A:221:ARG:HH11	1.91	0.84
1:B:330:MET:HG3	1:B:331:LEU:HD13	1.59	0.84
1:B:308:GLY:HA2	1:B:372:THR:CB	2.07	0.84
3:K:170:ASP:HB2	3:K:180:GLU:CB	2.06	0.84
1:B:12:CYS:O	1:B:16:ILE:HG13	1.76	0.84
2:A:12:ALA:HA	2:A:15:GLN:NE2	1.92	0.84
1:B:21:TRP:CE3	1:B:21:TRP:HA	2.10	0.84
2:A:48:SER:HB2	2:A:243:ARG:CD	2.06	0.84
2:A:310:GLY:HA3	2:A:381:THR:HB	1.56	0.84
3:K:162:GLU:OE2	3:K:223:THR:HG23	1.77	0.84
1:B:274:THR:HB	1:B:279:GLN:CB	2.04	0.84
1:B:286:VAL:HG11	1:B:325:GLU:CB	2.07	0.84
3:K:269:SER:HB3	3:K:288:ILE:CD1	2.07	0.84
1:B:292:GLN:O	1:B:298:ASN:HB2	1.78	0.84
3:K:17:LYS:CG	3:K:363:PRO:HG2	2.07	0.84
1:B:12:CYS:SG	1:B:138:SER:HB3	2.17	0.84
2:A:320:ARG:CG	2:A:374:ALA:HB3	2.07	0.84
1:B:350:LYS:HG3	2:A:179:THR:HG22	1.57	0.84
2:A:24:TYR:HB3	2:A:52:PHE:CD1	2.13	0.84
3:K:224:ALA:HB3	3:K:234:ARG:HG2	1.59	0.84
1:B:293:MET:HE1	1:B:367:PHE:HA	1.58	0.83
2:A:23:LEU:HD12	2:A:363:VAL:CA	2.06	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:36:MET:HE3	2:A:38:SER:HB3	1.59	0.83
2:A:81:GLY:HA3	2:A:83:TYR:CZ	2.12	0.83
2:A:163:LYS:HE3	2:A:164:LYS:H	1.43	0.83
3:K:234:ARG:NH2	3:K:284:GLU:HG3	1.92	0.83
1:B:17:GLY:N	1:B:136:THR:HG21	1.93	0.83
2:A:71:GLU:HB3	2:A:98:ASP:CG	1.99	0.83
2:A:215:ARG:NH1	2:A:216:ASN:HA	1.93	0.83
2:A:216:ASN:CB	2:A:280:LYS:HD2	2.08	0.83
1:B:21:TRP:CD1	1:B:63:ALA:HB2	2.13	0.83
3:K:162:GLU:CD	3:K:235:SER:CB	2.44	0.83
3:K:269:SER:HB3	3:K:288:ILE:CG1	2.09	0.83
1:B:324:LYS:CG	2:A:220:GLU:O	2.27	0.83
3:K:160:LEU:HG	3:K:171:LEU:CD1	2.07	0.83
3:K:168:LEU:HD12	3:K:182:LEU:HB3	1.59	0.83
1:B:64:ILE:HD12	1:B:119:VAL:HG21	1.61	0.83
1:B:260:PHE:CD1	2:A:404:PHE:CD2	2.62	0.83
2:A:70:LEU:HD13	2:A:145:THR:CG2	2.07	0.83
2:A:125:LEU:O	2:A:128:GLN:HG3	1.78	0.83
2:A:434:GLU:O	2:A:437:VAL:HG22	1.79	0.83
3:K:180:GLU:HG3	3:K:199:LEU:HD13	1.60	0.83
3:K:321:GLN:HA	3:K:324:LEU:HD23	1.59	0.83
1:B:42:LEU:HA	1:B:45:GLU:OE1	1.79	0.83
3:K:94:ILE:HG12	3:K:147:LEU:HD21	1.61	0.83
2:A:387:ALA:HA	2:A:390:ARG:CD	2.09	0.83
3:K:26:ARG:HD2	3:K:29:ASN:ND2	1.94	0.83
3:K:140:LEU:HD13	3:K:210:VAL:CG1	2.09	0.83
1:B:10:GLY:H	1:B:147:MET:HE1	1.43	0.82
3:K:168:LEU:HD13	3:K:182:LEU:HG	1.60	0.82
1:B:325:GLU:O	1:B:328:GLU:HG3	1.80	0.82
2:A:256:GLN:HA	2:A:259:LEU:CD1	2.08	0.82
2:A:385:ALA:HB1	2:A:429:GLU:OE1	1.79	0.82
3:K:322:ASP:O	3:K:326:GLY:HA3	1.79	0.82
1:B:273:LEU:HD22	1:B:274:THR:N	1.93	0.82
1:B:327:ASP:HA	1:B:330:MET:SD	2.18	0.82
2:A:19:ALA:HB1	2:A:229:ARG:HH22	1.43	0.82
2:A:273:ALA:HB3	2:A:375:VAL:CG2	2.09	0.82
2:A:286:LEU:CD1	2:A:373:ARG:HG3	2.07	0.82
2:A:317:LEU:HB2	2:A:353:VAL:CB	2.09	0.82
3:K:72:PHE:CD1	3:K:76:THR:HG21	2.14	0.82
1:B:139:LEU:HD11	1:B:171:PRO:HD3	1.59	0.82
2:A:23:LEU:HA	2:A:364:PRO:CG	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:117:LEU:O	2:A:121:ARG:HG3	1.78	0.82
2:A:409:VAL:CG1	3:K:290:GLN:N	2.42	0.82
1:B:139:LEU:CD1	1:B:185:ALA:HB1	2.10	0.82
1:B:379:LYS:HD3	1:B:419:VAL:HB	1.60	0.82
2:A:28:HIS:CE1	2:A:49:PHE:HA	2.15	0.82
2:A:70:LEU:CD1	2:A:145:THR:HG23	2.08	0.82
3:K:55:GLY:CA	3:K:60:LYS:HA	2.10	0.82
1:B:23:VAL:HA	1:B:26:ASP:OD2	1.79	0.82
1:B:51:TYR:CE1	1:B:61:PRO:HA	2.14	0.82
1:B:222:TYR:O	1:B:225:LEU:HG	1.79	0.82
2:A:286:LEU:HB2	2:A:291:ILE:CG1	2.08	0.82
2:A:320:ARG:CD	2:A:360:PRO:HA	2.10	0.82
2:A:383:ALA:CA	2:A:386:GLU:HG2	2.10	0.82
3:K:55:GLY:HA3	3:K:60:LYS:CE	2.05	0.82
2:A:153:LEU:HD12	2:A:156:ARG:NH1	1.95	0.82
2:A:277:SER:CB	2:A:280:LYS:HG3	2.10	0.82
1:B:97:ALA:HB2	1:B:143:THR:HG23	1.61	0.82
1:B:100:ASN:HB3	1:B:401:GLU:OE2	1.79	0.82
1:B:204:ASN:O	1:B:207:LEU:HG	1.80	0.82
1:B:318:ARG:HB3	1:B:358:PRO:HD3	1.60	0.82
2:A:181:VAL:HG11	2:A:404:PHE:CE1	2.14	0.82
2:A:189:LEU:HD22	2:A:418:PHE:HE2	1.42	0.82
2:A:247:ALA:HB3	2:A:355:ILE:CB	2.05	0.82
2:A:251:ASP:CB	2:A:254:GLU:HB3	2.09	0.82
3:K:41:VAL:CG2	3:K:338:PRO:HA	2.10	0.82
2:A:64:ARG:HH21	2:A:64:ARG:HA	1.45	0.82
3:K:82:TYR:CE2	3:K:86:VAL:HG11	2.15	0.82
3:K:171:LEU:HB3	3:K:220:LYS:HB3	1.60	0.82
1:B:152:ILE:HG13	1:B:192:LEU:CD2	2.09	0.82
1:B:389:PHE:O	1:B:392:LYS:HG3	1.79	0.82
1:B:392:LYS:HB3	1:B:395:LEU:CD1	2.08	0.82
2:A:275:VAL:HB	2:A:300:ASN:HA	1.62	0.82
2:A:409:VAL:CG2	3:K:293:LEU:HD23	1.98	0.82
1:B:67:ASP:OD2	1:B:73:MET:HB3	1.79	0.81
1:B:422:TYR:HA	1:B:425:TYR:CD2	2.15	0.81
2:A:232:SER:HB3	2:A:363:VAL:CG1	2.09	0.81
1:B:314:ALA:HB3	1:B:368:ILE:CG1	2.09	0.81
2:A:75:ILE:HG23	2:A:92:LEU:HD11	1.60	0.81
2:A:195:LEU:HD13	2:A:201:ALA:CB	2.10	0.81
3:K:329:ARG:CB	3:K:363:PRO:HB3	2.09	0.81
1:B:101:TRP:CZ2	1:B:403:MET:HG3	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:MET:O	1:B:419:VAL:HG13	1.79	0.81
2:A:117:LEU:HD22	2:A:117:LEU:H	1.44	0.81
2:A:255:PHE:CZ	2:A:352:LYS:HB3	2.15	0.81
2:A:307:PRO:HD2	2:A:308:ARG:CZ	2.10	0.81
1:B:323:MET:HE1	1:B:326:VAL:HG21	1.63	0.81
2:A:50:ASN:O	2:A:64:ARG:HD3	1.80	0.81
2:A:153:LEU:HD11	2:A:157:LEU:HD11	1.62	0.81
2:A:405:VAL:HG12	2:A:409:VAL:CG2	2.11	0.81
2:A:3:GLU:HA	2:A:51:THR:HA	1.61	0.81
2:A:107:HIS:HB2	2:A:148:GLY:CA	2.09	0.81
2:A:135:PHE:CE1	2:A:166:LYS:HA	2.16	0.81
2:A:154:MET:HE1	2:A:166:LYS:CE	2.09	0.81
2:A:242:LEU:HD23	2:A:252:LEU:CG	2.10	0.81
2:A:319:TYR:HB3	2:A:355:ILE:HG23	1.61	0.81
3:K:157:LYS:HB3	3:K:201:GLU:CB	2.09	0.81
3:K:227:LEU:HG	3:K:228:MET:HE3	1.60	0.81
1:B:65:LEU:HD13	1:B:90:PHE:HB3	1.63	0.81
1:B:260:PHE:HD1	2:A:404:PHE:CD2	1.95	0.81
1:B:324:LYS:HE3	2:A:222:PRO:HD2	1.62	0.81
2:A:41:THR:CG2	2:A:49:PHE:HB2	2.11	0.81
2:A:310:GLY:HA3	2:A:381:THR:CG2	2.11	0.81
2:A:279:GLU:HB3	2:A:283:HIS:CE1	2.15	0.81
3:K:246:LYS:CE	3:K:254:GLU:OE2	2.27	0.81
2:A:204:VAL:CG2	2:A:209:ILE:HD12	2.11	0.81
2:A:256:GLN:HA	2:A:259:LEU:HG	1.61	0.81
2:A:320:ARG:HG3	2:A:374:ALA:CB	2.09	0.81
3:K:181:ARG:NH2	3:K:197:LYS:CD	2.43	0.81
1:B:362:LYS:HA	1:B:362:LYS:HE3	1.61	0.81
2:A:45:GLY:HA2	2:A:49:PHE:CD2	2.15	0.81
2:A:84:ARG:HH11	2:A:85:GLN:HB3	1.45	0.81
2:A:205:ASP:CB	2:A:208:ALA:HB3	2.10	0.81
2:A:268:PRO:CB	2:A:378:LEU:HB3	2.09	0.81
2:A:318:LEU:HD11	2:A:320:ARG:HG2	1.62	0.81
2:A:414:GLU:O	2:A:417:GLU:HG2	1.80	0.81
3:K:47:ARG:NH1	3:K:47:ARG:HA	1.96	0.81
3:K:68:PHE:HB2	3:K:71:VAL:CG2	2.11	0.81
1:B:154:LYS:CE	1:B:157:GLU:HB3	2.11	0.81
1:B:260:PHE:CD1	2:A:406:HIS:CD2	2.67	0.81
2:A:48:SER:CB	2:A:243:ARG:HD3	2.08	0.81
2:A:81:GLY:O	2:A:84:ARG:HB3	1.81	0.81
2:A:212:ILE:O	2:A:215:ARG:HG3	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:344:VAL:HG23	2:A:347:CYS:H	1.46	0.81
3:K:77:LYS:NZ	3:K:78:GLN:HG3	1.95	0.81
3:K:304:GLU:CG	3:K:306:THR:HB	2.10	0.81
1:B:140:GLY:HA2	1:B:185:ALA:HB2	1.63	0.80
1:B:324:LYS:H	2:A:221:ARG:HG3	1.44	0.80
1:B:326:VAL:CG1	1:B:330:MET:HE1	2.07	0.80
1:B:421:GLU:HG3	1:B:425:TYR:CE1	2.14	0.80
2:A:5:ILE:HG23	2:A:65:ALA:HA	1.62	0.80
3:K:144:PHE:CD2	3:K:207:LYS:HA	2.16	0.80
3:K:199:LEU:HD12	3:K:200:GLU:H	1.44	0.80
1:B:278:SER:HA	1:B:282:ARG:HH11	1.45	0.80
2:A:392:ASP:OD2	2:A:422:ARG:HD3	1.80	0.80
3:K:258:ILE:O	3:K:368:LYS:HE2	1.81	0.80
3:K:212:GLN:O	3:K:216:LYS:HG2	1.82	0.80
1:B:280:GLN:HG3	1:B:281:TYR:CD1	2.16	0.80
1:B:285:THR:CG2	1:B:288:GLU:HB2	2.11	0.80
1:B:372:THR:HA	1:B:375:GLN:OE1	1.80	0.80
1:B:101:TRP:HA	1:B:146:GLY:CA	2.11	0.80
1:B:144:GLY:HA2	1:B:147:MET:SD	2.22	0.80
1:B:152:ILE:HA	1:B:155:ILE:HD11	1.63	0.80
1:B:214:THR:HB	1:B:276:ARG:N	1.96	0.80
1:B:269:GLY:CA	1:B:367:PHE:HB3	2.10	0.80
1:B:342:VAL:HA	1:B:429:THR:C	2.02	0.80
2:A:102:ASN:HB3	2:A:105:ARG:HB3	1.63	0.80
2:A:313:MET:HA	2:A:344:VAL:CG2	2.11	0.80
3:K:171:LEU:HD13	3:K:221:ARG:CA	2.11	0.80
1:B:258:VAL:HG12	1:B:263:LEU:CD1	2.11	0.80
1:B:258:VAL:HG21	1:B:261:PRO:HA	1.64	0.80
2:A:7:ILE:CG2	2:A:137:VAL:HA	2.12	0.80
2:A:224:TYR:CE1	4:A:501:G2P:C5	2.64	0.80
2:A:277:SER:HB3	2:A:280:LYS:HG3	1.62	0.80
3:K:177:ASP:HB2	3:K:179:SER:O	1.81	0.80
3:K:180:GLU:O	3:K:182:LEU:HD22	1.81	0.80
1:B:99:ASN:CA	1:B:142:GLY:HA3	2.12	0.80
1:B:345:ILE:HG12	1:B:346:PRO:O	1.81	0.80
2:A:156:ARG:NH1	2:A:156:ARG:HB3	1.96	0.80
2:A:237:SER:HA	2:A:320:ARG:NH1	1.96	0.80
3:K:29:ASN:CB	3:K:32:GLU:HG2	2.12	0.80
1:B:242:PHE:CE2	1:B:356:ILE:HD11	2.16	0.80
1:B:322:SER:HB3	1:B:325:GLU:HG3	1.63	0.80
2:A:229:ARG:HA	2:A:229:ARG:CZ	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:405:VAL:O	2:A:409:VAL:HG23	1.82	0.80
1:B:51:TYR:CD2	1:B:59:TYR:HB3	2.16	0.80
1:B:272:PRO:HB2	1:B:279:GLN:HE22	1.44	0.80
1:B:276:ARG:HG3	1:B:277:GLY:N	1.95	0.80
2:A:35:GLN:HB2	2:A:60:LYS:HE2	1.63	0.80
2:A:269:LEU:HD23	2:A:384:ILE:CD1	2.12	0.80
2:A:215:ARG:HH11	2:A:216:ASN:HD22	1.27	0.79
3:K:140:LEU:HD13	3:K:210:VAL:HG12	1.61	0.79
3:K:320:LEU:CD1	3:K:323:SER:HB2	2.12	0.79
2:A:46:ASP:OD1	2:A:48:SER:HB3	1.83	0.79
2:A:63:PRO:HG3	2:A:86:LEU:HD21	1.64	0.79
2:A:224:TYR:CZ	4:A:501:G2P:C4	2.65	0.79
2:A:431:ASP:HA	2:A:434:GLU:OE2	1.81	0.79
1:B:276:ARG:HD2	1:B:280:GLN:NE2	1.98	0.79
2:A:104:ALA:CB	2:A:411:GLU:HG3	2.13	0.79
2:A:224:TYR:CE2	4:A:501:G2P:C5	2.56	0.79
2:A:231:ILE:O	2:A:234:ILE:HG13	1.81	0.79
2:A:242:LEU:CD2	2:A:252:LEU:HG	2.09	0.79
2:A:121:ARG:O	2:A:124:LYS:HG3	1.83	0.79
3:K:274:ARG:NH1	3:K:274:ARG:HA	1.96	0.79
3:K:281:ARG:O	3:K:284:GLU:HG2	1.82	0.79
1:B:45:GLU:HB2	1:B:46:ARG:HH21	1.46	0.79
1:B:102:ALA:HB3	1:B:401:GLU:CD	2.03	0.79
2:A:192:HIS:CE1	2:A:421:ALA:HB2	2.17	0.79
2:A:217:LEU:HB3	2:A:219:ILE:CG1	2.12	0.79
2:A:278:ALA:HB1	2:A:282:TYR:OH	1.82	0.79
2:A:288:VAL:HG21	2:A:327:ASP:HB3	1.64	0.79
1:B:178:THR:HG23	1:B:181:GLU:N	1.98	0.79
1:B:318:ARG:HG2	1:B:354:CYS:HB2	1.65	0.79
2:A:8:HIS:CD2	2:A:17:GLY:HA3	2.18	0.79
3:K:28:PHE:HB3	3:K:33:ARG:NE	1.98	0.79
3:K:31:ALA:HB1	3:K:34:LYS:HE2	1.65	0.79
1:B:46:ARG:O	1:B:49:VAL:HG22	1.83	0.79
1:B:151:LEU:HD12	1:B:152:ILE:N	1.98	0.79
2:A:31:GLN:HB3	2:A:33:ASP:OD2	1.83	0.79
2:A:45:GLY:HA2	2:A:49:PHE:HD2	1.48	0.79
2:A:79:ARG:CZ	2:A:92:LEU:HG	2.13	0.79
2:A:311:LYS:HA	2:A:342:GLN:CG	2.11	0.79
3:K:40:ILE:HG12	3:K:338:PRO:O	1.80	0.79
1:B:321:MET:HG2	1:B:322:SER:O	1.83	0.79
1:B:321:MET:CG	1:B:325:GLU:HB2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:140:SER:HA	2:A:171:ILE:HG22	1.63	0.79
2:A:240:ALA:HA	2:A:243:ARG:HG2	1.62	0.79
3:K:95:MET:HE1	3:K:97:TYR:HB2	1.62	0.79
1:B:117:LEU:O	1:B:121:ARG:HG2	1.82	0.79
1:B:309:ARG:CB	1:B:426:GLN:HA	2.10	0.79
1:B:316:VAL:N	1:B:366:THR:HG22	1.97	0.79
1:B:416:ASN:O	1:B:419:VAL:HG22	1.83	0.79
2:A:246:GLY:CA	2:A:356:ASN:HA	2.10	0.79
2:A:287:SER:CB	2:A:290:GLU:HG3	2.13	0.79
1:B:215:LEU:O	1:B:276:ARG:HG2	1.83	0.79
2:A:8:HIS:NE2	2:A:17:GLY:HA3	1.98	0.79
2:A:221:ARG:HD3	2:A:222:PRO:CD	2.12	0.79
3:K:233:SER:OG	3:K:267:ALA:HA	1.82	0.79
2:A:30:ILE:CA	2:A:36:MET:HB3	2.07	0.78
2:A:213:CYS:O	2:A:217:LEU:HG	1.83	0.78
2:A:216:ASN:CG	2:A:280:LYS:HD2	2.04	0.78
3:K:95:MET:HE2	3:K:97:TYR:CD2	2.18	0.78
1:B:156:ARG:HH21	1:B:157:GLU:HA	1.47	0.78
1:B:341:PHE:CE2	1:B:346:PRO:HA	2.17	0.78
1:B:376:GLU:O	1:B:379:LYS:HG2	1.82	0.78
2:A:70:LEU:HD22	2:A:99:ALA:HB2	1.65	0.78
2:A:344:VAL:HB	2:A:346:TRP:HD1	1.43	0.78
3:K:158:VAL:C	3:K:201:GLU:HG2	2.03	0.78
3:K:173:ASN:HB3	3:K:175:SER:OG	1.82	0.78
1:B:103:LYS:NZ	1:B:103:LYS:HA	1.98	0.78
1:B:139:LEU:HD21	1:B:170:VAL:HG12	1.66	0.78
2:A:88:HIS:HB2	2:A:91:GLN:HE22	1.48	0.78
2:A:320:ARG:NE	2:A:360:PRO:HA	1.99	0.78
2:A:431:ASP:HA	2:A:434:GLU:CD	2.04	0.78
3:K:339:ALA:HB1	3:K:341:LEU:HD13	1.62	0.78
1:B:293:MET:HA	1:B:298:ASN:CG	2.03	0.78
2:A:184:PRO:O	2:A:188:ILE:HD13	1.82	0.78
3:K:155:SER:CB	3:K:203:THR:HG21	2.05	0.78
1:B:33:THR:HG23	1:B:35:SER:N	1.97	0.78
1:B:103:LYS:HD2	1:B:401:GLU:HG2	1.65	0.78
1:B:246:LEU:HD12	1:B:352:ALA:CA	2.12	0.78
1:B:293:MET:HE3	1:B:367:PHE:HB2	1.64	0.78
2:A:30:ILE:HD11	2:A:34:GLY:O	1.83	0.78
2:A:56:THR:HG22	2:A:57:GLY:H	1.46	0.78
2:A:243:ARG:HD2	2:A:244:PHE:CD2	2.18	0.78
2:A:388:TRP:HB2	2:A:425:MET:CE	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:411:GLU:HB2	2:A:413:MET:HG2	1.64	0.78
3:K:190:ASN:HB3	3:K:193:GLY:CA	2.13	0.78
1:B:120:VAL:HG23	1:B:121:ARG:NE	1.97	0.78
2:A:320:ARG:NH1	2:A:361:THR:HG23	1.99	0.78
2:A:383:ALA:HA	2:A:386:GLU:CG	2.13	0.78
3:K:311:TYR:HE1	3:K:324:LEU:HG	1.47	0.78
1:B:103:LYS:HG2	1:B:401:GLU:OE2	1.84	0.78
1:B:172:SER:CB	1:B:205:GLU:HB3	2.13	0.78
2:A:320:ARG:HH12	2:A:361:THR:HG23	1.48	0.78
3:K:144:PHE:HB2	3:K:207:LYS:HZ3	1.49	0.78
3:K:257:LYS:HA	3:K:368:LYS:HD3	1.65	0.78
2:A:70:LEU:HG	2:A:110:ILE:CG2	2.13	0.78
2:A:320:ARG:HB2	2:A:360:PRO:HG3	1.64	0.78
2:A:320:ARG:HD3	2:A:360:PRO:HA	1.66	0.78
1:B:211:CYS:SG	1:B:220:PRO:HB3	2.24	0.78
1:B:376:GLU:HB3	1:B:380:ARG:NH1	1.98	0.78
2:A:8:HIS:HB3	2:A:13:GLY:C	2.03	0.78
2:A:328:VAL:O	2:A:332:ILE:HG12	1.82	0.78
2:A:339:ARG:HG3	2:A:340:SER:N	1.97	0.78
3:K:227:LEU:HD23	3:K:227:LEU:H	1.48	0.78
1:B:139:LEU:HD23	1:B:168:SER:HB2	1.65	0.78
1:B:316:VAL:O	1:B:365:ALA:HA	1.82	0.78
2:A:84:ARG:NH1	2:A:85:GLN:HB3	1.99	0.78
2:A:223:THR:HG22	2:A:225:THR:H	1.49	0.78
2:A:9:VAL:HG11	2:A:146:GLY:HA2	1.63	0.77
2:A:171:ILE:HA	2:A:204:VAL:CG1	2.14	0.77
2:A:185:TYR:CZ	2:A:398:MET:HB3	2.18	0.77
2:A:288:VAL:HG21	2:A:327:ASP:CB	2.14	0.77
3:K:55:GLY:HA2	3:K:59:ASP:O	1.83	0.77
2:A:208:ALA:O	2:A:212:ILE:HG12	1.84	0.77
2:A:224:TYR:CE2	4:A:501:G2P:N1	2.52	0.77
2:A:286:LEU:HB2	2:A:291:ILE:HG12	1.65	0.77
2:A:287:SER:OG	2:A:290:GLU:HG3	1.82	0.77
2:A:306:ASP:HB2	2:A:309:HIS:CG	2.19	0.77
2:A:310:GLY:HA3	2:A:381:THR:CB	2.13	0.77
1:B:43:GLN:O	1:B:47:ILE:HG12	1.82	0.77
1:B:154:LYS:HE2	1:B:154:LYS:HA	1.67	0.77
1:B:208:TYR:CE2	1:B:220:PRO:HB2	2.19	0.77
2:A:56:THR:C	2:A:58:ALA:HA	2.03	0.77
3:K:192:ARG:HB2	3:K:322:ASP:OD1	1.84	0.77
3:K:354:HIS:O	3:K:357:LYS:HG2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:CYS:SG	1:B:16:ILE:HD11	2.24	0.77
1:B:46:ARG:HA	1:B:46:ARG:CZ	2.15	0.77
1:B:148:GLY:HA2	1:B:151:LEU:CD2	2.14	0.77
2:A:176:GLN:HE21	2:A:207:GLU:HA	1.48	0.77
2:A:247:ALA:HA	2:A:357:TYR:CE1	2.20	0.77
3:K:246:LYS:HE3	3:K:254:GLU:OE1	1.83	0.77
1:B:15:GLN:O	1:B:19:LYS:HG2	1.85	0.77
1:B:70:PRO:HB3	1:B:92:PHE:HE2	1.50	0.77
1:B:314:ALA:O	1:B:368:ILE:HG12	1.84	0.77
2:A:69:ASP:OD2	2:A:71:GLU:HG2	1.84	0.77
2:A:256:GLN:HA	2:A:259:LEU:CG	2.15	0.77
2:A:313:MET:HE2	2:A:344:VAL:CG1	2.13	0.77
3:K:274:ARG:HA	3:K:274:ARG:CZ	2.14	0.77
1:B:41:ASP:CA	1:B:44:LEU:HD23	2.07	0.77
1:B:159:TYR:HB2	1:B:162:ARG:HG2	1.66	0.77
1:B:375:GLN:OE1	1:B:422:TYR:HB3	1.83	0.77
2:A:278:ALA:HA	2:A:368:LEU:CA	2.11	0.77
1:B:139:LEU:HD12	1:B:185:ALA:HB1	1.65	0.77
1:B:190:HIS:CE1	1:B:411:ALA:HA	2.20	0.77
1:B:213:ARG:NH1	1:B:213:ARG:HB2	2.00	0.77
1:B:262:ARG:HD3	1:B:262:ARG:H	1.50	0.77
1:B:277:GLY:HA2	1:B:280:GLN:NE2	1.99	0.77
1:B:303:CYS:SG	1:B:371:SER:HB3	2.25	0.77
2:A:6:SER:HB3	2:A:138:PHE:CZ	2.19	0.77
2:A:84:ARG:HD2	2:A:85:GLN:N	1.99	0.77
2:A:119:LEU:HD12	2:A:120:ASP:N	1.98	0.77
2:A:384:ILE:HD11	2:A:432:TYR:CE2	2.19	0.77
1:B:51:TYR:CZ	1:B:61:PRO:HA	2.20	0.77
1:B:65:LEU:H	1:B:90:PHE:HB2	1.47	0.77
1:B:381:ILE:HA	1:B:384:GLN:CD	2.04	0.77
2:A:31:GLN:HB2	2:A:37:PRO:CD	2.14	0.77
2:A:166:LYS:HG2	2:A:199:ASP:OD2	1.85	0.77
2:A:281:ALA:CB	2:A:369:ALA:HB3	2.15	0.77
2:A:286:LEU:HD12	2:A:286:LEU:O	1.84	0.77
2:A:405:VAL:HG12	2:A:409:VAL:HG23	1.66	0.77
1:B:159:TYR:CD2	1:B:162:ARG:HG2	2.20	0.77
1:B:214:THR:O	1:B:216:LYS:HD2	1.85	0.77
1:B:376:GLU:HG3	1:B:379:LYS:NZ	2.00	0.77
2:A:30:ILE:HA	2:A:36:MET:CB	2.09	0.77
2:A:154:MET:CG	2:A:197:HIS:HB2	2.15	0.77
1:B:99:ASN:C	1:B:142:GLY:HA3	2.05	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:LEU:HD11	1:B:265:PHE:O	1.86	0.77
1:B:342:VAL:HB	1:B:348:ASN:HD21	1.50	0.77
1:B:414:ASN:O	1:B:418:LEU:HD23	1.84	0.77
2:A:64:ARG:N	2:A:64:ARG:HD2	2.00	0.77
2:A:103:TYR:HE2	2:A:151:SER:HB3	1.50	0.77
2:A:152:LEU:HA	2:A:155:GLU:OE1	1.85	0.76
2:A:273:ALA:CB	2:A:295:CYS:HB2	2.15	0.76
2:A:410:GLY:HA3	3:K:290:GLN:NE2	1.98	0.76
3:K:257:LYS:HD3	3:K:367:GLN:HE22	1.50	0.76
1:B:5:VAL:HA	1:B:62:ARG:HG3	1.66	0.76
1:B:6:HIS:O	1:B:63:ALA:HA	1.84	0.76
1:B:105:HIS:CE1	1:B:150:LEU:HD23	2.20	0.76
1:B:413:SER:HA	1:B:416:ASN:ND2	2.00	0.76
2:A:78:VAL:HA	2:A:83:TYR:HE1	1.49	0.76
2:A:189:LEU:HD13	2:A:418:PHE:HD2	1.46	0.76
2:A:320:ARG:HB2	2:A:374:ALA:N	2.00	0.76
2:A:360:PRO:HB3	2:A:374:ALA:HB2	1.67	0.76
3:K:135:ILE:HD12	3:K:136:ILE:N	2.00	0.76
3:K:155:SER:HB3	3:K:203:THR:CG2	2.05	0.76
3:K:256:VAL:O	3:K:368:LYS:HB2	1.85	0.76
1:B:145:SER:OG	1:B:185:ALA:HA	1.85	0.76
1:B:183:TYR:HA	1:B:385:PHE:CE1	2.20	0.76
1:B:331:LEU:HA	1:B:334:GLN:NE2	2.00	0.76
2:A:214:ARG:CZ	2:A:215:ARG:HA	2.16	0.76
2:A:409:VAL:CG1	3:K:289:ASN:HD22	1.95	0.76
3:K:26:ARG:CG	3:K:109:THR:HA	2.15	0.76
2:A:23:LEU:CD1	2:A:363:VAL:HA	2.11	0.76
2:A:26:LEU:CD2	2:A:364:PRO:HB3	2.15	0.76
2:A:306:ASP:HA	2:A:308:ARG:HH21	1.51	0.76
2:A:315:CYS:HA	2:A:378:LEU:O	1.84	0.76
2:A:317:LEU:HD23	2:A:377:MET:HG3	1.66	0.76
3:K:15:LYS:HE2	3:K:362:LYS:HE2	1.68	0.76
3:K:96:GLY:O	3:K:366:ASN:HB2	1.86	0.76
1:B:212:PHE:HB2	1:B:220:PRO:CD	2.15	0.76
2:A:262:TYR:HE2	2:A:435:VAL:HG23	1.50	0.76
3:K:312:ARG:CA	3:K:318:ARG:HD2	2.16	0.76
3:K:365:VAL:CG1	3:K:367:GLN:HG2	2.14	0.76
1:B:3:GLU:CD	1:B:50:TYR:HA	2.06	0.76
1:B:20:PHE:CE1	1:B:24:ILE:HD11	2.20	0.76
1:B:97:ALA:HB3	1:B:143:THR:CA	2.16	0.76
1:B:327:ASP:O	1:B:330:MET:HG2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:103:TYR:HB2	2:A:147:SER:CB	2.16	0.76
2:A:326:LYS:HA	2:A:329:ASN:ND2	2.00	0.76
1:B:308:GLY:HA2	1:B:372:THR:H	1.51	0.76
1:B:377:LEU:HD12	1:B:377:LEU:O	1.86	0.76
2:A:386:GLU:O	2:A:390:ARG:HG3	1.86	0.76
3:K:31:ALA:HB1	3:K:34:LYS:CE	2.16	0.76
3:K:92:GLU:O	3:K:97:TYR:HB2	1.84	0.76
1:B:140:GLY:CA	1:B:171:PRO:HG3	2.15	0.76
1:B:350:LYS:CG	2:A:179:THR:CG2	2.63	0.76
2:A:273:ALA:HB2	2:A:295:CYS:HB2	1.68	0.76
3:K:32:GLU:HB3	3:K:33:ARG:HH21	1.50	0.76
3:K:156:VAL:N	3:K:203:THR:HG23	2.01	0.76
1:B:147:MET:HG2	1:B:148:GLY:N	2.00	0.76
2:A:17:GLY:HA2	2:A:20:CYS:SG	2.25	0.76
2:A:174:ALA:HB2	2:A:207:GLU:H	1.50	0.76
2:A:370:LYS:NZ	2:A:372:GLN:HA	2.01	0.76
3:K:114:THR:O	3:K:135:ILE:HG23	1.86	0.76
1:B:217:LEU:HD12	1:B:219:THR:O	1.85	0.76
1:B:253:LEU:HD12	1:B:254:ALA:N	2.01	0.76
2:A:154:MET:HE2	2:A:154:MET:O	1.86	0.76
2:A:174:ALA:HB1	2:A:207:GLU:CB	2.16	0.76
2:A:396:ASP:HA	2:A:422:ARG:NH2	2.00	0.76
1:B:210:ILE:O	1:B:213:ARG:HG3	1.85	0.75
2:A:31:GLN:HG2	2:A:32:PRO:CD	2.14	0.75
2:A:53:PHE:HB3	2:A:62:VAL:C	2.07	0.75
2:A:319:TYR:CB	2:A:355:ILE:HG23	2.15	0.75
2:A:321:GLY:HA3	2:A:372:GLN:HE21	1.50	0.75
3:K:159:SER:HA	3:K:172:LEU:CD1	2.08	0.75
1:B:137:HIS:O	1:B:168:SER:HA	1.85	0.75
2:A:163:LYS:HE3	2:A:164:LYS:N	2.01	0.75
2:A:391:LEU:HA	2:A:394:LYS:HE2	1.68	0.75
1:B:149:THR:CG2	1:B:188:SER:HA	2.17	0.75
1:B:183:TYR:O	1:B:186:THR:HG22	1.86	0.75
2:A:9:VAL:HB	2:A:139:HIS:HB2	1.68	0.75
1:B:122:LYS:HA	1:B:125:GLU:OE1	1.86	0.75
1:B:203:ASP:OD2	1:B:301:ALA:HA	1.87	0.75
2:A:176:GLN:CG	2:A:207:GLU:HB2	2.14	0.75
2:A:282:TYR:HE1	2:A:369:ALA:HB2	1.49	0.75
2:A:427:ALA:HB1	3:K:57:LEU:CD2	1.75	0.75
2:A:390:ARG:HA	2:A:393:HIS:CD2	2.21	0.75
1:B:101:TRP:CD1	1:B:149:THR:HG21	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:35:GLN:CB	2:A:60:LYS:HE2	2.17	0.75
2:A:119:LEU:O	2:A:122:ILE:HG13	1.85	0.75
2:A:189:LEU:HD22	2:A:418:PHE:CE2	2.21	0.75
1:B:46:ARG:CB	1:B:241:ARG:HD3	2.16	0.75
1:B:103:LYS:NZ	1:B:401:GLU:HA	2.01	0.75
1:B:156:ARG:HH12	1:B:160:PRO:HA	1.50	0.75
1:B:251:ARG:HD3	2:A:105:ARG:HH21	1.52	0.75
2:A:396:ASP:HA	2:A:422:ARG:CZ	2.17	0.75
1:B:178:THR:OG1	1:B:180:VAL:HG22	1.87	0.75
1:B:217:LEU:HD13	1:B:218:THR:N	2.01	0.75
2:A:55:GLU:HG2	2:A:61:HIS:CD2	2.21	0.75
2:A:427:ALA:HB2	3:K:57:LEU:HD22	0.76	0.75
2:A:96:LYS:O	2:A:96:LYS:HD3	1.86	0.75
2:A:381:THR:O	2:A:384:ILE:HG12	1.86	0.75
3:K:168:LEU:HB3	3:K:182:LEU:HD23	1.69	0.75
2:A:211:ASP:O	2:A:214:ARG:HG3	1.87	0.74
1:B:2:ARG:HG3	1:B:131:GLN:N	2.02	0.74
1:B:81:PHE:O	1:B:84:ILE:HG22	1.86	0.74
1:B:367:PHE:O	1:B:368:ILE:HD13	1.86	0.74
2:A:331:ALA:O	2:A:335:ILE:HG12	1.87	0.74
3:K:15:LYS:CE	3:K:362:LYS:HE2	2.17	0.74
1:B:36:TYR:CZ	1:B:38:GLY:HA3	2.22	0.74
1:B:112:LEU:HD11	1:B:151:LEU:CB	2.17	0.74
1:B:112:LEU:CD1	1:B:151:LEU:HB3	2.18	0.74
1:B:272:PRO:HG3	1:B:284:LEU:HD11	1.69	0.74
1:B:308:GLY:CA	1:B:372:THR:H	1.99	0.74
3:K:34:LYS:HG2	3:K:35:ALA:N	2.01	0.74
3:K:171:LEU:HA	3:K:220:LYS:HD3	1.69	0.74
1:B:99:ASN:HA	1:B:142:GLY:HA3	1.70	0.74
2:A:30:ILE:CD1	2:A:61:HIS:HB2	2.17	0.74
2:A:214:ARG:NH1	2:A:215:ARG:HA	2.02	0.74
2:A:256:GLN:HA	2:A:259:LEU:HD12	1.67	0.74
2:A:288:VAL:O	2:A:292:THR:HG23	1.87	0.74
2:A:324:VAL:HG21	2:A:326:LYS:HZ1	1.51	0.74
2:A:326:LYS:HA	2:A:329:ASN:HD22	1.53	0.74
3:K:187:ASP:HB2	3:K:189:ARG:HD3	1.69	0.74
1:B:20:PHE:HA	1:B:230:SER:CB	2.16	0.74
1:B:186:THR:CG2	1:B:187:LEU:HD22	2.18	0.74
1:B:381:ILE:HA	1:B:384:GLN:NE2	2.01	0.74
2:A:171:ILE:CA	2:A:204:VAL:HG12	2.15	0.74
3:K:77:LYS:HG3	3:K:79:ILE:HG22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:191:LYS:H	3:K:191:LYS:HZ2	1.36	0.74
1:B:2:ARG:HA	1:B:129:CYS:O	1.87	0.74
1:B:71:GLY:HA2	1:B:74:ASP:OD1	1.86	0.74
1:B:181:GLU:HB3	1:B:182:PRO:HD3	1.69	0.74
1:B:323:MET:CA	2:A:221:ARG:HG3	2.18	0.74
1:B:337:ASN:HB3	1:B:340:TYR:HB2	1.68	0.74
2:A:174:ALA:HB1	2:A:207:GLU:HB2	1.70	0.74
2:A:321:GLY:CA	2:A:359:PRO:HA	2.18	0.74
3:K:95:MET:HE2	3:K:97:TYR:HB2	0.76	0.74
3:K:95:MET:HG2	3:K:97:TYR:H	1.52	0.74
3:K:97:TYR:CE1	3:K:329:ARG:HB2	2.22	0.74
2:A:175:PRO:HG2	2:A:304:LYS:CE	2.18	0.74
2:A:245:ASP:HA	2:A:249:ASN:HB2	1.70	0.74
2:A:381:THR:OG1	2:A:384:ILE:HG23	1.87	0.74
3:K:157:LYS:HG2	3:K:203:THR:CA	2.18	0.74
2:A:90:GLU:HA	2:A:121:ARG:HH21	1.51	0.74
2:A:276:ILE:CG2	2:A:281:ALA:HB2	2.18	0.74
3:K:68:PHE:HB2	3:K:71:VAL:HG22	1.68	0.74
1:B:3:GLU:HG3	1:B:50:TYR:HA	1.69	0.74
1:B:121:ARG:HB2	1:B:122:LYS:HZ3	1.52	0.74
2:A:116:ASP:HA	2:A:119:LEU:CD2	2.16	0.74
3:K:54:THR:C	3:K:60:LYS:HG3	2.08	0.74
1:B:336:LYS:HA	1:B:336:LYS:HE3	1.68	0.74
2:A:78:VAL:HA	2:A:83:TYR:CE1	2.21	0.74
2:A:409:VAL:CG1	3:K:293:LEU:CD2	2.66	0.74
3:K:160:LEU:H	3:K:172:LEU:HB3	1.51	0.74
1:B:43:GLN:HA	1:B:242:PHE:HZ	1.52	0.73
1:B:284:LEU:HD13	1:B:289:LEU:CG	2.18	0.73
1:B:324:LYS:N	2:A:221:ARG:CG	2.50	0.73
3:K:16:GLY:CA	3:K:362:LYS:HA	2.15	0.73
1:B:330:MET:CG	1:B:331:LEU:HD13	2.17	0.73
2:A:86:LEU:HD12	2:A:86:LEU:O	1.88	0.73
2:A:210:TYR:CE1	2:A:227:LEU:HB2	2.23	0.73
2:A:409:VAL:HG23	3:K:293:LEU:HG	1.69	0.73
3:K:95:MET:O	3:K:367:GLN:HA	1.88	0.73
1:B:112:LEU:HD13	1:B:150:LEU:HD12	1.70	0.73
3:K:146:LYS:HA	3:K:149:ASP:OD2	1.88	0.73
3:K:173:ASN:HB2	3:K:176:SER:CB	2.18	0.73
3:K:312:ARG:HA	3:K:318:ARG:HG2	1.68	0.73
1:B:46:ARG:HH12	1:B:49:VAL:HG11	1.51	0.73
1:B:424:GLN:NE2	1:B:427:ASP:HB2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:430:LYS:HZ2	2:A:433:GLU:HB3	1.51	0.73
1:B:100:ASN:CB	1:B:103:LYS:HB2	2.17	0.73
1:B:323:MET:HB2	2:A:221:ARG:NE	2.03	0.73
2:A:185:TYR:HA	2:A:395:PHE:CE2	2.22	0.73
3:K:17:LYS:N	3:K:363:PRO:HD2	2.03	0.73
3:K:95:MET:CE	3:K:97:TYR:CB	2.31	0.73
1:B:375:GLN:CD	1:B:422:TYR:HB3	2.08	0.73
2:A:67:PHE:HB2	2:A:92:LEU:CD1	2.19	0.73
2:A:105:ARG:HA	2:A:411:GLU:OE1	1.89	0.73
2:A:210:TYR:CD1	2:A:227:LEU:HD13	2.24	0.73
2:A:276:ILE:CG1	2:A:371:VAL:HG11	2.17	0.73
3:K:181:ARG:HH21	3:K:197:LYS:HG2	1.48	0.73
1:B:21:TRP:HA	1:B:21:TRP:HE3	1.53	0.73
1:B:215:LEU:HD22	1:B:217:LEU:CB	2.18	0.73
1:B:215:LEU:HD13	1:B:217:LEU:CB	2.18	0.73
1:B:324:LYS:CD	2:A:221:ARG:HH11	1.99	0.73
2:A:102:ASN:CB	2:A:105:ARG:HB3	2.19	0.73
1:B:5:VAL:HA	1:B:62:ARG:CG	2.18	0.73
1:B:23:VAL:HG11	1:B:230:SER:OG	1.88	0.73
1:B:65:LEU:HB2	1:B:90:PHE:CD1	2.24	0.73
1:B:288:GLU:HG2	1:B:291:GLN:OE1	1.88	0.73
1:B:308:GLY:HA2	1:B:372:THR:HB	1.69	0.73
2:A:8:HIS:CB	2:A:14:VAL:HA	2.19	0.73
2:A:20:CYS:HB3	2:A:24:TYR:OH	1.88	0.73
2:A:60:LYS:HD3	2:A:61:HIS:H	1.52	0.73
2:A:226:ASN:HA	2:A:229:ARG:CG	2.17	0.73
2:A:313:MET:HA	2:A:344:VAL:CG1	2.19	0.73
2:A:316:CYS:O	2:A:377:MET:HA	1.89	0.73
3:K:181:ARG:HH22	3:K:197:LYS:HE2	1.54	0.73
1:B:122:LYS:HA	1:B:125:GLU:CD	2.08	0.73
1:B:372:THR:O	1:B:375:GLN:HG2	1.89	0.73
1:B:392:LYS:HA	1:B:395:LEU:HD21	1.71	0.73
2:A:263:PRO:HD2	2:A:264:ARG:HD3	1.70	0.73
3:K:258:ILE:H	3:K:368:LYS:CE	2.02	0.73
2:A:35:GLN:N	2:A:60:LYS:HE2	2.04	0.73
2:A:224:TYR:CZ	4:A:501:G2P:N7	2.49	0.73
2:A:243:ARG:HG3	2:A:244:PHE:N	2.04	0.73
3:K:78:GLN:NE2	3:K:113:PHE:CD2	2.57	0.73
3:K:162:GLU:HG3	3:K:235:SER:HB2	1.66	0.73
1:B:41:ASP:CG	1:B:42:LEU:HD22	2.10	0.72
1:B:190:HIS:NE2	1:B:411:ALA:HA	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:SER:CB	3:K:308:HIS:HE1	2.00	0.72
2:A:205:ASP:OD2	2:A:303:VAL:HG23	1.89	0.72
2:A:277:SER:H	2:A:280:LYS:CB	1.99	0.72
1:B:250:LEU:HD12	1:B:253:LEU:CD1	2.05	0.72
2:A:5:ILE:H	2:A:132:LEU:CD2	2.02	0.72
2:A:8:HIS:HB3	2:A:14:VAL:N	2.03	0.72
2:A:200:CYS:HA	2:A:266:HIS:CB	1.99	0.72
2:A:306:ASP:HA	2:A:308:ARG:NH2	2.04	0.72
2:A:387:ALA:HA	2:A:390:ARG:NE	2.05	0.72
3:K:26:ARG:HB3	3:K:109:THR:HA	1.70	0.72
1:B:141:GLY:HA3	4:B:501:G2P:O5'	1.89	0.72
2:A:21:TRP:CZ2	2:A:65:ALA:HB2	2.24	0.72
2:A:132:LEU:HB3	2:A:134:GLY:O	1.89	0.72
3:K:147:LEU:O	3:K:150:ASN:HB2	1.89	0.72
3:K:162:GLU:CD	3:K:223:THR:HG22	2.10	0.72
1:B:103:LYS:O	1:B:107:THR:HG22	1.88	0.72
1:B:258:VAL:O	2:A:404:PHE:CE2	2.41	0.72
1:B:363:MET:H	1:B:363:MET:HE3	1.54	0.72
2:A:188:ILE:HB	2:A:395:PHE:CD1	2.24	0.72
1:B:12:CYS:CB	1:B:138:SER:HB3	2.19	0.72
3:K:311:TYR:CD2	3:K:321:GLN:HG3	2.24	0.72
1:B:97:ALA:HA	1:B:104:GLY:HA3	1.70	0.72
2:A:164:LYS:HA	2:A:164:LYS:CE	2.19	0.72
2:A:205:ASP:HB3	2:A:208:ALA:HB3	1.71	0.72
3:K:15:LYS:CD	3:K:362:LYS:HB3	2.19	0.72
1:B:190:HIS:O	1:B:193:VAL:HG12	1.90	0.72
1:B:285:THR:H	1:B:288:GLU:HB2	1.55	0.72
2:A:388:TRP:HB2	2:A:425:MET:HE1	1.71	0.72
3:K:23:VAL:HG21	3:K:68:PHE:CE1	2.24	0.72
3:K:171:LEU:HA	3:K:220:LYS:CD	2.20	0.72
3:K:181:ARG:HH22	3:K:197:LYS:CE	2.00	0.72
1:B:350:LYS:HG3	2:A:179:THR:CG2	2.19	0.72
1:B:392:LYS:O	1:B:395:LEU:HG	1.90	0.72
2:A:33:ASP:O	2:A:86:LEU:HA	1.90	0.72
2:A:215:ARG:HD3	2:A:216:ASN:ND2	2.04	0.72
1:B:3:GLU:CG	1:B:50:TYR:HA	2.20	0.72
1:B:43:GLN:HA	1:B:242:PHE:CZ	2.25	0.72
1:B:179:VAL:O	1:B:182:PRO:HD2	1.90	0.72
1:B:215:LEU:HA	1:B:276:ARG:CG	2.19	0.72
1:B:267:MET:HG3	1:B:369:GLY:O	1.90	0.72
1:B:285:THR:HG23	1:B:288:GLU:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:LYS:H	2:A:221:ARG:CG	2.03	0.72
2:A:265:ILE:HD12	2:A:432:TYR:CE1	2.25	0.72
3:K:172:LEU:HG	3:K:173:ASN:N	2.05	0.72
3:K:269:SER:HB3	3:K:288:ILE:HG13	1.71	0.72
1:B:15:GLN:O	1:B:19:LYS:HE2	1.89	0.71
2:A:90:GLU:HA	2:A:121:ARG:NH2	2.05	0.71
3:K:144:PHE:HB2	3:K:207:LYS:HG3	1.71	0.71
1:B:159:TYR:CB	1:B:162:ARG:HG2	2.20	0.71
1:B:167:PHE:CD1	1:B:200:TYR:HB2	2.25	0.71
1:B:313:VAL:O	1:B:349:VAL:HA	1.91	0.71
1:B:405:GLU:HA	1:B:408:PHE:HD1	1.54	0.71
2:A:346:TRP:O	2:A:348:PRO:HD3	1.89	0.71
1:B:140:GLY:HA2	1:B:171:PRO:HG3	1.71	0.71
1:B:322:SER:O	1:B:326:VAL:HG23	1.90	0.71
1:B:420:SER:CB	3:K:308:HIS:CE1	2.73	0.71
2:A:233:GLN:HE21	2:A:234:ILE:CG2	2.02	0.71
2:A:288:VAL:CG1	2:A:331:ALA:HB2	2.19	0.71
3:K:97:TYR:CE2	3:K:365:VAL:HG22	2.25	0.71
3:K:226:THR:HG23	3:K:232:SER:OG	1.89	0.71
3:K:255:LEU:HA	3:K:369:LEU:OXT	1.90	0.71
2:A:224:TYR:CZ	4:A:501:G2P:C6	2.56	0.71
2:A:274:PRO:HG3	2:A:291:ILE:CG1	2.17	0.71
3:K:181:ARG:HH21	3:K:197:LYS:HG3	0.55	0.71
1:B:97:ALA:CB	1:B:143:THR:HG23	2.20	0.71
2:A:70:LEU:HB3	2:A:97:GLU:O	1.91	0.71
2:A:276:ILE:CD1	2:A:371:VAL:HG11	2.20	0.71
3:K:156:VAL:O	3:K:203:THR:HA	1.91	0.71
3:K:311:TYR:HE1	3:K:324:LEU:CG	2.04	0.71
1:B:64:ILE:CD1	1:B:119:VAL:HG21	2.21	0.71
3:K:162:GLU:CG	3:K:235:SER:HB3	2.01	0.71
1:B:339:SER:HA	1:B:429:THR:HB	1.73	0.71
1:B:375:GLN:CG	1:B:422:TYR:HB3	2.21	0.71
1:B:419:VAL:HA	1:B:422:TYR:CE2	2.25	0.71
2:A:185:TYR:OH	2:A:398:MET:HB3	1.90	0.71
2:A:225:THR:O	2:A:229:ARG:HG2	1.90	0.71
2:A:262:TYR:HE2	2:A:435:VAL:CG2	2.03	0.71
2:A:275:VAL:CB	2:A:300:ASN:HD22	2.02	0.71
3:K:159:SER:OG	3:K:240:SER:OG	2.08	0.71
1:B:11:GLN:H	4:B:501:G2P:PB	2.14	0.71
1:B:67:ASP:HB3	1:B:69:GLU:O	1.90	0.71
1:B:86:ARG:HB3	1:B:88:ASP:OD1	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ALA:HB1	1:B:403:MET:SD	2.31	0.71
1:B:375:GLN:HG3	1:B:422:TYR:HB3	1.71	0.71
2:A:3:GLU:CA	2:A:51:THR:HA	2.20	0.71
2:A:317:LEU:HG	2:A:353:VAL:HG11	1.72	0.71
3:K:37:ALA:HB1	3:K:339:ALA:CB	2.21	0.71
3:K:52:VAL:HG11	3:K:346:THR:HG21	1.71	0.71
1:B:20:PHE:CD1	1:B:230:SER:HB2	2.22	0.71
1:B:198:GLU:OE1	1:B:265:PHE:HB2	1.90	0.71
2:A:115:ILE:HD12	2:A:152:LEU:HD21	1.72	0.71
2:A:206:ASN:O	2:A:210:TYR:HB2	1.91	0.71
2:A:242:LEU:HB2	2:A:252:LEU:HD11	1.73	0.71
2:A:275:VAL:HG13	2:A:280:LYS:HE3	1.73	0.71
3:K:48:LYS:CE	3:K:71:VAL:H	2.04	0.71
3:K:304:GLU:HG2	3:K:306:THR:HB	1.72	0.71
3:K:320:LEU:CD2	3:K:324:LEU:HD11	2.21	0.71
1:B:6:HIS:HB3	1:B:62:ARG:O	1.90	0.71
1:B:161:ASP:OD1	1:B:162:ARG:HD2	1.91	0.71
1:B:190:HIS:CD2	1:B:411:ALA:HA	2.24	0.71
1:B:273:LEU:CB	1:B:298:ASN:HA	2.21	0.71
1:B:274:THR:CG2	1:B:278:SER:HB2	2.18	0.71
1:B:304:ASP:OD1	1:B:306:ARG:HB3	1.90	0.71
3:K:136:ILE:HG21	3:K:214:LEU:HD11	1.72	0.71
3:K:212:GLN:HA	3:K:215:GLU:OE2	1.91	0.71
3:K:272:ILE:H	3:K:272:ILE:HD13	1.55	0.71
3:K:311:TYR:CG	3:K:321:GLN:HG3	2.25	0.71
1:B:215:LEU:HA	1:B:276:ARG:HG2	1.70	0.70
1:B:275:SER:HB3	1:B:278:SER:OG	1.91	0.70
2:A:176:GLN:HE21	2:A:207:GLU:CA	2.03	0.70
2:A:405:VAL:HG11	3:K:293:LEU:CG	2.14	0.70
1:B:16:ILE:HG12	1:B:226:ASN:ND2	2.06	0.70
1:B:152:ILE:HA	1:B:155:ILE:CD1	2.20	0.70
1:B:250:LEU:HA	1:B:253:LEU:CD2	2.20	0.70
2:A:5:ILE:HG23	2:A:65:ALA:CA	2.21	0.70
2:A:132:LEU:CD2	2:A:135:PHE:HB3	2.20	0.70
2:A:277:SER:N	2:A:280:LYS:HB2	2.05	0.70
3:K:246:LYS:HE2	3:K:254:GLU:OE2	1.90	0.70
1:B:42:LEU:HD22	1:B:42:LEU:H	1.55	0.70
1:B:105:HIS:HD1	1:B:106:TYR:HD2	1.36	0.70
2:A:4:CYS:N	2:A:51:THR:HA	2.06	0.70
2:A:8:HIS:CE1	2:A:21:TRP:HE1	2.09	0.70
2:A:23:LEU:HD12	2:A:363:VAL:HG12	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:217:LEU:CB	2:A:219:ILE:HG12	2.20	0.70
2:A:240:ALA:HA	2:A:243:ARG:CG	2.20	0.70
3:K:157:LYS:HG2	3:K:203:THR:N	2.06	0.70
3:K:227:LEU:HD21	3:K:270:GLU:OE2	1.90	0.70
1:B:101:TRP:CH2	1:B:187:LEU:HG	2.26	0.70
2:A:8:HIS:HE1	2:A:21:TRP:HE1	1.38	0.70
2:A:64:ARG:HH21	2:A:64:ARG:CA	2.03	0.70
2:A:66:VAL:HG21	2:A:122:ILE:HG22	1.74	0.70
2:A:212:ILE:HG22	2:A:216:ASN:OD1	1.91	0.70
3:K:187:ASP:CG	3:K:195:ILE:HG13	2.09	0.70
1:B:8:GLN:NE2	1:B:14:ASN:HA	2.05	0.70
1:B:421:GLU:OE1	1:B:424:GLN:HB3	1.92	0.70
2:A:255:PHE:O	2:A:259:LEU:HG	1.91	0.70
2:A:268:PRO:HG2	2:A:378:LEU:CD1	2.14	0.70
2:A:318:LEU:HD13	2:A:319:TYR:N	2.06	0.70
3:K:170:ASP:H	3:K:180:GLU:H	1.39	0.70
1:B:251:ARG:HG3	1:B:252:LYS:N	2.07	0.70
2:A:11:GLN:O	2:A:14:VAL:HG22	1.91	0.70
2:A:332:ILE:O	2:A:336:LYS:HG2	1.91	0.70
3:K:170:ASP:HB2	3:K:180:GLU:CA	2.22	0.70
1:B:1:MET:SD	1:B:3:GLU:HG2	2.32	0.70
1:B:143:THR:HG22	1:B:147:MET:CE	2.22	0.70
2:A:7:ILE:HG23	2:A:137:VAL:HA	1.73	0.70
2:A:204:VAL:HG23	2:A:209:ILE:CD1	2.20	0.70
1:B:47:ILE:HG22	1:B:59:TYR:CD1	2.27	0.70
1:B:135:LEU:HB2	1:B:166:THR:HG23	1.73	0.70
1:B:266:PHE:CZ	1:B:369:GLY:HA2	2.26	0.70
1:B:279:GLN:NE2	1:B:284:LEU:HD21	2.06	0.70
2:A:24:TYR:O	2:A:27:GLU:HG3	1.91	0.70
2:A:269:LEU:CD2	2:A:384:ILE:HD12	2.21	0.70
1:B:299:MET:HG3	1:B:301:ALA:O	1.92	0.70
2:A:351:PHE:HB2	2:A:352:LYS:NZ	2.07	0.70
3:K:221:ARG:HH22	3:K:233:SER:HB2	1.56	0.70
1:B:145:SER:HG	1:B:185:ALA:HA	1.57	0.70
1:B:215:LEU:CA	1:B:276:ARG:HG2	2.22	0.70
2:A:36:MET:CE	2:A:38:SER:HB3	2.22	0.70
2:A:269:LEU:O	2:A:378:LEU:HA	1.92	0.70
2:A:402:ARG:HG3	2:A:405:VAL:HG21	1.73	0.70
3:K:40:ILE:HD13	3:K:340:SER:HA	1.73	0.70
1:B:46:ARG:HG3	1:B:242:PHE:CD1	2.27	0.69
1:B:51:TYR:HB2	1:B:59:TYR:CD1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LEU:HD13	1:B:90:PHE:CB	2.21	0.69
1:B:160:PRO:HB2	3:K:283:ARG:HH22	1.56	0.69
2:A:210:TYR:CE1	2:A:227:LEU:HD13	2.26	0.69
3:K:47:ARG:HB3	3:K:49:GLU:CG	2.22	0.69
3:K:257:LYS:HD3	3:K:367:GLN:NE2	2.06	0.69
1:B:34:GLY:HA3	1:B:58:LYS:HG3	1.74	0.69
1:B:113:VAL:O	1:B:117:LEU:HD23	1.92	0.69
1:B:323:MET:HA	1:B:323:MET:CE	2.21	0.69
1:B:323:MET:HA	1:B:326:VAL:HG23	1.72	0.69
2:A:60:LYS:HD3	2:A:61:HIS:N	2.07	0.69
2:A:286:LEU:HD13	2:A:291:ILE:CD1	2.16	0.69
3:K:66:TYR:HE2	3:K:68:PHE:HA	1.57	0.69
3:K:157:LYS:HG2	3:K:203:THR:OG1	1.88	0.69
1:B:342:VAL:HA	1:B:429:THR:OXT	1.91	0.69
1:B:375:GLN:HG3	1:B:422:TYR:CB	2.22	0.69
2:A:41:THR:HG21	2:A:49:PHE:CB	2.22	0.69
2:A:103:TYR:CD1	2:A:189:LEU:HD23	2.27	0.69
2:A:346:TRP:NE1	2:A:438:ASP:HA	2.07	0.69
3:K:172:LEU:O	3:K:174:PRO:HD3	1.91	0.69
1:B:81:PHE:HA	1:B:83:GLN:OE1	1.92	0.69
2:A:259:LEU:O	2:A:261:PRO:HD3	1.93	0.69
3:K:32:GLU:O	3:K:35:ALA:HB3	1.93	0.69
3:K:221:ARG:HD3	3:K:237:SER:HB3	1.72	0.69
1:B:19:LYS:HA	1:B:22:GLU:OE2	1.92	0.69
1:B:20:PHE:CZ	1:B:24:ILE:HD11	2.26	0.69
1:B:23:VAL:HG22	1:B:27:GLU:OE1	1.93	0.69
1:B:148:GLY:O	1:B:152:ILE:HG12	1.92	0.69
1:B:267:MET:CG	1:B:370:ASN:HA	2.22	0.69
1:B:289:LEU:H	1:B:289:LEU:HD12	1.56	0.69
1:B:293:MET:HE1	1:B:366:THR:O	1.93	0.69
1:B:375:GLN:HG3	1:B:422:TYR:CD2	2.28	0.69
3:K:171:LEU:CA	3:K:220:LYS:HD3	2.23	0.69
3:K:221:ARG:CD	3:K:237:SER:HB3	2.20	0.69
2:A:243:ARG:HG3	2:A:244:PHE:H	1.55	0.69
2:A:301:GLN:OE1	2:A:307:PRO:HG3	1.92	0.69
2:A:318:LEU:O	2:A:375:VAL:HA	1.93	0.69
3:K:169:PHE:CA	3:K:179:SER:HA	2.17	0.69
1:B:30:ILE:HD12	1:B:59:TYR:HB2	1.73	0.69
1:B:181:GLU:OE2	4:B:501:G2P:H3'	1.93	0.69
2:A:1:MET:HG2	2:A:47:ASP:CA	2.22	0.69
2:A:52:PHE:HB3	2:A:53:PHE:CE1	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:101:ASN:CA	2:A:144:GLY:HA3	2.20	0.69
2:A:286:LEU:HD22	2:A:291:ILE:CD1	2.23	0.69
3:K:17:LYS:HD3	3:K:363:PRO:CB	2.22	0.69
1:B:65:LEU:HD23	1:B:73:MET:SD	2.33	0.69
1:B:270:PHE:HB3	1:B:300:MET:SD	2.32	0.69
2:A:4:CYS:H	2:A:51:THR:CA	2.05	0.69
2:A:172:TYR:H	2:A:204:VAL:HG12	1.56	0.69
2:A:272:TYR:CE1	2:A:374:ALA:HB1	2.26	0.69
2:A:311:LYS:HG3	2:A:342:GLN:NE2	2.08	0.69
3:K:48:LYS:O	3:K:71:VAL:HG21	1.91	0.69
3:K:144:PHE:CB	3:K:207:LYS:HZ3	2.06	0.69
3:K:237:SER:OG	3:K:265:ASP:HB3	1.91	0.69
1:B:148:GLY:HA2	1:B:151:LEU:CG	2.22	0.69
1:B:251:ARG:NH2	2:A:101:ASN:N	2.29	0.69
1:B:296:ALA:HA	1:B:305:PRO:HG3	1.73	0.69
1:B:334:GLN:HG2	1:B:335:ASN:N	2.08	0.69
2:A:318:LEU:HD22	2:A:319:TYR:N	2.06	0.69
3:K:321:GLN:HA	3:K:324:LEU:CD2	2.23	0.69
1:B:112:LEU:HD21	1:B:116:VAL:HG11	1.74	0.69
1:B:273:LEU:HD11	1:B:297:LYS:CD	2.07	0.69
1:B:288:GLU:HA	1:B:291:GLN:CD	2.13	0.69
2:A:170:SER:HB3	2:A:202:PHE:O	1.93	0.69
1:B:205:GLU:HG3	1:B:206:ALA:N	2.08	0.68
1:B:206:ALA:O	1:B:210:ILE:HG13	1.93	0.68
1:B:330:MET:HG3	1:B:331:LEU:CD1	2.23	0.68
1:B:341:PHE:CE1	1:B:348:ASN:HB2	2.28	0.68
2:A:247:ALA:CB	2:A:355:ILE:HB	2.13	0.68
2:A:302:MET:H	2:A:302:MET:CE	2.07	0.68
3:K:25:CYS:O	3:K:74:ALA:HA	1.93	0.68
3:K:157:LYS:CD	3:K:203:THR:OG1	2.40	0.68
3:K:174:PRO:HA	3:K:220:LYS:HZ2	1.57	0.68
1:B:59:TYR:O	1:B:61:PRO:HD3	1.94	0.68
1:B:139:LEU:CD1	1:B:171:PRO:HD3	2.24	0.68
1:B:278:SER:HA	1:B:282:ARG:NH1	2.06	0.68
2:A:5:ILE:N	2:A:132:LEU:HD21	2.05	0.68
2:A:85:GLN:HG3	2:A:86:LEU:N	2.07	0.68
2:A:298:PRO:HA	2:A:301:GLN:HG3	1.75	0.68
2:A:302:MET:H	2:A:302:MET:HE3	1.58	0.68
3:K:246:LYS:HE2	3:K:254:GLU:CD	2.14	0.68
1:B:214:THR:HB	1:B:276:ARG:H	1.58	0.68
1:B:245:GLN:HE21	1:B:353:VAL:HG23	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:SER:O	1:B:374:ILE:HG22	1.93	0.68
2:A:3:GLU:HA	2:A:51:THR:CA	2.22	0.68
3:K:26:ARG:HD3	3:K:109:THR:N	2.08	0.68
3:K:77:LYS:CE	3:K:78:GLN:H	2.05	0.68
1:B:7:ILE:H	1:B:134:GLN:HE22	1.42	0.68
1:B:187:LEU:HD11	1:B:408:PHE:CD2	2.28	0.68
1:B:250:LEU:O	1:B:253:LEU:HG	1.93	0.68
2:A:41:THR:HG22	2:A:42:ILE:H	1.57	0.68
2:A:155:GLU:O	2:A:159:VAL:HG23	1.93	0.68
2:A:273:ALA:O	2:A:375:VAL:HG22	1.93	0.68
3:K:66:TYR:HD2	3:K:68:PHE:CE2	2.12	0.68
3:K:160:LEU:HD21	3:K:221:ARG:HB2	1.75	0.68
1:B:313:VAL:HA	1:B:368:ILE:O	1.93	0.68
2:A:8:HIS:HA	2:A:138:PHE:HB2	1.75	0.68
2:A:265:ILE:HD11	2:A:435:VAL:HG11	1.73	0.68
2:A:384:ILE:CD1	2:A:432:TYR:HE2	2.04	0.68
3:K:17:LYS:CE	3:K:329:ARG:HD3	2.21	0.68
3:K:78:GLN:NE2	3:K:113:PHE:CE2	2.62	0.68
1:B:4:ILE:HG23	1:B:133:PHE:CA	2.21	0.68
1:B:339:SER:HA	1:B:429:THR:CB	2.23	0.68
2:A:9:VAL:HG22	2:A:149:PHE:CD1	2.29	0.68
2:A:217:LEU:HD12	2:A:222:PRO:HG3	1.75	0.68
2:A:414:GLU:CG	3:K:344:GLU:HB3	2.05	0.68
3:K:48:LYS:HD2	3:K:71:VAL:H	1.59	0.68
3:K:327:ARG:O	3:K:363:PRO:HA	1.93	0.68
1:B:414:ASN:HD21	3:K:312:ARG:HD3	1.57	0.68
2:A:270:ALA:HB2	2:A:378:LEU:CD2	2.24	0.68
2:A:294:ALA:HA	2:A:297:GLU:OE2	1.94	0.68
3:K:226:THR:HG23	3:K:232:SER:CB	2.24	0.68
3:K:329:ARG:CA	3:K:363:PRO:HB3	2.24	0.68
1:B:315:ALA:HA	1:B:366:THR:O	1.94	0.68
2:A:1:MET:HB2	2:A:47:ASP:HA	1.74	0.68
2:A:46:ASP:N	2:A:49:PHE:HB3	2.09	0.68
2:A:126:ALA:HA	2:A:129:CYS:SG	2.33	0.68
2:A:430:LYS:NZ	2:A:433:GLU:HB3	2.09	0.68
3:K:192:ARG:CD	3:K:327:ARG:HH12	2.07	0.68
3:K:192:ARG:NE	3:K:322:ASP:HA	2.09	0.68
1:B:186:THR:HG21	1:B:385:PHE:CD1	2.28	0.68
1:B:289:LEU:HA	1:B:292:GLN:NE2	2.09	0.68
2:A:301:GLN:CD	2:A:307:PRO:HG3	2.14	0.68
2:A:358:GLN:HG2	2:A:359:PRO:HD2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:169:PHE:HB3	3:K:178:VAL:O	1.93	0.68
1:B:30:ILE:HG22	1:B:36:TYR:CD1	2.29	0.68
2:A:96:LYS:HA	2:A:96:LYS:HZ2	1.58	0.68
2:A:260:VAL:CG1	2:A:268:PRO:HD3	2.24	0.68
2:A:287:SER:H	2:A:290:GLU:HB2	1.59	0.68
2:A:8:HIS:HB3	2:A:14:VAL:HA	1.75	0.67
2:A:156:ARG:HB3	2:A:156:ARG:CZ	2.25	0.67
1:B:245:GLN:HB2	1:B:353:VAL:CG2	2.24	0.67
2:A:26:LEU:HD23	2:A:364:PRO:HB3	1.75	0.67
2:A:205:ASP:CG	2:A:303:VAL:HA	2.14	0.67
2:A:390:ARG:HA	2:A:393:HIS:NE2	2.09	0.67
1:B:103:LYS:CD	1:B:401:GLU:HG2	2.23	0.67
1:B:143:THR:HB	4:B:501:G2P:PB	2.34	0.67
2:A:5:ILE:HD13	2:A:125:LEU:HD23	1.77	0.67
2:A:9:VAL:HG12	2:A:146:GLY:HA2	1.76	0.67
2:A:181:VAL:O	2:A:184:PRO:HD2	1.94	0.67
3:K:41:VAL:HG23	3:K:338:PRO:HA	1.74	0.67
3:K:199:LEU:HD12	3:K:200:GLU:N	2.09	0.67
3:K:312:ARG:NH1	3:K:318:ARG:NH2	2.42	0.67
1:B:293:MET:HA	1:B:298:ASN:OD1	1.95	0.67
2:A:6:SER:HB2	2:A:21:TRP:CZ2	2.29	0.67
2:A:36:MET:HG3	2:A:38:SER:O	1.94	0.67
2:A:133:GLN:OE1	2:A:242:LEU:HG	1.94	0.67
2:A:164:LYS:HA	2:A:164:LYS:NZ	2.09	0.67
2:A:176:GLN:HE21	2:A:207:GLU:CB	2.07	0.67
3:K:167:GLU:HA	3:K:167:GLU:OE1	1.94	0.67
3:K:312:ARG:NH1	3:K:318:ARG:HH21	1.92	0.67
1:B:3:GLU:HA	1:B:3:GLU:OE2	1.95	0.67
1:B:58:LYS:HG2	1:B:59:TYR:N	2.10	0.67
1:B:121:ARG:HB2	1:B:122:LYS:NZ	2.08	0.67
1:B:183:TYR:HB3	1:B:398:TYR:OH	1.95	0.67
1:B:200:TYR:CG	1:B:268:PRO:HG3	2.30	0.67
1:B:379:LYS:HD3	1:B:419:VAL:CB	2.24	0.67
2:A:21:TRP:CE2	2:A:65:ALA:HB2	2.30	0.67
2:A:147:SER:HB3	2:A:190:THR:OG1	1.95	0.67
2:A:256:GLN:CA	2:A:259:LEU:HG	2.23	0.67
3:K:171:LEU:CB	3:K:220:LYS:HB3	2.25	0.67
1:B:97:ALA:HB3	1:B:143:THR:OG1	1.94	0.67
1:B:103:LYS:HA	1:B:103:LYS:HZ2	1.56	0.67
1:B:324:LYS:CD	2:A:221:ARG:NH1	2.57	0.67
2:A:79:ARG:CD	2:A:92:LEU:HD23	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:102:ASN:HB2	2:A:407:TRP:NE1	2.09	0.67
2:A:210:TYR:CE1	2:A:227:LEU:HD22	2.29	0.67
2:A:271:THR:HG21	2:A:295:CYS:SG	2.35	0.67
3:K:227:LEU:HG	3:K:228:MET:CE	2.23	0.67
1:B:132:GLY:HA3	1:B:163:ILE:O	1.95	0.67
1:B:7:ILE:H	1:B:134:GLN:NE2	1.92	0.67
1:B:170:VAL:HG23	1:B:203:ASP:HA	1.75	0.67
2:A:200:CYS:HB3	2:A:266:HIS:O	1.95	0.67
3:K:95:MET:HB2	3:K:365:VAL:HG11	1.76	0.67
3:K:170:ASP:H	3:K:180:GLU:N	1.92	0.67
1:B:187:LEU:HD11	1:B:408:PHE:HD2	1.60	0.67
1:B:204:ASN:HA	1:B:207:LEU:HD23	1.77	0.67
1:B:285:THR:HG23	1:B:288:GLU:N	2.08	0.67
2:A:152:LEU:HD23	2:A:152:LEU:O	1.95	0.67
2:A:223:THR:HB	2:A:226:ASN:CG	2.15	0.67
1:B:4:ILE:HG13	1:B:132:GLY:O	1.95	0.67
1:B:11:GLN:N	4:B:501:G2P:O1B	2.28	0.67
1:B:24:ILE:HG22	1:B:28:HIS:NE2	2.10	0.67
1:B:142:GLY:HA2	1:B:184:ASN:ND2	2.10	0.67
2:A:221:ARG:CD	2:A:222:PRO:HD2	2.24	0.67
3:K:77:LYS:NZ	3:K:78:GLN:CG	2.57	0.67
1:B:44:LEU:HG	1:B:45:GLU:N	2.10	0.66
1:B:101:TRP:HA	1:B:146:GLY:HA2	1.77	0.66
1:B:110:ALA:O	1:B:113:VAL:HG22	1.95	0.66
2:A:210:TYR:HE1	2:A:227:LEU:HB2	1.60	0.66
2:A:262:TYR:HB3	2:A:264:ARG:NE	2.10	0.66
2:A:294:ALA:HA	2:A:297:GLU:CD	2.14	0.66
3:K:29:ASN:O	3:K:32:GLU:HB2	1.96	0.66
1:B:156:ARG:NH1	1:B:160:PRO:HA	2.10	0.66
1:B:341:PHE:HE2	1:B:346:PRO:HA	1.56	0.66
2:A:23:LEU:CD1	2:A:363:VAL:HG12	2.25	0.66
2:A:263:PRO:HD2	2:A:264:ARG:HH11	1.58	0.66
2:A:273:ALA:HB1	2:A:274:PRO:HA	1.77	0.66
2:A:281:ALA:HB1	2:A:369:ALA:HB3	1.76	0.66
2:A:313:MET:HA	2:A:344:VAL:HG22	1.77	0.66
2:A:321:GLY:N	2:A:359:PRO:HA	2.10	0.66
2:A:334:THR:O	2:A:338:LYS:HG2	1.95	0.66
3:K:171:LEU:HA	3:K:220:LYS:HG2	1.77	0.66
3:K:171:LEU:HA	3:K:220:LYS:CB	2.24	0.66
2:A:96:LYS:HA	2:A:96:LYS:NZ	2.10	0.66
3:K:172:LEU:HG	3:K:173:ASN:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LYS:HA	1:B:336:LYS:CE	2.25	0.66
1:B:404:ASP:O	1:B:407:GLU:HG3	1.95	0.66
2:A:2:ARG:O	2:A:51:THR:HG23	1.95	0.66
2:A:270:ALA:HA	2:A:378:LEU:HD23	1.76	0.66
2:A:320:ARG:O	2:A:373:ARG:HA	1.96	0.66
3:K:15:LYS:HD3	3:K:362:LYS:HD2	1.77	0.66
3:K:135:ILE:CD1	3:K:136:ILE:HG13	2.26	0.66
3:K:271:ASN:HD22	3:K:274:ARG:H	1.44	0.66
3:K:365:VAL:HG12	3:K:367:GLN:HG2	1.78	0.66
1:B:322:SER:H	1:B:325:GLU:CD	1.99	0.66
2:A:79:ARG:HD3	2:A:92:LEU:CD2	2.24	0.66
2:A:133:GLN:HE21	2:A:253:THR:HG23	1.61	0.66
3:K:298:VAL:HG23	3:K:310:PRO:CD	2.26	0.66
3:K:302:LEU:O	3:K:305:ARG:HD2	1.95	0.66
1:B:70:PRO:HG3	1:B:94:GLN:HA	1.78	0.66
1:B:179:VAL:CG2	1:B:388:MET:HG3	2.26	0.66
1:B:245:GLN:HB2	1:B:353:VAL:HG21	1.77	0.66
2:A:9:VAL:HB	2:A:139:HIS:HB3	1.76	0.66
2:A:104:ALA:HB2	2:A:413:MET:HG3	1.78	0.66
2:A:276:ILE:HG13	2:A:371:VAL:CG1	2.24	0.66
3:K:192:ARG:HE	3:K:327:ARG:HH22	1.42	0.66
1:B:276:ARG:HD2	1:B:280:GLN:HE22	1.61	0.66
1:B:313:VAL:HB	1:B:349:VAL:HG22	1.77	0.66
1:B:342:VAL:HA	1:B:429:THR:O	1.94	0.66
2:A:69:ASP:OD2	2:A:74:VAL:HG22	1.95	0.66
2:A:318:LEU:O	2:A:375:VAL:HG12	1.95	0.66
3:K:168:LEU:CD1	3:K:182:LEU:HG	2.25	0.66
3:K:327:ARG:HA	3:K:364:GLU:OE1	1.95	0.66
1:B:17:GLY:CA	1:B:136:THR:HG21	2.26	0.66
1:B:47:ILE:HG22	1:B:59:TYR:CE1	2.31	0.66
1:B:200:TYR:HB3	1:B:268:PRO:HG3	1.76	0.66
1:B:203:ASP:OD2	1:B:206:ALA:HB3	1.95	0.66
3:K:31:ALA:HB1	3:K:34:LYS:NZ	2.10	0.66
3:K:168:LEU:HB3	3:K:182:LEU:CD2	2.26	0.66
3:K:169:PHE:HD1	3:K:179:SER:HB2	1.59	0.66
3:K:303:VAL:CG1	3:K:358:ASN:HD22	2.09	0.66
1:B:200:TYR:CB	1:B:268:PRO:HG3	2.26	0.66
1:B:210:ILE:O	1:B:214:THR:HG23	1.95	0.66
1:B:323:MET:HA	1:B:326:VAL:CG2	2.25	0.66
1:B:390:ARG:HA	1:B:390:ARG:CZ	2.25	0.66
3:K:26:ARG:CD	3:K:109:THR:HA	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:VAL:HG11	1:B:325:GLU:CG	2.26	0.66
2:A:33:ASP:HA	2:A:85:GLN:CD	2.17	0.66
2:A:54:SER:CB	2:A:64:ARG:HH11	2.08	0.66
2:A:171:ILE:HD13	4:A:501:G2P:H1'	1.77	0.66
2:A:270:ALA:HA	2:A:377:MET:O	1.96	0.66
2:A:320:ARG:CB	2:A:374:ALA:H	2.09	0.66
2:A:333:ALA:O	2:A:337:THR:HG22	1.95	0.66
2:A:428:LEU:HA	2:A:431:ASP:OD1	1.95	0.66
2:A:8:HIS:CD2	2:A:14:VAL:HA	2.32	0.65
2:A:243:ARG:HD2	2:A:244:PHE:CE2	2.31	0.65
3:K:15:LYS:HD3	3:K:362:LYS:HB3	1.78	0.65
3:K:27:PRO:CA	3:K:74:ALA:HB1	2.26	0.65
3:K:160:LEU:H	3:K:172:LEU:CD2	2.08	0.65
1:B:34:GLY:C	1:B:58:LYS:HA	2.16	0.65
1:B:215:LEU:C	1:B:276:ARG:HG2	2.16	0.65
1:B:251:ARG:HG3	1:B:252:LYS:H	1.59	0.65
1:B:324:LYS:CG	2:A:220:GLU:C	2.64	0.65
1:B:382:SER:O	1:B:385:PHE:HB2	1.96	0.65
2:A:5:ILE:CD1	2:A:125:LEU:HD23	2.27	0.65
2:A:56:THR:HG22	2:A:57:GLY:N	2.11	0.65
2:A:288:VAL:HG12	2:A:331:ALA:CB	2.24	0.65
2:A:430:LYS:O	2:A:430:LYS:HD3	1.95	0.65
3:K:26:ARG:CB	3:K:109:THR:HA	2.25	0.65
3:K:256:VAL:H	3:K:369:LEU:C	1.99	0.65
1:B:6:HIS:O	1:B:7:ILE:HD13	1.95	0.65
1:B:156:ARG:NH2	1:B:157:GLU:HA	2.11	0.65
1:B:262:ARG:NE	3:K:297:ARG:NH1	2.45	0.65
1:B:289:LEU:HD21	1:B:363:MET:HB2	1.78	0.65
1:B:376:GLU:CB	1:B:379:LYS:HE2	2.25	0.65
2:A:308:ARG:H	2:A:308:ARG:NE	1.94	0.65
2:A:321:GLY:HA2	2:A:359:PRO:HA	1.79	0.65
2:A:401:LYS:HA	2:A:401:LYS:NZ	2.12	0.65
2:A:57:GLY:N	2:A:58:ALA:HA	2.09	0.65
3:K:356:ALA:O	3:K:359:ILE:HG22	1.95	0.65
1:B:103:LYS:HG2	1:B:401:GLU:HG2	1.78	0.65
1:B:167:PHE:CE1	1:B:200:TYR:HD2	2.15	0.65
3:K:95:MET:CE	3:K:97:TYR:CD2	2.80	0.65
3:K:301:ALA:HB1	3:K:306:THR:HG21	1.79	0.65
1:B:67:ASP:OD2	1:B:70:PRO:HA	1.97	0.65
2:A:25:CYS:HA	2:A:30:ILE:CG2	2.27	0.65
2:A:75:ILE:HD12	2:A:92:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:75:ILE:HG22	2:A:79:ARG:HE	1.62	0.65
2:A:102:ASN:HB3	2:A:105:ARG:CD	2.27	0.65
2:A:189:LEU:HD13	2:A:418:PHE:CE2	2.31	0.65
2:A:251:ASP:HB3	2:A:254:GLU:OE1	1.97	0.65
2:A:288:VAL:CG2	2:A:327:ASP:HB3	2.26	0.65
3:K:136:ILE:O	3:K:139:THR:HG22	1.96	0.65
1:B:5:VAL:HG22	1:B:133:PHE:CD1	2.31	0.65
1:B:46:ARG:HA	1:B:46:ARG:NH1	2.12	0.65
2:A:32:PRO:O	2:A:86:LEU:HB2	1.97	0.65
3:K:50:VAL:HB	3:K:68:PHE:CZ	2.32	0.65
3:K:225:ALA:HB1	3:K:230:ALA:O	1.97	0.65
1:B:52:ASN:H	1:B:62:ARG:HH22	1.44	0.65
1:B:97:ALA:HA	1:B:104:GLY:CA	2.26	0.65
1:B:143:THR:HG22	1:B:147:MET:HE3	1.79	0.65
1:B:215:LEU:HD13	1:B:217:LEU:HB2	1.76	0.65
1:B:274:THR:HG22	1:B:275:SER:H	1.61	0.65
1:B:288:GLU:HA	1:B:291:GLN:OE1	1.97	0.65
1:B:361:LEU:HD23	1:B:361:LEU:O	1.97	0.65
1:B:379:LYS:HA	1:B:415:MET:SD	2.36	0.65
2:A:46:ASP:H	2:A:49:PHE:HB3	1.62	0.65
2:A:102:ASN:ND2	2:A:105:ARG:HB3	2.11	0.65
2:A:188:ILE:HG12	2:A:395:PHE:HD1	1.62	0.65
2:A:242:LEU:HD23	2:A:252:LEU:H	1.61	0.65
2:A:409:VAL:CB	3:K:293:LEU:HD23	2.26	0.65
3:K:144:PHE:HE2	3:K:210:VAL:HG21	1.61	0.65
3:K:172:LEU:H	3:K:172:LEU:HD23	1.61	0.65
1:B:1:MET:HE2	1:B:1:MET:HA	1.76	0.65
1:B:99:ASN:HA	1:B:142:GLY:CA	2.27	0.65
1:B:238:THR:O	1:B:241:ARG:HG3	1.97	0.65
1:B:271:ALA:HB3	1:B:365:ALA:O	1.97	0.65
2:A:132:LEU:HD22	2:A:135:PHE:HB3	1.78	0.65
3:K:31:ALA:CA	3:K:34:LYS:HD3	2.22	0.65
3:K:82:TYR:OH	3:K:86:VAL:CG1	2.44	0.65
3:K:301:ALA:HB1	3:K:306:THR:CG2	2.27	0.65
1:B:9:ALA:O	1:B:137:HIS:HA	1.97	0.65
1:B:25:SER:O	1:B:28:HIS:HB2	1.97	0.65
1:B:139:LEU:HD12	1:B:140:GLY:N	2.12	0.65
1:B:320:ARG:HB3	1:B:320:ARG:NH1	2.11	0.65
1:B:321:MET:HG3	1:B:325:GLU:OE1	1.97	0.65
2:A:7:ILE:HG22	2:A:136:LEU:O	1.97	0.65
2:A:147:SER:O	2:A:150:THR:HG22	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:231:ILE:O	2:A:235:VAL:HG23	1.97	0.65
2:A:324:VAL:HG21	2:A:326:LYS:NZ	2.12	0.65
1:B:327:ASP:O	1:B:331:LEU:HD22	1.97	0.64
2:A:3:GLU:O	2:A:132:LEU:HA	1.97	0.64
2:A:78:VAL:CG1	2:A:92:LEU:HD22	2.27	0.64
2:A:311:LYS:HA	2:A:342:GLN:CD	2.17	0.64
2:A:375:VAL:HG21	2:A:377:MET:HE1	1.79	0.64
3:K:189:ARG:CD	3:K:189:ARG:H	2.09	0.64
3:K:329:ARG:HD2	3:K:363:PRO:CG	2.27	0.64
3:K:341:LEU:H	3:K:341:LEU:HD12	1.62	0.64
1:B:377:LEU:HA	1:B:380:ARG:CZ	2.27	0.64
2:A:174:ALA:HB1	2:A:176:GLN:HG2	1.77	0.64
3:K:66:TYR:HD2	3:K:68:PHE:CD2	2.14	0.64
3:K:192:ARG:HB3	3:K:322:ASP:HA	1.79	0.64
1:B:116:VAL:O	1:B:120:VAL:HG13	1.97	0.64
1:B:159:TYR:HD2	1:B:162:ARG:HG2	1.60	0.64
2:A:103:TYR:CE2	2:A:151:SER:HB3	2.32	0.64
2:A:209:ILE:CG1	2:A:302:MET:HB2	2.27	0.64
2:A:318:LEU:CD1	2:A:320:ARG:HG2	2.27	0.64
2:A:388:TRP:HZ3	2:A:428:LEU:HG	1.61	0.64
3:K:168:LEU:CB	3:K:182:LEU:HD23	2.26	0.64
3:K:221:ARG:NE	3:K:237:SER:HB3	2.12	0.64
1:B:11:GLN:HA	1:B:14:ASN:HB2	1.79	0.64
1:B:317:PHE:HA	1:B:364:SER:O	1.97	0.64
2:A:49:PHE:CE1	2:A:53:PHE:HD1	2.16	0.64
2:A:214:ARG:HG3	2:A:215:ARG:N	2.12	0.64
3:K:173:ASN:CB	3:K:176:SER:H	2.11	0.64
1:B:214:THR:CG2	1:B:275:SER:HA	2.27	0.64
2:A:28:HIS:HE1	2:A:49:PHE:HA	1.58	0.64
3:K:17:LYS:HD3	3:K:363:PRO:HG2	1.77	0.64
3:K:109:THR:CB	3:K:335:THR:HB	2.27	0.64
3:K:144:PHE:CG	3:K:207:LYS:HG3	2.32	0.64
3:K:156:VAL:H	3:K:203:THR:HG23	1.60	0.64
3:K:164:TYR:HB2	3:K:235:SER:OG	1.97	0.64
1:B:21:TRP:HD1	1:B:85:PHE:HE2	1.44	0.64
1:B:27:GLU:HA	1:B:359:ARG:NH1	2.12	0.64
1:B:45:GLU:HB2	1:B:46:ARG:NH2	2.12	0.64
1:B:183:TYR:CZ	1:B:385:PHE:HB3	2.31	0.64
1:B:244:GLY:HA2	1:B:355:ASP:H	1.63	0.64
1:B:258:VAL:HG11	1:B:263:LEU:O	1.98	0.64
2:A:1:MET:CB	2:A:47:ASP:HA	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:123:ARG:CZ	2:A:123:ARG:HB2	2.27	0.64
2:A:236:SER:HB2	2:A:361:THR:OG1	1.98	0.64
2:A:240:ALA:CA	2:A:243:ARG:HG2	2.27	0.64
2:A:287:SER:O	2:A:291:ILE:HG13	1.97	0.64
2:A:312:TYR:CE2	2:A:341:ILE:HD12	2.31	0.64
3:K:48:LYS:HD2	3:K:71:VAL:N	2.12	0.64
3:K:94:ILE:HD13	3:K:150:ASN:HD21	1.63	0.64
1:B:4:ILE:HG23	1:B:132:GLY:O	1.98	0.64
1:B:244:GLY:HA2	1:B:355:ASP:CA	2.27	0.64
1:B:245:GLN:OE1	1:B:355:ASP:HA	1.98	0.64
1:B:269:GLY:HA3	1:B:367:PHE:CB	2.23	0.64
1:B:329:GLN:OE1	1:B:330:MET:HE3	1.98	0.64
1:B:379:LYS:CB	1:B:419:VAL:HG11	2.27	0.64
2:A:45:GLY:CA	2:A:49:PHE:HD2	2.11	0.64
2:A:53:PHE:HA	2:A:64:ARG:HD2	1.80	0.64
3:K:33:ARG:CZ	3:K:33:ARG:HA	2.28	0.64
3:K:171:LEU:HA	3:K:220:LYS:HB3	1.79	0.64
3:K:174:PRO:HA	3:K:220:LYS:NZ	2.12	0.64
3:K:227:LEU:HG	3:K:228:MET:SD	2.37	0.64
3:K:234:ARG:HE	3:K:281:ARG:HH21	1.44	0.64
3:K:312:ARG:HA	3:K:318:ARG:HG3	1.77	0.64
1:B:291:GLN:HG2	1:B:292:GLN:N	2.13	0.64
2:A:274:PRO:O	2:A:276:ILE:HG12	1.98	0.64
2:A:311:LYS:HG3	2:A:342:GLN:CD	2.18	0.64
2:A:339:ARG:HH22	2:A:342:GLN:HB3	1.62	0.64
2:A:397:LEU:O	2:A:397:LEU:HD23	1.98	0.64
1:B:28:HIS:HA	1:B:43:GLN:OE1	1.98	0.64
1:B:63:ALA:O	1:B:64:ILE:HD13	1.97	0.64
1:B:67:ASP:HB3	1:B:69:GLU:C	2.18	0.64
1:B:245:GLN:NE2	1:B:245:GLN:H	1.95	0.64
2:A:78:VAL:HG11	2:A:92:LEU:HD22	1.80	0.64
3:K:55:GLY:C	3:K:62:SER:HB2	2.18	0.64
3:K:366:ASN:O	3:K:368:LYS:HD2	1.97	0.64
1:B:135:LEU:HD22	1:B:135:LEU:N	2.13	0.64
1:B:347:ASN:OD1	2:A:179:THR:C	2.36	0.64
2:A:189:LEU:CD2	2:A:418:PHE:HE2	2.11	0.64
2:A:281:ALA:HB3	2:A:369:ALA:HB3	1.80	0.64
3:K:26:ARG:HD3	3:K:109:THR:CA	2.28	0.64
3:K:258:ILE:H	3:K:368:LYS:HE2	1.62	0.64
1:B:271:ALA:HB2	1:B:293:MET:SD	2.38	0.63
1:B:274:THR:HG22	1:B:275:SER:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:35:GLN:HB2	2:A:60:LYS:CE	2.28	0.63
2:A:154:MET:SD	2:A:197:HIS:HB2	2.38	0.63
2:A:412:GLY:HA3	3:K:271:ASN:OD1	1.98	0.63
3:K:157:LYS:HG3	3:K:203:THR:HG1	1.59	0.63
3:K:192:ARG:HB3	3:K:322:ASP:CA	2.28	0.63
3:K:192:ARG:O	3:K:194:VAL:HG13	1.98	0.63
1:B:66:VAL:HG11	1:B:147:MET:HE2	1.79	0.63
1:B:178:THR:CG2	1:B:181:GLU:HB2	2.28	0.63
2:A:116:ASP:O	2:A:119:LEU:HG	1.98	0.63
2:A:253:THR:O	2:A:257:THR:HG23	1.99	0.63
2:A:317:LEU:CG	2:A:353:VAL:HG11	2.28	0.63
1:B:97:ALA:HB3	1:B:143:THR:CB	2.28	0.63
1:B:149:THR:CA	1:B:191:GLN:HE22	2.05	0.63
1:B:320:ARG:NH1	1:B:320:ARG:H	1.95	0.63
1:B:342:VAL:HB	1:B:348:ASN:ND2	2.13	0.63
2:A:164:LYS:HA	2:A:164:LYS:HE2	1.80	0.63
2:A:205:ASP:CG	2:A:303:VAL:HG23	2.19	0.63
2:A:411:GLU:HB3	2:A:413:MET:SD	2.38	0.63
3:K:94:ILE:O	3:K:245:MET:CE	2.45	0.63
3:K:158:VAL:HG12	3:K:241:VAL:HG22	1.79	0.63
3:K:171:LEU:CA	3:K:220:LYS:HB3	2.28	0.63
3:K:285:ALA:O	3:K:288:ILE:HG12	1.99	0.63
3:K:298:VAL:O	3:K:302:LEU:HD13	1.97	0.63
1:B:272:PRO:HG3	1:B:284:LEU:CD1	2.27	0.63
1:B:318:ARG:CB	1:B:358:PRO:HD3	2.29	0.63
2:A:8:HIS:CG	2:A:14:VAL:HA	2.33	0.63
3:K:25:CYS:SG	3:K:41:VAL:HG11	2.38	0.63
3:K:212:GLN:HA	3:K:215:GLU:CD	2.18	0.63
1:B:101:TRP:H	1:B:184:ASN:HB2	1.64	0.63
1:B:127:CYS:SG	1:B:130:LEU:HG	2.38	0.63
1:B:253:LEU:HB2	1:B:257:MET:HE2	1.77	0.63
1:B:286:VAL:CG1	1:B:325:GLU:HB3	2.19	0.63
1:B:303:CYS:CB	1:B:371:SER:HB3	2.29	0.63
1:B:309:ARG:HD2	1:B:429:THR:HA	1.79	0.63
2:A:70:LEU:HD23	2:A:99:ALA:HA	1.79	0.63
3:K:227:LEU:HG	3:K:228:MET:N	2.13	0.63
3:K:258:ILE:H	3:K:368:LYS:HD3	1.64	0.63
1:B:70:PRO:HB3	1:B:92:PHE:CE2	2.33	0.63
1:B:167:PHE:CE1	1:B:200:TYR:HB2	2.34	0.63
1:B:48:ASN:HA	1:B:59:TYR:CE1	2.33	0.63
1:B:77:ARG:HH11	1:B:82:GLY:CA	2.09	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLN:HE21	1:B:353:VAL:CG2	2.11	0.63
1:B:357:PRO:HB3	1:B:362:LYS:O	1.98	0.63
2:A:102:ASN:HD22	2:A:105:ARG:HB3	1.63	0.63
2:A:409:VAL:HG22	3:K:293:LEU:CG	2.19	0.63
3:K:92:GLU:HB3	3:K:97:TYR:CD2	2.34	0.63
3:K:144:PHE:CE2	3:K:210:VAL:HG21	2.34	0.63
3:K:365:VAL:HG11	3:K:367:GLN:HG2	1.78	0.63
1:B:103:LYS:CD	1:B:401:GLU:HA	2.25	0.63
1:B:103:LYS:HZ2	1:B:401:GLU:HA	1.61	0.63
1:B:193:VAL:HG13	1:B:194:GLU:N	2.14	0.63
1:B:199:THR:HG23	1:B:265:PHE:CD2	2.34	0.63
1:B:215:LEU:CD1	1:B:217:LEU:HB2	2.28	0.63
2:A:124:LYS:HD2	2:A:125:LEU:N	2.14	0.63
2:A:143:GLY:HA2	4:A:501:G2P:H3A1	1.80	0.63
2:A:188:ILE:HB	2:A:395:PHE:CE1	2.33	0.63
2:A:247:ALA:HA	2:A:357:TYR:HE1	1.62	0.63
2:A:286:LEU:HD21	2:A:373:ARG:H	1.64	0.63
2:A:305:CYS:O	2:A:307:PRO:HD3	1.98	0.63
3:K:47:ARG:HA	3:K:47:ARG:CZ	2.29	0.63
1:B:46:ARG:HG3	1:B:241:ARG:HD2	1.80	0.63
1:B:98:GLY:C	4:B:501:G2P:O3G	2.37	0.63
1:B:404:ASP:HB3	1:B:406:MET:HG2	1.81	0.63
2:A:9:VAL:O	2:A:139:HIS:HA	1.98	0.63
2:A:242:LEU:O	2:A:242:LEU:HD13	1.98	0.63
2:A:261:PRO:HB2	2:A:262:TYR:CE1	2.34	0.63
2:A:430:LYS:NZ	2:A:430:LYS:HA	2.13	0.63
1:B:251:ARG:HD3	2:A:105:ARG:NH2	2.14	0.62
2:A:385:ALA:HA	2:A:388:TRP:CZ2	2.33	0.62
3:K:25:CYS:SG	3:K:338:PRO:HG3	2.38	0.62
3:K:191:LYS:HD3	3:K:191:LYS:N	2.13	0.62
3:K:204:VAL:HG11	3:K:209:GLU:CB	2.29	0.62
1:B:4:ILE:HD11	1:B:131:GLN:CB	2.23	0.62
1:B:159:TYR:HB3	1:B:161:ASP:CG	2.19	0.62
1:B:210:ILE:HG23	1:B:297:LYS:HE3	1.81	0.62
1:B:258:VAL:HB	1:B:260:PHE:O	1.98	0.62
1:B:275:SER:HG	1:B:276:ARG:N	1.97	0.62
3:K:55:GLY:HA2	3:K:59:ASP:C	2.20	0.62
3:K:320:LEU:HG	3:K:324:LEU:HD22	1.80	0.62
1:B:102:ALA:HB1	1:B:401:GLU:HB3	1.82	0.62
1:B:309:ARG:NH2	1:B:309:ARG:HA	2.15	0.62
2:A:8:HIS:HB3	2:A:14:VAL:CA	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:214:ARG:O	2:A:217:LEU:HB2	1.98	0.62
2:A:430:LYS:HD3	2:A:430:LYS:C	2.19	0.62
1:B:65:LEU:HD22	1:B:90:PHE:CG	2.35	0.62
1:B:103:LYS:HA	1:B:103:LYS:CE	2.29	0.62
1:B:215:LEU:CA	1:B:276:ARG:HB3	2.25	0.62
2:A:7:ILE:HD12	2:A:8:HIS:H	1.63	0.62
2:A:30:ILE:HD11	2:A:61:HIS:HB2	1.80	0.62
2:A:214:ARG:HA	2:A:222:PRO:HG3	1.80	0.62
3:K:342:ASN:ND2	3:K:345:GLU:H	1.96	0.62
1:B:12:CYS:C	1:B:16:ILE:HG13	2.19	0.62
1:B:271:ALA:HB3	1:B:365:ALA:C	2.20	0.62
1:B:320:ARG:HB3	1:B:320:ARG:HH11	1.63	0.62
2:A:31:GLN:CB	2:A:37:PRO:HD3	2.26	0.62
2:A:104:ALA:HB1	2:A:413:MET:SD	2.39	0.62
2:A:139:HIS:HE1	2:A:141:PHE:CD2	2.17	0.62
2:A:191:THR:HG23	2:A:192:HIS:N	2.15	0.62
2:A:368:LEU:HD12	2:A:368:LEU:O	1.98	0.62
3:K:144:PHE:CB	3:K:207:LYS:HG3	2.29	0.62
3:K:227:LEU:HD23	3:K:227:LEU:N	2.15	0.62
3:K:327:ARG:HD3	3:K:327:ARG:N	2.13	0.62
1:B:112:LEU:CD2	1:B:116:VAL:HG11	2.29	0.62
1:B:260:PHE:HE2	2:A:406:HIS:N	1.54	0.62
2:A:217:LEU:HD11	2:A:222:PRO:HB3	1.81	0.62
2:A:275:VAL:CG1	2:A:280:LYS:HE3	2.28	0.62
2:A:286:LEU:HD21	2:A:371:VAL:HB	1.78	0.62
3:K:96:GLY:HA3	3:K:366:ASN:O	1.98	0.62
3:K:181:ARG:HG3	3:K:181:ARG:O	1.98	0.62
1:B:10:GLY:N	1:B:147:MET:HE1	2.15	0.62
1:B:191:GLN:HG2	1:B:195:ASN:ND2	2.14	0.62
1:B:289:LEU:HD12	1:B:289:LEU:N	2.15	0.62
2:A:117:LEU:HD22	2:A:117:LEU:N	2.14	0.62
3:K:94:ILE:HG12	3:K:147:LEU:CD2	2.28	0.62
3:K:109:THR:HB	3:K:335:THR:HB	1.81	0.62
1:B:97:ALA:CA	1:B:104:GLY:HA3	2.30	0.62
1:B:138:SER:CB	1:B:169:VAL:HG22	2.29	0.62
1:B:155:ILE:O	1:B:158:GLU:HG3	1.99	0.62
1:B:304:ASP:HB3	1:B:307:HIS:CD2	2.33	0.62
2:A:72:PRO:HA	2:A:94:THR:OG1	2.00	0.62
1:B:341:PHE:HZ	1:B:347:ASN:N	1.97	0.62
1:B:361:LEU:HG	1:B:363:MET:O	2.00	0.62
2:A:19:ALA:HA	2:A:22:GLU:OE1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:31:GLN:NE2	2:A:33:ASP:HB3	2.15	0.62
2:A:240:ALA:O	2:A:243:ARG:HG3	2.00	0.62
3:K:17:LYS:CD	3:K:363:PRO:HG2	2.28	0.62
3:K:160:LEU:N	3:K:172:LEU:HD22	2.12	0.62
3:K:227:LEU:CG	3:K:228:MET:HE3	2.30	0.62
1:B:240:LEU:HD12	1:B:247:ASN:OD1	2.00	0.62
2:A:224:TYR:CG	4:A:501:G2P:O6	2.53	0.62
2:A:234:ILE:HD12	2:A:235:VAL:N	2.15	0.62
2:A:274:PRO:N	2:A:291:ILE:HG23	2.15	0.62
1:B:70:PRO:CD	1:B:94:GLN:HG2	2.30	0.61
1:B:363:MET:H	1:B:363:MET:CE	2.12	0.61
1:B:421:GLU:O	1:B:424:GLN:HB3	1.99	0.61
2:A:103:TYR:HE2	2:A:151:SER:CB	2.12	0.61
2:A:180:ALA:HB3	2:A:183:GLU:HG3	1.82	0.61
3:K:115:MET:HE1	3:K:135:ILE:HD11	1.80	0.61
3:K:173:ASN:HB2	3:K:176:SER:HB2	1.81	0.61
1:B:323:MET:CE	1:B:326:VAL:HG21	2.29	0.61
1:B:323:MET:C	2:A:221:ARG:HG3	2.20	0.61
1:B:404:ASP:OD1	1:B:406:MET:HE2	2.00	0.61
2:A:176:GLN:HE21	2:A:207:GLU:HB2	1.64	0.61
3:K:200:GLU:O	3:K:200:GLU:HG2	1.98	0.61
3:K:202:ILE:HD12	3:K:203:THR:N	2.15	0.61
1:B:116:VAL:O	1:B:120:VAL:HG22	2.00	0.61
1:B:200:TYR:CD1	1:B:268:PRO:HG3	2.36	0.61
1:B:214:THR:HG22	1:B:275:SER:HA	1.82	0.61
1:B:285:THR:HG22	1:B:288:GLU:CB	2.17	0.61
1:B:305:PRO:HB3	1:B:310:TYR:OH	1.99	0.61
2:A:9:VAL:HG13	2:A:149:PHE:HD1	1.65	0.61
2:A:310:GLY:CA	2:A:381:THR:HB	2.28	0.61
3:K:78:GLN:CD	3:K:113:PHE:CE2	2.74	0.61
1:B:101:TRP:HB2	1:B:145:SER:HB3	1.81	0.61
1:B:170:VAL:HG13	1:B:201:CYS:HB2	1.80	0.61
1:B:318:ARG:NH2	1:B:356:ILE:HG13	2.14	0.61
1:B:321:MET:HG3	1:B:325:GLU:HB2	1.82	0.61
2:A:143:GLY:CA	4:A:501:G2P:H3A1	2.30	0.61
2:A:324:VAL:HG23	2:A:327:ASP:H	1.65	0.61
3:K:93:VAL:O	3:K:259:GLY:HA3	2.00	0.61
3:K:269:SER:CB	3:K:288:ILE:HD11	2.29	0.61
1:B:1:MET:HA	1:B:49:VAL:HB	1.82	0.61
1:B:30:ILE:HA	1:B:36:TYR:HD1	1.65	0.61
1:B:234:SER:O	1:B:238:THR:HG23	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:LEU:O	1:B:292:GLN:HB3	1.99	0.61
1:B:288:GLU:HA	1:B:291:GLN:NE2	2.16	0.61
1:B:362:LYS:HA	1:B:362:LYS:CE	2.30	0.61
2:A:22:GLU:HA	2:A:25:CYS:SG	2.40	0.61
2:A:46:ASP:OD2	2:A:49:PHE:HB2	2.00	0.61
2:A:75:ILE:HG22	2:A:79:ARG:NE	2.15	0.61
2:A:210:TYR:HB3	2:A:221:ARG:HH21	1.65	0.61
2:A:312:TYR:CD2	2:A:341:ILE:HG23	2.35	0.61
2:A:427:ALA:HB2	3:K:57:LEU:CG	2.23	0.61
2:A:430:LYS:O	2:A:434:GLU:HG3	1.99	0.61
3:K:48:LYS:CD	3:K:71:VAL:H	2.13	0.61
3:K:329:ARG:HA	3:K:363:PRO:HB3	1.83	0.61
1:B:20:PHE:HD1	1:B:230:SER:CB	2.10	0.61
1:B:140:GLY:HA3	1:B:171:PRO:HG3	1.80	0.61
1:B:273:LEU:HG	1:B:298:ASN:CA	2.23	0.61
1:B:347:ASN:OD1	2:A:179:THR:O	2.18	0.61
2:A:163:LYS:HB2	2:A:163:LYS:NZ	2.16	0.61
3:K:361:ASN:CG	3:K:363:PRO:HD3	2.20	0.61
1:B:107:THR:HG23	1:B:108:GLU:N	2.15	0.61
1:B:186:THR:HG21	1:B:385:PHE:HD1	1.64	0.61
1:B:204:ASN:HA	1:B:207:LEU:CD2	2.31	0.61
1:B:259:PRO:HG2	1:B:262:ARG:HH12	1.64	0.61
2:A:122:ILE:HD12	2:A:123:ARG:N	2.15	0.61
3:K:115:MET:CE	3:K:135:ILE:HD11	2.31	0.61
3:K:181:ARG:HB2	3:K:181:ARG:NH1	2.12	0.61
1:B:42:LEU:HD22	1:B:42:LEU:N	2.16	0.61
1:B:143:THR:CG2	1:B:147:MET:HE3	2.31	0.61
1:B:314:ALA:H	1:B:368:ILE:CB	2.06	0.61
1:B:318:ARG:CD	1:B:358:PRO:HG3	2.31	0.61
2:A:63:PRO:CG	2:A:86:LEU:HD21	2.31	0.61
2:A:224:TYR:HH	4:A:501:G2P:C4	2.12	0.61
2:A:307:PRO:HD2	2:A:308:ARG:NH2	2.15	0.61
2:A:431:ASP:O	2:A:435:VAL:HG12	2.00	0.61
3:K:159:SER:CB	3:K:199:LEU:HD21	2.22	0.61
3:K:270:GLU:CD	3:K:275:SER:HB2	2.20	0.61
3:K:311:TYR:O	3:K:318:ARG:HG3	2.00	0.61
1:B:381:ILE:HA	1:B:384:GLN:CG	2.29	0.61
2:A:248:LEU:HD23	2:A:249:ASN:N	2.16	0.61
2:A:277:SER:H	2:A:280:LYS:CG	2.14	0.61
3:K:54:THR:HG23	3:K:55:GLY:N	2.16	0.61
3:K:68:PHE:CG	3:K:71:VAL:HG22	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:GLU:HG3	1:B:46:ARG:NE	2.13	0.61
1:B:108:GLU:HA	1:B:111:GLU:OE2	2.01	0.61
1:B:162:ARG:HA	1:B:162:ARG:NE	2.16	0.61
1:B:421:GLU:CD	1:B:424:GLN:HB3	2.21	0.61
2:A:101:ASN:O	2:A:182:VAL:HG11	2.00	0.61
2:A:130:THR:HG23	2:A:131:GLY:N	2.15	0.61
2:A:140:SER:HA	2:A:171:ILE:CG2	2.31	0.61
2:A:172:TYR:HE2	2:A:391:LEU:HD23	1.66	0.61
2:A:344:VAL:HA	2:A:438:ASP:CG	2.21	0.61
3:K:26:ARG:HD3	3:K:109:THR:HA	1.81	0.61
3:K:303:VAL:HG13	3:K:358:ASN:HD22	1.66	0.61
3:K:320:LEU:HD21	3:K:324:LEU:HD11	1.83	0.61
1:B:140:GLY:HA2	1:B:185:ALA:CB	2.31	0.60
1:B:208:TYR:CD2	1:B:220:PRO:HG2	2.36	0.60
1:B:347:ASN:HD22	2:A:177:VAL:CG2	2.14	0.60
2:A:23:LEU:HD12	2:A:363:VAL:CG1	2.30	0.60
2:A:78:VAL:HG13	2:A:83:TYR:CE1	2.36	0.60
2:A:183:GLU:HB2	2:A:184:PRO:HD3	1.83	0.60
3:K:28:PHE:CD2	3:K:32:GLU:HB3	2.36	0.60
3:K:77:LYS:HB3	3:K:80:ASP:OD2	2.00	0.60
1:B:215:LEU:O	1:B:215:LEU:HD23	2.01	0.60
2:A:409:VAL:HG11	3:K:289:ASN:C	2.22	0.60
3:K:17:LYS:HD3	3:K:363:PRO:CG	2.30	0.60
3:K:189:ARG:NH1	3:K:193:GLY:HA3	2.15	0.60
1:B:108:GLU:OE1	1:B:147:MET:HA	2.01	0.60
1:B:151:LEU:O	1:B:155:ILE:HG12	2.01	0.60
1:B:244:GLY:HA2	1:B:355:ASP:HB2	1.81	0.60
1:B:246:LEU:H	1:B:353:VAL:CG2	2.14	0.60
2:A:78:VAL:HB	2:A:92:LEU:HD21	1.82	0.60
2:A:210:TYR:HB3	2:A:221:ARG:NH2	2.15	0.60
2:A:229:ARG:O	2:A:363:VAL:HG11	2.00	0.60
2:A:274:PRO:HB2	2:A:276:ILE:HD11	1.83	0.60
3:K:272:ILE:HB	3:K:282:ALA:HB1	1.83	0.60
1:B:46:ARG:HH12	1:B:49:VAL:CG1	2.14	0.60
1:B:139:LEU:HD13	1:B:185:ALA:HB1	1.81	0.60
1:B:271:ALA:HB3	1:B:365:ALA:HB3	1.82	0.60
1:B:382:SER:HB3	1:B:415:MET:HE1	1.84	0.60
3:K:15:LYS:HE2	3:K:362:LYS:CE	2.31	0.60
3:K:55:GLY:N	3:K:60:LYS:HA	2.15	0.60
2:A:26:LEU:HD22	2:A:364:PRO:HB3	1.81	0.60
2:A:155:GLU:HG2	2:A:156:ARG:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:317:LEU:HD22	2:A:377:MET:CE	2.31	0.60
2:A:321:GLY:HA3	2:A:372:GLN:O	2.01	0.60
3:K:228:MET:HA	3:K:228:MET:HE2	1.83	0.60
1:B:1:MET:HA	1:B:1:MET:CE	2.30	0.60
1:B:151:LEU:HD12	1:B:152:ILE:CA	2.32	0.60
1:B:337:ASN:OD1	1:B:339:SER:HB3	2.02	0.60
2:A:70:LEU:CG	2:A:110:ILE:HG21	2.19	0.60
2:A:216:ASN:HB3	2:A:280:LYS:CD	2.31	0.60
2:A:221:ARG:HH11	2:A:221:ARG:HA	1.66	0.60
2:A:407:TRP:HA	2:A:407:TRP:HE3	1.66	0.60
3:K:190:ASN:HD22	3:K:191:LYS:N	1.99	0.60
1:B:101:TRP:CH2	1:B:403:MET:HG3	2.36	0.60
2:A:115:ILE:HG23	2:A:116:ASP:N	2.17	0.60
2:A:154:MET:HE2	2:A:154:MET:CA	2.31	0.60
2:A:271:THR:O	2:A:376:CYS:HA	2.02	0.60
2:A:287:SER:HB3	2:A:290:GLU:HG3	1.83	0.60
3:K:215:GLU:OE2	3:K:216:LYS:HE3	2.01	0.60
3:K:246:LYS:NZ	3:K:254:GLU:OE2	2.35	0.60
1:B:67:ASP:CG	1:B:73:MET:HB3	2.22	0.60
1:B:225:LEU:HD12	1:B:226:ASN:N	2.17	0.60
1:B:262:ARG:NE	3:K:297:ARG:HH12	1.98	0.60
1:B:293:MET:CE	1:B:367:PHE:HA	2.31	0.60
1:B:318:ARG:NH2	1:B:358:PRO:HA	2.16	0.60
2:A:31:GLN:HE22	2:A:33:ASP:HB3	1.65	0.60
3:K:77:LYS:HE3	3:K:78:GLN:HB2	1.83	0.60
3:K:145:GLU:HG2	3:K:207:LYS:NZ	2.17	0.60
3:K:170:ASP:OD2	3:K:180:GLU:HG2	2.02	0.60
1:B:36:TYR:CD2	1:B:44:LEU:HB2	2.37	0.60
1:B:90:PHE:HE1	1:B:92:PHE:CE1	2.19	0.60
1:B:241:ARG:HD2	1:B:242:PHE:N	2.17	0.60
2:A:16:ILE:HG23	2:A:17:GLY:N	2.16	0.60
2:A:135:PHE:HE1	2:A:166:LYS:HA	1.66	0.60
2:A:317:LEU:HD22	2:A:377:MET:HE3	1.84	0.60
3:K:48:LYS:NZ	3:K:70:MET:HG3	2.16	0.60
3:K:152:THR:O	3:K:154:PHE:HD2	1.85	0.60
3:K:215:GLU:HG2	3:K:216:LYS:N	2.17	0.60
1:B:381:ILE:HA	1:B:384:GLN:HG3	1.82	0.60
2:A:171:ILE:HG13	2:A:204:VAL:CG1	2.32	0.60
2:A:204:VAL:HG13	2:A:206:ASN:OD1	2.01	0.60
2:A:255:PHE:HZ	2:A:352:LYS:H	1.50	0.60
2:A:259:LEU:CD1	2:A:378:LEU:HD12	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:326:LYS:NZ	2:A:326:LYS:HB3	2.17	0.60
1:B:154:LYS:HE2	1:B:157:GLU:CB	2.26	0.59
1:B:272:PRO:HB3	1:B:292:GLN:HE22	1.67	0.59
1:B:318:ARG:CZ	1:B:358:PRO:HA	2.31	0.59
2:A:78:VAL:O	2:A:84:ARG:HB2	2.02	0.59
2:A:103:TYR:HD2	2:A:147:SER:C	2.05	0.59
2:A:105:ARG:HB2	2:A:411:GLU:OE2	2.01	0.59
2:A:174:ALA:HB2	2:A:207:GLU:N	2.15	0.59
2:A:349:THR:HG1	2:A:351:PHE:HD1	1.50	0.59
3:K:16:GLY:CA	3:K:363:PRO:HD2	2.31	0.59
3:K:102:PHE:HD1	3:K:264:VAL:CG1	2.15	0.59
1:B:84:ILE:HG23	1:B:85:PHE:CD1	2.37	0.59
1:B:217:LEU:HD13	1:B:218:THR:H	1.65	0.59
1:B:323:MET:CA	1:B:326:VAL:HG23	2.33	0.59
2:A:409:VAL:CB	3:K:290:GLN:HA	2.30	0.59
3:K:77:LYS:CD	3:K:78:GLN:H	2.15	0.59
3:K:226:THR:HG23	3:K:232:SER:HB3	1.84	0.59
3:K:329:ARG:HA	3:K:363:PRO:HG3	1.84	0.59
1:B:113:VAL:HG23	1:B:114:ASP:N	2.17	0.59
1:B:137:HIS:HE1	1:B:166:THR:CG2	2.15	0.59
1:B:404:ASP:OD1	1:B:406:MET:HG2	2.02	0.59
2:A:189:LEU:HD12	2:A:192:HIS:HE1	1.66	0.59
2:A:294:ALA:HA	2:A:297:GLU:OE1	2.02	0.59
3:K:59:ASP:HA	3:K:60:LYS:NZ	2.17	0.59
3:K:204:VAL:HG11	3:K:209:GLU:HB3	1.84	0.59
1:B:9:ALA:HB1	1:B:147:MET:SD	2.42	0.59
1:B:118:ASP:O	1:B:122:LYS:HD2	2.03	0.59
1:B:141:GLY:HA3	4:B:501:G2P:C5'	2.32	0.59
1:B:167:PHE:HE1	1:B:200:TYR:CD2	2.20	0.59
1:B:170:VAL:HG22	1:B:203:ASP:HA	1.83	0.59
1:B:178:THR:CG2	1:B:180:VAL:HG22	2.32	0.59
2:A:6:SER:HB2	2:A:21:TRP:HZ2	1.68	0.59
2:A:274:PRO:CD	2:A:291:ILE:HG23	2.32	0.59
2:A:276:ILE:HG22	2:A:277:SER:O	2.02	0.59
3:K:60:LYS:H	3:K:60:LYS:HD2	1.67	0.59
3:K:192:ARG:CB	3:K:322:ASP:HA	2.32	0.59
1:B:131:GLN:NE2	1:B:131:GLN:HA	2.17	0.59
1:B:160:PRO:CB	3:K:283:ARG:HH22	2.14	0.59
1:B:276:ARG:O	1:B:280:GLN:HG2	2.03	0.59
1:B:324:LYS:HD2	2:A:221:ARG:NH1	2.16	0.59
2:A:408:TYR:O	2:A:411:GLU:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:41:VAL:HB	3:K:338:PRO:HA	1.85	0.59
3:K:184:MET:SD	3:K:194:VAL:HG21	2.42	0.59
3:K:258:ILE:H	3:K:368:LYS:CD	2.16	0.59
1:B:68:LEU:O	1:B:68:LEU:HD23	2.03	0.59
1:B:272:PRO:CG	1:B:284:LEU:HD11	2.33	0.59
1:B:375:GLN:HG3	1:B:376:GLU:OE2	2.03	0.59
2:A:4:CYS:SG	2:A:135:PHE:HA	2.42	0.59
2:A:188:ILE:CG2	2:A:421:ALA:HB1	2.31	0.59
2:A:242:LEU:HB2	2:A:252:LEU:CD1	2.31	0.59
2:A:280:LYS:HA	2:A:283:HIS:HD2	1.66	0.59
3:K:82:TYR:CZ	3:K:86:VAL:CB	2.85	0.59
1:B:145:SER:HB3	1:B:188:SER:OG	2.02	0.59
1:B:167:PHE:HE1	1:B:200:TYR:HD2	1.49	0.59
1:B:221:THR:HG22	1:B:223:GLY:H	1.66	0.59
1:B:243:PRO:C	1:B:355:ASP:HB2	2.23	0.59
1:B:306:ARG:HH21	1:B:309:ARG:NH2	2.00	0.59
2:A:277:SER:HB3	2:A:280:LYS:H	1.67	0.59
3:K:23:VAL:HG21	3:K:68:PHE:HE1	1.66	0.59
3:K:66:TYR:HB3	3:K:68:PHE:CZ	2.37	0.59
2:A:11:GLN:HG3	2:A:71:GLU:OE1	2.03	0.59
2:A:78:VAL:HB	2:A:92:LEU:CD2	2.32	0.59
2:A:214:ARG:HH21	2:A:219:ILE:N	2.00	0.59
3:K:15:LYS:O	3:K:362:LYS:HA	2.02	0.59
1:B:53:GLU:HA	1:B:58:LYS:O	2.03	0.59
1:B:303:CYS:HB2	1:B:371:SER:HB3	1.83	0.59
2:A:295:CYS:HA	2:A:300:ASN:CG	2.22	0.59
3:K:48:LYS:HA	3:K:71:VAL:HB	1.85	0.59
3:K:157:LYS:CB	3:K:201:GLU:HB3	2.21	0.59
3:K:181:ARG:HH22	3:K:183:GLN:HB2	1.68	0.59
3:K:228:MET:CE	3:K:228:MET:HA	2.33	0.59
3:K:284:GLU:HA	3:K:287:ASN:HD22	1.67	0.59
1:B:34:GLY:HA2	1:B:84:ILE:HD13	1.84	0.59
1:B:215:LEU:HD23	1:B:276:ARG:NE	2.17	0.59
2:A:97:GLU:CD	2:A:105:ARG:HH22	2.07	0.59
2:A:146:GLY:O	2:A:150:THR:HG22	2.03	0.59
2:A:229:ARG:HH21	2:A:363:VAL:HB	1.68	0.59
2:A:351:PHE:HB2	2:A:352:LYS:HZ3	1.68	0.59
3:K:171:LEU:N	3:K:171:LEU:HD23	2.18	0.59
3:K:272:ILE:HD13	3:K:272:ILE:N	2.17	0.59
1:B:20:PHE:CE1	1:B:233:MET:HB2	2.37	0.58
1:B:139:LEU:HD11	1:B:171:PRO:CD	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ARG:CD	1:B:262:ARG:H	2.14	0.58
1:B:272:PRO:HA	1:B:292:GLN:HE22	1.67	0.58
1:B:309:ARG:HB2	1:B:426:GLN:CA	2.19	0.58
2:A:171:ILE:HG13	2:A:204:VAL:HG11	1.84	0.58
3:K:321:GLN:CA	3:K:324:LEU:HD23	2.31	0.58
1:B:20:PHE:O	1:B:23:VAL:HG12	2.04	0.58
1:B:140:GLY:CA	1:B:185:ALA:HB2	2.32	0.58
1:B:277:GLY:CA	1:B:280:GLN:HE21	2.08	0.58
1:B:376:GLU:HB2	1:B:380:ARG:HH22	1.68	0.58
2:A:141:PHE:HB2	2:A:171:ILE:O	2.03	0.58
2:A:239:THR:O	2:A:243:ARG:HG2	2.03	0.58
2:A:428:LEU:HD12	2:A:428:LEU:O	2.03	0.58
3:K:191:LYS:H	3:K:191:LYS:NZ	2.01	0.58
1:B:156:ARG:HE	1:B:157:GLU:HA	1.67	0.58
1:B:174:LYS:HD2	1:B:175:VAL:HG23	1.86	0.58
1:B:339:SER:HA	1:B:429:THR:HG22	1.84	0.58
1:B:392:LYS:CA	1:B:395:LEU:HD21	2.33	0.58
2:A:93:ILE:CD1	2:A:118:VAL:HG12	2.33	0.58
2:A:287:SER:HB3	2:A:290:GLU:OE2	2.02	0.58
2:A:420:GLU:OE1	2:A:420:GLU:HA	2.02	0.58
3:K:26:ARG:HH21	3:K:337:SER:HB2	1.67	0.58
3:K:95:MET:HB2	3:K:365:VAL:CG1	2.32	0.58
3:K:109:THR:HG21	3:K:336:ILE:H	1.65	0.58
1:B:228:LEU:HD21	1:B:300:MET:HE1	1.85	0.58
1:B:251:ARG:CD	2:A:105:ARG:HE	2.16	0.58
1:B:318:ARG:HD3	1:B:358:PRO:HG3	1.85	0.58
2:A:78:VAL:CA	2:A:83:TYR:HE1	2.15	0.58
2:A:217:LEU:HD23	2:A:277:SER:OG	2.03	0.58
2:A:423:GLU:CD	3:K:57:LEU:HD13	2.22	0.58
3:K:48:LYS:C	3:K:71:VAL:HG21	2.23	0.58
3:K:92:GLU:HB3	3:K:97:TYR:CG	2.38	0.58
1:B:190:HIS:CG	1:B:411:ALA:HB1	2.38	0.58
1:B:246:LEU:O	1:B:352:ALA:HB1	2.04	0.58
2:A:114:ILE:HG23	2:A:115:ILE:N	2.18	0.58
3:K:84:SER:CB	3:K:84:SER:HG	1.24	0.58
3:K:109:THR:HB	3:K:335:THR:CB	2.34	0.58
3:K:170:ASP:HB3	3:K:177:ASP:O	2.03	0.58
3:K:202:ILE:HD12	3:K:203:THR:H	1.68	0.58
3:K:275:SER:OG	3:K:277:ALA:HB2	2.03	0.58
3:K:311:TYR:CE1	3:K:324:LEU:HD23	2.39	0.58
1:B:119:VAL:HG12	1:B:123:GLU:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ALA:HB2	1:B:305:PRO:CD	2.33	0.58
2:A:156:ARG:NH1	2:A:157:LEU:HG	2.18	0.58
2:A:215:ARG:HH11	2:A:216:ASN:HA	1.69	0.58
2:A:216:ASN:ND2	2:A:280:LYS:HD2	2.18	0.58
3:K:48:LYS:HE3	3:K:70:MET:CA	2.25	0.58
3:K:191:LYS:HZ2	3:K:191:LYS:N	2.01	0.58
1:B:309:ARG:HD2	1:B:429:THR:CA	2.33	0.58
2:A:360:PRO:HG3	2:A:374:ALA:N	2.18	0.58
3:K:15:LYS:HD3	3:K:362:LYS:CD	2.33	0.58
3:K:180:GLU:CD	3:K:199:LEU:HA	2.24	0.58
3:K:190:ASN:HB3	3:K:193:GLY:H	1.69	0.58
1:B:21:TRP:HH2	1:B:50:TYR:CZ	2.22	0.58
1:B:54:ALA:CB	1:B:58:LYS:HB3	2.24	0.58
1:B:323:MET:HA	1:B:323:MET:HE3	1.86	0.58
1:B:362:LYS:HD2	1:B:362:LYS:N	2.17	0.58
2:A:78:VAL:HG13	2:A:83:TYR:HE1	1.69	0.58
2:A:174:ALA:CB	2:A:176:GLN:HG2	2.33	0.58
2:A:217:LEU:HA	2:A:277:SER:OG	2.03	0.58
2:A:339:ARG:HH22	2:A:342:GLN:CB	2.17	0.58
3:K:68:PHE:CB	3:K:71:VAL:HG22	2.33	0.58
1:B:111:GLU:HA	1:B:114:ASP:OD2	2.04	0.58
1:B:260:PHE:C	1:B:262:ARG:HD3	2.25	0.58
2:A:8:HIS:O	2:A:68:VAL:HG22	2.04	0.58
2:A:67:PHE:HB2	2:A:92:LEU:HD12	1.85	0.58
2:A:67:PHE:HB2	2:A:92:LEU:HD13	1.85	0.58
3:K:236:HIS:N	3:K:267:ALA:HB2	2.19	0.58
1:B:45:GLU:HG2	1:B:46:ARG:N	2.18	0.58
1:B:138:SER:O	1:B:144:GLY:HA3	2.04	0.58
2:A:430:LYS:HD3	2:A:434:GLU:HG3	1.84	0.58
3:K:44:ASP:OD2	3:K:47:ARG:HG2	2.04	0.58
3:K:190:ASN:HB3	3:K:193:GLY:N	2.19	0.58
3:K:235:SER:C	3:K:267:ALA:HB2	2.24	0.58
1:B:44:LEU:O	1:B:48:ASN:HB2	2.03	0.57
1:B:191:GLN:HG2	1:B:195:ASN:HD21	1.69	0.57
1:B:213:ARG:HE	1:B:214:THR:HG22	1.68	0.57
1:B:410:GLU:HA	1:B:410:GLU:OE2	2.03	0.57
2:A:2:ARG:HG3	2:A:131:GLY:O	2.04	0.57
2:A:11:GLN:HB3	2:A:74:VAL:HG11	1.86	0.57
2:A:272:TYR:HE1	2:A:374:ALA:CB	2.15	0.57
3:K:222:THR:HG23	3:K:231:TYR:CE2	2.39	0.57
1:B:139:LEU:HD12	1:B:185:ALA:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:SER:OG	1:B:188:SER:HB2	2.04	0.57
1:B:151:LEU:CD1	1:B:152:ILE:HG12	2.34	0.57
2:A:9:VAL:HG23	2:A:138:PHE:O	2.04	0.57
2:A:156:ARG:HH12	2:A:157:LEU:HG	1.68	0.57
2:A:429:GLU:OE1	2:A:429:GLU:HA	2.04	0.57
3:K:136:ILE:CG2	3:K:214:LEU:HD11	2.34	0.57
1:B:67:ASP:H	1:B:92:PHE:HB2	1.68	0.57
1:B:288:GLU:O	1:B:292:GLN:HG3	2.04	0.57
2:A:5:ILE:CG2	2:A:65:ALA:HA	2.34	0.57
2:A:185:TYR:HB3	2:A:408:TYR:HE1	1.68	0.57
2:A:260:VAL:HG23	2:A:260:VAL:O	2.04	0.57
2:A:268:PRO:HB3	2:A:380:ASN:OD1	2.05	0.57
2:A:388:TRP:CZ3	2:A:428:LEU:HD21	2.39	0.57
3:K:272:ILE:HG12	3:K:273:GLY:N	2.19	0.57
1:B:108:GLU:OE2	1:B:147:MET:HB3	2.04	0.57
1:B:324:LYS:HE3	2:A:221:ARG:NH1	2.15	0.57
1:B:337:ASN:HB3	1:B:340:TYR:CB	2.32	0.57
2:A:12:ALA:HA	2:A:15:GLN:HE22	1.70	0.57
2:A:67:PHE:O	2:A:93:ILE:HG12	2.03	0.57
2:A:273:ALA:HB3	2:A:375:VAL:HG21	1.86	0.57
2:A:319:TYR:CB	2:A:355:ILE:HA	2.08	0.57
3:K:92:GLU:HB3	3:K:97:TYR:CB	2.34	0.57
3:K:189:ARG:HH11	3:K:193:GLY:HA3	1.70	0.57
3:K:227:LEU:H	3:K:227:LEU:CD2	2.16	0.57
1:B:32:PRO:HG3	1:B:81:PHE:CE1	2.40	0.57
1:B:112:LEU:O	1:B:116:VAL:HG13	2.03	0.57
1:B:284:LEU:HD22	1:B:288:GLU:OE1	2.04	0.57
1:B:309:ARG:HD2	1:B:429:THR:O	2.04	0.57
1:B:326:VAL:O	1:B:329:GLN:HG3	2.04	0.57
2:A:176:GLN:NE2	2:A:207:GLU:HA	2.18	0.57
2:A:246:GLY:HA3	2:A:355:ILE:O	2.03	0.57
3:K:110:GLY:HA3	3:K:113:PHE:HB3	1.87	0.57
3:K:215:GLU:HG3	3:K:216:LYS:HE3	1.85	0.57
3:K:327:ARG:H	3:K:327:ARG:NH2	1.99	0.57
2:A:105:ARG:HD2	2:A:407:TRP:HZ2	1.70	0.57
2:A:223:THR:HG22	2:A:224:TYR:N	2.19	0.57
3:K:223:THR:HG21	3:K:235:SER:N	2.11	0.57
3:K:327:ARG:HA	3:K:362:LYS:O	2.05	0.57
1:B:186:THR:HG23	1:B:187:LEU:N	2.19	0.57
1:B:271:ALA:CB	1:B:365:ALA:HB3	2.34	0.57
2:A:97:GLU:OE2	2:A:110:ILE:HD11	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:SD	1:B:127:CYS:HB3	2.44	0.57
1:B:20:PHE:O	1:B:24:ILE:HG12	2.04	0.57
1:B:62:ARG:NH1	1:B:62:ARG:HA	2.19	0.57
1:B:217:LEU:HD13	1:B:219:THR:H	1.69	0.57
1:B:240:LEU:HD13	1:B:248:ALA:O	2.05	0.57
1:B:244:GLY:CA	1:B:355:ASP:HB2	2.34	0.57
2:A:11:GLN:CB	2:A:74:VAL:HG11	2.34	0.57
2:A:35:GLN:OE1	2:A:35:GLN:HA	2.03	0.57
2:A:70:LEU:HD22	2:A:99:ALA:CB	2.35	0.57
2:A:248:LEU:HB3	2:A:354:GLY:HA2	1.87	0.57
2:A:282:TYR:CD1	2:A:369:ALA:HB2	2.39	0.57
2:A:319:TYR:CD2	2:A:375:VAL:HG12	2.40	0.57
3:K:54:THR:HG23	3:K:56:GLY:N	2.19	0.57
3:K:109:THR:HG21	3:K:335:THR:HB	1.83	0.57
3:K:162:GLU:OE2	3:K:235:SER:HB2	2.05	0.57
1:B:103:LYS:CG	1:B:401:GLU:HG2	2.34	0.57
2:A:30:ILE:HD12	2:A:61:HIS:CG	2.40	0.57
2:A:33:ASP:CG	2:A:35:GLN:H	2.08	0.57
2:A:41:THR:HG22	2:A:46:ASP:OD2	2.05	0.57
2:A:187:SER:O	2:A:191:THR:HG22	2.05	0.57
2:A:246:GLY:HA2	2:A:357:TYR:N	2.17	0.57
2:A:275:VAL:HG13	2:A:275:VAL:O	2.05	0.57
2:A:388:TRP:HB2	2:A:425:MET:HE2	1.87	0.57
1:B:245:GLN:NE2	1:B:355:ASP:HA	2.20	0.57
2:A:4:CYS:N	2:A:51:THR:HG22	2.19	0.57
2:A:153:LEU:HD11	2:A:157:LEU:CD1	2.33	0.57
2:A:176:GLN:HG3	2:A:177:VAL:H	1.69	0.57
2:A:278:ALA:HB1	2:A:282:TYR:CZ	2.40	0.57
2:A:409:VAL:CB	3:K:293:LEU:CD2	2.80	0.57
2:A:410:GLY:CA	3:K:290:GLN:NE2	2.58	0.57
3:K:26:ARG:HE	3:K:337:SER:CB	2.17	0.57
3:K:43:CYS:C	3:K:45:PRO:HD3	2.26	0.57
1:B:19:LYS:HZ3	1:B:19:LYS:N	2.02	0.56
1:B:187:LEU:HG	1:B:408:PHE:CE2	2.40	0.56
1:B:266:PHE:CE2	1:B:311:LEU:HG	2.40	0.56
2:A:108:TYR:O	2:A:112:LYS:HG2	2.05	0.56
2:A:112:LYS:O	2:A:115:ILE:HG22	2.04	0.56
2:A:122:ILE:HD12	2:A:123:ARG:HA	1.86	0.56
2:A:311:LYS:HA	2:A:342:GLN:NE2	2.20	0.56
2:A:395:PHE:HA	2:A:398:MET:HG2	1.87	0.56
2:A:401:LYS:HA	2:A:401:LYS:HZ3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:181:ARG:HH22	3:K:197:LYS:NZ	2.03	0.56
3:K:303:VAL:HG22	3:K:358:ASN:HB2	1.87	0.56
3:K:343:LEU:H	3:K:343:LEU:CD2	2.10	0.56
3:K:347:LEU:O	3:K:347:LEU:HD23	2.04	0.56
3:K:361:ASN:OD1	3:K:363:PRO:HG3	2.05	0.56
1:B:81:PHE:HA	1:B:83:GLN:HE22	1.70	0.56
1:B:116:VAL:HG23	1:B:117:LEU:N	2.20	0.56
1:B:183:TYR:CE1	1:B:385:PHE:HB3	2.40	0.56
1:B:216:LYS:HE2	1:B:277:GLY:CA	2.31	0.56
2:A:9:VAL:HG11	2:A:149:PHE:HB3	1.87	0.56
2:A:317:LEU:HG	2:A:353:VAL:CG1	2.34	0.56
2:A:358:GLN:HG2	2:A:359:PRO:CD	2.35	0.56
3:K:41:VAL:CB	3:K:338:PRO:HA	2.34	0.56
3:K:221:ARG:HD2	3:K:221:ARG:O	2.05	0.56
3:K:361:ASN:C	3:K:363:PRO:HD3	2.25	0.56
1:B:4:ILE:CG2	1:B:133:PHE:HA	2.24	0.56
1:B:102:ALA:HB3	1:B:401:GLU:OE1	2.03	0.56
1:B:149:THR:HG21	1:B:188:SER:HA	1.87	0.56
1:B:216:LYS:HD3	1:B:276:ARG:NH1	2.20	0.56
1:B:260:PHE:CB	3:K:297:ARG:HH22	2.18	0.56
1:B:284:LEU:HD13	1:B:289:LEU:CD2	2.36	0.56
1:B:308:GLY:HA2	1:B:372:THR:N	2.20	0.56
1:B:327:ASP:O	1:B:331:LEU:HD13	2.05	0.56
1:B:374:ILE:HG13	1:B:378:PHE:CZ	2.40	0.56
2:A:5:ILE:HD11	2:A:125:LEU:HG	1.87	0.56
2:A:102:ASN:CB	2:A:105:ARG:HD2	2.35	0.56
2:A:172:TYR:N	2:A:204:VAL:HG12	2.18	0.56
2:A:188:ILE:CG1	2:A:395:PHE:HD1	2.18	0.56
2:A:246:GLY:HA3	2:A:356:ASN:CA	2.18	0.56
2:A:263:PRO:HD2	2:A:264:ARG:CD	2.33	0.56
2:A:275:VAL:HB	2:A:300:ASN:ND2	2.18	0.56
2:A:387:ALA:HA	2:A:390:ARG:HD2	1.85	0.56
3:K:26:ARG:NH1	3:K:338:PRO:HD2	2.20	0.56
3:K:68:PHE:HB2	3:K:71:VAL:HG23	1.85	0.56
3:K:290:GLN:HA	3:K:293:LEU:HD23	1.86	0.56
3:K:341:LEU:HD12	3:K:341:LEU:N	2.19	0.56
1:B:322:SER:HB3	1:B:325:GLU:CG	2.34	0.56
2:A:262:TYR:HD2	2:A:265:ILE:HG12	1.70	0.56
2:A:275:VAL:HG13	2:A:280:LYS:CE	2.35	0.56
2:A:390:ARG:O	2:A:394:LYS:HD2	2.04	0.56
3:K:32:GLU:CB	3:K:33:ARG:HH21	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:GLN:NE2	1:B:83:GLN:H	2.04	0.56
2:A:1:MET:HB2	2:A:47:ASP:CB	2.35	0.56
2:A:4:CYS:CA	2:A:132:LEU:HG	2.04	0.56
2:A:205:ASP:HB3	2:A:208:ALA:CB	2.36	0.56
2:A:409:VAL:HG12	3:K:290:GLN:N	2.19	0.56
3:K:43:CYS:O	3:K:45:PRO:HD3	2.06	0.56
1:B:42:LEU:O	1:B:45:GLU:HG2	2.05	0.56
1:B:84:ILE:HG23	1:B:85:PHE:N	2.19	0.56
1:B:266:PHE:CE1	1:B:369:GLY:HA2	2.40	0.56
1:B:320:ARG:H	1:B:320:ARG:CZ	2.19	0.56
1:B:324:LYS:N	1:B:324:LYS:HD3	2.19	0.56
1:B:377:LEU:HA	1:B:380:ARG:HG3	1.88	0.56
1:B:384:GLN:O	1:B:388:MET:HG2	2.05	0.56
2:A:63:PRO:CD	2:A:86:LEU:HD11	2.30	0.56
2:A:117:LEU:H	2:A:117:LEU:CD2	2.17	0.56
2:A:240:ALA:HA	2:A:243:ARG:NE	2.20	0.56
3:K:135:ILE:HD11	3:K:136:ILE:HG13	1.88	0.56
3:K:272:ILE:CD1	3:K:272:ILE:H	2.18	0.56
1:B:2:ARG:HG3	1:B:131:GLN:H	1.70	0.56
1:B:208:TYR:HE2	1:B:225:LEU:HD23	1.69	0.56
2:A:71:GLU:HB3	2:A:98:ASP:CB	2.36	0.56
2:A:150:THR:HG23	2:A:151:SER:N	2.21	0.56
2:A:191:THR:O	2:A:194:THR:HG22	2.06	0.56
2:A:235:VAL:HA	2:A:238:ILE:HD12	1.87	0.56
2:A:313:MET:HA	2:A:344:VAL:HG13	1.87	0.56
3:K:48:LYS:NZ	3:K:71:VAL:H	2.03	0.56
1:B:15:GLN:OE1	1:B:19:LYS:HE3	2.05	0.56
1:B:31:ASP:HB2	1:B:33:THR:HG22	1.88	0.56
1:B:130:LEU:HD12	1:B:130:LEU:N	2.20	0.56
1:B:213:ARG:HG3	1:B:214:THR:H	1.70	0.56
2:A:125:LEU:HD12	2:A:128:GLN:CG	2.36	0.56
2:A:172:TYR:H	2:A:204:VAL:CG1	2.19	0.56
2:A:288:VAL:HG21	2:A:327:ASP:HB2	1.88	0.56
2:A:305:CYS:SG	2:A:383:ALA:HB3	2.45	0.56
2:A:323:VAL:HB	2:A:355:ILE:HG21	1.86	0.56
3:K:321:GLN:O	3:K:324:LEU:HD23	2.06	0.56
1:B:3:GLU:OE1	1:B:49:VAL:HG23	2.05	0.56
1:B:284:LEU:CD1	1:B:361:LEU:HD12	2.32	0.56
2:A:53:PHE:CD2	2:A:63:PRO:HA	2.41	0.56
2:A:163:LYS:HB2	2:A:163:LYS:HZ1	1.69	0.56
2:A:402:ARG:HG3	2:A:405:VAL:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:26:ARG:NH2	3:K:32:GLU:HG3	2.20	0.56
3:K:97:TYR:HA	3:K:366:ASN:H	1.70	0.56
1:B:192:LEU:HD13	1:B:192:LEU:C	2.26	0.56
1:B:214:THR:HB	1:B:275:SER:HA	1.87	0.56
1:B:379:LYS:HB3	1:B:419:VAL:HG11	1.88	0.56
1:B:382:SER:HB3	1:B:415:MET:CE	2.36	0.56
2:A:154:MET:HA	2:A:154:MET:CE	2.36	0.56
2:A:233:GLN:HB3	2:A:363:VAL:HG13	1.88	0.56
2:A:427:ALA:CA	3:K:57:LEU:HD22	2.33	0.56
3:K:82:TYR:CE2	3:K:86:VAL:CB	2.88	0.56
3:K:95:MET:CG	3:K:365:VAL:CG1	2.79	0.56
3:K:172:LEU:HD21	3:K:199:LEU:CD1	2.35	0.56
1:B:11:GLN:N	4:B:501:G2P:O2A	2.39	0.55
1:B:28:HIS:HB3	1:B:30:ILE:HG23	1.86	0.55
1:B:139:LEU:HG	1:B:169:VAL:O	2.06	0.55
1:B:215:LEU:CG	1:B:217:LEU:HB2	2.36	0.55
2:A:75:ILE:HG23	2:A:92:LEU:CD1	2.35	0.55
2:A:182:VAL:HG12	2:A:186:ASN:OD1	2.06	0.55
3:K:15:LYS:HG2	3:K:16:GLY:N	2.20	0.55
3:K:94:ILE:HA	3:K:245:MET:HE1	1.87	0.55
1:B:35:SER:HA	1:B:57:ASN:O	2.05	0.55
1:B:175:VAL:HG12	1:B:176:SER:N	2.21	0.55
2:A:52:PHE:O	2:A:63:PRO:HA	2.06	0.55
2:A:137:VAL:HB	2:A:168:GLU:HA	1.88	0.55
2:A:233:GLN:NE2	2:A:234:ILE:HA	2.20	0.55
2:A:271:THR:CG2	2:A:377:MET:HB2	2.36	0.55
3:K:226:THR:CG2	3:K:232:SER:HB3	2.37	0.55
3:K:303:VAL:CG2	3:K:358:ASN:HD22	2.19	0.55
1:B:42:LEU:HA	1:B:45:GLU:CD	2.27	0.55
1:B:62:ARG:HA	1:B:62:ARG:HH11	1.71	0.55
1:B:112:LEU:HD23	1:B:112:LEU:C	2.27	0.55
1:B:113:VAL:HG23	1:B:114:ASP:OD1	2.07	0.55
1:B:245:GLN:CD	1:B:355:ASP:HA	2.26	0.55
2:A:31:GLN:H	2:A:36:MET:HA	1.71	0.55
2:A:118:VAL:HG23	2:A:119:LEU:N	2.21	0.55
2:A:171:ILE:HD12	4:A:501:G2P:N3	2.22	0.55
2:A:311:LYS:HG2	2:A:438:ASP:OD2	2.05	0.55
2:A:321:GLY:HA3	2:A:372:GLN:NE2	2.20	0.55
3:K:15:LYS:HD3	3:K:362:LYS:CG	2.36	0.55
3:K:15:LYS:HE3	3:K:364:GLU:CD	2.26	0.55
3:K:172:LEU:CD1	3:K:199:LEU:HD11	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:187:ASP:OD1	3:K:195:ILE:HG12	1.99	0.55
3:K:312:ARG:CA	3:K:318:ARG:CG	2.71	0.55
3:K:360:LEU:HD12	3:K:360:LEU:N	2.20	0.55
1:B:3:GLU:HG3	1:B:50:TYR:CA	2.37	0.55
1:B:11:GLN:CA	1:B:14:ASN:HB2	2.37	0.55
1:B:43:GLN:CA	1:B:242:PHE:HZ	2.19	0.55
1:B:142:GLY:HA2	1:B:184:ASN:OD1	2.06	0.55
1:B:199:THR:O	1:B:265:PHE:HD2	1.90	0.55
2:A:121:ARG:NH1	2:A:121:ARG:HG2	2.22	0.55
2:A:189:LEU:CD1	2:A:417:GLU:HG3	2.37	0.55
2:A:409:VAL:CG1	3:K:289:ASN:C	2.75	0.55
3:K:26:ARG:NH1	3:K:28:PHE:HA	2.18	0.55
1:B:1:MET:HG3	1:B:2:ARG:H	1.72	0.55
1:B:81:PHE:HA	1:B:83:GLN:NE2	2.22	0.55
1:B:259:PRO:HB2	1:B:262:ARG:NH1	2.22	0.55
1:B:263:LEU:HD22	1:B:264:HIS:N	2.21	0.55
2:A:4:CYS:O	2:A:64:ARG:HB2	2.07	0.55
2:A:52:PHE:HB3	2:A:53:PHE:CZ	2.40	0.55
2:A:230:LEU:HD23	2:A:230:LEU:C	2.27	0.55
3:K:29:ASN:H	3:K:32:GLU:HG3	1.71	0.55
3:K:134:GLY:CA	3:K:138:ARG:HG2	2.37	0.55
3:K:140:LEU:HD22	3:K:210:VAL:HG11	1.89	0.55
1:B:225:LEU:O	1:B:229:VAL:HG23	2.06	0.55
1:B:306:ARG:HA	1:B:340:TYR:HE1	1.70	0.55
1:B:375:GLN:HG2	1:B:376:GLU:N	2.21	0.55
1:B:398:TYR:O	1:B:401:GLU:HB2	2.07	0.55
2:A:70:LEU:CD2	2:A:99:ALA:HA	2.36	0.55
2:A:177:VAL:HG22	2:A:178:SER:N	2.20	0.55
2:A:259:LEU:HD13	2:A:378:LEU:CD1	2.31	0.55
2:A:414:GLU:CB	3:K:344:GLU:HG2	2.37	0.55
3:K:16:GLY:HA3	3:K:363:PRO:HD2	1.87	0.55
3:K:136:ILE:HG21	3:K:214:LEU:CD1	2.37	0.55
3:K:145:GLU:HG2	3:K:207:LYS:HZ1	1.70	0.55
1:B:3:GLU:C	1:B:4:ILE:HD12	2.27	0.55
1:B:23:VAL:HG11	1:B:230:SER:CB	2.37	0.55
1:B:46:ARG:HG3	1:B:241:ARG:CD	2.35	0.55
1:B:246:LEU:H	1:B:353:VAL:HG22	1.70	0.55
1:B:307:HIS:O	1:B:426:GLN:HG3	2.07	0.55
1:B:308:GLY:HA2	1:B:372:THR:OG1	2.06	0.55
1:B:396:HIS:O	1:B:399:THR:HB	2.06	0.55
2:A:1:MET:CG	2:A:47:ASP:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:104:ALA:HB3	2:A:411:GLU:CG	2.23	0.55
2:A:210:TYR:HA	2:A:213:CYS:SG	2.46	0.55
2:A:229:ARG:HG2	2:A:229:ARG:HH11	1.72	0.55
2:A:317:LEU:HB2	2:A:353:VAL:CG1	2.36	0.55
3:K:82:TYR:CE2	3:K:86:VAL:CG1	2.87	0.55
3:K:102:PHE:CD1	3:K:264:VAL:CG1	2.90	0.55
3:K:115:MET:SD	3:K:135:ILE:HG12	2.46	0.55
3:K:223:THR:OG1	3:K:233:SER:HA	2.06	0.55
1:B:86:ARG:HB2	1:B:89:ASN:OD1	2.06	0.55
1:B:178:THR:HG22	1:B:181:GLU:HB2	1.89	0.55
1:B:214:THR:CB	1:B:275:SER:HA	2.37	0.55
1:B:321:MET:HG2	1:B:325:GLU:HB2	1.89	0.55
2:A:34:GLY:HA2	2:A:86:LEU:HD13	1.89	0.55
2:A:224:TYR:OH	4:A:501:G2P:N9	2.40	0.55
2:A:286:LEU:HD22	2:A:291:ILE:HD11	1.87	0.55
2:A:370:LYS:HE2	2:A:371:VAL:O	2.07	0.55
3:K:224:ALA:HB3	3:K:234:ARG:CG	2.33	0.55
3:K:271:ASN:ND2	3:K:274:ARG:H	2.05	0.55
1:B:101:TRP:HB2	1:B:188:SER:OG	2.07	0.55
2:A:205:ASP:OD1	2:A:303:VAL:HG23	2.07	0.55
2:A:262:TYR:HB2	2:A:265:ILE:H	1.72	0.55
2:A:318:LEU:HD13	2:A:318:LEU:C	2.27	0.55
3:K:144:PHE:HD2	3:K:207:LYS:HG3	1.64	0.55
3:K:311:TYR:CE1	3:K:324:LEU:HG	2.36	0.55
1:B:41:ASP:OD1	1:B:42:LEU:HD22	2.07	0.55
1:B:215:LEU:HD13	1:B:217:LEU:HB3	1.87	0.55
1:B:341:PHE:CZ	1:B:346:PRO:HA	2.41	0.55
1:B:421:GLU:HA	1:B:421:GLU:OE2	2.05	0.55
2:A:115:ILE:HD12	2:A:152:LEU:CD2	2.37	0.55
2:A:271:THR:HG22	2:A:377:MET:HB2	1.89	0.55
2:A:344:VAL:HA	2:A:438:ASP:OD1	2.06	0.55
2:A:358:GLN:CG	2:A:359:PRO:HD2	2.35	0.55
2:A:401:LYS:HG3	2:A:403:ALA:HB2	1.88	0.55
3:K:144:PHE:HB2	3:K:207:LYS:CG	2.37	0.55
3:K:172:LEU:HD21	3:K:199:LEU:HD11	1.87	0.55
1:B:415:MET:HG2	1:B:419:VAL:HG13	1.89	0.54
2:A:274:PRO:HB2	2:A:276:ILE:CD1	2.37	0.54
1:B:8:GLN:HE22	1:B:14:ASN:HA	1.72	0.54
1:B:11:GLN:O	1:B:14:ASN:HB2	2.07	0.54
1:B:15:GLN:HG3	1:B:19:LYS:CG	2.37	0.54
1:B:36:TYR:HD2	1:B:44:LEU:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:HD21	1:B:300:MET:CE	2.37	0.54
2:A:101:ASN:HD22	2:A:144:GLY:CA	2.20	0.54
2:A:317:LEU:N	2:A:353:VAL:HG12	2.22	0.54
2:A:388:TRP:CH2	2:A:432:TYR:CE2	2.95	0.54
1:B:149:THR:HA	1:B:191:GLN:NE2	2.09	0.54
1:B:154:LYS:NZ	1:B:157:GLU:HG3	2.23	0.54
1:B:214:THR:HA	1:B:275:SER:OG	2.07	0.54
2:A:16:ILE:HD11	2:A:231:ILE:HB	1.89	0.54
2:A:172:TYR:CG	2:A:203:MET:HB2	2.43	0.54
2:A:298:PRO:HA	2:A:301:GLN:CG	2.37	0.54
2:A:311:LYS:N	2:A:311:LYS:HE3	2.22	0.54
2:A:385:ALA:HA	2:A:388:TRP:CE3	2.42	0.54
3:K:55:GLY:HA2	3:K:60:LYS:CA	2.35	0.54
3:K:190:ASN:HD22	3:K:192:ARG:H	1.55	0.54
1:B:113:VAL:O	1:B:116:VAL:HG22	2.08	0.54
1:B:253:LEU:O	1:B:257:MET:HG2	2.07	0.54
1:B:262:ARG:HD3	1:B:262:ARG:N	2.20	0.54
1:B:266:PHE:CD1	1:B:368:ILE:HG22	2.43	0.54
1:B:280:GLN:HG3	1:B:281:TYR:N	2.23	0.54
1:B:376:GLU:OE2	1:B:422:TYR:HB2	2.07	0.54
2:A:154:MET:HE2	2:A:154:MET:HA	1.90	0.54
2:A:155:GLU:HG2	2:A:156:ARG:H	1.71	0.54
2:A:189:LEU:HD13	2:A:417:GLU:HG3	1.90	0.54
2:A:221:ARG:HD3	2:A:222:PRO:N	2.22	0.54
2:A:250:VAL:HG22	2:A:251:ASP:N	2.23	0.54
2:A:294:ALA:O	2:A:300:ASN:HB2	2.07	0.54
2:A:349:THR:HG21	2:A:351:PHE:CD1	2.43	0.54
2:A:394:LYS:HD2	2:A:394:LYS:H	1.73	0.54
2:A:433:GLU:O	2:A:437:VAL:HG13	2.08	0.54
3:K:162:GLU:HG3	3:K:221:ARG:NH1	2.22	0.54
3:K:191:LYS:H	3:K:191:LYS:HD3	1.71	0.54
1:B:45:GLU:HG2	1:B:46:ARG:H	1.71	0.54
1:B:214:THR:C	1:B:276:ARG:H	2.11	0.54
1:B:255:VAL:HG13	1:B:256:ASN:N	2.23	0.54
2:A:46:ASP:OD1	2:A:244:PHE:HZ	1.90	0.54
2:A:391:LEU:HA	2:A:394:LYS:CE	2.37	0.54
3:K:171:LEU:HD13	3:K:221:ARG:CB	2.37	0.54
1:B:102:ALA:HB3	1:B:401:GLU:CB	2.32	0.54
1:B:306:ARG:HA	1:B:340:TYR:CE1	2.43	0.54
2:A:143:GLY:HA3	4:A:501:G2P:O1B	2.07	0.54
2:A:270:ALA:HB2	2:A:378:LEU:HD21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:307:PRO:HB3	2:A:312:TYR:OH	2.08	0.54
2:A:319:TYR:HB3	2:A:323:VAL:HG21	1.90	0.54
2:A:323:VAL:HG12	2:A:324:VAL:N	2.23	0.54
3:K:158:VAL:O	3:K:201:GLU:HG2	2.07	0.54
1:B:139:LEU:H	1:B:168:SER:HB3	1.71	0.54
1:B:155:ILE:HG13	1:B:156:ARG:N	2.23	0.54
1:B:213:ARG:HE	1:B:214:THR:CG2	2.21	0.54
1:B:232:THR:HG23	1:B:270:PHE:HD1	1.72	0.54
2:A:102:ASN:HB3	2:A:105:ARG:HD2	1.89	0.54
3:K:102:PHE:HD1	3:K:264:VAL:HB	1.72	0.54
1:B:178:THR:HG21	1:B:180:VAL:CG2	2.38	0.54
1:B:186:THR:HB	1:B:385:PHE:HE1	1.72	0.54
1:B:372:THR:HA	1:B:375:GLN:CD	2.28	0.54
2:A:24:TYR:HB3	2:A:52:PHE:CG	2.42	0.54
2:A:101:ASN:HB2	4:A:501:G2P:O3G	2.07	0.54
2:A:270:ALA:CA	2:A:378:LEU:HD23	2.38	0.54
2:A:298:PRO:HB3	2:A:301:GLN:HE21	1.72	0.54
2:A:407:TRP:HA	2:A:407:TRP:CE3	2.42	0.54
3:K:50:VAL:HG23	3:K:71:VAL:CG1	2.38	0.54
1:B:70:PRO:HA	1:B:92:PHE:CE2	2.43	0.54
1:B:154:LYS:O	1:B:158:GLU:HG3	2.08	0.54
1:B:309:ARG:HD2	1:B:429:THR:C	2.28	0.54
2:A:23:LEU:HA	2:A:364:PRO:HG2	1.89	0.54
2:A:23:LEU:HD23	2:A:23:LEU:C	2.27	0.54
2:A:174:ALA:HB1	2:A:207:GLU:HB3	1.90	0.54
2:A:346:TRP:HD1	2:A:346:TRP:H	1.55	0.54
3:K:102:PHE:CZ	3:K:266:LEU:HB2	2.43	0.54
3:K:140:LEU:HD13	3:K:210:VAL:HG11	1.90	0.54
3:K:144:PHE:HB3	3:K:207:LYS:HD2	1.90	0.54
1:B:41:ASP:OD2	1:B:42:LEU:HD22	2.08	0.54
1:B:70:PRO:HG3	1:B:94:GLN:CB	2.38	0.54
1:B:154:LYS:O	1:B:154:LYS:HD3	2.08	0.54
1:B:263:LEU:C	1:B:263:LEU:HD13	2.28	0.54
1:B:374:ILE:HG23	1:B:375:GLN:N	2.23	0.54
2:A:1:MET:HB2	2:A:47:ASP:CA	2.38	0.54
2:A:74:VAL:HG23	2:A:75:ILE:N	2.23	0.54
2:A:136:LEU:N	2:A:136:LEU:HD22	2.23	0.54
3:K:181:ARG:CG	3:K:198:GLY:HA3	2.38	0.54
1:B:24:ILE:CA	1:B:27:GLU:HG2	2.36	0.53
1:B:72:THR:O	1:B:76:VAL:HG23	2.08	0.53
1:B:90:PHE:HE1	1:B:92:PHE:HE1	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLY:O	1:B:151:LEU:HG	2.07	0.53
1:B:221:THR:HG22	1:B:222:TYR:N	2.23	0.53
1:B:228:LEU:HD23	1:B:228:LEU:C	2.29	0.53
1:B:267:MET:HE2	1:B:370:ASN:C	2.29	0.53
1:B:278:SER:HB3	1:B:282:ARG:HD2	1.91	0.53
1:B:418:LEU:HB3	1:B:422:TYR:CZ	2.43	0.53
2:A:107:HIS:HD2	2:A:152:LEU:HB2	1.63	0.53
2:A:202:PHE:HE1	2:A:267:PHE:CB	2.22	0.53
2:A:217:LEU:CD1	2:A:222:PRO:HG3	2.37	0.53
2:A:286:LEU:HB2	2:A:291:ILE:HG13	1.87	0.53
2:A:317:LEU:HD13	2:A:319:TYR:OH	2.08	0.53
3:K:17:LYS:HE3	3:K:329:ARG:CD	2.26	0.53
3:K:134:GLY:HA2	3:K:138:ARG:HG2	1.89	0.53
1:B:15:GLN:HG3	1:B:19:LYS:CD	2.38	0.53
1:B:154:LYS:HZ3	1:B:158:GLU:N	2.06	0.53
1:B:155:ILE:HA	1:B:158:GLU:OE1	2.08	0.53
1:B:159:TYR:HB3	1:B:161:ASP:OD1	2.08	0.53
1:B:238:THR:O	1:B:242:PHE:HB2	2.08	0.53
1:B:388:MET:O	1:B:391:ARG:HB2	2.09	0.53
2:A:99:ALA:HB2	2:A:145:THR:HA	1.89	0.53
2:A:194:THR:HG23	2:A:195:LEU:N	2.23	0.53
2:A:234:ILE:O	2:A:238:ILE:HG13	2.08	0.53
2:A:273:ALA:HA	2:A:274:PRO:C	2.29	0.53
2:A:370:LYS:CE	2:A:372:GLN:HA	2.37	0.53
2:A:414:GLU:HB2	3:K:344:GLU:HG2	1.90	0.53
3:K:284:GLU:HA	3:K:287:ASN:ND2	2.23	0.53
1:B:32:PRO:HG3	1:B:81:PHE:HE1	1.74	0.53
1:B:215:LEU:HB3	1:B:217:LEU:H	1.73	0.53
1:B:249:ASP:OD2	1:B:251:ARG:HG2	2.07	0.53
1:B:306:ARG:NH2	1:B:339:SER:HB3	2.23	0.53
2:A:53:PHE:HA	2:A:63:PRO:HA	1.89	0.53
2:A:53:PHE:HD2	2:A:63:PRO:CA	2.20	0.53
3:K:48:LYS:HZ1	3:K:70:MET:HG3	1.73	0.53
3:K:66:TYR:CD2	3:K:68:PHE:CE1	2.95	0.53
3:K:215:GLU:HG2	3:K:216:LYS:HE3	1.85	0.53
3:K:312:ARG:HH11	3:K:318:ARG:NH2	2.05	0.53
1:B:1:MET:HA	1:B:3:GLU:OE1	2.09	0.53
1:B:246:LEU:HD12	1:B:352:ALA:CB	2.38	0.53
1:B:259:PRO:HD2	1:B:262:ARG:HH22	1.74	0.53
1:B:285:THR:H	1:B:288:GLU:CB	2.20	0.53
2:A:276:ILE:HG21	2:A:281:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:409:VAL:HB	3:K:290:GLN:HG2	1.90	0.53
3:K:66:TYR:CE2	3:K:68:PHE:HA	2.41	0.53
3:K:66:TYR:CD2	3:K:68:PHE:CZ	2.96	0.53
3:K:162:GLU:CD	3:K:235:SER:HG	2.11	0.53
1:B:145:SER:HB2	1:B:184:ASN:OD1	2.09	0.53
1:B:156:ARG:NE	1:B:157:GLU:HA	2.24	0.53
1:B:251:ARG:HD3	2:A:105:ARG:HE	1.74	0.53
1:B:419:VAL:HG23	1:B:420:SER:N	2.24	0.53
2:A:62:VAL:HG13	2:A:62:VAL:O	2.08	0.53
2:A:93:ILE:HG21	2:A:121:ARG:CD	2.38	0.53
2:A:115:ILE:O	2:A:118:VAL:HG22	2.07	0.53
2:A:195:LEU:CD1	2:A:201:ALA:HB2	2.29	0.53
2:A:209:ILE:CD1	2:A:302:MET:HB2	2.39	0.53
3:K:29:ASN:H	3:K:32:GLU:CG	2.21	0.53
3:K:37:ALA:HB1	3:K:339:ALA:HB1	1.88	0.53
3:K:96:GLY:HA2	3:K:258:ILE:O	2.09	0.53
3:K:221:ARG:CZ	3:K:237:SER:HB3	2.39	0.53
1:B:11:GLN:C	1:B:14:ASN:HB2	2.29	0.53
1:B:150:LEU:C	1:B:150:LEU:HD13	2.28	0.53
1:B:207:LEU:HD12	1:B:208:TYR:N	2.23	0.53
1:B:271:ALA:HB2	1:B:293:MET:HG2	1.90	0.53
1:B:289:LEU:H	1:B:289:LEU:CD1	2.22	0.53
1:B:304:ASP:HB3	1:B:307:HIS:ND1	2.23	0.53
2:A:242:LEU:CD2	2:A:252:LEU:H	2.21	0.53
2:A:251:ASP:CG	2:A:254:GLU:H	2.12	0.53
3:K:31:ALA:O	3:K:34:LYS:HG2	2.09	0.53
3:K:43:CYS:SG	3:K:73:GLY:HA2	2.48	0.53
1:B:2:ARG:HD2	1:B:131:GLN:HA	1.91	0.53
1:B:4:ILE:HG13	1:B:132:GLY:H	1.73	0.53
1:B:225:LEU:HD11	4:B:501:G2P:H2N1	1.72	0.53
1:B:246:LEU:HD13	1:B:246:LEU:C	2.29	0.53
1:B:260:PHE:HB2	3:K:297:ARG:HH22	1.72	0.53
1:B:286:VAL:HG21	1:B:325:GLU:CD	2.29	0.53
1:B:323:MET:CB	2:A:221:ARG:NE	2.69	0.53
1:B:388:MET:CE	1:B:388:MET:HA	2.39	0.53
2:A:21:TRP:HD1	2:A:67:PHE:HZ	1.56	0.53
2:A:260:VAL:HG13	2:A:268:PRO:HD3	1.91	0.53
2:A:265:ILE:HG23	2:A:432:TYR:OH	2.08	0.53
2:A:317:LEU:CD2	2:A:377:MET:HG3	2.36	0.53
2:A:368:LEU:HD12	2:A:368:LEU:C	2.29	0.53
1:B:73:MET:HG2	1:B:92:PHE:HE1	1.65	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASP:OD2	1:B:119:VAL:HG23	2.09	0.53
1:B:121:ARG:O	1:B:125:GLU:HG3	2.08	0.53
1:B:152:ILE:O	1:B:155:ILE:HG12	2.08	0.53
1:B:379:LYS:HB2	1:B:419:VAL:HG11	1.90	0.53
2:A:298:PRO:HB3	2:A:301:GLN:NE2	2.24	0.53
3:K:357:LYS:HG3	3:K:358:ASN:OD1	2.08	0.53
1:B:73:MET:HG3	1:B:74:ASP:N	2.24	0.53
1:B:207:LEU:HD12	1:B:207:LEU:C	2.29	0.53
1:B:334:GLN:HG2	1:B:335:ASN:ND2	2.24	0.53
1:B:339:SER:CA	1:B:429:THR:HB	2.38	0.53
2:A:63:PRO:HB2	2:A:87:PHE:CZ	2.44	0.53
2:A:103:TYR:HD1	2:A:189:LEU:HD23	1.72	0.53
2:A:124:LYS:HZ3	2:A:125:LEU:HB2	1.73	0.53
2:A:143:GLY:HA3	4:A:501:G2P:C3A	2.38	0.53
2:A:153:LEU:CD1	2:A:157:LEU:HG	2.39	0.53
2:A:337:THR:HG23	2:A:338:LYS:N	2.24	0.53
2:A:360:PRO:HG2	2:A:371:VAL:HG23	1.90	0.53
1:B:5:VAL:HG12	1:B:123:GLU:HG3	1.91	0.53
1:B:6:HIS:HA	1:B:134:GLN:OE1	2.08	0.53
2:A:3:GLU:HB3	2:A:64:ARG:HG2	1.91	0.53
2:A:144:GLY:HA2	2:A:186:ASN:ND2	2.25	0.53
2:A:430:LYS:HD3	2:A:434:GLU:CG	2.39	0.53
3:K:50:VAL:HB	3:K:68:PHE:CE2	2.44	0.53
3:K:278:VAL:HG12	3:K:279:ASP:N	2.23	0.53
1:B:172:SER:HB2	1:B:205:GLU:CB	2.24	0.52
1:B:318:ARG:HA	1:B:354:CYS:CB	2.39	0.52
1:B:376:GLU:CB	1:B:380:ARG:HH22	2.22	0.52
2:A:19:ALA:HB1	2:A:229:ARG:NH2	2.21	0.52
2:A:21:TRP:HA	2:A:24:TYR:CD2	2.44	0.52
2:A:21:TRP:CE3	2:A:24:TYR:HD2	2.27	0.52
2:A:176:GLN:HG3	2:A:177:VAL:N	2.24	0.52
2:A:214:ARG:HB2	2:A:222:PRO:HD3	1.91	0.52
2:A:221:ARG:NH1	2:A:222:PRO:HD2	2.24	0.52
2:A:256:GLN:HE22	2:A:260:VAL:CG1	2.22	0.52
3:K:16:GLY:C	3:K:363:PRO:HD2	2.29	0.52
3:K:102:PHE:CD1	3:K:264:VAL:HG12	2.43	0.52
3:K:135:ILE:HD12	3:K:136:ILE:HG13	1.90	0.52
3:K:173:ASN:HB2	3:K:176:SER:H	1.75	0.52
3:K:326:GLY:HA2	3:K:362:LYS:NZ	2.24	0.52
1:B:42:LEU:H	1:B:42:LEU:CD2	2.21	0.52
1:B:77:ARG:HD3	1:B:82:GLY:CA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:VAL:HG23	1:B:117:LEU:CD2	2.36	0.52
1:B:213:ARG:HB2	1:B:213:ARG:HH11	1.70	0.52
1:B:244:GLY:HA2	1:B:355:ASP:CB	2.39	0.52
1:B:284:LEU:HB3	1:B:289:LEU:CD1	2.38	0.52
1:B:334:GLN:HG2	1:B:335:ASN:H	1.73	0.52
1:B:358:PRO:HG2	1:B:364:SER:OG	2.09	0.52
1:B:422:TYR:HD1	1:B:425:TYR:CZ	2.27	0.52
2:A:84:ARG:HD2	2:A:85:GLN:CA	2.38	0.52
2:A:256:GLN:HE22	2:A:260:VAL:HG13	1.73	0.52
2:A:387:ALA:HA	2:A:390:ARG:CZ	2.39	0.52
3:K:320:LEU:HD21	3:K:324:LEU:CD1	2.39	0.52
1:B:97:ALA:CB	1:B:143:THR:CA	2.75	0.52
1:B:97:ALA:H	1:B:143:THR:CG2	2.22	0.52
1:B:280:GLN:HG3	1:B:281:TYR:CE1	2.44	0.52
2:A:188:ILE:HG22	2:A:421:ALA:HB1	1.90	0.52
2:A:255:PHE:HZ	2:A:352:LYS:N	2.08	0.52
2:A:430:LYS:HZ2	2:A:430:LYS:HA	1.72	0.52
3:K:60:LYS:HD2	3:K:60:LYS:N	2.24	0.52
3:K:147:LEU:HD11	3:K:243:ILE:HD13	1.90	0.52
3:K:187:ASP:HB2	3:K:189:ARG:NE	2.25	0.52
3:K:246:LYS:CE	3:K:254:GLU:OE1	2.50	0.52
1:B:120:VAL:CG2	1:B:121:ARG:HH21	2.22	0.52
1:B:293:MET:HE1	1:B:367:PHE:CA	2.36	0.52
1:B:293:MET:HA	1:B:298:ASN:CB	2.38	0.52
1:B:308:GLY:HA3	1:B:372:THR:H	1.73	0.52
2:A:122:ILE:HD12	2:A:123:ARG:CA	2.39	0.52
2:A:306:ASP:CA	2:A:308:ARG:HH21	2.21	0.52
3:K:26:ARG:CZ	3:K:32:GLU:HG3	2.39	0.52
3:K:64:LYS:HD3	3:K:350:LEU:HG	1.91	0.52
3:K:172:LEU:HD11	3:K:173:ASN:HD21	1.75	0.52
3:K:206:ASN:ND2	3:K:209:GLU:H	2.08	0.52
3:K:327:ARG:NH2	3:K:327:ARG:HG2	2.24	0.52
1:B:65:LEU:O	1:B:92:PHE:HB3	2.10	0.52
1:B:101:TRP:CA	1:B:146:GLY:HA2	2.39	0.52
1:B:101:TRP:O	1:B:146:GLY:HA2	2.09	0.52
1:B:159:TYR:HB3	1:B:161:ASP:OD2	2.09	0.52
1:B:284:LEU:HB2	1:B:289:LEU:HD11	1.92	0.52
1:B:322:SER:OG	1:B:324:LYS:HG2	2.09	0.52
1:B:337:ASN:HB3	1:B:340:TYR:CG	2.45	0.52
1:B:375:GLN:HG2	1:B:376:GLU:H	1.75	0.52
2:A:223:THR:HG22	2:A:225:THR:N	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:417:GLU:HG3	2:A:418:PHE:CD2	2.44	0.52
3:K:173:ASN:HB2	3:K:176:SER:OG	2.09	0.52
3:K:192:ARG:HD3	3:K:327:ARG:HH12	1.74	0.52
1:B:273:LEU:C	1:B:273:LEU:HD13	2.30	0.52
1:B:285:THR:N	1:B:288:GLU:HB2	2.25	0.52
2:A:111:GLY:O	2:A:114:ILE:HG22	2.09	0.52
2:A:263:PRO:CD	2:A:264:ARG:HH11	2.22	0.52
2:A:355:ILE:HG22	2:A:356:ASN:N	2.25	0.52
1:B:277:GLY:O	1:B:280:GLN:HG2	2.08	0.52
2:A:205:ASP:HB2	2:A:208:ALA:HB3	1.88	0.52
2:A:219:ILE:HG22	2:A:220:GLU:N	2.25	0.52
3:K:68:PHE:CD2	3:K:71:VAL:HG22	2.45	0.52
3:K:236:HIS:CE1	3:K:267:ALA:HB3	2.45	0.52
1:B:203:ASP:OD1	1:B:206:ALA:HB2	2.09	0.52
1:B:240:LEU:HA	1:B:247:ASN:HD21	1.75	0.52
2:A:16:ILE:HA	2:A:228:ASN:ND2	2.17	0.52
2:A:140:SER:OG	2:A:143:GLY:HA3	2.10	0.52
2:A:174:ALA:HB2	2:A:206:ASN:HB2	1.92	0.52
2:A:233:GLN:HG3	2:A:234:ILE:N	2.25	0.52
2:A:286:LEU:CG	2:A:291:ILE:HD11	2.39	0.52
2:A:339:ARG:HG3	2:A:340:SER:CA	2.40	0.52
3:K:27:PRO:HA	3:K:74:ALA:HB1	1.91	0.52
3:K:48:LYS:CE	3:K:70:MET:HG3	2.39	0.52
3:K:144:PHE:CE1	3:K:156:VAL:HG21	2.44	0.52
3:K:181:ARG:NH2	3:K:197:LYS:NZ	2.58	0.52
1:B:363:MET:HE3	1:B:363:MET:N	2.23	0.52
1:B:422:TYR:CD1	1:B:425:TYR:CE2	2.97	0.52
2:A:23:LEU:HA	2:A:364:PRO:HG3	1.89	0.52
2:A:276:ILE:HG23	2:A:281:ALA:CA	2.40	0.52
2:A:286:LEU:HD11	2:A:372:GLN:HB3	1.92	0.52
2:A:313:MET:O	2:A:347:CYS:HB3	2.09	0.52
3:K:15:LYS:HG2	3:K:364:GLU:OE2	2.10	0.52
3:K:25:CYS:HB3	3:K:43:CYS:SG	2.50	0.52
3:K:160:LEU:H	3:K:172:LEU:CB	2.23	0.52
3:K:311:TYR:CD1	3:K:321:GLN:HG3	2.44	0.52
1:B:12:CYS:SG	4:B:501:G2P:C4	2.98	0.52
1:B:34:GLY:HA3	1:B:58:LYS:CG	2.37	0.52
1:B:34:GLY:HA2	1:B:84:ILE:CD1	2.40	0.52
1:B:208:TYR:CE2	1:B:225:LEU:HD23	2.44	0.52
2:A:41:THR:HG22	2:A:42:ILE:N	2.24	0.52
2:A:214:ARG:HG3	2:A:215:ARG:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:214:ARG:CB	2:A:222:PRO:HD3	2.40	0.52
2:A:215:ARG:HH11	2:A:216:ASN:ND2	2.04	0.52
3:K:212:GLN:O	3:K:215:GLU:HG2	2.10	0.52
1:B:23:VAL:HG13	1:B:24:ILE:N	2.24	0.51
1:B:167:PHE:CE1	1:B:200:TYR:CD2	2.96	0.51
1:B:174:LYS:CD	1:B:175:VAL:HG23	2.40	0.51
1:B:299:MET:HE2	1:B:299:MET:HA	1.92	0.51
1:B:313:VAL:O	1:B:349:VAL:HG13	2.10	0.51
1:B:345:ILE:HG23	1:B:345:ILE:O	2.10	0.51
2:A:30:ILE:HD12	2:A:61:HIS:HB2	1.92	0.51
2:A:189:LEU:HD11	2:A:417:GLU:OE2	2.10	0.51
3:K:110:GLY:HA2	3:K:113:PHE:H	1.74	0.51
1:B:1:MET:HE2	1:B:49:VAL:CA	2.41	0.51
1:B:14:ASN:CB	1:B:72:THR:HG21	2.40	0.51
1:B:272:PRO:CB	1:B:292:GLN:HE22	2.23	0.51
2:A:3:GLU:C	2:A:51:THR:HG22	2.30	0.51
2:A:7:ILE:HD12	2:A:8:HIS:N	2.24	0.51
3:K:192:ARG:HG2	3:K:192:ARG:NH1	2.26	0.51
3:K:240:SER:HB3	3:K:262:ASN:OD1	2.10	0.51
1:B:1:MET:HG3	1:B:127:CYS:CB	2.34	0.51
1:B:361:LEU:HD21	1:B:364:SER:OG	2.11	0.51
2:A:26:LEU:HD23	2:A:364:PRO:CB	2.40	0.51
2:A:90:GLU:CA	2:A:121:ARG:HH21	2.21	0.51
2:A:145:THR:HB	4:A:501:G2P:O1B	2.11	0.51
2:A:233:GLN:CA	2:A:363:VAL:HG13	2.40	0.51
3:K:93:VAL:CG1	3:K:243:ILE:HD12	2.40	0.51
1:B:1:MET:CG	1:B:127:CYS:HB2	2.33	0.51
1:B:179:VAL:HG13	1:B:180:VAL:N	2.24	0.51
1:B:260:PHE:HB3	1:B:262:ARG:CD	2.40	0.51
2:A:317:LEU:CB	2:A:353:VAL:HB	2.25	0.51
2:A:332:ILE:HG22	2:A:336:LYS:HG2	1.93	0.51
2:A:399:TYR:HB2	2:A:422:ARG:NH2	2.26	0.51
3:K:15:LYS:HE3	3:K:364:GLU:OE2	2.09	0.51
3:K:68:PHE:CD2	3:K:71:VAL:CG2	2.94	0.51
3:K:189:ARG:CZ	3:K:189:ARG:HB2	2.39	0.51
1:B:47:ILE:HG22	1:B:59:TYR:HD1	1.76	0.51
1:B:117:LEU:O	1:B:120:VAL:HG22	2.10	0.51
1:B:159:TYR:HD2	1:B:162:ARG:CG	2.23	0.51
1:B:225:LEU:HD12	1:B:225:LEU:C	2.31	0.51
1:B:376:GLU:HG3	1:B:379:LYS:HZ3	1.75	0.51
2:A:54:SER:O	2:A:61:HIS:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:344:VAL:HG12	2:A:438:ASP:OD2	2.10	0.51
3:K:26:ARG:NH1	3:K:26:ARG:HG3	2.25	0.51
3:K:180:GLU:HG3	3:K:199:LEU:CD1	2.36	0.51
1:B:193:VAL:HG13	1:B:194:GLU:H	1.76	0.51
2:A:20:CYS:HB3	2:A:24:TYR:CZ	2.45	0.51
2:A:132:LEU:HD23	2:A:134:GLY:O	2.11	0.51
2:A:215:ARG:HD3	2:A:216:ASN:N	2.25	0.51
2:A:416:GLY:O	2:A:420:GLU:HG2	2.11	0.51
1:B:189:VAL:HG13	1:B:190:HIS:N	2.26	0.51
1:B:272:PRO:CA	1:B:292:GLN:HE22	2.24	0.51
1:B:273:LEU:O	1:B:273:LEU:HD13	2.11	0.51
1:B:323:MET:HG3	2:A:210:TYR:CE2	2.46	0.51
2:A:188:ILE:O	2:A:191:THR:HG22	2.10	0.51
2:A:382:THR:HG22	2:A:433:GLU:HA	1.92	0.51
3:K:154:PHE:CE2	3:K:205:HIS:HE1	2.29	0.51
3:K:168:LEU:CD1	3:K:182:LEU:HB3	2.38	0.51
3:K:257:LYS:CA	3:K:368:LYS:HD3	2.38	0.51
1:B:33:THR:CG2	1:B:35:SER:H	2.13	0.51
1:B:210:ILE:HA	1:B:213:ARG:HG2	1.92	0.51
1:B:414:ASN:ND2	3:K:312:ARG:HD3	2.25	0.51
2:A:14:VAL:HG23	2:A:15:GLN:N	2.25	0.51
2:A:115:ILE:O	2:A:119:LEU:HG	2.11	0.51
2:A:188:ILE:HG22	2:A:421:ALA:CB	2.40	0.51
2:A:286:LEU:CD2	2:A:291:ILE:HD11	2.41	0.51
2:A:370:LYS:HZ3	2:A:372:GLN:HA	1.74	0.51
2:A:397:LEU:HD23	2:A:397:LEU:C	2.30	0.51
3:K:19:ILE:HB	3:K:361:ASN:HB2	1.93	0.51
3:K:341:LEU:H	3:K:341:LEU:CD1	2.23	0.51
1:B:77:ARG:NH1	1:B:82:GLY:HA2	2.11	0.51
1:B:113:VAL:HA	1:B:116:VAL:HG22	1.93	0.51
1:B:213:ARG:HG3	1:B:214:THR:N	2.24	0.51
1:B:392:LYS:CG	1:B:395:LEU:HD11	2.41	0.51
2:A:35:GLN:CA	2:A:60:LYS:HE2	2.41	0.51
2:A:153:LEU:HD12	2:A:156:ARG:CZ	2.40	0.51
2:A:277:SER:HB2	2:A:280:LYS:HG3	1.92	0.51
3:K:17:LYS:CD	3:K:17:LYS:H	2.24	0.51
3:K:97:TYR:HB3	3:K:99:CYS:SG	2.50	0.51
1:B:101:TRP:HD1	1:B:149:THR:HG21	1.74	0.51
2:A:272:TYR:H	2:A:302:MET:HE1	1.76	0.51
2:A:273:ALA:HB2	2:A:295:CYS:CB	2.40	0.51
2:A:316:CYS:O	2:A:317:LEU:HD23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:349:THR:HG21	2:A:351:PHE:CE1	2.46	0.51
3:K:31:ALA:CB	3:K:34:LYS:HE2	2.40	0.51
3:K:190:ASN:ND2	3:K:192:ARG:H	2.09	0.51
3:K:327:ARG:HD3	3:K:362:LYS:HZ1	1.76	0.51
1:B:117:LEU:HA	1:B:120:VAL:HG22	1.93	0.50
1:B:148:GLY:HA2	1:B:151:LEU:HG	1.92	0.50
1:B:306:ARG:HH21	1:B:309:ARG:CZ	2.24	0.50
2:A:11:GLN:HG2	2:A:74:VAL:CG1	2.41	0.50
2:A:21:TRP:CE3	2:A:24:TYR:CD2	2.99	0.50
2:A:30:ILE:N	2:A:36:MET:HE1	2.26	0.50
2:A:54:SER:HB2	2:A:64:ARG:HE	1.76	0.50
2:A:153:LEU:CD1	2:A:157:LEU:HD11	2.37	0.50
2:A:154:MET:HE2	2:A:154:MET:C	2.31	0.50
3:K:271:ASN:HD22	3:K:274:ARG:N	2.09	0.50
1:B:52:ASN:H	1:B:62:ARG:NH2	2.08	0.50
1:B:143:THR:HB	4:B:501:G2P:O2B	2.10	0.50
1:B:279:GLN:HE22	1:B:284:LEU:HD21	1.76	0.50
2:A:9:VAL:HG22	2:A:149:PHE:CE1	2.46	0.50
2:A:123:ARG:HG3	2:A:127:ASP:OD1	2.12	0.50
2:A:295:CYS:HA	2:A:300:ASN:OD1	2.12	0.50
2:A:395:PHE:HB3	2:A:422:ARG:HH12	1.75	0.50
2:A:401:LYS:CG	2:A:403:ALA:HB2	2.42	0.50
2:A:402:ARG:HD2	2:A:415:GLU:OE1	2.12	0.50
3:K:15:LYS:HD3	3:K:362:LYS:CB	2.39	0.50
3:K:192:ARG:HG2	3:K:192:ARG:HH11	1.76	0.50
3:K:215:GLU:CD	3:K:216:LYS:HE3	2.31	0.50
3:K:314:SER:HB3	3:K:317:THR:OG1	2.10	0.50
1:B:28:HIS:HE1	1:B:51:TYR:CZ	2.29	0.50
1:B:143:THR:HG22	1:B:147:MET:SD	2.52	0.50
2:A:65:ALA:HB3	2:A:87:PHE:CE2	2.47	0.50
2:A:217:LEU:HD12	2:A:222:PRO:CG	2.40	0.50
2:A:417:GLU:O	2:A:420:GLU:HB2	2.11	0.50
3:K:157:LYS:HE3	3:K:203:THR:HG1	1.73	0.50
3:K:311:TYR:CE2	3:K:321:GLN:HG3	2.46	0.50
3:K:350:LEU:HD13	3:K:350:LEU:C	2.31	0.50
1:B:47:ILE:HD13	1:B:241:ARG:HH12	1.75	0.50
1:B:309:ARG:HG2	1:B:428:ALA:O	2.11	0.50
2:A:24:TYR:HB3	2:A:52:PHE:CE1	2.46	0.50
2:A:316:CYS:SG	2:A:377:MET:HA	2.52	0.50
3:K:33:ARG:HG3	3:K:33:ARG:HH11	1.76	0.50
3:K:33:ARG:HG3	3:K:33:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASN:HB2	1:B:59:TYR:OH	2.12	0.50
1:B:286:VAL:CB	1:B:287:PRO:HD3	2.38	0.50
1:B:321:MET:HG2	1:B:322:SER:N	2.26	0.50
2:A:47:ASP:OD2	2:A:243:ARG:HA	2.10	0.50
2:A:90:GLU:OE1	2:A:121:ARG:HB3	2.11	0.50
2:A:96:LYS:HD3	2:A:96:LYS:C	2.30	0.50
2:A:237:SER:HB3	2:A:320:ARG:HD2	1.93	0.50
2:A:385:ALA:HB2	2:A:432:TYR:CD2	2.45	0.50
3:K:221:ARG:NH2	3:K:233:SER:HB2	2.25	0.50
3:K:233:SER:HG	3:K:267:ALA:HA	1.76	0.50
1:B:151:LEU:O	1:B:155:ILE:HG23	2.12	0.50
1:B:205:GLU:HG3	1:B:206:ALA:H	1.76	0.50
2:A:118:VAL:O	2:A:122:ILE:HG23	2.11	0.50
2:A:312:TYR:CD2	2:A:341:ILE:CG2	2.95	0.50
3:K:32:GLU:HA	3:K:32:GLU:OE2	2.11	0.50
3:K:301:ALA:O	3:K:304:GLU:HB3	2.12	0.50
3:K:320:LEU:O	3:K:324:LEU:HD22	2.12	0.50
1:B:4:ILE:HD12	1:B:4:ILE:N	2.26	0.50
1:B:97:ALA:HB2	1:B:143:THR:HA	1.84	0.50
1:B:214:THR:HB	1:B:275:SER:CA	2.42	0.50
1:B:273:LEU:HD22	1:B:274:THR:H	1.73	0.50
1:B:311:LEU:O	1:B:342:VAL:HG21	2.12	0.50
2:A:9:VAL:HG13	2:A:149:PHE:CD1	2.47	0.50
2:A:76:ASP:HA	2:A:79:ARG:HG2	1.94	0.50
2:A:224:TYR:CE1	4:A:501:G2P:C8	2.93	0.50
2:A:275:VAL:CA	2:A:300:ASN:HD22	2.23	0.50
3:K:54:THR:HG23	3:K:56:GLY:H	1.77	0.50
3:K:104:TYR:CD2	3:K:266:LEU:HG	2.47	0.50
3:K:170:ASP:HB2	3:K:180:GLU:N	2.27	0.50
3:K:170:ASP:N	3:K:180:GLU:H	2.06	0.50
3:K:171:LEU:HD13	3:K:221:ARG:HB2	1.93	0.50
1:B:51:TYR:CD1	1:B:61:PRO:HA	2.46	0.50
1:B:99:ASN:O	1:B:142:GLY:HA3	2.11	0.50
1:B:271:ALA:HB2	1:B:293:MET:CG	2.41	0.50
1:B:323:MET:HG3	2:A:210:TYR:HE2	1.76	0.50
2:A:9:VAL:HG22	2:A:149:PHE:HD1	1.75	0.50
2:A:319:TYR:HB2	2:A:355:ILE:HG23	1.94	0.50
3:K:16:GLY:HA3	3:K:363:PRO:CD	2.41	0.50
3:K:66:TYR:HD2	3:K:68:PHE:CZ	2.30	0.50
1:B:13:GLY:HA2	1:B:16:ILE:HB	1.93	0.50
1:B:59:TYR:O	1:B:84:ILE:HD11	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:TRP:CG	1:B:102:ALA:N	2.78	0.50
1:B:342:VAL:HG12	1:B:344:TRP:H	1.76	0.50
1:B:353:VAL:HG23	1:B:353:VAL:O	2.12	0.50
2:A:164:LYS:HA	2:A:164:LYS:HZ1	1.76	0.50
2:A:188:ILE:HD12	2:A:188:ILE:N	2.27	0.50
2:A:223:THR:HB	2:A:226:ASN:H	1.77	0.50
3:K:23:VAL:CG2	3:K:68:PHE:CD1	2.95	0.50
1:B:2:ARG:CG	1:B:131:GLN:HB2	2.42	0.49
1:B:14:ASN:CG	1:B:72:THR:HG21	2.32	0.49
1:B:379:LYS:HB2	1:B:415:MET:SD	2.52	0.49
2:A:72:PRO:HG3	2:A:96:LYS:HZ2	1.77	0.49
3:K:48:LYS:HZ1	3:K:70:MET:CG	2.25	0.49
1:B:148:GLY:CA	1:B:151:LEU:HD21	2.35	0.49
2:A:4:CYS:H	2:A:51:THR:CB	2.25	0.49
2:A:101:ASN:HA	2:A:144:GLY:N	2.27	0.49
2:A:240:ALA:HA	2:A:243:ARG:HE	1.77	0.49
2:A:310:GLY:HA3	2:A:381:THR:HG22	1.91	0.49
3:K:44:ASP:HB3	3:K:47:ARG:HB2	1.94	0.49
1:B:6:HIS:HB3	1:B:21:TRP:CE2	2.46	0.49
1:B:45:GLU:CG	1:B:46:ARG:HE	2.16	0.49
1:B:156:ARG:HA	1:B:164:MET:CE	2.43	0.49
1:B:186:THR:HB	1:B:385:PHE:CE1	2.47	0.49
1:B:272:PRO:CB	1:B:279:GLN:HE22	2.19	0.49
1:B:396:HIS:H	1:B:396:HIS:CD2	2.28	0.49
1:B:405:GLU:HA	1:B:408:PHE:CD1	2.43	0.49
1:B:418:LEU:HB3	1:B:422:TYR:OH	2.12	0.49
2:A:3:GLU:HA	2:A:51:THR:N	2.26	0.49
2:A:150:THR:CG2	2:A:190:THR:HG21	2.42	0.49
2:A:166:LYS:HD2	2:A:198:SER:CA	2.21	0.49
2:A:232:SER:HB3	2:A:363:VAL:HG12	1.90	0.49
2:A:430:LYS:HD3	2:A:434:GLU:OE1	2.13	0.49
3:K:369:LEU:HD22	3:K:369:LEU:N	2.27	0.49
1:B:137:HIS:HB2	1:B:144:GLY:CA	2.42	0.49
1:B:266:PHE:CE2	1:B:370:ASN:HB3	2.48	0.49
1:B:313:VAL:HG13	1:B:367:PHE:CE2	2.48	0.49
1:B:339:SER:O	1:B:429:THR:HB	2.12	0.49
1:B:422:TYR:HD1	1:B:425:TYR:CE2	2.31	0.49
2:A:8:HIS:HB2	2:A:14:VAL:HG12	1.94	0.49
2:A:153:LEU:HG	2:A:157:LEU:CD1	2.42	0.49
2:A:171:ILE:O	2:A:171:ILE:HG23	2.11	0.49
2:A:256:GLN:OE1	2:A:259:LEU:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:29:ASN:HB2	3:K:32:GLU:H	1.78	0.49
3:K:181:ARG:HG3	3:K:198:GLY:HA3	1.95	0.49
1:B:46:ARG:CG	1:B:242:PHE:CE1	2.95	0.49
1:B:148:GLY:CA	1:B:151:LEU:HG	2.42	0.49
1:B:157:GLU:HA	1:B:157:GLU:OE1	2.12	0.49
1:B:260:PHE:CD2	2:A:404:PHE:N	2.66	0.49
1:B:375:GLN:HG3	1:B:422:TYR:CG	2.47	0.49
2:A:6:SER:CB	2:A:21:TRP:CZ2	2.95	0.49
2:A:265:ILE:CD1	2:A:432:TYR:CE1	2.95	0.49
3:K:82:TYR:CE1	3:K:86:VAL:HB	2.47	0.49
3:K:168:LEU:HB2	3:K:182:LEU:CB	2.42	0.49
3:K:329:ARG:HA	3:K:363:PRO:CB	2.42	0.49
1:B:252:LYS:O	1:B:255:VAL:HG12	2.13	0.49
1:B:318:ARG:CB	1:B:358:PRO:HG3	2.43	0.49
1:B:320:ARG:HG2	1:B:321:MET:N	2.21	0.49
1:B:350:LYS:HG2	2:A:179:THR:HG22	1.89	0.49
2:A:99:ALA:HB2	2:A:145:THR:CA	2.42	0.49
2:A:388:TRP:CZ3	2:A:428:LEU:CD2	2.95	0.49
3:K:181:ARG:NE	3:K:197:LYS:HG3	2.27	0.49
1:B:137:HIS:HB2	1:B:144:GLY:HA2	1.94	0.49
1:B:149:THR:HG23	1:B:188:SER:CB	2.43	0.49
1:B:154:LYS:HE2	1:B:154:LYS:CA	2.39	0.49
1:B:419:VAL:HA	1:B:422:TYR:CG	2.45	0.49
2:A:9:VAL:CG1	2:A:149:PHE:HD1	2.25	0.49
2:A:23:LEU:HA	2:A:364:PRO:CD	2.42	0.49
2:A:124:LYS:NZ	2:A:125:LEU:HB2	2.28	0.49
2:A:219:ILE:HG22	2:A:220:GLU:OE1	2.13	0.49
2:A:255:PHE:HZ	2:A:352:LYS:CA	2.26	0.49
3:K:39:SER:HA	3:K:338:PRO:HB2	1.93	0.49
3:K:66:TYR:HD2	3:K:68:PHE:CG	2.31	0.49
3:K:157:LYS:HE2	3:K:203:THR:OG1	2.07	0.49
3:K:283:ARG:HG2	3:K:287:ASN:HD21	1.78	0.49
1:B:151:LEU:HD12	1:B:152:ILE:HG12	1.95	0.49
1:B:180:VAL:HG23	1:B:181:GLU:N	2.28	0.49
1:B:208:TYR:CE2	1:B:225:LEU:CD2	2.95	0.49
1:B:306:ARG:HH22	1:B:339:SER:HB3	1.77	0.49
1:B:331:LEU:HA	1:B:334:GLN:HE22	1.74	0.49
1:B:342:VAL:HG12	1:B:344:TRP:N	2.28	0.49
2:A:23:LEU:HD22	2:A:24:TYR:CD1	2.47	0.49
2:A:286:LEU:HD12	2:A:286:LEU:C	2.32	0.49
2:A:411:GLU:OE1	2:A:411:GLU:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:430:LYS:CD	2:A:434:GLU:HG3	2.43	0.49
3:K:50:VAL:H	3:K:68:PHE:HE2	1.59	0.49
1:B:27:GLU:HA	1:B:27:GLU:OE2	2.12	0.49
1:B:390:ARG:HA	1:B:390:ARG:NH1	2.27	0.49
2:A:35:GLN:HG2	2:A:59:GLY:O	2.13	0.49
2:A:72:PRO:HG3	2:A:96:LYS:HA	1.95	0.49
2:A:102:ASN:HB3	2:A:105:ARG:CB	2.38	0.49
3:K:28:PHE:CD2	3:K:32:GLU:CB	2.96	0.49
3:K:59:ASP:HA	3:K:60:LYS:HZ2	1.76	0.49
3:K:192:ARG:HH21	3:K:326:GLY:HA3	1.77	0.49
1:B:120:VAL:HG23	1:B:121:ARG:N	2.28	0.49
1:B:156:ARG:HH21	1:B:157:GLU:CA	2.21	0.49
1:B:186:THR:CG2	1:B:385:PHE:CE1	2.96	0.49
1:B:249:ASP:O	1:B:253:LEU:HD23	2.13	0.49
1:B:418:LEU:HB3	1:B:422:TYR:CE1	2.48	0.49
2:A:7:ILE:HG22	2:A:137:VAL:HA	1.95	0.49
2:A:12:ALA:O	2:A:16:ILE:HG22	2.13	0.49
2:A:388:TRP:CH2	2:A:432:TYR:CD2	3.01	0.49
2:A:401:LYS:O	2:A:401:LYS:HE3	2.13	0.49
3:K:66:TYR:CD2	3:K:68:PHE:CG	3.01	0.49
1:B:24:ILE:O	1:B:27:GLU:HB2	2.13	0.48
1:B:47:ILE:CG2	1:B:59:TYR:CE1	2.96	0.48
1:B:156:ARG:HA	1:B:164:MET:SD	2.53	0.48
2:A:111:GLY:HA3	2:A:152:LEU:CD1	2.42	0.48
2:A:130:THR:HG23	2:A:131:GLY:H	1.78	0.48
2:A:226:ASN:O	2:A:229:ARG:HB2	2.12	0.48
2:A:311:LYS:HG3	2:A:342:GLN:OE1	2.13	0.48
2:A:358:GLN:HG2	2:A:359:PRO:N	2.28	0.48
2:A:407:TRP:CE3	2:A:407:TRP:CA	2.96	0.48
3:K:320:LEU:HD23	3:K:324:LEU:HD11	1.95	0.48
1:B:36:TYR:CD2	1:B:44:LEU:CB	2.95	0.48
1:B:46:ARG:HG2	1:B:242:PHE:CE1	2.48	0.48
1:B:156:ARG:HB2	1:B:164:MET:HE3	1.95	0.48
1:B:390:ARG:O	1:B:392:LYS:HE2	2.13	0.48
2:A:113:GLU:CD	2:A:113:GLU:H	2.16	0.48
2:A:154:MET:HG2	2:A:197:HIS:HB2	1.93	0.48
2:A:200:CYS:CB	2:A:267:PHE:HB3	2.33	0.48
2:A:267:PHE:N	2:A:267:PHE:CD2	2.81	0.48
2:A:349:THR:CG2	2:A:351:PHE:HD1	2.25	0.48
2:A:385:ALA:HB1	2:A:429:GLU:CD	2.32	0.48
2:A:387:ALA:HB2	2:A:390:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:277:ALA:HB1	3:K:281:ARG:HB2	1.93	0.48
1:B:156:ARG:HA	1:B:164:MET:HE1	1.95	0.48
2:A:214:ARG:HH22	2:A:218:ASP:HA	1.78	0.48
2:A:243:ARG:HD3	2:A:244:PHE:CZ	2.49	0.48
2:A:338:LYS:HZ3	2:A:338:LYS:HA	1.78	0.48
3:K:170:ASP:OD2	3:K:176:SER:HB2	2.12	0.48
1:B:33:THR:HG23	1:B:34:GLY:N	2.29	0.48
1:B:208:TYR:CG	1:B:220:PRO:HG2	2.47	0.48
1:B:258:VAL:O	1:B:258:VAL:HG23	2.13	0.48
1:B:318:ARG:HG2	1:B:354:CYS:CB	2.40	0.48
1:B:345:ILE:HG23	1:B:348:ASN:ND2	2.29	0.48
2:A:42:ILE:O	2:A:46:ASP:HB3	2.13	0.48
2:A:221:ARG:NH1	2:A:221:ARG:HG2	2.27	0.48
2:A:420:GLU:O	2:A:424:ASP:HB3	2.13	0.48
3:K:78:GLN:CG	3:K:113:PHE:HE2	2.27	0.48
1:B:31:ASP:OD1	1:B:37:HIS:HB2	2.13	0.48
1:B:81:PHE:HA	1:B:83:GLN:CD	2.33	0.48
1:B:242:PHE:HD1	1:B:242:PHE:HA	1.51	0.48
1:B:376:GLU:HG3	1:B:379:LYS:HZ1	1.75	0.48
2:A:141:PHE:HD2	2:A:141:PHE:HA	1.57	0.48
2:A:174:ALA:CB	2:A:207:GLU:H	2.22	0.48
2:A:243:ARG:CD	2:A:244:PHE:CE2	2.95	0.48
3:K:77:LYS:HE3	3:K:78:GLN:H	1.75	0.48
3:K:78:GLN:CG	3:K:113:PHE:CE2	2.96	0.48
3:K:347:LEU:HD23	3:K:347:LEU:C	2.34	0.48
1:B:111:GLU:H	1:B:111:GLU:CD	2.16	0.48
1:B:117:LEU:CA	1:B:120:VAL:HG22	2.44	0.48
1:B:166:THR:O	1:B:167:PHE:HD1	1.96	0.48
1:B:225:LEU:HD11	1:B:226:ASN:ND2	2.28	0.48
1:B:228:LEU:HD23	1:B:229:VAL:N	2.29	0.48
1:B:371:SER:CB	1:B:374:ILE:HG22	2.34	0.48
1:B:394:PHE:HD1	1:B:396:HIS:NE2	2.10	0.48
2:A:2:ARG:HE	2:A:132:LEU:C	2.17	0.48
2:A:52:PHE:CB	2:A:53:PHE:CE1	2.96	0.48
2:A:339:ARG:HG3	2:A:340:SER:HA	1.95	0.48
2:A:368:LEU:HD13	2:A:369:ALA:O	2.13	0.48
2:A:408:TYR:CD1	2:A:418:PHE:CZ	3.01	0.48
3:K:345:GLU:O	3:K:349:THR:HG23	2.13	0.48
1:B:343:GLU:HG2	1:B:344:TRP:N	2.29	0.48
1:B:377:LEU:CA	1:B:380:ARG:HG3	2.43	0.48
1:B:394:PHE:HA	1:B:396:HIS:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:91:GLN:NE2	2:A:91:GLN:H	2.10	0.48
2:A:174:ALA:HB3	2:A:176:GLN:CG	2.43	0.48
2:A:210:TYR:HD1	2:A:213:CYS:SG	2.36	0.48
2:A:360:PRO:HB3	2:A:374:ALA:CB	2.40	0.48
2:A:391:LEU:O	2:A:394:LYS:HD3	2.14	0.48
3:K:117:GLY:HA2	3:K:134:GLY:O	2.14	0.48
3:K:181:ARG:HH22	3:K:183:GLN:N	2.12	0.48
3:K:243:ILE:HG22	3:K:245:MET:HG3	1.95	0.48
3:K:320:LEU:HD12	3:K:320:LEU:O	2.13	0.48
1:B:167:PHE:CE2	1:B:233:MET:SD	3.07	0.48
1:B:169:VAL:O	1:B:169:VAL:HG23	2.14	0.48
1:B:183:TYR:CD1	1:B:385:PHE:CD1	3.02	0.48
3:K:27:PRO:HA	3:K:74:ALA:CB	2.44	0.48
3:K:94:ILE:HD13	3:K:150:ASN:ND2	2.27	0.48
3:K:168:LEU:HB3	3:K:182:LEU:HG	1.96	0.48
3:K:206:ASN:CG	3:K:209:GLU:HG3	2.33	0.48
3:K:323:SER:HA	3:K:328:THR:HB	1.95	0.48
1:B:45:GLU:O	1:B:49:VAL:HG13	2.14	0.48
1:B:148:GLY:C	1:B:151:LEU:HG	2.34	0.48
1:B:150:LEU:HD13	1:B:150:LEU:O	2.13	0.48
1:B:380:ARG:O	1:B:383:GLU:HB3	2.14	0.48
2:A:21:TRP:HE3	2:A:24:TYR:HD2	1.62	0.48
2:A:274:PRO:HG2	2:A:286:LEU:HD23	1.95	0.48
3:K:66:TYR:CD2	3:K:68:PHE:CD1	3.01	0.48
3:K:190:ASN:HD22	3:K:192:ARG:N	2.12	0.48
3:K:234:ARG:CZ	3:K:284:GLU:HG3	2.44	0.48
3:K:288:ILE:O	3:K:291:SER:HB3	2.14	0.48
1:B:262:ARG:HE	3:K:297:ARG:NH1	2.12	0.48
1:B:276:ARG:HG3	1:B:276:ARG:HH11	1.79	0.48
1:B:337:ASN:HB3	1:B:340:TYR:CD2	2.49	0.48
1:B:413:SER:HA	1:B:416:ASN:HD22	1.77	0.48
2:A:188:ILE:CB	2:A:395:PHE:HD1	2.27	0.48
2:A:210:TYR:OH	2:A:224:TYR:HA	2.14	0.48
3:K:28:PHE:CE2	3:K:37:ALA:HB3	2.49	0.48
3:K:159:SER:HB2	3:K:199:LEU:CD2	2.26	0.48
3:K:312:ARG:HH12	3:K:318:ARG:HH21	1.60	0.48
1:B:152:ILE:HA	1:B:155:ILE:CG1	2.43	0.47
1:B:258:VAL:HG12	1:B:263:LEU:HB3	1.96	0.47
1:B:267:MET:SD	1:B:299:MET:HE1	2.53	0.47
1:B:313:VAL:HG22	1:B:368:ILE:O	2.14	0.47
1:B:415:MET:HG2	1:B:419:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:49:PHE:CE1	2:A:53:PHE:CD1	3.00	0.47
2:A:176:GLN:NE2	2:A:207:GLU:HB2	2.29	0.47
2:A:188:ILE:CB	2:A:395:PHE:CD1	2.95	0.47
2:A:286:LEU:CB	2:A:291:ILE:HG12	2.40	0.47
3:K:25:CYS:CB	3:K:43:CYS:SG	3.02	0.47
3:K:139:THR:HG23	3:K:140:LEU:N	2.28	0.47
3:K:170:ASP:OD1	3:K:172:LEU:HD23	2.14	0.47
3:K:178:VAL:HA	3:K:220:LYS:CE	2.33	0.47
1:B:149:THR:HB	1:B:191:GLN:OE1	2.14	0.47
1:B:217:LEU:CD1	1:B:219:THR:H	2.27	0.47
1:B:219:THR:HB	1:B:220:PRO:HD2	1.95	0.47
1:B:271:ALA:HA	1:B:272:PRO:C	2.34	0.47
1:B:307:HIS:O	1:B:372:THR:HB	2.14	0.47
2:A:262:TYR:CD1	2:A:264:ARG:CZ	2.97	0.47
2:A:317:LEU:H	2:A:353:VAL:HG12	1.79	0.47
2:A:343:PHE:HD2	2:A:343:PHE:HA	1.49	0.47
2:A:387:ALA:HA	2:A:390:ARG:CG	2.44	0.47
3:K:104:TYR:HD2	3:K:105:GLY:H	1.60	0.47
3:K:157:LYS:HG2	3:K:203:THR:HA	1.92	0.47
3:K:181:ARG:CD	3:K:198:GLY:HA3	2.45	0.47
3:K:311:TYR:CG	3:K:321:GLN:CG	2.95	0.47
1:B:2:ARG:HG2	1:B:131:GLN:HB2	1.95	0.47
1:B:18:ALA:C	1:B:19:LYS:HZ3	2.18	0.47
1:B:30:ILE:CD1	1:B:59:TYR:HB2	2.43	0.47
1:B:51:TYR:CB	1:B:59:TYR:HB3	2.45	0.47
1:B:105:HIS:HD2	1:B:149:THR:CB	2.26	0.47
2:A:1:MET:CE	2:A:1:MET:HA	2.45	0.47
2:A:275:VAL:CB	2:A:300:ASN:HA	2.38	0.47
2:A:303:VAL:HG22	2:A:304:LYS:N	2.28	0.47
2:A:435:VAL:HG13	2:A:436:GLY:N	2.30	0.47
3:K:97:TYR:CD2	3:K:365:VAL:HA	2.50	0.47
3:K:222:THR:CG2	3:K:231:TYR:HE2	2.28	0.47
1:B:266:PHE:CZ	1:B:311:LEU:HG	2.49	0.47
2:A:4:CYS:SG	2:A:136:LEU:HD22	2.55	0.47
2:A:63:PRO:HD2	2:A:87:PHE:CD1	2.50	0.47
2:A:105:ARG:CB	2:A:407:TRP:CZ2	2.96	0.47
2:A:115:ILE:HA	2:A:118:VAL:HG22	1.96	0.47
2:A:122:ILE:HD12	2:A:122:ILE:C	2.35	0.47
2:A:234:ILE:HD12	2:A:234:ILE:C	2.35	0.47
3:K:24:ARG:NH1	3:K:109:THR:O	2.48	0.47
3:K:47:ARG:CD	3:K:49:GLU:OE2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:95:MET:CE	3:K:97:TYR:HD2	2.27	0.47
3:K:160:LEU:O	3:K:172:LEU:HD23	2.14	0.47
3:K:347:LEU:HD23	3:K:351:GLU:HG2	1.95	0.47
1:B:5:VAL:CG2	1:B:133:PHE:HB3	2.44	0.47
1:B:21:TRP:NE1	1:B:63:ALA:HB2	2.30	0.47
1:B:69:GLU:OE2	1:B:94:GLN:HG2	2.15	0.47
1:B:102:ALA:HB2	1:B:403:MET:CG	2.45	0.47
1:B:191:GLN:CG	1:B:195:ASN:HD21	2.27	0.47
1:B:262:ARG:CG	3:K:297:ARG:NH1	2.77	0.47
2:A:233:GLN:N	2:A:363:VAL:HG13	2.29	0.47
2:A:338:LYS:HZ2	2:A:338:LYS:HB3	1.78	0.47
2:A:351:PHE:CB	2:A:352:LYS:HA	2.41	0.47
2:A:370:LYS:HE2	2:A:372:GLN:HA	1.95	0.47
3:K:26:ARG:HE	3:K:337:SER:HB3	1.79	0.47
3:K:329:ARG:HD2	3:K:363:PRO:HG2	1.97	0.47
3:K:343:LEU:HG	3:K:344:GLU:N	2.28	0.47
1:B:192:LEU:HD21	1:B:196:THR:OG1	2.14	0.47
1:B:269:GLY:C	1:B:367:PHE:HB3	2.35	0.47
2:A:64:ARG:HA	2:A:64:ARG:NH2	2.20	0.47
2:A:90:GLU:CD	2:A:124:LYS:HE3	2.35	0.47
2:A:189:LEU:HD21	2:A:417:GLU:OE2	2.15	0.47
2:A:410:GLY:N	3:K:290:GLN:HG2	2.30	0.47
1:B:65:LEU:HD22	1:B:90:PHE:CD1	2.50	0.47
1:B:70:PRO:HG3	1:B:94:GLN:HB2	1.96	0.47
1:B:70:PRO:HG3	1:B:94:GLN:CA	2.42	0.47
1:B:101:TRP:O	1:B:105:HIS:HB2	2.15	0.47
1:B:139:LEU:HD12	1:B:140:GLY:CA	2.45	0.47
1:B:139:LEU:O	1:B:185:ALA:HB2	2.14	0.47
1:B:212:PHE:CB	1:B:220:PRO:HG3	2.44	0.47
1:B:260:PHE:O	1:B:262:ARG:HD3	2.13	0.47
1:B:270:PHE:CG	1:B:271:ALA:N	2.83	0.47
1:B:380:ARG:HG2	1:B:380:ARG:HH11	1.80	0.47
2:A:9:VAL:CG2	2:A:149:PHE:CD1	2.97	0.47
2:A:53:PHE:HB3	2:A:62:VAL:O	2.14	0.47
2:A:53:PHE:HD2	2:A:63:PRO:CG	2.28	0.47
2:A:75:ILE:HG21	2:A:79:ARG:NH2	2.30	0.47
2:A:102:ASN:CB	2:A:407:TRP:HE1	2.21	0.47
2:A:103:TYR:CD2	2:A:148:GLY:HA2	2.49	0.47
2:A:111:GLY:HA3	2:A:152:LEU:HD12	1.96	0.47
2:A:205:ASP:O	2:A:209:ILE:HB	2.15	0.47
2:A:220:GLU:CD	2:A:221:ARG:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:245:ASP:OD1	2:A:249:ASN:HB2	2.15	0.47
2:A:270:ALA:CB	2:A:378:LEU:HD23	2.45	0.47
3:K:180:GLU:C	3:K:182:LEU:HD22	2.34	0.47
3:K:204:VAL:HG11	3:K:209:GLU:HB2	1.97	0.47
1:B:99:ASN:N	4:B:501:G2P:PG	2.88	0.47
1:B:143:THR:CG2	1:B:147:MET:CE	2.91	0.47
1:B:159:TYR:CG	1:B:162:ARG:HG2	2.49	0.47
1:B:217:LEU:HD13	1:B:218:THR:OG1	2.14	0.47
1:B:284:LEU:CB	1:B:289:LEU:HD11	2.45	0.47
1:B:318:ARG:HB3	1:B:358:PRO:CD	2.39	0.47
2:A:1:MET:HG2	2:A:47:ASP:H	1.74	0.47
2:A:30:ILE:HG23	2:A:30:ILE:O	2.15	0.47
2:A:93:ILE:HD13	2:A:118:VAL:HG12	1.96	0.47
2:A:192:HIS:NE2	2:A:193:THR:HG23	2.29	0.47
3:K:17:LYS:O	3:K:361:ASN:HB3	2.15	0.47
1:B:28:HIS:CE1	1:B:47:ILE:HG23	2.49	0.47
1:B:67:ASP:N	1:B:92:PHE:HB2	2.29	0.47
1:B:377:LEU:O	1:B:380:ARG:HG3	2.15	0.47
1:B:394:PHE:HD1	1:B:396:HIS:CE1	2.33	0.47
1:B:419:VAL:O	1:B:422:TYR:HB2	2.14	0.47
2:A:88:HIS:H	2:A:88:HIS:CD2	2.33	0.47
2:A:360:PRO:HG2	2:A:371:VAL:O	2.14	0.47
3:K:37:ALA:HB1	3:K:339:ALA:HB2	1.95	0.47
3:K:168:LEU:HB3	3:K:182:LEU:CG	2.45	0.47
3:K:311:TYR:HE1	3:K:324:LEU:CD2	2.26	0.47
1:B:46:ARG:CG	1:B:242:PHE:CD1	2.98	0.47
1:B:149:THR:HG23	1:B:188:SER:OG	2.14	0.47
1:B:151:LEU:HD12	1:B:152:ILE:CG1	2.45	0.47
1:B:162:ARG:HA	1:B:162:ARG:NH1	2.29	0.47
1:B:347:ASN:ND2	2:A:177:VAL:CG2	2.78	0.47
2:A:1:MET:HA	2:A:1:MET:HE3	1.97	0.47
2:A:102:ASN:CG	2:A:105:ARG:H	2.18	0.47
2:A:141:PHE:H	2:A:171:ILE:CG2	2.28	0.47
2:A:406:HIS:O	3:K:290:GLN:HG2	2.14	0.47
3:K:72:PHE:HB3	3:K:76:THR:OG1	2.14	0.47
3:K:311:TYR:CE1	3:K:324:LEU:CD2	2.98	0.47
1:B:49:VAL:HG23	1:B:50:TYR:N	2.30	0.46
1:B:214:THR:CB	1:B:276:ARG:H	2.26	0.46
1:B:371:SER:HB2	1:B:374:ILE:HG21	1.91	0.46
2:A:83:TYR:O	2:A:86:LEU:HB3	2.15	0.46
3:K:26:ARG:NH2	3:K:337:SER:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:47:ARG:O	3:K:48:LYS:HB2	2.16	0.46
3:K:102:PHE:CE1	3:K:264:VAL:HG12	2.50	0.46
1:B:3:GLU:HG3	1:B:50:TYR:O	2.15	0.46
1:B:3:GLU:OE2	1:B:50:TYR:HA	2.15	0.46
1:B:103:LYS:HG2	1:B:401:GLU:CG	2.43	0.46
1:B:245:GLN:NE2	1:B:353:VAL:HG23	2.28	0.46
1:B:291:GLN:HE21	1:B:291:GLN:HB3	1.38	0.46
1:B:321:MET:HG3	1:B:325:GLU:CB	2.45	0.46
1:B:331:LEU:HD12	1:B:334:GLN:HE22	1.80	0.46
1:B:377:LEU:HD12	1:B:377:LEU:C	2.34	0.46
1:B:394:PHE:CZ	1:B:397:TRP:CH2	3.03	0.46
2:A:9:VAL:CG1	2:A:149:PHE:HB3	2.46	0.46
2:A:53:PHE:HD2	2:A:63:PRO:CB	2.27	0.46
2:A:233:GLN:NE2	2:A:234:ILE:HG22	2.20	0.46
3:K:288:ILE:HG13	3:K:289:ASN:N	2.31	0.46
1:B:97:ALA:H	1:B:143:THR:HG23	1.80	0.46
1:B:102:ALA:O	1:B:105:HIS:HB3	2.16	0.46
1:B:152:ILE:C	1:B:155:ILE:HG12	2.36	0.46
1:B:251:ARG:NH2	2:A:101:ASN:H	2.09	0.46
1:B:343:GLU:HG2	1:B:344:TRP:CD1	2.50	0.46
2:A:78:VAL:CG1	2:A:83:TYR:HE1	2.28	0.46
2:A:121:ARG:HG2	2:A:121:ARG:HH11	1.80	0.46
2:A:321:GLY:HA2	2:A:359:PRO:CA	2.46	0.46
3:K:68:PHE:CD2	3:K:68:PHE:N	2.83	0.46
3:K:171:LEU:C	3:K:220:LYS:HD3	2.36	0.46
3:K:204:VAL:HG12	3:K:209:GLU:OE1	2.16	0.46
3:K:286:GLY:O	3:K:290:GLN:HG3	2.14	0.46
3:K:365:VAL:HG11	3:K:367:GLN:CG	2.44	0.46
1:B:103:LYS:HD2	1:B:401:GLU:CG	2.40	0.46
1:B:284:LEU:HB3	1:B:289:LEU:HD12	1.96	0.46
1:B:341:PHE:HZ	1:B:346:PRO:C	2.19	0.46
2:A:1:MET:HB2	2:A:47:ASP:HB2	1.97	0.46
2:A:48:SER:HB3	2:A:244:PHE:CZ	2.51	0.46
3:K:41:VAL:HB	3:K:338:PRO:HB3	1.97	0.46
3:K:204:VAL:CG2	3:K:210:VAL:HG22	2.45	0.46
1:B:186:THR:O	1:B:189:VAL:HG12	2.16	0.46
1:B:252:LYS:CD	2:A:101:ASN:HB2	2.19	0.46
1:B:273:LEU:HD22	1:B:273:LEU:C	2.34	0.46
2:A:30:ILE:HD12	2:A:61:HIS:CB	2.45	0.46
2:A:192:HIS:ND1	2:A:421:ALA:HB2	2.30	0.46
2:A:324:VAL:HG22	2:A:327:ASP:CG	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:389:ALA:O	2:A:392:ASP:HB3	2.16	0.46
3:K:50:VAL:HG23	3:K:71:VAL:HG13	1.97	0.46
1:B:215:LEU:HD23	1:B:276:ARG:HE	1.81	0.46
1:B:321:MET:SD	1:B:326:VAL:HA	2.55	0.46
2:A:349:THR:CG2	2:A:351:PHE:CD1	2.99	0.46
3:K:112:THR:O	3:K:116:GLU:HG3	2.16	0.46
3:K:161:LEU:HA	3:K:171:LEU:HG	1.98	0.46
3:K:211:TYR:O	3:K:214:LEU:HB3	2.16	0.46
3:K:255:LEU:HD22	3:K:369:LEU:HA	1.95	0.46
1:B:7:ILE:N	1:B:134:GLN:HE22	2.12	0.46
1:B:45:GLU:CB	1:B:46:ARG:HH21	2.23	0.46
1:B:152:ILE:CA	1:B:155:ILE:HG12	2.46	0.46
2:A:108:TYR:CE2	2:A:413:MET:SD	3.09	0.46
2:A:143:GLY:HA3	4:A:501:G2P:H3A1	1.98	0.46
2:A:223:THR:HB	2:A:226:ASN:OD1	2.14	0.46
2:A:298:PRO:HA	2:A:301:GLN:NE2	2.31	0.46
3:K:55:GLY:N	3:K:60:LYS:HG3	2.30	0.46
3:K:97:TYR:CD2	3:K:365:VAL:HG22	2.51	0.46
3:K:317:THR:HA	3:K:320:LEU:HB3	1.98	0.46
3:K:327:ARG:HH21	3:K:327:ARG:N	2.01	0.46
3:K:357:LYS:HG3	3:K:358:ASN:N	2.31	0.46
1:B:34:GLY:CA	1:B:84:ILE:HD13	2.46	0.46
1:B:242:PHE:HD1	1:B:243:PRO:HD3	1.81	0.46
1:B:331:LEU:HD13	1:B:331:LEU:N	2.31	0.46
1:B:381:ILE:HG23	1:B:384:GLN:OE1	2.15	0.46
2:A:2:ARG:NH1	2:A:131:GLY:HA3	2.31	0.46
2:A:7:ILE:HD11	2:A:68:VAL:HG22	1.95	0.46
2:A:63:PRO:HB2	2:A:87:PHE:CE1	2.50	0.46
2:A:104:ALA:CB	2:A:413:MET:HG3	2.43	0.46
2:A:308:ARG:H	2:A:308:ARG:HE	1.63	0.46
2:A:318:LEU:HD11	2:A:320:ARG:CG	2.41	0.46
3:K:77:LYS:HA	3:K:77:LYS:HD2	1.76	0.46
3:K:350:LEU:HD13	3:K:354:HIS:CD2	2.51	0.46
1:B:3:GLU:HG3	1:B:50:TYR:HD1	1.81	0.46
1:B:154:LYS:NZ	1:B:157:GLU:HB3	2.31	0.46
1:B:154:LYS:HZ3	1:B:157:GLU:C	2.18	0.46
1:B:251:ARG:CD	2:A:105:ARG:NE	2.79	0.46
1:B:324:LYS:HD2	2:A:221:ARG:HH11	1.74	0.46
2:A:75:ILE:HG21	2:A:79:ARG:HH21	1.80	0.46
2:A:209:ILE:HG22	2:A:227:LEU:HD11	1.98	0.46
2:A:288:VAL:HG11	2:A:328:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:334:THR:O	2:A:337:THR:HG22	2.16	0.46
2:A:384:ILE:HG13	2:A:385:ALA:N	2.30	0.46
3:K:144:PHE:CB	3:K:207:LYS:HD2	2.46	0.46
1:B:5:VAL:HA	1:B:62:ARG:HG2	1.97	0.46
1:B:200:TYR:HD1	1:B:268:PRO:HD3	1.81	0.46
1:B:253:LEU:HD12	1:B:254:ALA:CA	2.46	0.46
2:A:351:PHE:HB2	2:A:352:LYS:HZ2	1.80	0.46
2:A:388:TRP:HH2	2:A:432:TYR:CE2	2.31	0.46
2:A:404:PHE:CD2	2:A:404:PHE:N	2.82	0.46
1:B:28:HIS:CG	1:B:47:ILE:CG2	2.99	0.45
1:B:44:LEU:C	1:B:44:LEU:HD12	2.36	0.45
1:B:138:SER:HA	1:B:169:VAL:HG22	1.97	0.45
1:B:323:MET:O	1:B:326:VAL:HB	2.16	0.45
2:A:2:ARG:CZ	2:A:131:GLY:HA3	2.46	0.45
2:A:86:LEU:HD12	2:A:86:LEU:C	2.37	0.45
2:A:248:LEU:HD23	2:A:248:LEU:C	2.36	0.45
2:A:264:ARG:HD3	2:A:264:ARG:N	2.18	0.45
2:A:291:ILE:CD1	2:A:373:ARG:HB2	2.46	0.45
2:A:351:PHE:HD2	2:A:352:LYS:HZ3	1.63	0.45
2:A:402:ARG:O	2:A:405:VAL:HG23	2.16	0.45
3:K:102:PHE:HD1	3:K:264:VAL:CB	2.29	0.45
3:K:109:THR:HG23	3:K:336:ILE:O	2.16	0.45
3:K:221:ARG:HD3	3:K:237:SER:CB	2.42	0.45
3:K:293:LEU:HD22	3:K:293:LEU:N	2.32	0.45
1:B:12:CYS:O	1:B:15:GLN:HB3	2.17	0.45
1:B:77:ARG:HD3	1:B:82:GLY:HA3	1.98	0.45
1:B:102:ALA:CB	1:B:403:MET:CG	2.94	0.45
1:B:159:TYR:CD2	1:B:162:ARG:CG	2.98	0.45
1:B:214:THR:CG2	1:B:297:LYS:CE	2.95	0.45
1:B:222:TYR:CG	4:B:501:G2P:C6	2.98	0.45
1:B:262:ARG:HH21	1:B:263:LEU:H	1.64	0.45
1:B:266:PHE:HD2	1:B:266:PHE:HA	1.40	0.45
1:B:318:ARG:HA	1:B:354:CYS:HB3	1.97	0.45
1:B:358:PRO:HD2	1:B:362:LYS:O	2.15	0.45
1:B:422:TYR:HA	1:B:425:TYR:CZ	2.49	0.45
2:A:49:PHE:CD1	2:A:53:PHE:HD1	2.34	0.45
2:A:273:ALA:C	2:A:375:VAL:HG22	2.36	0.45
2:A:306:ASP:HB2	2:A:309:HIS:CD2	2.51	0.45
3:K:189:ARG:HD3	3:K:189:ARG:H	1.80	0.45
3:K:191:LYS:HZ2	3:K:191:LYS:HB2	1.81	0.45
3:K:236:HIS:ND1	3:K:267:ALA:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:PRO:HD3	1:B:94:GLN:HA	1.98	0.45
1:B:106:TYR:N	1:B:106:TYR:CD2	2.82	0.45
1:B:211:CYS:O	1:B:215:LEU:HB2	2.16	0.45
1:B:299:MET:CE	1:B:367:PHE:HD1	2.30	0.45
1:B:325:GLU:O	1:B:329:GLN:HG3	2.16	0.45
2:A:49:PHE:CZ	2:A:61:HIS:HD2	2.33	0.45
2:A:53:PHE:CD2	2:A:63:PRO:CA	2.99	0.45
2:A:70:LEU:CD2	2:A:99:ALA:CA	2.95	0.45
2:A:175:PRO:HG2	2:A:304:LYS:NZ	2.31	0.45
2:A:281:ALA:HB3	2:A:369:ALA:H	1.81	0.45
2:A:375:VAL:CG2	2:A:377:MET:CE	2.95	0.45
2:A:409:VAL:HG12	3:K:290:GLN:CA	2.43	0.45
3:K:29:ASN:CG	3:K:32:GLU:HG2	2.37	0.45
3:K:181:ARG:HH22	3:K:183:GLN:CB	2.28	0.45
1:B:5:VAL:HG23	1:B:5:VAL:O	2.15	0.45
1:B:12:CYS:CB	1:B:138:SER:CB	2.93	0.45
1:B:260:PHE:CB	1:B:262:ARG:CD	2.95	0.45
1:B:299:MET:CE	1:B:367:PHE:CD1	3.00	0.45
1:B:342:VAL:CB	1:B:348:ASN:HD21	2.23	0.45
2:A:21:TRP:CZ2	2:A:65:ALA:CB	2.97	0.45
2:A:152:LEU:HD23	2:A:152:LEU:C	2.36	0.45
2:A:279:GLU:HB3	2:A:283:HIS:NE2	2.31	0.45
2:A:298:PRO:HA	2:A:301:GLN:HE21	1.81	0.45
3:K:50:VAL:CG2	3:K:71:VAL:HG13	2.46	0.45
3:K:204:VAL:HG23	3:K:204:VAL:O	2.17	0.45
1:B:123:GLU:HA	1:B:123:GLU:OE2	2.16	0.45
1:B:186:THR:HA	1:B:189:VAL:HG12	1.99	0.45
1:B:266:PHE:HE1	1:B:312:THR:CG2	2.29	0.45
1:B:326:VAL:O	1:B:330:MET:HE3	2.16	0.45
1:B:341:PHE:CE1	1:B:348:ASN:CB	2.98	0.45
2:A:172:TYR:HB3	2:A:204:VAL:O	2.16	0.45
2:A:317:LEU:CB	2:A:353:VAL:CG1	2.95	0.45
2:A:391:LEU:N	2:A:391:LEU:HD22	2.32	0.45
1:B:70:PRO:CG	1:B:94:GLN:HA	2.47	0.45
1:B:97:ALA:CB	1:B:143:THR:CG2	2.94	0.45
1:B:213:ARG:HH21	1:B:214:THR:HA	1.81	0.45
2:A:25:CYS:O	2:A:30:ILE:HG22	2.17	0.45
2:A:28:HIS:CE1	2:A:52:PHE:HD1	2.35	0.45
2:A:71:GLU:HB3	2:A:98:ASP:OD2	2.17	0.45
2:A:147:SER:HA	2:A:190:THR:HG21	1.98	0.45
2:A:150:THR:CG2	2:A:190:THR:CG2	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:172:TYR:H	2:A:204:VAL:H	1.65	0.45
2:A:202:PHE:HE1	2:A:267:PHE:HB2	1.80	0.45
2:A:212:ILE:HG21	2:A:299:ALA:O	2.16	0.45
2:A:233:GLN:CB	2:A:363:VAL:HG13	2.47	0.45
3:K:15:LYS:CD	3:K:362:LYS:HD2	2.46	0.45
3:K:15:LYS:HG2	3:K:362:LYS:HB3	1.99	0.45
3:K:37:ALA:CB	3:K:341:LEU:HD13	2.47	0.45
3:K:191:LYS:H	3:K:191:LYS:CD	2.29	0.45
3:K:303:VAL:HG13	3:K:358:ASN:ND2	2.31	0.45
3:K:311:TYR:CD2	3:K:321:GLN:CG	2.98	0.45
1:B:105:HIS:HD2	1:B:149:THR:HB	1.82	0.45
1:B:154:LYS:HD3	1:B:154:LYS:C	2.37	0.45
1:B:252:LYS:NZ	2:A:102:ASN:CB	2.79	0.45
1:B:271:ALA:HB1	1:B:272:PRO:HA	1.99	0.45
2:A:5:ILE:HG22	2:A:6:SER:N	2.31	0.45
2:A:62:VAL:CG2	2:A:88:HIS:HD2	2.30	0.45
2:A:104:ALA:CB	2:A:413:MET:CG	2.94	0.45
3:K:209:GLU:O	3:K:213:ILE:HG12	2.17	0.45
1:B:1:MET:CG	1:B:2:ARG:H	2.27	0.45
1:B:81:PHE:CA	1:B:83:GLN:HE22	2.29	0.45
1:B:108:GLU:OE2	1:B:143:THR:HG23	2.17	0.45
1:B:266:PHE:HE2	1:B:370:ASN:HB3	1.81	0.45
1:B:267:MET:CE	1:B:367:PHE:HE1	2.30	0.45
1:B:288:GLU:O	1:B:291:GLN:HG2	2.17	0.45
2:A:54:SER:HB3	2:A:64:ARG:NH1	2.20	0.45
2:A:102:ASN:OD1	2:A:408:TYR:HE2	1.99	0.45
2:A:132:LEU:HD23	2:A:135:PHE:HA	1.99	0.45
2:A:136:LEU:HD12	2:A:169:PHE:HE1	1.82	0.45
2:A:188:ILE:CG2	2:A:421:ALA:CB	2.95	0.45
2:A:255:PHE:O	2:A:258:ASN:HB3	2.16	0.45
3:K:15:LYS:HE3	3:K:362:LYS:HE2	1.94	0.45
3:K:109:THR:HB	3:K:335:THR:OG1	2.17	0.45
3:K:145:GLU:CG	3:K:207:LYS:HZ1	2.30	0.45
3:K:203:THR:HG22	3:K:204:VAL:N	2.32	0.45
1:B:112:LEU:CD2	1:B:116:VAL:CG1	2.95	0.45
1:B:180:VAL:O	1:B:183:TYR:HB2	2.17	0.45
1:B:242:PHE:CE2	1:B:356:ILE:CD1	2.96	0.45
1:B:331:LEU:HA	1:B:334:GLN:CD	2.37	0.45
1:B:331:LEU:O	1:B:334:GLN:HG2	2.16	0.45
1:B:376:GLU:CD	1:B:422:TYR:HB2	2.37	0.45
2:A:4:CYS:HG	2:A:135:PHE:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:24:TYR:HA	2:A:27:GLU:CG	2.47	0.45
2:A:50:ASN:HA	2:A:53:PHE:O	2.17	0.45
2:A:62:VAL:CG2	2:A:88:HIS:CD2	3.00	0.45
2:A:316:CYS:O	2:A:377:MET:HG3	2.17	0.45
3:K:144:PHE:CD1	3:K:154:PHE:HE1	2.34	0.45
1:B:138:SER:HB2	1:B:169:VAL:CG2	2.47	0.45
1:B:151:LEU:HD11	1:B:152:ILE:HG12	1.98	0.45
1:B:207:LEU:HG	1:B:208:TYR:N	2.32	0.45
1:B:310:TYR:N	1:B:310:TYR:CD2	2.82	0.45
2:A:26:LEU:O	2:A:26:LEU:HD12	2.17	0.45
2:A:70:LEU:N	2:A:70:LEU:HD12	2.31	0.45
2:A:153:LEU:HD12	2:A:156:ARG:NH2	2.32	0.45
2:A:383:ALA:C	2:A:386:GLU:HG2	2.37	0.45
3:K:23:VAL:CG2	3:K:68:PHE:CE1	2.98	0.45
3:K:72:PHE:HB3	3:K:76:THR:CB	2.47	0.45
1:B:422:TYR:CD1	1:B:422:TYR:N	2.82	0.44
2:A:153:LEU:CG	2:A:157:LEU:CD1	2.95	0.44
2:A:352:LYS:HG3	2:A:353:VAL:H	1.82	0.44
1:B:58:LYS:HZ2	1:B:86:ARG:HE	1.65	0.44
1:B:121:ARG:HE	1:B:121:ARG:N	2.15	0.44
1:B:322:SER:OG	2:A:221:ARG:HB2	2.16	0.44
2:A:154:MET:CA	2:A:154:MET:CE	2.95	0.44
2:A:174:ALA:CB	2:A:176:GLN:CG	2.95	0.44
2:A:174:ALA:CB	2:A:207:GLU:HB2	2.42	0.44
2:A:176:GLN:OE1	2:A:177:VAL:HG12	2.18	0.44
2:A:256:GLN:OE1	2:A:259:LEU:HB2	2.18	0.44
2:A:287:SER:HB3	2:A:290:GLU:CG	2.47	0.44
2:A:311:LYS:O	2:A:312:TYR:HD1	2.00	0.44
2:A:411:GLU:C	3:K:272:ILE:CD1	2.79	0.44
3:K:28:PHE:CG	3:K:33:ARG:NH2	2.85	0.44
3:K:246:LYS:NZ	3:K:254:GLU:CD	2.69	0.44
1:B:21:TRP:HH2	1:B:50:TYR:OH	1.98	0.44
1:B:166:THR:HG22	1:B:167:PHE:N	2.32	0.44
2:A:204:VAL:HG22	2:A:205:ASP:N	2.32	0.44
2:A:211:ASP:HA	2:A:214:ARG:HG2	1.99	0.44
2:A:274:PRO:HD3	2:A:291:ILE:HD13	1.98	0.44
1:B:61:PRO:HB2	1:B:85:PHE:CE2	2.53	0.44
1:B:202:ILE:O	1:B:202:ILE:HG13	2.17	0.44
1:B:291:GLN:HG2	1:B:292:GLN:H	1.80	0.44
1:B:330:MET:HG2	1:B:331:LEU:HD13	1.98	0.44
2:A:46:ASP:H	2:A:49:PHE:CB	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:211:ASP:OD1	2:A:212:ILE:HD13	2.17	0.44
2:A:267:PHE:H	2:A:267:PHE:HD2	1.64	0.44
2:A:360:PRO:HG3	2:A:373:ARG:C	2.38	0.44
3:K:66:TYR:CD2	3:K:68:PHE:CE2	3.00	0.44
3:K:303:VAL:HG22	3:K:358:ASN:ND2	2.32	0.44
1:B:20:PHE:CE1	1:B:24:ILE:CD1	2.97	0.44
1:B:24:ILE:HD11	1:B:234:SER:HA	1.98	0.44
1:B:154:LYS:HZ3	1:B:157:GLU:HB3	1.82	0.44
1:B:194:GLU:H	1:B:194:GLU:CD	2.21	0.44
1:B:199:THR:CG2	1:B:265:PHE:CD2	3.00	0.44
1:B:200:TYR:HB3	1:B:268:PRO:CG	2.45	0.44
1:B:225:LEU:CD1	4:B:501:G2P:H2N1	2.30	0.44
1:B:251:ARG:HD3	2:A:105:ARG:NE	2.31	0.44
1:B:347:ASN:OD1	1:B:350:LYS:HD3	2.14	0.44
1:B:381:ILE:CA	1:B:384:GLN:HG3	2.46	0.44
2:A:28:HIS:CD2	2:A:41:THR:CG2	3.00	0.44
2:A:103:TYR:CD1	2:A:104:ALA:N	2.86	0.44
2:A:105:ARG:CD	2:A:407:TRP:HZ2	2.31	0.44
2:A:107:HIS:CE1	2:A:108:TYR:HE1	2.34	0.44
2:A:141:PHE:H	2:A:171:ILE:HG23	1.81	0.44
2:A:312:TYR:HB2	2:A:342:GLN:O	2.18	0.44
2:A:370:LYS:HD3	2:A:371:VAL:C	2.38	0.44
2:A:402:ARG:CZ	2:A:402:ARG:HB2	2.47	0.44
3:K:15:LYS:CE	3:K:362:LYS:HB3	2.46	0.44
3:K:82:TYR:CZ	3:K:86:VAL:HB	2.51	0.44
3:K:135:ILE:HD12	3:K:136:ILE:CA	2.48	0.44
3:K:191:LYS:HZ2	3:K:191:LYS:CB	2.31	0.44
3:K:228:MET:CE	3:K:228:MET:CA	2.96	0.44
3:K:258:ILE:N	3:K:368:LYS:HD3	2.32	0.44
1:B:65:LEU:HD22	1:B:90:PHE:CD2	2.52	0.44
1:B:112:LEU:O	1:B:116:VAL:HG22	2.18	0.44
1:B:383:GLU:O	1:B:386:THR:HB	2.17	0.44
1:B:396:HIS:CE1	1:B:397:TRP:CD1	3.05	0.44
1:B:398:TYR:HA	1:B:398:TYR:HD1	1.41	0.44
2:A:24:TYR:C	2:A:27:GLU:HG3	2.38	0.44
2:A:175:PRO:HG2	2:A:304:LYS:HE2	1.96	0.44
3:K:87:CYS:HB2	3:K:88:PRO:HD3	2.00	0.44
3:K:115:MET:SD	3:K:135:ILE:CG1	3.05	0.44
3:K:211:TYR:HD2	3:K:211:TYR:HA	1.41	0.44
3:K:255:LEU:HB3	3:K:369:LEU:HD13	1.94	0.44
3:K:304:GLU:HG3	3:K:306:THR:CA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:OD1	1:B:73:MET:HB3	2.18	0.44
1:B:139:LEU:HD23	1:B:168:SER:CB	2.43	0.44
1:B:187:LEU:HD22	1:B:187:LEU:H	1.83	0.44
1:B:246:LEU:CD1	1:B:352:ALA:CB	2.95	0.44
1:B:263:LEU:HD22	1:B:264:HIS:H	1.82	0.44
2:A:23:LEU:HG	2:A:364:PRO:HD3	2.00	0.44
2:A:123:ARG:HH11	2:A:123:ARG:HG2	1.82	0.44
2:A:176:GLN:HG2	2:A:207:GLU:CB	2.22	0.44
2:A:319:TYR:HD2	2:A:375:VAL:HG12	1.83	0.44
2:A:375:VAL:HB	2:A:377:MET:HE3	1.99	0.44
3:K:15:LYS:HE3	3:K:362:LYS:HB3	1.99	0.44
3:K:329:ARG:HA	3:K:363:PRO:CG	2.46	0.44
1:B:33:THR:HG21	1:B:35:SER:HB2	1.99	0.44
1:B:190:HIS:CD2	1:B:411:ALA:CA	2.99	0.44
2:A:21:TRP:CD1	2:A:67:PHE:CZ	3.06	0.44
2:A:102:ASN:HD21	2:A:411:GLU:CG	2.31	0.44
2:A:153:LEU:CD1	2:A:157:LEU:CD1	2.96	0.44
2:A:345:ASP:H	2:A:438:ASP:HB3	1.83	0.44
2:A:387:ALA:HA	2:A:390:ARG:HG3	2.00	0.44
3:K:15:LYS:HD3	3:K:15:LYS:N	2.32	0.44
3:K:15:LYS:CG	3:K:362:LYS:HB3	2.48	0.44
3:K:19:ILE:N	3:K:361:ASN:HB3	2.33	0.44
3:K:26:ARG:NE	3:K:337:SER:HA	2.33	0.44
3:K:50:VAL:HG23	3:K:71:VAL:HG11	2.00	0.44
3:K:157:LYS:HG2	3:K:203:THR:CB	2.47	0.44
3:K:168:LEU:CB	3:K:182:LEU:HG	2.48	0.44
1:B:2:ARG:HE	1:B:2:ARG:HB2	1.68	0.44
1:B:30:ILE:HB	1:B:35:SER:O	2.18	0.44
1:B:117:LEU:C	1:B:120:VAL:HG22	2.39	0.44
1:B:244:GLY:N	1:B:355:ASP:HB2	2.32	0.44
2:A:24:TYR:HA	2:A:27:GLU:HG3	1.99	0.44
2:A:234:ILE:HD12	2:A:235:VAL:CA	2.48	0.44
2:A:301:GLN:HE22	2:A:307:PRO:HD3	1.83	0.44
2:A:311:LYS:HD3	2:A:436:GLY:O	2.18	0.44
3:K:26:ARG:CG	3:K:26:ARG:HH11	2.29	0.44
3:K:54:THR:CG2	3:K:56:GLY:H	2.31	0.44
3:K:222:THR:CG2	3:K:231:TYR:CE2	3.00	0.44
3:K:327:ARG:HH21	3:K:327:ARG:HG2	1.82	0.44
1:B:2:ARG:O	1:B:4:ILE:HD12	2.18	0.43
1:B:113:VAL:CA	1:B:116:VAL:HG22	2.47	0.43
1:B:260:PHE:CD2	3:K:297:ARG:NH2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:SER:HA	1:B:429:THR:HG21	1.97	0.43
2:A:1:MET:HG2	2:A:47:ASP:CB	2.48	0.43
2:A:5:ILE:CD1	2:A:125:LEU:CD2	2.96	0.43
2:A:103:TYR:CE2	2:A:151:SER:CB	2.95	0.43
2:A:185:TYR:H	2:A:185:TYR:HD2	1.66	0.43
2:A:391:LEU:HA	2:A:394:LYS:CD	2.48	0.43
2:A:411:GLU:C	3:K:272:ILE:HD11	2.22	0.43
3:K:109:THR:HG21	3:K:335:THR:C	2.38	0.43
3:K:324:LEU:HD22	3:K:324:LEU:N	2.33	0.43
1:B:15:GLN:HG3	1:B:19:LYS:HD2	1.99	0.43
1:B:40:SER:O	1:B:44:LEU:HB3	2.18	0.43
1:B:105:HIS:HD2	1:B:149:THR:OG1	2.01	0.43
1:B:106:TYR:CZ	1:B:403:MET:SD	3.11	0.43
1:B:151:LEU:CD1	1:B:152:ILE:CD1	2.96	0.43
1:B:178:THR:HG21	1:B:180:VAL:HG22	1.96	0.43
1:B:222:TYR:CD1	4:B:501:G2P:C6	3.01	0.43
1:B:263:LEU:HG	1:B:311:LEU:CD1	2.47	0.43
1:B:275:SER:HG	1:B:276:ARG:H	1.66	0.43
1:B:390:ARG:HA	1:B:392:LYS:NZ	2.33	0.43
2:A:102:ASN:HB2	2:A:105:ARG:HD2	1.99	0.43
2:A:276:ILE:HG23	2:A:281:ALA:HA	2.00	0.43
3:K:168:LEU:CB	3:K:182:LEU:CG	2.95	0.43
3:K:358:ASN:O	3:K:360:LEU:HD12	2.18	0.43
1:B:12:CYS:HB2	1:B:138:SER:OG	2.17	0.43
1:B:58:LYS:HG2	1:B:59:TYR:H	1.80	0.43
1:B:70:PRO:HD3	1:B:94:GLN:HG2	1.98	0.43
1:B:216:LYS:HD3	1:B:276:ARG:CZ	2.48	0.43
1:B:269:GLY:HA3	1:B:367:PHE:CD1	2.52	0.43
1:B:319:GLY:H	1:B:354:CYS:HB3	1.83	0.43
2:A:8:HIS:CE1	2:A:67:PHE:CE1	3.06	0.43
2:A:70:LEU:HD22	2:A:99:ALA:CA	2.48	0.43
2:A:98:ASP:OD1	4:A:501:G2P:O2G	2.36	0.43
3:K:40:ILE:HG23	3:K:340:SER:HB2	2.01	0.43
3:K:136:ILE:CG2	3:K:214:LEU:CD1	2.96	0.43
3:K:303:VAL:HG22	3:K:358:ASN:HD22	1.81	0.43
1:B:85:PHE:CD1	1:B:85:PHE:N	2.86	0.43
1:B:199:THR:HG22	1:B:265:PHE:CB	2.48	0.43
1:B:222:TYR:HB3	4:B:501:G2P:O6	2.18	0.43
1:B:299:MET:HE1	1:B:367:PHE:HD1	1.83	0.43
2:A:25:CYS:HB3	2:A:30:ILE:HG23	2.00	0.43
2:A:240:ALA:HA	2:A:243:ARG:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:375:VAL:HG21	2:A:377:MET:CE	2.46	0.43
3:K:48:LYS:HE3	3:K:70:MET:HG3	2.00	0.43
3:K:144:PHE:CB	3:K:207:LYS:CD	2.96	0.43
1:B:48:ASN:HD21	1:B:53:GLU:CG	2.31	0.43
1:B:288:GLU:OE2	1:B:292:GLN:HG2	2.18	0.43
1:B:309:ARG:HG3	1:B:310:TYR:N	2.33	0.43
1:B:309:ARG:NH1	1:B:426:GLN:HG2	2.34	0.43
1:B:310:TYR:CD1	1:B:313:VAL:CG2	3.01	0.43
1:B:385:PHE:HA	1:B:388:MET:HG2	2.01	0.43
1:B:405:GLU:O	1:B:408:PHE:HB2	2.18	0.43
2:A:21:TRP:HA	2:A:21:TRP:CE3	2.54	0.43
2:A:70:LEU:CG	2:A:110:ILE:HG13	2.47	0.43
2:A:105:ARG:HA	2:A:411:GLU:CD	2.39	0.43
2:A:185:TYR:CD2	2:A:185:TYR:N	2.87	0.43
2:A:278:ALA:HB2	2:A:367:ASP:O	2.18	0.43
2:A:296:PHE:CE1	2:A:335:ILE:HG23	2.54	0.43
2:A:318:LEU:HD13	2:A:374:ALA:O	2.18	0.43
2:A:320:ARG:HB2	2:A:360:PRO:CG	2.41	0.43
3:K:169:PHE:HA	3:K:179:SER:CA	2.24	0.43
1:B:21:TRP:HD1	1:B:85:PHE:CE2	2.29	0.43
1:B:117:LEU:HA	1:B:120:VAL:CG2	2.48	0.43
1:B:156:ARG:CZ	1:B:157:GLU:HA	2.48	0.43
1:B:303:CYS:HB2	1:B:371:SER:CB	2.48	0.43
2:A:430:LYS:CD	2:A:434:GLU:CG	2.96	0.43
3:K:40:ILE:HG13	3:K:41:VAL:N	2.34	0.43
3:K:47:ARG:CZ	3:K:47:ARG:CA	2.95	0.43
1:B:34:GLY:CA	1:B:84:ILE:CD1	2.96	0.43
1:B:143:THR:HG22	1:B:143:THR:O	2.18	0.43
1:B:147:MET:O	1:B:151:LEU:HG	2.18	0.43
2:A:26:LEU:HB3	2:A:364:PRO:HG3	2.00	0.43
2:A:185:TYR:HB3	2:A:408:TYR:CE1	2.50	0.43
2:A:218:ASP:OD2	2:A:279:GLU:HG2	2.19	0.43
2:A:234:ILE:CG1	2:A:235:VAL:N	2.82	0.43
2:A:246:GLY:CA	2:A:356:ASN:HD22	2.32	0.43
2:A:312:TYR:C	2:A:344:VAL:HG13	2.39	0.43
2:A:375:VAL:CG2	2:A:377:MET:HE1	2.47	0.43
3:K:93:VAL:HG12	3:K:243:ILE:HD12	2.00	0.43
3:K:215:GLU:HG2	3:K:216:LYS:H	1.81	0.43
3:K:350:LEU:HD13	3:K:350:LEU:O	2.19	0.43
3:K:361:ASN:ND2	3:K:363:PRO:HD3	2.33	0.43
3:K:367:GLN:HE21	3:K:367:GLN:HB3	1.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PHE:CD1	1:B:368:ILE:CG2	3.02	0.43
1:B:284:LEU:CB	1:B:289:LEU:CD1	2.96	0.43
1:B:313:VAL:CG1	1:B:367:PHE:CE2	3.01	0.43
1:B:327:ASP:C	1:B:331:LEU:HD22	2.39	0.43
2:A:102:ASN:ND2	2:A:407:TRP:CE2	2.87	0.43
3:K:54:THR:CG2	3:K:55:GLY:N	2.82	0.43
3:K:78:GLN:NE2	3:K:113:PHE:O	2.45	0.43
1:B:49:VAL:CG2	1:B:50:TYR:N	2.82	0.43
1:B:198:GLU:OE1	1:B:198:GLU:HA	2.19	0.43
2:A:21:TRP:CD1	2:A:67:PHE:HZ	2.35	0.43
2:A:123:ARG:HD3	2:A:127:ASP:OD2	2.18	0.43
2:A:262:TYR:CD1	2:A:264:ARG:NH2	2.87	0.43
3:K:72:PHE:CD1	3:K:76:THR:CG2	2.97	0.43
3:K:95:MET:HG3	3:K:365:VAL:CG1	2.28	0.43
3:K:95:MET:CB	3:K:365:VAL:CG1	2.95	0.43
3:K:304:GLU:HG3	3:K:306:THR:HB	1.98	0.43
1:B:9:ALA:CB	1:B:147:MET:SD	3.07	0.43
1:B:178:THR:CG2	1:B:180:VAL:CG2	2.95	0.43
1:B:252:LYS:HG2	2:A:100:ALA:HB1	1.59	0.43
1:B:315:ALA:HB1	1:B:365:ALA:HB1	2.01	0.43
2:A:31:GLN:NE2	2:A:33:ASP:H	2.16	0.43
2:A:49:PHE:HE1	2:A:53:PHE:CD1	2.37	0.43
2:A:153:LEU:HG	2:A:157:LEU:HD12	2.00	0.43
2:A:172:TYR:CE2	2:A:391:LEU:HD23	2.51	0.43
2:A:223:THR:CG2	2:A:224:TYR:N	2.82	0.43
2:A:280:LYS:NZ	2:A:280:LYS:HB3	2.34	0.43
2:A:388:TRP:CZ3	2:A:428:LEU:HG	2.48	0.43
3:K:172:LEU:HG	3:K:173:ASN:ND2	2.34	0.43
1:B:21:TRP:HE1	1:B:62:ARG:N	2.16	0.42
1:B:48:ASN:HD21	1:B:53:GLU:HG3	1.84	0.42
1:B:70:PRO:CB	1:B:92:PHE:HE2	2.24	0.42
1:B:103:LYS:HD2	1:B:401:GLU:N	2.30	0.42
1:B:345:ILE:HD11	2:A:181:VAL:HA	1.72	0.42
1:B:398:TYR:CA	1:B:401:GLU:HG3	2.40	0.42
2:A:174:ALA:HB3	2:A:176:GLN:HG3	2.01	0.42
2:A:233:GLN:N	2:A:363:VAL:CG1	2.82	0.42
3:K:26:ARG:HG3	3:K:26:ARG:HH11	1.83	0.42
3:K:28:PHE:CE1	3:K:39:SER:N	2.86	0.42
3:K:314:SER:O	3:K:318:ARG:HG3	2.19	0.42
1:B:1:MET:CG	1:B:127:CYS:CB	2.95	0.42
1:B:107:THR:CG2	1:B:108:GLU:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PHE:HB2	1:B:220:PRO:CG	2.48	0.42
1:B:241:ARG:NE	1:B:242:PHE:CG	2.86	0.42
1:B:274:THR:CG2	1:B:279:GLN:N	2.83	0.42
1:B:280:GLN:CG	1:B:281:TYR:N	2.81	0.42
1:B:293:MET:CE	1:B:367:PHE:CA	2.96	0.42
1:B:394:PHE:CZ	1:B:397:TRP:CZ3	3.07	0.42
2:A:3:GLU:OE1	2:A:54:SER:HB2	2.19	0.42
2:A:139:HIS:HE1	2:A:141:PHE:CE2	2.37	0.42
2:A:163:LYS:HE3	2:A:163:LYS:N	2.33	0.42
2:A:233:GLN:CG	2:A:234:ILE:N	2.83	0.42
2:A:248:LEU:HD13	2:A:353:VAL:O	2.19	0.42
2:A:302:MET:HG2	2:A:303:VAL:H	1.84	0.42
2:A:313:MET:CA	2:A:344:VAL:HG13	2.48	0.42
2:A:387:ALA:O	2:A:391:LEU:HD23	2.19	0.42
3:K:139:THR:CG2	3:K:140:LEU:N	2.82	0.42
3:K:191:LYS:N	3:K:191:LYS:CD	2.82	0.42
3:K:202:ILE:HG23	3:K:202:ILE:O	2.18	0.42
3:K:204:VAL:HG21	3:K:209:GLU:HB2	2.00	0.42
3:K:255:LEU:CD2	3:K:369:LEU:CA	2.77	0.42
1:B:30:ILE:HA	1:B:36:TYR:CD1	2.50	0.42
1:B:149:THR:CG2	1:B:188:SER:CA	2.95	0.42
1:B:273:LEU:HD21	1:B:297:LYS:CD	2.49	0.42
2:A:71:GLU:HA	2:A:72:PRO:HD3	1.82	0.42
2:A:99:ALA:CB	2:A:145:THR:N	2.82	0.42
2:A:111:GLY:HA2	2:A:114:ILE:HG22	2.01	0.42
2:A:135:PHE:O	2:A:135:PHE:HD1	2.02	0.42
2:A:185:TYR:HB2	2:A:408:TYR:OH	2.19	0.42
2:A:229:ARG:HE	2:A:363:VAL:HB	1.85	0.42
2:A:286:LEU:HD22	2:A:291:ILE:HD13	2.00	0.42
2:A:310:GLY:C	2:A:311:LYS:HE3	2.40	0.42
2:A:342:GLN:O	2:A:342:GLN:HG3	2.19	0.42
2:A:347:CYS:SG	2:A:349:THR:CG2	3.07	0.42
2:A:413:MET:HB3	2:A:413:MET:HE2	1.95	0.42
3:K:135:ILE:HD12	3:K:136:ILE:CG1	2.49	0.42
3:K:226:THR:CG2	3:K:232:SER:CB	2.95	0.42
3:K:320:LEU:CD2	3:K:324:LEU:CD1	2.95	0.42
1:B:9:ALA:HA	1:B:66:VAL:HB	2.02	0.42
1:B:15:GLN:OE1	1:B:15:GLN:HA	2.19	0.42
1:B:29:GLY:O	1:B:37:HIS:HB3	2.19	0.42
1:B:97:ALA:CB	1:B:143:THR:CB	2.95	0.42
1:B:151:LEU:CD1	1:B:152:ILE:HD13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LYS:CE	1:B:154:LYS:HA	2.44	0.42
1:B:267:MET:SD	1:B:299:MET:CE	3.07	0.42
1:B:292:GLN:HA	1:B:295:ASP:OD1	2.19	0.42
2:A:226:ASN:HB3	2:A:367:ASP:OD2	2.20	0.42
2:A:312:TYR:CD2	2:A:315:CYS:SG	3.12	0.42
3:K:16:GLY:HA3	3:K:362:LYS:C	2.37	0.42
3:K:33:ARG:CZ	3:K:33:ARG:CA	2.97	0.42
3:K:255:LEU:HD23	3:K:369:LEU:HB3	1.06	0.42
1:B:36:TYR:CE1	1:B:38:GLY:N	2.84	0.42
1:B:58:LYS:HZ2	1:B:86:ARG:HG2	1.84	0.42
1:B:101:TRP:HB3	1:B:184:ASN:O	2.19	0.42
1:B:113:VAL:CG2	1:B:114:ASP:N	2.82	0.42
1:B:155:ILE:CG1	1:B:156:ARG:N	2.83	0.42
1:B:187:LEU:CD1	1:B:408:PHE:CD2	3.00	0.42
1:B:241:ARG:CD	1:B:242:PHE:N	2.82	0.42
1:B:276:ARG:HH11	1:B:280:GLN:NE2	2.18	0.42
1:B:314:ALA:HB3	1:B:368:ILE:HG12	1.99	0.42
1:B:374:ILE:CG2	1:B:375:GLN:N	2.81	0.42
1:B:381:ILE:HG12	1:B:384:GLN:NE2	2.33	0.42
1:B:382:SER:CB	1:B:415:MET:CE	2.98	0.42
2:A:4:CYS:SG	2:A:132:LEU:HD23	2.59	0.42
2:A:5:ILE:CG1	2:A:64:ARG:HB3	2.32	0.42
2:A:161:TYR:O	2:A:163:LYS:HD3	2.19	0.42
2:A:229:ARG:HG2	2:A:229:ARG:NH1	2.34	0.42
2:A:274:PRO:CB	2:A:276:ILE:HD11	2.49	0.42
3:K:272:ILE:CB	3:K:282:ALA:HB1	2.48	0.42
3:K:298:VAL:HG13	3:K:299:ILE:N	2.34	0.42
3:K:327:ARG:HH21	3:K:327:ARG:CG	2.33	0.42
1:B:1:MET:CG	1:B:2:ARG:N	2.83	0.42
1:B:116:VAL:CG2	1:B:117:LEU:N	2.82	0.42
1:B:154:LYS:HZ3	1:B:157:GLU:CB	2.32	0.42
1:B:210:ILE:HG23	1:B:297:LYS:CE	2.45	0.42
1:B:267:MET:HA	1:B:268:PRO:HD3	1.76	0.42
1:B:362:LYS:CE	1:B:362:LYS:CA	2.96	0.42
2:A:14:VAL:CG2	2:A:15:GLN:N	2.82	0.42
2:A:135:PHE:HE1	2:A:166:LYS:CB	2.33	0.42
2:A:138:PHE:O	2:A:139:HIS:HB3	2.20	0.42
2:A:202:PHE:CD1	2:A:267:PHE:CD1	3.07	0.42
2:A:234:ILE:HD12	2:A:235:VAL:HA	2.02	0.42
2:A:255:PHE:HZ	2:A:352:LYS:HB3	1.78	0.42
2:A:351:PHE:HA	2:A:352:LYS:HA	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:27:PRO:CA	3:K:74:ALA:CB	2.97	0.42
3:K:60:LYS:N	3:K:60:LYS:CD	2.83	0.42
3:K:312:ARG:CA	3:K:318:ARG:HG2	2.43	0.42
1:B:181:GLU:OE2	4:B:501:G2P:H5'1	2.20	0.42
1:B:187:LEU:HD22	1:B:187:LEU:N	2.34	0.42
1:B:207:LEU:CG	1:B:208:TYR:N	2.83	0.42
1:B:260:PHE:HB3	1:B:262:ARG:HD2	2.01	0.42
1:B:294:PHE:N	1:B:294:PHE:CD2	2.87	0.42
1:B:306:ARG:NH2	1:B:340:TYR:CD1	2.88	0.42
1:B:386:THR:O	1:B:389:PHE:HB3	2.19	0.42
2:A:53:PHE:CA	2:A:63:PRO:HA	2.49	0.42
2:A:62:VAL:HB	2:A:88:HIS:NE2	2.35	0.42
2:A:104:ALA:HB1	2:A:411:GLU:HB3	2.01	0.42
2:A:153:LEU:CD1	2:A:157:LEU:CG	2.97	0.42
2:A:305:CYS:SG	2:A:383:ALA:CB	3.08	0.42
2:A:314:ALA:HA	2:A:343:PHE:CE2	2.55	0.42
2:A:387:ALA:CA	2:A:390:ARG:CZ	2.97	0.42
2:A:411:GLU:CB	2:A:413:MET:HG2	2.42	0.42
3:K:40:ILE:CG1	3:K:41:VAL:N	2.83	0.42
1:B:65:LEU:N	1:B:65:LEU:CD1	2.83	0.42
1:B:138:SER:HB2	1:B:169:VAL:HG22	1.99	0.42
1:B:164:MET:HB2	1:B:164:MET:HE2	1.84	0.42
1:B:207:LEU:HD11	1:B:225:LEU:HD22	2.00	0.42
1:B:217:LEU:HD22	1:B:218:THR:H	1.85	0.42
1:B:258:VAL:CG1	1:B:263:LEU:HB3	2.49	0.42
2:A:11:GLN:NE2	4:A:501:G2P:H3A2	2.32	0.42
2:A:114:ILE:CG2	2:A:115:ILE:N	2.83	0.42
2:A:203:MET:SD	2:A:267:PHE:HZ	2.43	0.42
2:A:224:TYR:CZ	4:A:501:G2P:C8	3.03	0.42
2:A:254:GLU:OE2	2:A:255:PHE:HA	2.19	0.42
2:A:274:PRO:HG2	2:A:286:LEU:CD2	2.50	0.42
2:A:384:ILE:CG1	2:A:385:ALA:N	2.83	0.42
2:A:390:ARG:CA	2:A:393:HIS:CD2	2.99	0.42
2:A:413:MET:HB3	2:A:417:GLU:OE2	2.20	0.42
3:K:40:ILE:HB	3:K:53:ARG:HB2	2.01	0.42
3:K:136:ILE:HB	3:K:137:PRO:CD	2.50	0.42
3:K:321:GLN:C	3:K:324:LEU:HD23	2.40	0.42
1:B:2:ARG:HG3	1:B:2:ARG:O	2.20	0.42
1:B:14:ASN:HB3	1:B:72:THR:HG21	2.01	0.42
1:B:28:HIS:CG	1:B:47:ILE:HG23	2.55	0.42
1:B:105:HIS:NE2	1:B:150:LEU:HA	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:THR:N	1:B:288:GLU:CB	2.83	0.42
1:B:321:MET:CG	1:B:322:SER:N	2.83	0.42
1:B:343:GLU:H	1:B:343:GLU:CD	2.23	0.42
1:B:407:GLU:HG3	1:B:408:PHE:N	2.35	0.42
2:A:125:LEU:HD12	2:A:128:GLN:HG3	2.01	0.42
2:A:135:PHE:HE1	2:A:166:LYS:CA	2.33	0.42
2:A:244:PHE:N	2:A:244:PHE:CD1	2.85	0.42
3:K:28:PHE:HE1	3:K:39:SER:N	2.18	0.42
3:K:109:THR:HG22	3:K:335:THR:HB	1.93	0.42
1:B:4:ILE:N	1:B:4:ILE:CD1	2.83	0.42
1:B:36:TYR:CE1	1:B:38:GLY:HA3	2.53	0.42
1:B:152:ILE:HA	1:B:155:ILE:HG12	2.01	0.42
1:B:190:HIS:CG	1:B:411:ALA:CB	3.02	0.42
1:B:315:ALA:HA	1:B:366:THR:HG23	2.02	0.42
1:B:368:ILE:HG22	1:B:369:GLY:N	2.35	0.42
2:A:107:HIS:ND1	2:A:108:TYR:CE1	2.88	0.42
3:K:30:LEU:HD12	3:K:33:ARG:HB2	2.01	0.42
1:B:23:VAL:HG11	1:B:230:SER:HB2	2.01	0.41
1:B:250:LEU:C	1:B:253:LEU:HG	2.40	0.41
1:B:293:MET:HE3	1:B:367:PHE:CB	2.42	0.41
1:B:296:ALA:CB	1:B:305:PRO:HD3	2.50	0.41
1:B:313:VAL:HG13	1:B:367:PHE:CD2	2.55	0.41
2:A:122:ILE:CG1	2:A:123:ARG:N	2.83	0.41
2:A:188:ILE:CG1	2:A:395:PHE:CD1	3.02	0.41
2:A:306:ASP:CB	2:A:309:HIS:CE1	3.03	0.41
2:A:311:LYS:H	2:A:311:LYS:HD2	1.84	0.41
2:A:318:LEU:HD13	2:A:319:TYR:C	2.40	0.41
2:A:425:MET:SD	2:A:429:GLU:HG2	2.59	0.41
2:A:432:TYR:O	2:A:435:VAL:HG13	2.20	0.41
3:K:234:ARG:HD3	3:K:234:ARG:HA	1.52	0.41
3:K:298:VAL:HB	3:K:310:PRO:HG2	2.01	0.41
1:B:4:ILE:HG22	1:B:5:VAL:O	2.19	0.41
1:B:138:SER:OG	4:B:501:G2P:O2A	2.37	0.41
1:B:151:LEU:HD12	1:B:152:ILE:HA	2.02	0.41
1:B:172:SER:HB3	1:B:205:GLU:N	2.35	0.41
1:B:260:PHE:CD2	2:A:406:HIS:N	2.63	0.41
2:A:21:TRP:CE2	2:A:65:ALA:CB	3.00	0.41
2:A:188:ILE:N	2:A:188:ILE:CD1	2.83	0.41
2:A:318:LEU:CD1	2:A:320:ARG:CG	2.96	0.41
2:A:325:PRO:O	2:A:328:VAL:HB	2.20	0.41
2:A:411:GLU:CB	2:A:413:MET:SD	3.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:22:VAL:HG11	3:K:70:MET:HE2	2.01	0.41
3:K:92:GLU:CB	3:K:97:TYR:CD2	3.01	0.41
3:K:365:VAL:CG1	3:K:367:GLN:CG	2.95	0.41
1:B:23:VAL:CG1	1:B:24:ILE:N	2.83	0.41
1:B:99:ASN:HA	1:B:143:THR:N	2.34	0.41
1:B:165:ASN:ND2	1:B:167:PHE:CZ	2.89	0.41
1:B:263:LEU:O	1:B:263:LEU:HD13	2.20	0.41
2:A:171:ILE:HD12	4:A:501:G2P:H1'	1.94	0.41
2:A:250:VAL:HG22	2:A:254:GLU:OE1	2.20	0.41
2:A:255:PHE:C	2:A:259:LEU:HG	2.40	0.41
2:A:296:PHE:N	2:A:296:PHE:CD2	2.85	0.41
2:A:370:LYS:HD3	2:A:370:LYS:C	2.40	0.41
2:A:389:ALA:N	2:A:425:MET:CE	2.83	0.41
3:K:94:ILE:HA	3:K:245:MET:CE	2.50	0.41
3:K:159:SER:CB	3:K:172:LEU:HD13	2.47	0.41
3:K:173:ASN:HB3	3:K:176:SER:H	1.83	0.41
1:B:112:LEU:HD11	1:B:151:LEU:CA	2.49	0.41
1:B:323:MET:N	2:A:221:ARG:HG3	2.35	0.41
2:A:9:VAL:CG2	2:A:149:PHE:HD1	2.32	0.41
2:A:122:ILE:CD1	2:A:123:ARG:N	2.82	0.41
2:A:192:HIS:CD2	2:A:193:THR:HG23	2.55	0.41
2:A:210:TYR:CZ	2:A:227:LEU:HD22	2.55	0.41
2:A:275:VAL:HG13	2:A:280:LYS:NZ	2.34	0.41
2:A:311:LYS:N	2:A:311:LYS:CD	2.83	0.41
2:A:393:HIS:O	2:A:396:ASP:HB3	2.19	0.41
3:K:97:TYR:OH	3:K:363:PRO:HB2	2.20	0.41
3:K:272:ILE:CG2	3:K:282:ALA:HB1	2.50	0.41
3:K:342:ASN:C	3:K:342:ASN:HD22	2.23	0.41
1:B:186:THR:CG2	1:B:187:LEU:N	2.82	0.41
1:B:304:ASP:CB	1:B:307:HIS:CE1	3.04	0.41
2:A:36:MET:HB2	2:A:38:SER:HB3	2.03	0.41
2:A:79:ARG:NH1	2:A:92:LEU:HG	2.36	0.41
2:A:102:ASN:ND2	2:A:105:ARG:H	2.18	0.41
2:A:118:VAL:CG2	2:A:119:LEU:N	2.82	0.41
2:A:143:GLY:HA3	4:A:501:G2P:PB	2.60	0.41
2:A:262:TYR:CB	2:A:264:ARG:HD3	2.35	0.41
2:A:270:ALA:HB2	2:A:378:LEU:HD23	2.01	0.41
2:A:352:LYS:CG	2:A:353:VAL:N	2.83	0.41
3:K:162:GLU:HG3	3:K:235:SER:CB	2.29	0.41
3:K:272:ILE:HB	3:K:282:ALA:CB	2.50	0.41
1:B:192:LEU:HD13	1:B:192:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:MET:N	2:A:47:ASP:HA	2.36	0.41
2:A:13:GLY:O	2:A:16:ILE:HG22	2.20	0.41
2:A:210:TYR:CD2	2:A:221:ARG:NE	2.88	0.41
2:A:242:LEU:HB2	2:A:252:LEU:CG	2.50	0.41
2:A:253:THR:O	2:A:256:GLN:HB3	2.21	0.41
2:A:308:ARG:CD	2:A:308:ARG:N	2.83	0.41
2:A:321:GLY:CA	2:A:372:GLN:HE21	2.25	0.41
2:A:336:LYS:HD2	2:A:336:LYS:HA	1.76	0.41
3:K:28:PHE:CZ	3:K:37:ALA:C	2.93	0.41
3:K:227:LEU:CD1	3:K:228:MET:CE	2.98	0.41
3:K:258:ILE:N	3:K:368:LYS:HE2	2.33	0.41
1:B:47:ILE:CD1	1:B:241:ARG:HH12	2.33	0.41
1:B:106:TYR:HD2	1:B:106:TYR:N	2.18	0.41
1:B:137:HIS:HD2	1:B:144:GLY:O	2.04	0.41
1:B:183:TYR:CE1	1:B:385:PHE:CD1	3.09	0.41
1:B:190:HIS:CG	1:B:411:ALA:HA	2.56	0.41
1:B:271:ALA:CB	1:B:293:MET:SD	3.07	0.41
1:B:303:CYS:CB	1:B:371:SER:CB	2.99	0.41
1:B:324:LYS:HG2	2:A:221:ARG:HB2	1.12	0.41
1:B:410:GLU:CD	1:B:413:SER:HB2	2.41	0.41
1:B:414:ASN:HD21	3:K:312:ARG:CD	2.31	0.41
2:A:36:MET:HA	2:A:37:PRO:HD3	1.88	0.41
2:A:74:VAL:CG2	2:A:75:ILE:N	2.83	0.41
2:A:87:PHE:CE1	2:A:91:GLN:HG2	2.55	0.41
2:A:214:ARG:CG	2:A:215:ARG:N	2.82	0.41
2:A:272:TYR:CG	2:A:273:ALA:N	2.86	0.41
3:K:272:ILE:HG22	3:K:282:ALA:HA	2.01	0.41
3:K:343:LEU:HD23	3:K:343:LEU:N	2.12	0.41
1:B:154:LYS:O	1:B:157:GLU:HB3	2.21	0.41
1:B:221:THR:HG22	1:B:223:GLY:N	2.35	0.41
2:A:20:CYS:HA	2:A:232:SER:OG	2.21	0.41
2:A:108:TYR:C	2:A:112:LYS:HZ2	2.24	0.41
3:K:17:LYS:HG3	3:K:329:ARG:NE	2.35	0.41
3:K:97:TYR:HA	3:K:366:ASN:OD1	2.21	0.41
3:K:145:GLU:OE2	3:K:207:LYS:NZ	2.49	0.41
3:K:168:LEU:HB2	3:K:182:LEU:HB2	2.02	0.41
1:B:19:LYS:HA	1:B:19:LYS:NZ	2.36	0.41
1:B:31:ASP:OD1	1:B:37:HIS:HA	2.21	0.41
1:B:32:PRO:HB3	1:B:81:PHE:CE1	2.56	0.41
1:B:34:GLY:O	1:B:58:LYS:HA	2.20	0.41
1:B:94:GLN:HE21	1:B:94:GLN:HB3	1.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:CYS:SG	1:B:130:LEU:CD1	3.09	0.41
1:B:130:LEU:CD2	1:B:133:PHE:HE1	2.10	0.41
1:B:186:THR:HG21	1:B:385:PHE:CE1	2.56	0.41
1:B:196:THR:HG22	1:B:198:GLU:N	2.36	0.41
1:B:199:THR:HG23	1:B:199:THR:O	2.21	0.41
1:B:213:ARG:HB2	1:B:213:ARG:CZ	2.51	0.41
1:B:252:LYS:NZ	2:A:102:ASN:CA	2.48	0.41
1:B:255:VAL:CG1	1:B:256:ASN:N	2.83	0.41
1:B:258:VAL:O	2:A:404:PHE:CZ	2.73	0.41
1:B:266:PHE:HE1	1:B:312:THR:HG23	1.85	0.41
1:B:323:MET:HE1	1:B:326:VAL:CG2	2.44	0.41
1:B:337:ASN:CB	1:B:340:TYR:CD2	3.03	0.41
1:B:347:ASN:HB2	2:A:178:SER:H	1.86	0.41
2:A:24:TYR:CA	2:A:27:GLU:HG3	2.51	0.41
2:A:35:GLN:NE2	2:A:40:LYS:HE3	2.36	0.41
2:A:108:TYR:O	2:A:112:LYS:HD3	2.21	0.41
2:A:130:THR:CG2	2:A:131:GLY:N	2.82	0.41
2:A:150:THR:CG2	2:A:151:SER:N	2.82	0.41
2:A:234:ILE:CD1	2:A:235:VAL:N	2.82	0.41
2:A:245:ASP:CA	2:A:249:ASN:HB2	2.45	0.41
2:A:251:ASP:CG	2:A:254:GLU:HB3	2.40	0.41
2:A:262:TYR:CD2	2:A:265:ILE:HG12	2.54	0.41
2:A:298:PRO:CG	2:A:308:ARG:HH12	2.34	0.41
2:A:320:ARG:HD3	2:A:360:PRO:CA	2.43	0.41
2:A:347:CYS:SG	2:A:349:THR:HG23	2.61	0.41
2:A:351:PHE:HB2	2:A:352:LYS:HA	2.03	0.41
3:K:26:ARG:HG2	3:K:109:THR:HA	2.01	0.41
3:K:77:LYS:CE	3:K:78:GLN:HB2	2.51	0.41
3:K:134:GLY:CA	3:K:138:ARG:CG	2.99	0.41
3:K:139:THR:O	3:K:143:ILE:HG13	2.21	0.41
3:K:190:ASN:CB	3:K:193:GLY:H	2.32	0.41
1:B:24:ILE:CG2	1:B:28:HIS:NE2	2.82	0.41
1:B:269:GLY:HA3	1:B:367:PHE:HD1	1.86	0.41
2:A:7:ILE:O	2:A:138:PHE:CD1	2.74	0.41
2:A:28:HIS:CD2	2:A:41:THR:HG23	2.56	0.41
2:A:105:ARG:HG2	2:A:105:ARG:HH11	1.85	0.41
2:A:242:LEU:HD23	2:A:252:LEU:N	2.33	0.41
2:A:261:PRO:C	2:A:262:TYR:CD1	2.95	0.41
2:A:276:ILE:HB	2:A:368:LEU:HD22	2.03	0.41
2:A:278:ALA:O	2:A:282:TYR:CD1	2.74	0.41
2:A:306:ASP:CB	2:A:308:ARG:HH21	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:311:LYS:N	2:A:311:LYS:CE	2.83	0.41
2:A:318:LEU:O	2:A:319:TYR:CD2	2.74	0.41
3:K:54:THR:HG23	3:K:62:SER:HB2	2.02	0.41
3:K:54:THR:CB	3:K:56:GLY:H	2.34	0.41
3:K:59:ASP:C	3:K:61:SER:H	2.24	0.41
3:K:272:ILE:CG1	3:K:273:GLY:N	2.82	0.41
1:B:6:HIS:C	1:B:7:ILE:HD13	2.41	0.40
1:B:21:TRP:CZ2	1:B:62:ARG:O	2.74	0.40
1:B:152:ILE:HG21	1:B:192:LEU:CD2	2.51	0.40
1:B:175:VAL:CG1	1:B:176:SER:N	2.84	0.40
1:B:214:THR:HB	1:B:275:SER:C	2.40	0.40
1:B:245:GLN:HE22	1:B:355:ASP:HA	1.85	0.40
1:B:320:ARG:CZ	1:B:320:ARG:N	2.83	0.40
1:B:390:ARG:CZ	1:B:390:ARG:CA	2.96	0.40
2:A:102:ASN:CG	2:A:105:ARG:HB3	2.41	0.40
2:A:111:GLY:HA2	2:A:114:ILE:CG2	2.51	0.40
2:A:243:ARG:C	2:A:244:PHE:CD1	2.94	0.40
2:A:255:PHE:CD1	2:A:259:LEU:HD21	2.56	0.40
2:A:311:LYS:HA	2:A:342:GLN:HG2	1.99	0.40
3:K:16:GLY:HA3	3:K:363:PRO:N	2.35	0.40
3:K:141:HIS:HB2	3:K:211:TYR:OH	2.21	0.40
1:B:10:GLY:N	1:B:147:MET:SD	2.94	0.40
1:B:20:PHE:CZ	1:B:24:ILE:CD1	3.01	0.40
1:B:193:VAL:HG13	1:B:194:GLU:CD	2.41	0.40
1:B:250:LEU:HA	1:B:253:LEU:CG	2.51	0.40
1:B:256:ASN:HD21	2:A:181:VAL:H	1.69	0.40
1:B:309:ARG:HG2	1:B:425:TYR:O	2.22	0.40
1:B:378:PHE:O	1:B:381:ILE:HB	2.20	0.40
1:B:396:HIS:ND1	1:B:397:TRP:CD1	2.89	0.40
2:A:16:ILE:CG2	2:A:17:GLY:N	2.82	0.40
2:A:68:VAL:O	2:A:68:VAL:HG23	2.21	0.40
2:A:308:ARG:H	2:A:308:ARG:CD	2.34	0.40
3:K:19:ILE:HD11	3:K:332:ILE:HG13	2.03	0.40
1:B:99:ASN:HA	1:B:142:GLY:C	2.41	0.40
1:B:200:TYR:CD1	1:B:268:PRO:HD3	2.56	0.40
1:B:253:LEU:CB	1:B:257:MET:HE1	2.40	0.40
1:B:419:VAL:CG2	1:B:420:SER:N	2.83	0.40
2:A:63:PRO:O	2:A:87:PHE:CE1	2.75	0.40
2:A:102:ASN:HD22	2:A:105:ARG:CB	2.29	0.40
2:A:304:LYS:HG3	2:A:304:LYS:O	2.22	0.40
2:A:318:LEU:H	2:A:376:CYS:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:399:TYR:CE1	2:A:402:ARG:NE	2.89	0.40
3:K:50:VAL:CG2	3:K:71:VAL:CG1	2.99	0.40
3:K:144:PHE:CB	3:K:207:LYS:CG	2.97	0.40
1:B:51:TYR:CE2	1:B:61:PRO:HA	2.56	0.40
1:B:108:GLU:CD	1:B:147:MET:HA	2.41	0.40
1:B:186:THR:CG2	1:B:385:PHE:HE1	2.33	0.40
1:B:274:THR:CG2	1:B:275:SER:N	2.83	0.40
1:B:404:ASP:O	1:B:408:PHE:CD1	2.75	0.40
2:A:1:MET:CB	2:A:47:ASP:CA	2.96	0.40
2:A:3:GLU:HG2	2:A:50:ASN:C	2.41	0.40
2:A:5:ILE:HG23	2:A:65:ALA:N	2.36	0.40
2:A:10:GLY:HA2	2:A:145:THR:HB	2.03	0.40
2:A:153:LEU:HD11	2:A:157:LEU:CG	2.52	0.40
2:A:156:ARG:HB3	2:A:156:ARG:HH11	1.84	0.40
2:A:346:TRP:HZ2	2:A:437:VAL:O	2.04	0.40
2:A:349:THR:OG1	2:A:351:PHE:HD1	2.01	0.40
2:A:407:TRP:CE3	2:A:407:TRP:O	2.75	0.40
3:K:15:LYS:HE3	3:K:362:LYS:CB	2.50	0.40
3:K:27:PRO:N	3:K:74:ALA:HB1	2.37	0.40
3:K:105:GLY:HA3	3:K:335:THR:O	2.22	0.40
3:K:162:GLU:CD	3:K:235:SER:OG	2.59	0.40
3:K:255:LEU:CD2	3:K:369:LEU:HA	2.50	0.40
3:K:368:LYS:HD2	3:K:368:LYS:N	2.37	0.40
1:B:43:GLN:OE1	1:B:47:ILE:HD11	2.21	0.40
1:B:70:PRO:HD3	1:B:94:GLN:O	2.21	0.40
1:B:81:PHE:N	1:B:81:PHE:CD1	2.88	0.40
1:B:196:THR:HG22	1:B:198:GLU:H	1.86	0.40
2:A:36:MET:HB2	2:A:38:SER:H	1.85	0.40
2:A:56:THR:CG2	2:A:57:GLY:N	2.82	0.40
2:A:63:PRO:CB	2:A:87:PHE:CE1	3.04	0.40
2:A:215:ARG:CD	2:A:216:ASN:N	2.84	0.40
2:A:377:MET:N	2:A:377:MET:SD	2.95	0.40
2:A:406:HIS:O	2:A:409:VAL:HB	2.21	0.40
3:K:204:VAL:HG23	3:K:206:ASN:O	2.22	0.40
3:K:311:TYR:CD2	3:K:321:GLN:CD	2.95	0.40
3:K:369:LEU:N	3:K:369:LEU:CD2	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	B	427/429 (100%)	426 (100%)	1 (0%)	0	100	100
2	A	436/438 (100%)	434 (100%)	2 (0%)	0	100	100
3	K	328/391 (84%)	322 (98%)	6 (2%)	0	100	100
All	All	1191/1258 (95%)	1182 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	B	369/369 (100%)	303 (82%)	66 (18%)	1	9
2	A	369/369 (100%)	307 (83%)	62 (17%)	1	12
3	K	292/343 (85%)	256 (88%)	36 (12%)	4	19
All	All	1030/1081 (95%)	866 (84%)	164 (16%)	4	13

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	GLU
1	B	6	HIS
1	B	8	GLN
1	B	19	LYS
1	B	21	TRP

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Mol	Chain	Res	Type
1	B	22	GLU
1	B	31	ASP
1	B	37	HIS
1	B	43	GLN
1	B	44	LEU
1	B	50	TYR
1	B	73	MET
1	B	83	GLN
1	B	88	ASP
1	B	94	GLN
1	B	101	TRP
1	B	103	LYS
1	B	114	ASP
1	B	122	LYS
1	B	134	GLN
1	B	145	SER
1	B	147	MET
1	B	154	LYS
1	B	156	ARG
1	B	158	GLU
1	B	161	ASP
1	B	183	TYR
1	B	184	ASN
1	B	190	HIS
1	B	197	ASP
1	B	208	TYR
1	B	212	PHE
1	B	213	ARG
1	B	216	LYS
1	B	217	LEU
1	B	222	TYR
1	B	227	HIS
1	B	241	ARG
1	B	242	PHE
1	B	251	ARG
1	B	252	LYS
1	B	260	PHE
1	B	262	ARG
1	B	265	PHE
1	B	266	PHE
1	B	267	MET
1	B	273	LEU

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Mol	Chain	Res	Type
1	B	276	ARG
1	B	291	GLN
1	B	292	GLN
1	B	297	LYS
1	B	306	ARG
1	B	307	HIS
1	B	320	ARG
1	B	329	GLN
1	B	330	MET
1	B	331	LEU
1	B	336	LYS
1	B	343	GLU
1	B	361	LEU
1	B	363	MET
1	B	375	GLN
1	B	376	GLU
1	B	383	GLU
1	B	414	ASN
1	B	423	GLN
2	A	15	GLN
2	A	18	ASN
2	A	22	GLU
2	A	31	GLN
2	A	46	ASP
2	A	53	PHE
2	A	60	LYS
2	A	64	ARG
2	A	84	ARG
2	A	85	GLN
2	A	87	PHE
2	A	91	GLN
2	A	96	LYS
2	A	101	ASN
2	A	103	TYR
2	A	105	ARG
2	A	120	ASP
2	A	128	GLN
2	A	135	PHE
2	A	154	MET
2	A	156	ARG
2	A	163	LYS
2	A	164	LYS

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Mol	Chain	Res	Type
2	A	203	MET
2	A	210	TYR
2	A	211	ASP
2	A	214	ARG
2	A	215	ARG
2	A	218	ASP
2	A	220	GLU
2	A	221	ARG
2	A	224	TYR
2	A	229	ARG
2	A	242	LEU
2	A	243	ARG
2	A	254	GLU
2	A	255	PHE
2	A	264	ARG
2	A	267	PHE
2	A	285	GLN
2	A	302	MET
2	A	308	ARG
2	A	309	HIS
2	A	311	LYS
2	A	313	MET
2	A	320	ARG
2	A	326	LYS
2	A	339	ARG
2	A	343	PHE
2	A	346	TRP
2	A	351	PHE
2	A	352	LYS
2	A	392	ASP
2	A	394	LYS
2	A	396	ASP
2	A	401	LYS
2	A	406	HIS
2	A	407	TRP
2	A	423	GLU
2	A	424	ASP
2	A	430	LYS
2	A	432	TYR
3	K	15	LYS
3	K	17	LYS
3	K	28	PHE

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Mol	Chain	Res	Type
3	K	33	ARG
3	K	34	LYS
3	K	38	HIS
3	K	54	THR
3	K	60	LYS
3	K	77	LYS
3	K	84	SER
3	K	95	MET
3	K	97	TYR
3	K	104	TYR
3	K	171	LEU
3	K	172	LEU
3	K	181	ARG
3	K	182	LEU
3	K	187	ASP
3	K	189	ARG
3	K	190	ASN
3	K	191	LYS
3	K	202	ILE
3	K	207	LYS
3	K	208	ASP
3	K	228	MET
3	K	247	GLU
3	K	257	LYS
3	K	266	LEU
3	K	272	ILE
3	K	289	ASN
3	K	327	ARG
3	K	342	ASN
3	K	343	LEU
3	K	345	GLU
3	K	367	GLN
3	K	368	LYS

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

Mol	Chain	Res	Type
1	B	11	GLN
1	B	28	HIS
1	B	94	GLN
1	B	99	ASN
1	B	105	HIS

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Mol	Chain	Res	Type
1	B	131	GLN
1	B	226	ASN
1	B	245	GLN
1	B	256	ASN
1	B	279	GLN
1	B	280	GLN
1	B	291	GLN
1	B	292	GLN
1	B	334	GLN
1	B	335	ASN
1	B	348	ASN
1	B	375	GLN
1	B	414	ASN
1	B	424	GLN
1	B	426	GLN
2	A	8	HIS
2	A	15	GLN
2	A	31	GLN
2	A	61	HIS
2	A	88	HIS
2	A	91	GLN
2	A	101	ASN
2	A	139	HIS
2	A	176	GLN
2	A	186	ASN
2	A	216	ASN
2	A	228	ASN
2	A	233	GLN
2	A	283	HIS
2	A	285	GLN
2	A	300	ASN
2	A	301	GLN
2	A	329	ASN
2	A	342	GLN
2	A	358	GLN
3	K	98	ASN
3	K	150	ASN
3	K	173	ASN
3	K	190	ASN
3	K	205	HIS
3	K	287	ASN
3	K	289	ASN

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Mol	Chain	Res	Type
3	K	290	GLN
3	K	308	HIS
3	K	342	ASN
3	K	367	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
4	G2P	A	501	5	27,34,34	1.11	1 (3%)	33,54,54	1.99	5 (15%)
4	G2P	B	501	1,5	27,34,34	1.19	3 (11%)	33,54,54	2.13	7 (21%)
6	MZK	K	501	-	23,23,23	1.37	1 (4%)	34,34,34	1.15	3 (8%)

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
4	G2P	A	501	5	-	7/15/38/38	0/3/3/3
4	G2P	B	501	1,5	-	4/15/38/38	0/3/3/3
6	MZK	K	501	-	-	0/10/19/19	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	501	MZK	C7-N1	3.84	1.39	1.35
4	B	501	G2P	C6-N1	3.01	1.38	1.33
4	A	501	G2P	C6-N1	2.99	1.38	1.33
4	B	501	G2P	PA-O1A	-2.46	1.50	1.56
4	B	501	G2P	PB-O1B	-2.40	1.50	1.56

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	G2P	C5-C6-N1	-8.13	112.31	123.43
4	B	501	G2P	C5-C6-N1	-8.02	112.46	123.43
4	B	501	G2P	C2-N1-C6	5.73	125.04	115.93
4	A	501	G2P	C2-N1-C6	5.70	124.99	115.93
4	B	501	G2P	O1B-PB-C3A	3.17	119.55	106.58
4	B	501	G2P	N3-C2-N1	-3.05	123.15	127.22
4	B	501	G2P	O1A-PA-C3A	2.94	118.59	106.58
4	A	501	G2P	N3-C2-N1	-2.92	123.33	127.22
6	K	501	MZK	C2-C1-C3	2.86	121.19	118.55
6	K	501	MZK	C5-C1-C3	2.77	120.89	118.54
6	K	501	MZK	C14-C13-C16	2.61	124.12	119.97
4	B	501	G2P	C4-C5-C6	-2.47	118.44	120.80
4	A	501	G2P	C4-C5-C6	-2.45	118.46	120.80
4	B	501	G2P	C2-N3-C4	-2.26	112.77	115.36
4	A	501	G2P	C2-N3-C4	-2.17	112.88	115.36

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	A	501	G2P	PB-C3A-PA-O5'
4	A	501	G2P	C5'-O5'-PA-O1A
4	B	501	G2P	PB-O3B-PG-O3G
4	A	501	G2P	PB-O3B-PG-O3G
4	A	501	G2P	PB-O3B-PG-O2G

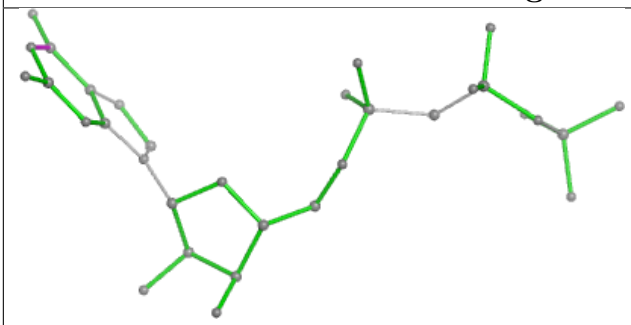
There are no ring outliers.

2 monomers are involved in 50 short contacts:

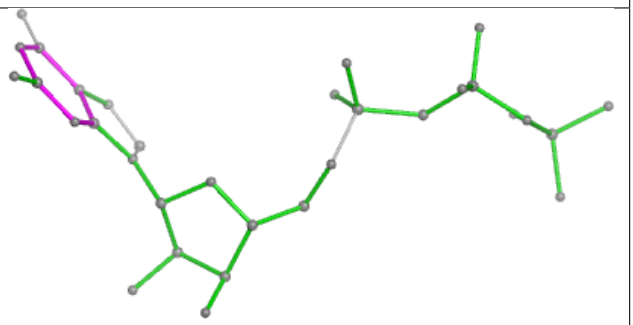
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	G2P	31	0
4	B	501	G2P	19	0

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

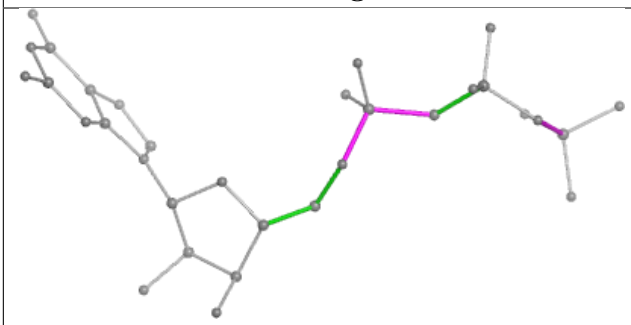
Ligand G2P A 501



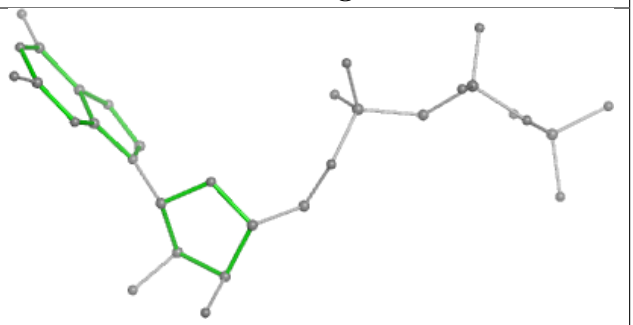
Bond lengths



Bond angles

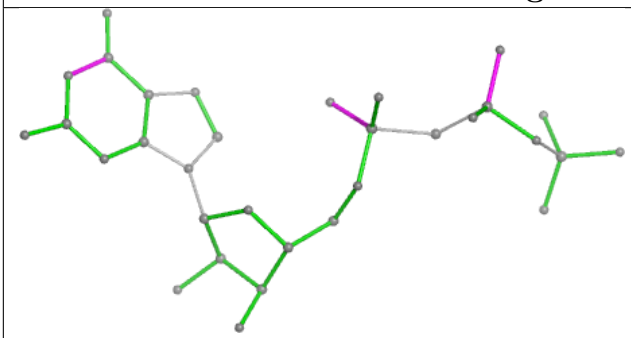


Torsions

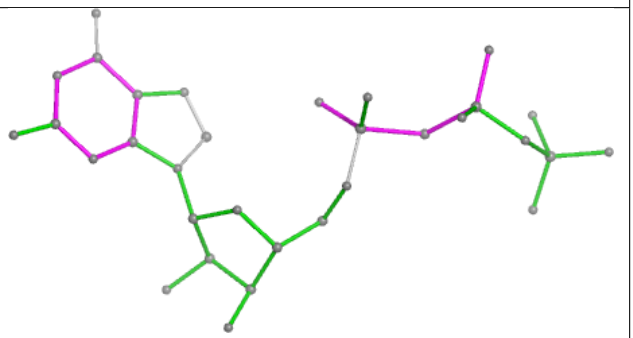


Rings

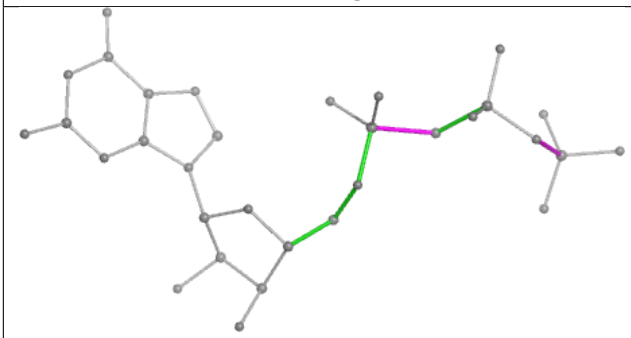
Ligand G2P B 501



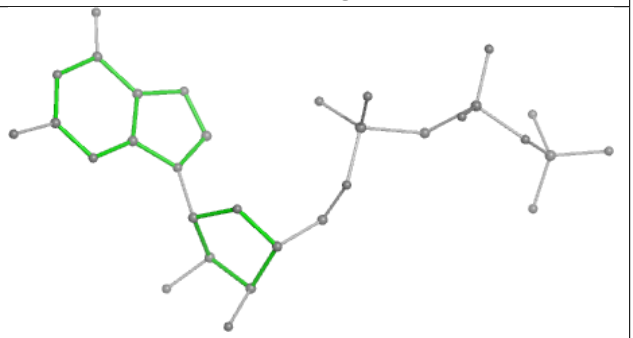
Bond lengths



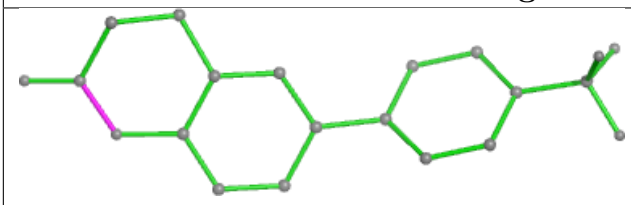
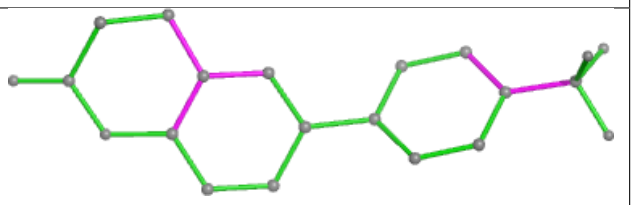
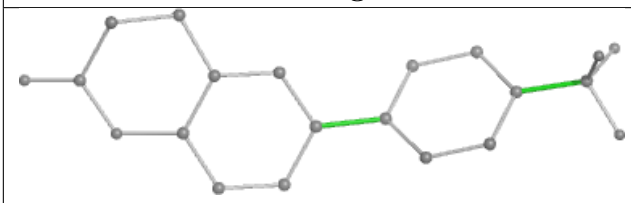
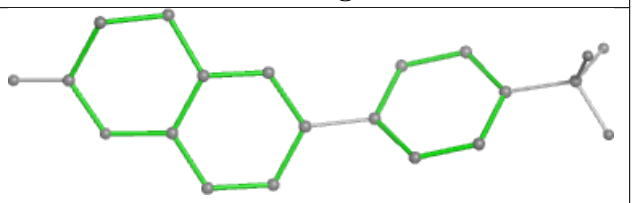
Bond angles



Torsions



Rings

Ligand MZK K 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 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.