



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 04:42 AM UTC

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

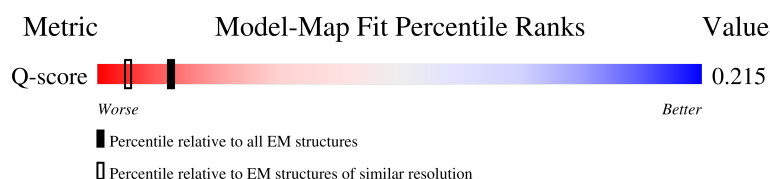
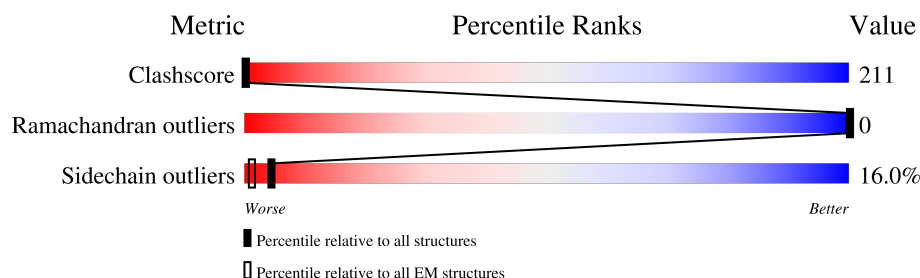
1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	429	9% 64% 25%
2	A	438	5% 6% 68% 24%
3	K	391	18% 15% 52% 15% 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

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
1	B	429	Total	C	N	O	S	0	0
			3372	2117	578	651	26		

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

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

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

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

There are 22 discrepancies between the modelled and reference sequences:

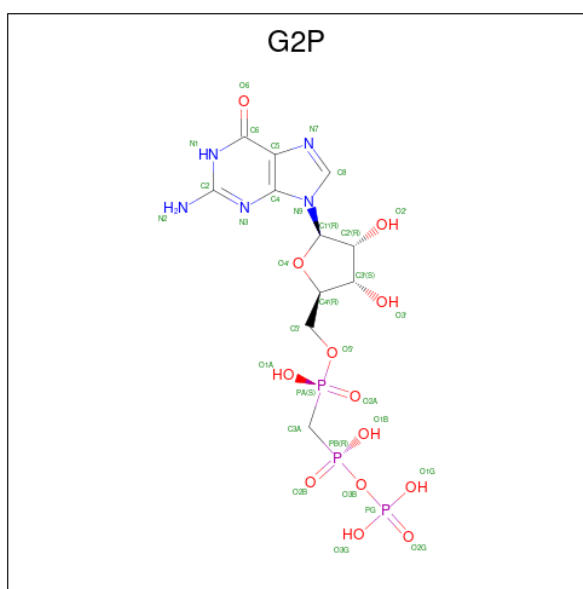
Chain	Residue	Modelled	Actual	Comment	Reference
K	-21	MET	-	initiating methionine	UNP P52732
K	-20	HIS	-	expression tag	UNP P52732
K	-19	HIS	-	expression tag	UNP P52732
K	-18	HIS	-	expression tag	UNP P52732
K	-17	HIS	-	expression tag	UNP P52732
K	-16	HIS	-	expression tag	UNP P52732
K	-15	HIS	-	expression tag	UNP P52732
K	-14	SER	-	expression tag	UNP P52732
K	-13	SER	-	expression tag	UNP P52732
K	-12	GLY	-	expression tag	UNP P52732
K	-11	VAL	-	expression tag	UNP P52732
K	-10	ASP	-	expression tag	UNP P52732
K	-9	LEU	-	expression tag	UNP P52732
K	-8	GLY	-	expression tag	UNP P52732
K	-7	THR	-	expression tag	UNP P52732

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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: $C_{11}H_{18}N_5O_{13}P_3$).



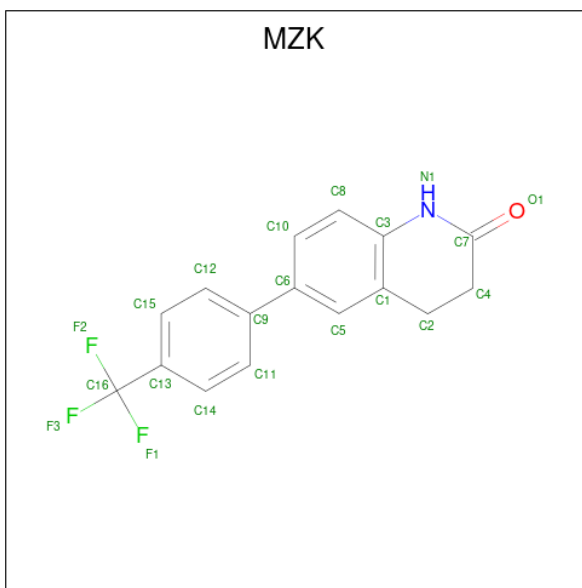
Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			32	11	5	13	3	
4	A	1	Total	C	N	O	P	0
			32	11	5	13	3	

- 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: C₁₆H₁₂F₃NO) (labeled as "Ligand of Interest" by depositor).

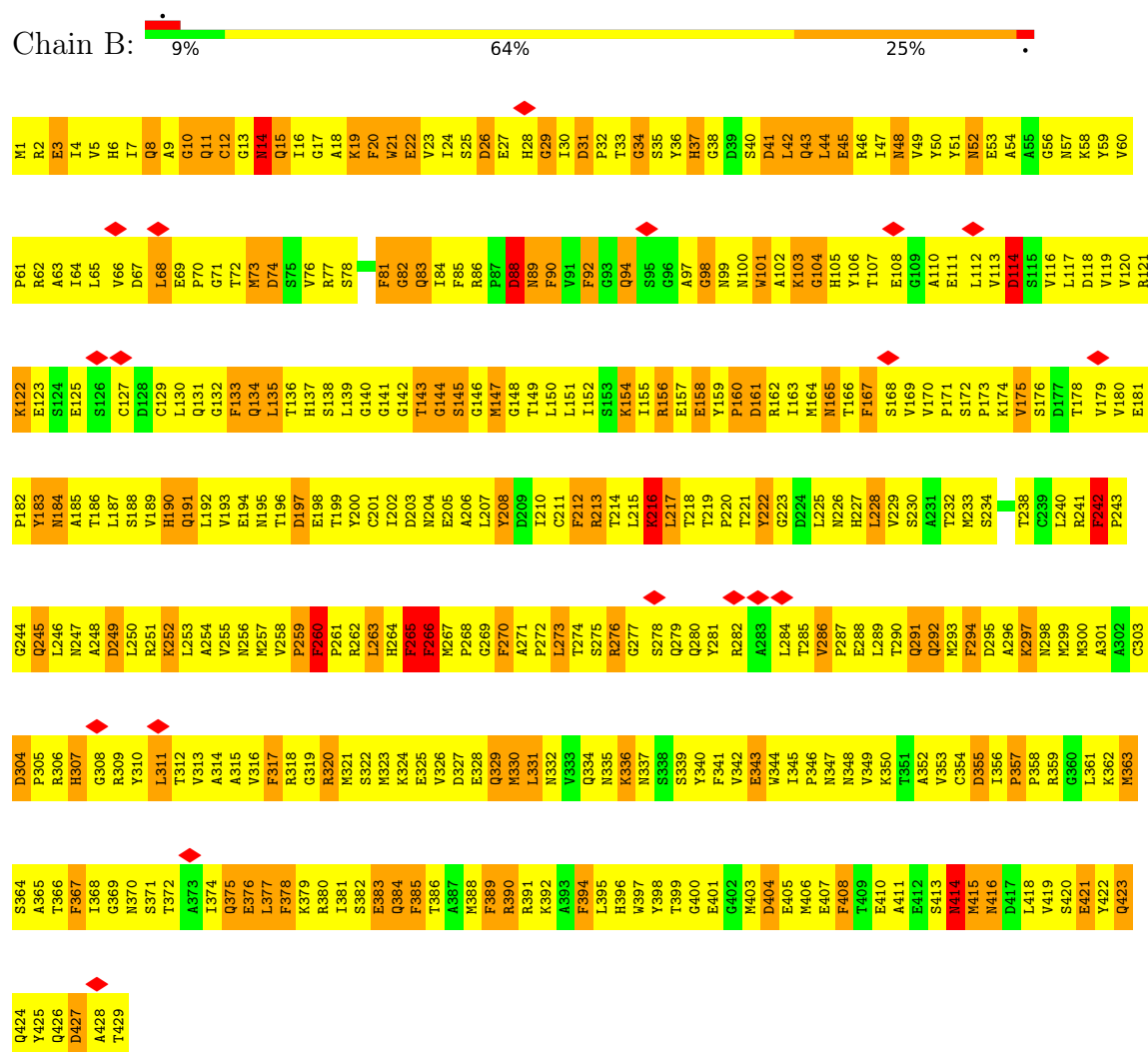


Mol	Chain	Residues	Atoms					AltConf
6	K	1	Total 21	C 16	F 3	N 1	O 1	0

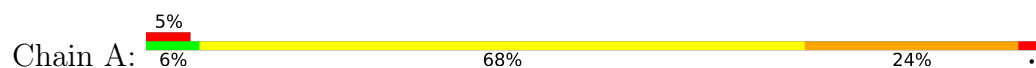
3 Residue-property plots

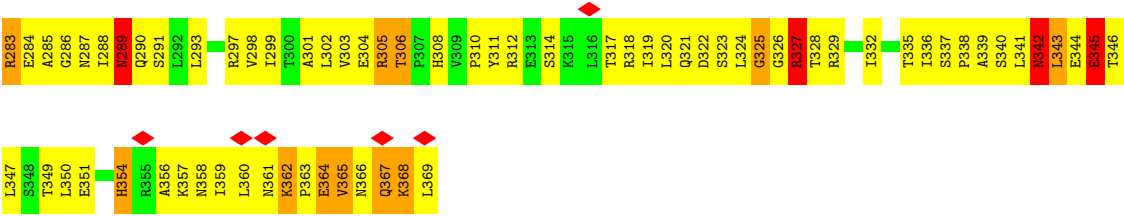
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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



- Molecule 2: Tubulin alpha-1B chain





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.7°, rise=8.9 Å, axial sym=C1	Depositor
Number of segments used	507219	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	555.9, 555.9, 555.9	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	B	1.57	4/3447 (0.1%)	1.86	72/4669 (1.5%)
2	A	1.55	3/3503 (0.1%)	1.76	67/4754 (1.4%)
3	K	1.68	20/2640 (0.8%)	1.70	55/3557 (1.5%)
All	All	1.59	27/9590 (0.3%)	1.78	194/12980 (1.5%)

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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	84	SER	CB-OG	-36.95	0.68	1.42
3	K	254	GLU	CB-CG	-15.31	1.06	1.52
3	K	306	THR	C-O	-11.95	1.08	1.23
3	K	260	LYS	CG-CD	-10.53	1.20	1.52
3	K	257	LYS	CB-CG	-9.54	1.23	1.52
3	K	247	GLU	CB-CG	-8.93	1.25	1.52
3	K	79	ILE	C-N	-8.00	1.23	1.33
1	B	286	VAL	CA-CB	-7.36	1.50	1.54
3	K	81	VAL	C-N	-7.31	1.24	1.33
3	K	81	VAL	CA-CB	-6.97	1.45	1.54
3	K	230	ALA	CA-C	-6.47	1.44	1.52
3	K	247	GLU	CD-OE1	-6.47	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	12	CYS	CA-C	-6.05	1.45	1.52
2	A	62	VAL	CA-CB	-5.76	1.50	1.54
3	K	79	ILE	N-CA	-5.73	1.39	1.46
3	K	80	ASP	N-CA	-5.64	1.39	1.46
3	K	186	ASP	C-O	-5.60	1.17	1.24
3	K	278	VAL	CA-CB	-5.56	1.48	1.54
1	B	60	VAL	CA-C	-5.56	1.48	1.53
3	K	79	ILE	CA-C	-5.50	1.45	1.52
3	K	19	ILE	CA-CB	-5.47	1.47	1.54
2	A	260	VAL	CA-C	-5.44	1.48	1.53
3	K	362	LYS	CA-C	-5.17	1.47	1.52
2	A	177	VAL	CA-CB	-5.16	1.50	1.55
3	K	283	ARG	NE-CZ	5.14	1.38	1.33
1	B	175	VAL	CA-CB	-5.05	1.47	1.55
3	K	271	ASN	CA-C	-5.02	1.46	1.52

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	GLY	O-C-N	-27.56	90.86	122.56
3	K	84	SER	CA-CB-OG	14.10	139.29	111.10
3	K	254	GLU	CA-CB-CG	12.76	139.62	114.10
3	K	289	ASN	N-CA-C	-11.06	99.23	111.07
3	K	257	LYS	CA-CB-CG	10.54	135.18	114.10
3	K	257	LYS	CB-CG-CD	10.05	134.43	111.30
3	K	254	GLU	CB-CG-CD	9.67	129.03	112.60
1	B	144	GLY	N-CA-C	-8.69	102.30	112.73
2	A	49	PHE	CA-CB-CG	-8.57	105.22	113.80
3	K	260	LYS	CG-CD-CE	8.41	130.64	111.30
1	B	92	PHE	CA-CB-CG	-8.37	105.43	113.80
1	B	12	CYS	N-CA-C	-8.29	101.93	110.97
1	B	133	PHE	CA-CB-CG	-8.29	105.51	113.80
3	K	97	TYR	CA-C-N	-8.21	111.39	122.72
3	K	97	TYR	C-N-CA	-8.21	111.39	122.72
1	B	12	CYS	CA-C-N	8.18	130.60	120.22
1	B	12	CYS	C-N-CA	8.18	130.60	120.22
2	A	161	TYR	CA-CB-CG	-8.12	99.28	113.90
1	B	378	PHE	CA-CB-CG	-8.03	105.77	113.80
3	K	61	SER	N-CA-C	-8.01	102.63	111.36
3	K	247	GLU	CB-CG-CD	7.96	126.13	112.60
1	B	385	PHE	CA-CB-CG	-7.88	105.92	113.80
1	B	389	PHE	CA-CB-CG	-7.87	105.93	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	GLN	CA-C-N	7.84	131.00	120.65
1	B	11	GLN	C-N-CA	7.84	131.00	120.65
1	B	317	PHE	CA-CB-CG	-7.78	106.02	113.80
2	A	141	PHE	CA-CB-CG	-7.71	106.09	113.80
2	A	255	PHE	CA-CB-CG	-7.68	106.12	113.80
2	A	202	PHE	CA-CB-CG	-7.62	106.18	113.80
2	A	296	PHE	CA-CB-CG	-7.56	106.24	113.80
1	B	90	PHE	CA-CB-CG	-7.33	106.47	113.80
1	B	143	THR	N-CA-CB	7.24	120.87	110.16
1	B	68	LEU	N-CA-C	-7.19	103.45	111.28
1	B	56	GLY	N-CA-C	-7.16	105.35	115.30
2	A	87	PHE	CA-CB-CG	-7.13	106.67	113.80
2	A	102	ASN	CA-CB-CG	-7.12	105.47	112.60
3	K	365	VAL	CA-C-N	-7.11	111.53	122.05
3	K	365	VAL	C-N-CA	-7.11	111.53	122.05
3	K	28	PHE	CA-CB-CG	-7.10	106.70	113.80
1	B	212	PHE	CA-CB-CG	-7.09	106.71	113.80
1	B	294	PHE	CA-CB-CG	-7.05	106.75	113.80
1	B	367	PHE	CA-CB-CG	-7.01	106.79	113.80
3	K	260	LYS	CB-CG-CD	6.87	127.11	111.30
2	A	138	PHE	CA-CB-CG	-6.86	106.94	113.80
1	B	266	PHE	CA-CB-CG	-6.83	106.97	113.80
3	K	211	TYR	CA-CB-CG	-6.74	101.77	113.90
2	A	135	PHE	CA-CB-CG	-6.73	107.07	113.80
1	B	34	GLY	N-CA-C	-6.73	106.17	114.92
1	B	20	PHE	CA-CB-CG	-6.72	107.08	113.80
2	A	29	GLY	N-CA-C	-6.69	106.00	115.43
2	A	133	GLN	N-CA-C	-6.69	103.99	111.28
2	A	356	ASN	CA-CB-CG	-6.65	105.95	112.60
3	K	29	ASN	CA-CB-CG	-6.64	105.96	112.60
1	B	81	PHE	CA-CB-CG	-6.56	107.24	113.80
3	K	59	ASP	CA-CB-CG	-6.54	106.06	112.60
3	K	55	GLY	N-CA-C	-6.53	105.47	114.67
3	K	174	PRO	N-CA-C	-6.52	104.84	113.65
1	B	29	GLY	N-CA-C	-6.52	106.23	115.30
1	B	242	PHE	CA-CB-CG	-6.52	107.28	113.80
3	K	18	ASN	CA-CB-CG	-6.52	106.08	112.60
1	B	260	PHE	CA-CB-CG	-6.43	107.37	113.80
3	K	208	ASP	CA-CB-CG	-6.39	106.21	112.60
1	B	304	ASP	CA-CB-CG	-6.39	106.21	112.60
2	A	50	ASN	CA-CB-CG	-6.38	106.22	112.60
1	B	114	ASP	CA-CB-CG	-6.29	106.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	408	PHE	CA-CB-CG	-6.28	107.52	113.80
2	A	116	ASP	CA-CB-CG	-6.23	106.37	112.60
2	A	244	PHE	CA-CB-CG	-6.21	107.59	113.80
2	A	263	PRO	N-CA-C	-6.20	105.77	113.84
2	A	418	PHE	CA-CB-CG	-6.17	107.63	113.80
1	B	14	ASN	N-CA-C	-6.16	104.57	111.28
1	B	332	ASN	CA-CB-CG	-6.14	106.46	112.60
1	B	98	GLY	N-CA-C	-6.13	106.24	115.32
3	K	86	VAL	N-CA-C	6.10	116.73	110.82
1	B	165	ASN	CA-CB-CG	-6.09	106.50	112.60
2	A	37	PRO	N-CA-C	-6.08	105.44	113.65
3	K	177	ASP	CA-CB-CG	-6.03	106.57	112.60
2	A	412	GLY	N-CA-C	-6.01	106.80	115.27
2	A	343	PHE	CA-CB-CG	-5.94	107.86	113.80
1	B	259	PRO	N-CA-C	-5.94	105.63	113.65
2	A	218	ASP	N-CA-C	-5.93	104.64	112.24
3	K	342	ASN	CA-CB-CG	-5.93	106.67	112.60
1	B	394	PHE	CA-CB-CG	-5.92	107.88	113.80
3	K	30	LEU	N-CA-C	-5.90	104.85	111.28
2	A	149	PHE	CA-CB-CG	-5.89	107.91	113.80
3	K	31	ALA	N-CA-C	-5.89	104.86	111.28
1	B	52	ASN	CA-CB-CG	-5.88	106.72	112.60
1	B	245	GLN	N-CA-C	-5.88	104.78	111.07
3	K	325	GLY	N-CA-C	-5.84	105.90	114.90
3	K	175	SER	N-CA-C	-5.83	104.83	111.07
1	B	144	GLY	CA-C-N	-5.83	112.51	120.44
1	B	144	GLY	C-N-CA	-5.83	112.51	120.44
2	A	404	PHE	CA-CB-CG	-5.83	107.97	113.80
3	K	151	GLY	N-CA-C	-5.83	107.28	115.32
2	A	175	PRO	N-CA-C	-5.82	106.28	113.84
1	B	10	GLY	N-CA-C	-5.82	105.44	112.48
2	A	211	ASP	CA-CB-CG	-5.80	106.80	112.60
1	B	10	GLY	CA-C-N	5.79	129.11	120.31
1	B	10	GLY	C-N-CA	5.79	129.11	120.31
2	A	39	ASP	CA-CB-CG	-5.78	106.82	112.60
1	B	167	PHE	CA-CB-CG	-5.75	108.05	113.80
2	A	395	PHE	CA-CB-CG	-5.75	108.05	113.80
1	B	82	GLY	N-CA-C	-5.73	105.85	112.73
2	A	224	TYR	N-CA-C	-5.73	105.03	111.28
3	K	247	GLU	CA-CB-CG	5.70	125.51	114.10
3	K	40	ILE	N-CA-C	-5.70	104.96	110.72
1	B	104	GLY	N-CA-C	-5.67	105.92	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	226	ASN	CA-CB-CG	-5.67	106.93	112.60
2	A	322	ASP	CA-CB-CG	-5.67	106.93	112.60
1	B	249	ASP	CA-CB-CG	-5.66	106.94	112.60
2	A	53	PHE	CA-CB-CG	-5.65	108.15	113.80
1	B	89	ASN	CA-CB-CG	-5.63	106.97	112.60
2	A	365	GLY	N-CA-C	-5.62	105.61	114.10
1	B	74	ASP	CA-CB-CG	-5.62	106.98	112.60
1	B	270	PHE	CA-CB-CG	-5.62	108.18	113.80
2	A	306	ASP	CA-CB-CG	-5.61	106.99	112.60
2	A	267	PHE	CA-CB-CG	-5.61	108.19	113.80
3	K	69	ASP	N-CA-C	-5.60	105.08	111.07
3	K	364	GLU	CA-C-N	-5.58	113.39	120.98
3	K	364	GLU	C-N-CA	-5.58	113.39	120.98
1	B	311	LEU	N-CA-C	-5.57	105.11	111.07
1	B	414	ASN	CA-CB-CG	-5.56	107.04	112.60
3	K	108	GLY	N-CA-C	-5.55	106.07	112.73
2	A	410	GLY	N-CA-C	-5.53	106.09	112.73
3	K	150	ASN	N-CA-C	-5.51	105.27	111.28
2	A	367	ASP	CA-CB-CG	-5.50	107.10	112.60
2	A	396	ASP	CA-CB-CG	-5.49	107.11	112.60
2	A	144	GLY	N-CA-C	-5.48	106.15	112.73
1	B	384	GLN	N-CA-C	-5.47	105.31	111.28
3	K	276	GLY	N-CA-C	-5.47	106.48	114.90
1	B	197	ASP	CA-CB-CG	-5.47	107.13	112.60
3	K	181	ARG	CA-C-N	-5.45	115.31	123.00
3	K	181	ARG	C-N-CA	-5.45	115.31	123.00
1	B	48	ASN	CA-CB-CG	-5.43	107.17	112.60
2	A	47	ASP	N-CA-C	-5.41	105.38	111.28
2	A	247	ALA	N-CA-C	-5.41	105.29	111.07
1	B	427	ASP	CA-CB-CG	-5.37	107.23	112.60
2	A	106	GLY	N-CA-C	-5.36	106.30	112.73
3	K	289	ASN	CA-CB-CG	-5.35	107.25	112.60
1	B	400	GLY	N-CA-C	-5.35	106.31	112.73
1	B	173	PRO	N-CA-C	-5.34	107.18	113.86
1	B	404	ASP	CA-CB-CG	-5.34	107.26	112.60
2	A	127	ASP	CA-CB-CG	-5.33	107.27	112.60
2	A	169	PHE	CA-CB-CG	-5.33	108.47	113.80
2	A	218	ASP	CA-CB-CG	-5.32	107.28	112.60
2	A	120	ASP	CA-CB-CG	-5.30	107.30	112.60
3	K	180	GLU	N-CA-C	-5.28	103.05	110.50
2	A	216	ASN	N-CA-C	-5.28	105.53	111.28
2	A	293	ASN	CA-CB-CG	-5.27	107.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ASP	CA-CB-CG	-5.26	107.34	112.60
2	A	34	GLY	N-CA-C	-5.26	107.74	114.37
2	A	278	ALA	N-CA-C	-5.26	105.44	111.07
1	B	78	SER	N-CA-C	-5.25	105.68	111.71
3	K	48	LYS	CA-C-N	-5.24	115.33	122.93
3	K	48	LYS	C-N-CA	-5.24	115.33	122.93
3	K	354	HIS	CE1-NE2-CD2	-5.24	103.76	109.00
2	A	319	TYR	CA-CB-CG	-5.23	104.49	113.90
3	K	306	THR	N-CA-C	-5.23	102.61	110.24
3	K	319	ILE	O-C-N	5.21	126.92	121.87
3	K	48	LYS	N-CA-C	-5.21	105.57	112.24
3	K	305	ARG	N-CA-C	-5.20	104.72	111.74
1	B	14	ASN	CA-CB-CG	-5.19	107.41	112.60
3	K	206	ASN	CA-CB-CG	-5.19	107.41	112.60
1	B	216	LYS	N-CA-C	-5.18	106.55	112.86
2	A	83	TYR	N-CA-C	-5.18	105.76	111.71
3	K	327	ARG	N-CA-C	-5.15	105.79	111.71
2	A	210	TYR	CA-CB-CG	-5.12	104.68	113.90
2	A	307	PRO	N-CA-C	-5.12	106.73	113.65
3	K	192	ARG	N-CA-C	-5.12	105.78	111.36
2	A	100	ALA	N-CA-C	-5.11	106.62	112.86
2	A	101	ASN	CA-C-N	-5.11	115.90	123.05
2	A	101	ASN	C-N-CA	-5.11	115.90	123.05
1	B	355	ASP	CA-CB-CG	-5.11	107.49	112.60
2	A	59	GLY	N-CA-C	-5.10	108.24	115.43
1	B	88	ASP	CA-CB-CG	-5.09	107.50	112.60
2	A	299	ALA	N-CA-C	-5.09	105.73	111.28
1	B	26	ASP	CA-CB-CG	-5.08	107.52	112.60
2	A	351	PHE	CA-CB-CG	-5.08	108.72	113.80
2	A	43	GLY	N-CA-C	-5.08	106.05	114.48
1	B	416	ASN	CA-CB-CG	-5.08	107.52	112.60
2	A	146	GLY	N-CA-C	-5.08	106.64	112.73
2	A	424	ASP	N-CA-C	-5.07	105.75	111.28
1	B	160	PRO	N-CA-C	-5.07	106.81	113.65
1	B	357	PRO	N-CA-CB	5.06	106.02	103.19
2	A	431	ASP	CA-CB-CG	-5.06	107.54	112.60
2	A	329	ASN	CA-CB-CG	-5.05	107.55	112.60
3	K	110	GLY	CA-C-N	-5.04	113.74	120.54
3	K	110	GLY	C-N-CA	-5.04	113.74	120.54
2	A	249	ASN	CA-CB-CG	-5.04	107.56	112.60
2	A	33	ASP	CA-CB-CG	-5.02	107.58	112.60
3	K	54	THR	N-CA-C	-5.02	105.52	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	CYS	O-C-N	5.01	127.25	122.03
1	B	423	GLN	N-CA-C	-5.01	105.82	111.28
1	B	265	PHE	CA-CB-CG	-5.00	108.80	113.80

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 ⓘ

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	1534	0
2	A	3425	0	3330	1620	0
3	K	2607	0	2670	978	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	3960	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 211.

All (3960) 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
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
3:K:95:MET:HE2	3:K:97:TYR:CB	1.54	1.35
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
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: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:252:LYS:CD	2:A:101:ASN:CB	1.96	1.20
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: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
1:B:260:PHE:CZ	2:A:406:HIS:N	2.11	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:K:162:GLU:CD	3:K:235:SER:HB2	1.73	1.14
1:B:253:LEU:HB2	1:B:257:MET:HE2	1.29	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
1:B:321:MET:HE3	1:B:326:VAL:HG22	1.17	1.11
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
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:246:LYS:CE	3:K:254:GLU:CD	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:K:246:LYS:HE3	3:K:254:GLU:CD	1.79	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
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
1:B:260:PHE:CD1	2:A:406:HIS:NE2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:MET:HE3	3:K:97:TYR:CD2	1.94	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
2:A:317:LEU:HD22	2:A:377:MET:HE3	1.41	1.01
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
1:B:323:MET:HA	1:B:323:MET:HE3	1.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LYS:HD2	1:B:401:GLU:HA	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:326:VAL:HG12	1:B:330:MET:HE1	1.45	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
3:K:223:THR:HG21	3:K:235:SER:H	1.29	0.97
1:B:382:SER:HB3	1:B:415:MET:HE1	1.47	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:375:VAL:HG21	2:A:377:MET:HE1	1.50	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
1:B:9:ALA:HB1	1:B:147:MET:HE2	1.47	0.93
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:154:MET:HA	2:A:154:MET:HE3	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:324:LYS:HG3	2:A:220:GLU:C	1.93	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:94:ILE:O	3:K:245:MET:HE1	1.69	0.91
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:142:GLY:HA2	1:B:184:ASN:CG	1.96	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
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
1:B:1:MET:HE2	1:B:49:VAL:HB	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:115:MET:HE1	3:K:135:ILE:HD11	1.52	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
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:51:TYR:HD2	1:B:59:TYR:HB3	1.38	0.88
1:B:253:LEU:HB2	1:B:257:MET:CE	2.02	0.88
2:A:71:GLU:HB3	2:A:98:ASP:CG	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:382:SER:CB	1:B:415:MET:HE1	2.04	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:228:MET:HA	3:K:228:MET:HE3	1.56	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
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
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
3:K:162:GLU:CD	3:K:235:SER:CB	2.44	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:45:GLU:HG3	1:B:46:ARG:HE	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:36:MET:HE2	2:A:38:SER:HB3	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
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
1:B:342:VAL:HA	1:B:429:THR:C	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:102:ALA:HB3	1:B:401:GLU:CD	2.03	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:156:ARG:CB	1:B:164:MET:HE1	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
2:A:23:LEU:HD12	2:A:363:VAL:CA	2.06	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: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: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
2:A:216:ASN:CG	2:A:280:LYS:HD2	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:158:VAL:C	3:K:201:GLU:HG2	2.03	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
1:B:293:MET:HA	1:B:298:ASN:CG	2.03	0.83
3:K:95:MET:HE3	3:K:97:TYR:HD2	1.40	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
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:313:MET:HE2	2:A:344:VAL:HG11	1.58	0.82
2:A:385:ALA:HB1	2:A:429:GLU:OE1	1.79	0.82
2:A:431:ASP:HA	2:A:434:GLU:CD	2.04	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
2:A:375:VAL:CG2	2:A:377:MET:HE1	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:8:HIS:HB3	2:A:13:GLY:C	2.03	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
3:K:144:PHE:HB2	3:K:207:LYS:HZ3	1.44	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:56:THR:C	2:A:58:ALA:HA	2.03	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:99:ASN:C	1:B:142:GLY:HA3	2.05	0.81
1:B:101:TRP:CZ2	1:B:403:MET:HG3	2.15	0.81
1:B:293:MET:HE3	1:B:367:PHE:HB2	1.62	0.81
1:B:381:ILE:HA	1:B:384:GLN:CD	2.04	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:3:GLU:CD	1:B:50:TYR:HA	2.06	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
1:B:323:MET:HE3	1:B:326:VAL:HG21	1.62	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
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:156:ARG:HB2	1:B:164:MET:HE1	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:LYS:H	2:A:221:ARG:HG3	1.44	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
2:A:53:PHE:HB3	2:A:62:VAL:C	2.07	0.80
1:B:372:THR:HA	1:B:375:GLN:OE1	1.80	0.80
2:A:1:MET:HE3	2:A:1:MET:HA	1.63	0.80
2:A:351:PHE:HB2	2:A:352:LYS:HZ2	1.47	0.80
3:K:95:MET:CE	3:K:97:TYR:CB	2.31	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
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
2:A:405:VAL:O	2:A:409:VAL:HG23	1.82	0.80
3:K:94:ILE:C	3:K:245:MET:HE1	2.06	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:10:GLY:H	1:B:147:MET:HE1	1.47	0.79
1:B:388:MET:HA	1:B:388:MET:HE3	1.64	0.79
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
1:B:1:MET:HE2	1:B:1:MET:HA	1.64	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
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
1:B:375:GLN:CD	1:B:422:TYR:HB3	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:K:54:THR:C	3:K:60:LYS:HG3	2.08	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: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
3:K:339:ALA:HB1	3:K:341:LEU:HD13	1.62	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:122:LYS:HA	1:B:125:GLU:CD	2.08	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:257:LYS:HA	3:K:368:LYS:HD3	1.65	0.78
1:B:293:MET:HE1	1:B:367:PHE:HA	1.66	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:K:162:GLU:CD	3:K:223:THR:HG22	2.10	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:167:PHE:CD2	1:B:233:MET:HE3	2.20	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
3:K:227:LEU:HD12	3:K:228:MET:HE1	1.67	0.77
1:B:41:ASP:CG	1:B:42:LEU:HD22	2.10	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
3:K:187:ASP:CG	3:K:195:ILE:HG13	2.09	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
2:A:388:TRP:HB2	2:A:425:MET:HE1	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:108:TYR:OH	2:A:413:MET:HE1	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:1:MET:HE1	1:B:49:VAL:O	1.88	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
2:A:116:ASP:HA	2:A:119:LEU:CD2	2.16	0.74
1:B:101:TRP:CD1	1:B:188:SER:HG	2.05	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
1:B:253:LEU:CB	1:B:257:MET:HE2	2.15	0.73
1:B:288:GLU:HA	1:B:291:GLN:CD	2.13	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ARG:HB2	1:B:122:LYS:HZ3	1.53	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
3:K:246:LYS:HE2	3:K:254:GLU:CD	2.14	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: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:190:HIS:NE2	1:B:411:ALA:HA	2.04	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:A:205:ASP:CG	2:A:303:VAL:HA	2.14	0.72
3:K:228:MET:HE3	3:K:228:MET:CA	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
2:A:301:GLN:CD	2:A:307:PRO:HG3	2.14	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
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:154:MET:HE1	2:A:166:LYS:CE	2.19	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:223:THR:HB	2:A:226:ASN:CG	2.15	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
2:A:302:MET:HE3	2:A:302:MET:H	1.55	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
2:A:294:ALA:HA	2:A:297:GLU:CD	2.14	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
3:K:191:LYS:H	3:K:191:LYS:HZ2	1.39	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
1:B:102:ALA:HB1	1:B:403:MET:SD	2.31	0.71
1:B:215:LEU:C	1:B:276:ARG:HG2	2.16	0.71
1:B:375:GLN:HG3	1:B:422:TYR:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:322:SER:H	1:B:325:GLU:CD	1.99	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
2:A:346:TRP:CD1	2:A:346:TRP:H	2.06	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:33:ASP:HA	2:A:85:GLN:CD	2.17	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
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
3:K:256:VAL:H	3:K:369:LEU:C	1.99	0.70
1:B:34:GLY:C	1:B:58:LYS:HA	2.16	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
1:B:324:LYS:CG	2:A:220:GLU:C	2.64	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:164:LYS:HA	2:A:164:LYS:HZ3	1.57	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
3:K:221:ARG:HH22	3:K:233:SER:HB2	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:TYR:HB2	1:B:59:TYR:CD1	2.26	0.69
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
2:A:324:VAL:HG21	2:A:326:LYS:HZ1	1.57	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: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
2:A:351:PHE:HB2	2:A:352:LYS:NZ	2.07	0.69
3:K:32:GLU:O	3:K:35:ALA:HB3	1.93	0.69
3:K:172:LEU:HG	3:K:173:ASN:N	2.05	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:375:GLN:HG3	1:B:422:TYR:CD2	2.28	0.69
2:A:29:GLY:C	2:A:36:MET:HE3	2.16	0.69
2:A:311:LYS:HA	2:A:342:GLN:CD	2.17	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
1:B:1:MET:CE	1:B:49:VAL:HB	2.22	0.69
1:B:251:ARG:HG3	1:B:252:LYS:N	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:318:LEU:O	2:A:375:VAL:HA	1.93	0.69
3:K:84:SER:HB3	3:K:84:SER:HG	1.18	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
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
1:B:329:GLN:OE1	1:B:330:MET:HE3	1.92	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: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:227:LEU:HG	3:K:228:MET:CE	2.23	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:404:ASP:OD1	1:B:406:MET:HE3	1.92	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
2:A:311:LYS:HG3	2:A:342:GLN:CD	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:HB3	1:B:69:GLU:C	2.18	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
1:B:346:PRO:HD2	2:A:398:MET:HE1	1.75	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
3:K:55:GLY:C	3:K:62:SER:HB2	2.18	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
1:B:347:ASN:OD1	2:A:179:THR:C	2.36	0.68
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
2:A:154:MET:HE2	2:A:158:SER:OG	1.93	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:212:GLN:HA	3:K:215:GLU:CD	2.18	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:205:ASP:CG	2:A:303:VAL:HG23	2.19	0.68
2:A:270:ALA:HB2	2:A:378:LEU:CD2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:299:MET:HE2	1:B:299:MET:HA	1.75	0.68
2:A:358:GLN:HG2	2:A:359:PRO:HD2	1.76	0.68
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:98:GLY:C	4:B:501:G2P:O3G	2.37	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: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:159:TYR:HB3	1:B:161:ASP:CG	2.19	0.67
1:B:271:ALA:HB3	1:B:365:ALA:C	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:55:GLY:HA2	3:K:59:ASP:C	2.20	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:103:LYS:HZ2	1:B:401:GLU:HA	1.60	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
2:A:430:LYS:C	2:A:430:LYS:HD3	2.19	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: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
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
1:B:12:CYS:C	1:B:16:ILE:HG13	2.19	0.67
1:B:132:GLY:HA3	1:B:163:ILE:O	1.95	0.67
1:B:267:MET:HE1	1:B:367:PHE:HE1	1.59	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
1:B:323:MET:HA	1:B:323:MET:CE	2.21	0.67
2:A:152:LEU:HD23	2:A:152:LEU:O	1.95	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:376:GLU:HG3	1:B:379:LYS:HZ3	1.59	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
1:B:323:MET:C	2:A:221:ARG:HG3	2.20	0.66
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
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
2:A:370:LYS:HZ3	2:A:372:GLN:HA	1.60	0.66
3:K:78:GLN:CD	3:K:113:PHE:CE2	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:270:GLU:CD	3:K:275:SER:HB2	2.20	0.66
1:B:103:LYS:HA	1:B:103:LYS:HZ2	1.57	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:144:PHE:CB	3:K:207:LYS:HZ3	2.09	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
3:K:361:ASN:CG	3:K:363:PRO:HD3	2.20	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
1:B:286:VAL:HG11	1:B:325:GLU:CG	2.26	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:251:ARG:HG3	1:B:252:LYS:H	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:430:LYS:HD3	2:A:430:LYS:O	1.95	0.65
3:K:26:ARG:CB	3:K:109:THR:HA	2.25	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
1:B:142:GLY:HA2	1:B:184:ASN:ND2	2.10	0.65
1:B:421:GLU:CD	1:B:424:GLN:HB3	2.21	0.65
2:A:57:GLY:N	2:A:58:ALA:HA	2.09	0.65
2:A:409:VAL:HG11	3:K:289:ASN:C	2.22	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:344:VAL:HA	2:A:438:ASP:CG	2.21	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: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:36:MET:HE2	2:A:38:SER:CB	2.26	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:67:ASP:CG	1:B:73:MET:HB3	2.22	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:103:TYR:HD2	2:A:147:SER:C	2.05	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:A:317:LEU:CD2	2:A:377:MET:HE3	2.25	0.64
3:K:366:ASN:O	3:K:368:LYS:HD2	1.97	0.64
1:B:101:TRP:CG	1:B:188:SER:HG	2.16	0.64
1:B:135:LEU:HD22	1:B:135:LEU:N	2.13	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
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:295:CYS:HA	2:A:300:ASN:CG	2.22	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:178:THR:CG2	1:B:181:GLU:HB2	2.28	0.63
1:B:326:VAL:O	1:B:330:MET:HE3	1.98	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:411:GLU:HB3	2:A:413:MET:SD	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:94:ILE:O	3:K:245:MET:CE	2.45	0.63
3:K:258:ILE:H	3:K:368:LYS:HD3	1.64	0.63
1:B:66:VAL:HG11	1:B:147:MET:HE2	1.79	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
2:A:423:GLU:CD	3:K:57:LEU:HD13	2.22	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
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:97:GLU:CD	2:A:105:ARG:HH22	2.07	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:430:LYS:NZ	2:A:430:LYS:HA	2.13	0.63
3:K:48:LYS:C	3:K:71:VAL:HG21	2.23	0.63
3:K:180:GLU:CD	3:K:199:LEU:HA	2.24	0.63
1:B:243:PRO:C	1:B:355:ASP:HB2	2.23	0.62
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
3:K:227:LEU:HG	3:K:228:MET:N	2.13	0.62
1:B:4:ILE:HD11	1:B:131:GLN:CB	2.23	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
1:B:363:MET:H	1:B:363:MET:CE	2.12	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
2:A:214:ARG:O	2:A:217:LEU:HB2	1.98	0.62
3:K:235:SER:C	3:K:267:ALA:HB2	2.24	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:70:MET:HE3	3:K:72:PHE:CE2	2.35	0.62
3:K:342:ASN:ND2	3:K:345:GLU:H	1.96	0.62
1:B:267:MET:HE3	1:B:369:GLY:C	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:B:240:LEU:HD12	1:B:247:ASN:OD1	2.00	0.62
1:B:260:PHE:C	1:B:262:ARG:HD3	2.25	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
2:A:313:MET:HE3	2:A:344:VAL:HG11	1.81	0.62
1:B:70:PRO:CD	1:B:94:GLN:HG2	2.30	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:173:ASN:HB2	3:K:176:SER:HB2	1.81	0.61
3:K:361:ASN:C	3:K:363:PRO:HD3	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:33:ASP:CG	2:A:35:GLN:H	2.08	0.61
2:A:310:GLY:CA	2:A:381:THR:HB	2.28	0.61
3:K:227:LEU:CD1	3:K:228:MET:HE1	2.30	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
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
1:B:363:MET:H	1:B:363:MET:HE2	1.65	0.61
2:A:22:GLU:HA	2:A:25:CYS:SG	2.40	0.61
2:A:30:ILE:HA	2:A:36:MET:HE3	1.82	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
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:22:VAL:HG11	3:K:70:MET:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:43:CYS:C	3:K:45:PRO:HD3	2.26	0.61
3:K:159:SER:CB	3:K:199:LEU:HD21	2.22	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:154:MET:HE3	2:A:154:MET:CA	2.27	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
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
2:A:30:ILE:N	2:A:36:MET:HE3	2.16	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:293:MET:HE1	1:B:366:THR:O	2.01	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:192:LEU:HD13	1:B:192:LEU:C	2.26	0.60
1:B:271:ALA:HB3	1:B:365:ALA:HB3	1.82	0.60
1:B:323:MET:CE	1:B:326:VAL:HG21	2.29	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
2:A:321:GLY:HA3	2:A:372:GLN:O	2.01	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:42:LEU:HA	1:B:45:GLU:CD	2.27	0.60
1:B:101:TRP:CH2	1:B:403:MET:HG3	2.36	0.60
1:B:112:LEU:HD23	1:B:112:LEU:C	2.27	0.60
2:A:115:ILE:HG23	2:A:116:ASP:N	2.17	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:15:LYS:HE3	3:K:364:GLU:CD	2.26	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: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
2:A:409:VAL:CG1	3:K:289:ASN:C	2.75	0.60
3:K:77:LYS:HE3	3:K:78:GLN:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:135:PHE:HE1	2:A:166:LYS:HA	1.66	0.60
2:A:230:LEU:HD23	2:A:230:LEU:C	2.27	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
1:B:1:MET:HA	1:B:1:MET:CE	2.30	0.60
1:B:1:MET:HE1	1:B:49:VAL:CA	2.32	0.60
1:B:245:GLN:CD	1:B:355:ASP:HA	2.26	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
2:A:326:LYS:NZ	2:A:326:LYS:HB3	2.17	0.60
1:B:3:GLU:C	1:B:4:ILE:HD12	2.27	0.59
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: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:318:LEU:HD13	2:A:318:LEU:C	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:K:215:GLU:HG2	3:K:216:LYS:N	2.17	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
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: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
3:K:84:SER:CB	3:K:84:SER:HG	1.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:214:THR:C	1:B:276:ARG:H	2.11	0.59
1:B:303:CYS:HB2	1:B:371:SER:HB3	1.83	0.59
3:K:48:LYS:HA	3:K:71:VAL:HB	1.85	0.59
3:K:95:MET:HE3	3:K:97:TYR:CG	2.38	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:284:GLU:HA	3:K:287:ASN:HD22	1.67	0.59
1:B:10:GLY:N	1:B:147:MET:HE1	2.18	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
1:B:263:LEU:C	1:B:263:LEU:HD13	2.28	0.59
2:A:16:ILE:HG23	2:A:17:GLY:N	2.16	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
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
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
1:B:372:THR:HA	1:B:375:GLN:CD	2.28	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:309:ARG:HD2	1:B:429:THR:C	2.28	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:23:LEU:HD23	2:A:23:LEU:C	2.27	0.58
2:A:93:ILE:CD1	2:A:118:VAL:HG12	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:287:SER:HB3	2:A:290:GLU:OE2	2.02	0.58
2:A:313:MET:HE2	2:A:344:VAL:CG1	2.32	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: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
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:95:MET:CE	3:K:97:TYR:CD2	2.80	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
1:B:296:ALA:HB2	1:B:305:PRO:CD	2.33	0.58
2:A:154:MET:HE2	2:A:158:SER:HG	1.67	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
1:B:309:ARG:HD2	1:B:429:THR:CA	2.33	0.58
2:A:273:ALA:HA	2:A:274:PRO:C	2.29	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: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:150:LEU:C	1:B:150:LEU:HD13	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLU:HA	1:B:114:ASP:OD2	2.04	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:11:GLN:C	1:B:14:ASN:HB2	2.29	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
1:B:228:LEU:HD23	1:B:228:LEU:C	2.29	0.58
1:B:246:LEU:HD13	1:B:246:LEU:C	2.29	0.58
2:A:251:ASP:CG	2:A:254:GLU:H	2.12	0.58
2:A:368:LEU:HD12	2:A:368:LEU:C	2.29	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
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:286:VAL:HG21	1:B:325:GLU:CD	2.29	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:92:GLU:C	3:K:97:TYR:HB2	2.21	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
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:207:LEU:C	1:B:207:LEU:HD12	2.29	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
2:A:394:LYS:C	2:A:398:MET:HE2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:16:GLY:C	3:K:363:PRO:HD2	2.29	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:154:MET:HE1	2:A:166:LYS:HD3	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:245:GLN:NE2	1:B:355:ASP:HA	2.20	0.57
1:B:273:LEU:C	1:B:273:LEU:HD13	2.30	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
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: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
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:143:THR:HG22	1:B:147:MET:HE3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:221:ARG:HD2	3:K:221:ARG:O	2.05	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:154:MET:HE1	2:A:166:LYS:HE2	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:394:LYS:O	2:A:398:MET:HE2	2.06	0.56
3:K:135:ILE:HD11	3:K:136:ILE:HG13	1.88	0.56
3:K:191:LYS:HZ2	3:K:191:LYS:N	2.04	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
2:A:397:LEU:HD23	2:A:397:LEU:C	2.30	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:30:ILE:CA	2:A:36:MET:HE3	2.37	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
2:A:311:LYS:HA	2:A:342:GLN:NE2	2.20	0.55
3:K:15:LYS:HG2	3:K:16:GLY:N	2.20	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
1:B:225:LEU:HD12	1:B:225:LEU:C	2.31	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:62:ARG:HA	1:B:62:ARG:HH11	1.71	0.55
1:B:113:VAL:HG23	1:B:114:ASP:OD1	2.07	0.55
1:B:324:LYS:CD	2:A:220:GLU:C	2.77	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:172:LEU:CD1	3:K:199:LEU:HD11	2.28	0.55
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:3:GLU:C	2:A:51:THR:HG22	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:K:215:GLU:CD	3:K:216:LYS:HE3	2.31	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:95:MET:CE	3:K:97:TYR:CG	2.89	0.55
3:K:136:ILE:HG21	3:K:214:LEU:CD1	2.37	0.55
1:B:1:MET:HE1	1:B:49:VAL:C	2.32	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
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:96:LYS:HD3	2:A:96:LYS:C	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:156:ARG:HA	1:B:164:MET:HE1	1.89	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
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
3:K:350:LEU:HD13	3:K:350:LEU:C	2.31	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
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
3:K:94:ILE:HA	3:K:245:MET:HE1	1.89	0.54
1:B:14:ASN:CG	1:B:72:THR:HG21	2.32	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:156:ARG:CA	1:B:164:MET:HE1	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:94:ILE:CA	3:K:245:MET:HE1	2.37	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
2:A:46:ASP:OD1	2:A:244:PHE:HZ	1.90	0.54
2:A:250:VAL:HG22	2:A:251:ASP:N	2.23	0.54
2:A:391:LEU:HA	2:A:394:LYS:CE	2.37	0.54
3:K:115:MET:CE	3:K:135:ILE:HD11	2.31	0.54
3:K:171:LEU:HD13	3:K:221:ARG:CB	2.37	0.54
3:K:228:MET:HA	3:K:228:MET:CE	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:A:23:LEU:HA	2:A:364:PRO:HG2	1.89	0.54
2:A:174:ALA:HB1	2:A:207:GLU:HB3	1.90	0.54
2:A:326:LYS:HB3	2:A:326:LYS:HZ2	1.72	0.54
2:A:346:TRP:HD1	2:A:346:TRP:H	1.55	0.54
2:A:388:TRP:HB2	2:A:425:MET:HE2	1.90	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
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
2:A:154:MET:HE1	2:A:166:LYS:CD	2.39	0.54
2:A:286:LEU:HD12	2:A:286:LEU:C	2.32	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:238:THR:O	1:B:242:PHE:HB2	2.08	0.53
1:B:293:MET:HE3	1:B:367:PHE:CB	2.36	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: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:66:TYR:CD2	3:K:68:PHE:CE1	2.95	0.53
3:K:206:ASN:CG	3:K:209:GLU:HG3	2.33	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
2:A:385:ALA:HB1	2:A:429:GLU:CD	2.32	0.53
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
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:255:VAL:HG13	1:B:256:ASN:N	2.23	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:113:GLU:CD	2:A:113:GLU:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:81:PHE:HA	1:B:83:GLN:CD	2.33	0.53
1:B:225:LEU:HD11	4:B:501:G2P:H2N1	1.72	0.53
1:B:260:PHE:HB2	3:K:297:ARG:HH22	1.72	0.53
1:B:323:MET:CB	2:A:221:ARG:NE	2.69	0.53
1:B:419:VAL:HG23	1:B:420:SER:N	2.24	0.53
2:A:2:ARG:HE	2:A:132:LEU:C	2.17	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
3:K:347:LEU:HD23	3:K:347:LEU:C	2.34	0.53
1:B:73:MET:HG2	1:B:92:PHE:HE1	1.65	0.53
1:B:111:GLU:H	1:B:111:GLU:CD	2.16	0.53
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:143:THR:CG2	1:B:147:MET:HE3	2.39	0.53
1:B:159:TYR:HB3	1:B:161:ASP:OD1	2.08	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:143:GLY:HA3	4:A:501:G2P:C3A	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:148:GLY:C	1:B:151:LEU:HG	2.34	0.52
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:271:ALA:HA	1:B:272:PRO:C	2.34	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:18:ALA:C	1:B:19:LYS:HZ3	2.18	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
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:285:THR:N	1:B:288:GLU:HB2	2.25	0.52
1:B:374:ILE:HG23	1:B:375:GLN:N	2.23	0.52
2:A:111:GLY:O	2:A:114:ILE:HG22	2.09	0.52
2:A:122:ILE:HD12	2:A:122:ILE:C	2.35	0.52
2:A:234:ILE:HD12	2:A:234:ILE:C	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:269:GLY:C	1:B:367:PHE:HB3	2.35	0.52
2:A:16:ILE:HA	2:A:228:ASN:ND2	2.17	0.52
2:A:90:GLU:CD	2:A:124:LYS:HE3	2.35	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: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:220:GLU:CD	2:A:221:ARG:H	2.18	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:180:GLU:C	3:K:182:LEU:HD22	2.34	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:411:GLU:C	3:K:272:ILE:HD11	2.22	0.51
3:K:110:GLY:HA2	3:K:113:PHE:H	1.74	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
1:B:273:LEU:HD22	1:B:273:LEU:C	2.34	0.51
1:B:284:LEU:HD12	1:B:363:MET:HE3	1.90	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:102:ASN:CG	2:A:105:ARG:H	2.18	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:377:LEU:HD12	1:B:377:LEU:C	2.34	0.51
2:A:54:SER:O	2:A:61:HIS:HA	2.11	0.51
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:58:LYS:HZ2	1:B:86:ARG:HG2	1.75	0.51
1:B:152:ILE:C	1:B:155:ILE:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:341:PHE:HZ	1:B:346:PRO:C	2.19	0.51
2:A:188:ILE:O	2:A:191:THR:HG22	2.10	0.51
2:A:272:TYR:H	2:A:302:MET:HE1	1.76	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:324:VAL:HG22	2:A:327:ASP:CG	2.36	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
3:K:171:LEU:C	3:K:220:LYS:HD3	2.36	0.51
1:B:101:TRP:HD1	1:B:149:THR:HG21	1.74	0.51
2:A:273:ALA:HB2	2:A:295:CYS:CB	2.40	0.51
2:A:278:ALA:HB1	2:A:282:TYR:HH	1.76	0.51
2:A:316:CYS:O	2:A:317:LEU:HD23	2.11	0.51
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
1:B:117:LEU:HA	1:B:120:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:154:LYS:HZ3	1:B:157:GLU:C	2.18	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: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
1:B:44:LEU:C	1:B:44:LEU:HD12	2.36	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:86:LEU:HD12	2:A:86:LEU:C	2.37	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
1:B:48:ASN:HB2	1:B:59:TYR:OH	2.12	0.50
1:B:167:PHE:CE2	1:B:233:MET:HE3	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:237:SER:HB3	2:A:320:ARG:HD2	1.93	0.50
2:A:248:LEU:HD23	2:A:248:LEU:C	2.36	0.50
2:A:273:ALA:C	2:A:375:VAL:HG22	2.36	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
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:29:ASN:CG	3:K:32:GLU:HG2	2.37	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
3:K:327:ARG:HD3	3:K:362:LYS:HZ1	1.77	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:299:MET:HE1	1:B:367:PHE:HD1	1.75	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:152:LEU:HD23	2:A:152:LEU:C	2.36	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:48:LYS:HZ2	3:K:71:VAL:H	1.58	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:154:LYS:HD3	1:B:154:LYS:C	2.37	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: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:326:VAL:CG1	1:B:330:MET:HE1	2.31	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:70:MET:HE3	3:K:72:PHE:HE2	1.73	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:331:LEU:HA	1:B:334:GLN:CD	2.37	0.49
1:B:376:GLU:CD	1:B:422:TYR:HB2	2.37	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:16:GLY:HA3	3:K:362:LYS:C	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:153:LEU:HG	2:A:157:LEU:CD1	2.42	0.49
2:A:154:MET:HE2	2:A:154:MET:O	2.12	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
2:A:383:ALA:C	2:A:386:GLU:HG2	2.37	0.49
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:191:LYS:HZ2	3:K:191:LYS:HB2	1.78	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
2:A:411:GLU:C	3:K:272:ILE:CD1	2.79	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:246:LYS:NZ	3:K:254:GLU:CD	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:360:PRO:HG3	2:A:373:ARG:C	2.38	0.49
2:A:411:GLU:OE1	2:A:411:GLU:HA	2.12	0.49
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:194:GLU:H	1:B:194:GLU:CD	2.21	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:95:MET:HE2	3:K:97:TYR:HB2	0.62	0.49
3:K:192:ARG:HH21	3:K:326:GLY:HA3	1.77	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:24:TYR:C	2:A:27:GLU:HG3	2.38	0.49
2:A:338:LYS:HZ2	2:A:338:LYS:HB3	1.77	0.49
2:A:370:LYS:HD3	2:A:371:VAL:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:390:ARG:O	1:B:392:LYS:HE2	2.13	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:387:ALA:HB2	2:A:390:ARG:NH1	2.28	0.48
3:K:277:ALA:HB1	3:K:281:ARG:HB2	1.93	0.48
1:B:117:LEU:C	1:B:120:VAL:HG22	2.39	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
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
3:K:109:THR:HG21	3:K:335:THR:C	2.38	0.48
1:B:31:ASP:OD1	1:B:37:HIS:HB2	2.13	0.48
1:B:242:PHE:HD1	1:B:242:PHE:HA	1.51	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
2:A:312:TYR:C	2:A:344:VAL:HG13	2.39	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
1:B:117:LEU:CA	1:B:120:VAL:HG22	2.44	0.48
1:B:120:VAL:HG23	1:B:121:ARG:N	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:228:MET:HE3	3:K:228:MET:N	2.28	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:388:MET:HA	1:B:388:MET:CE	2.39	0.48
1:B:394:PHE:HA	1:B:396:HIS:NE2	2.29	0.48
2:A:91:GLN:NE2	2:A:91:GLN:H	2.10	0.48
2:A:154:MET:CE	2:A:166:LYS:HE2	2.43	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
2:A:105:ARG:HA	2:A:411:GLU:CD	2.39	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: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: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:323:MET:HE3	1:B:326:VAL:CG2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:313:VAL:HG22	1:B:368:ILE:O	2.14	0.47
1:B:326:VAL:HG12	1:B:330:MET:HE3	1.88	0.47
1:B:327:ASP:C	1:B:331:LEU:HD22	2.39	0.47
1:B:415:MET:HG2	1:B:419:VAL:CG1	2.44	0.47
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: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: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: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
1:B:267:MET:HE1	1:B:299:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
2:A:64:ARG:HA	2:A:64:ARG:NH2	2.20	0.47
2:A:189:LEU:HD21	2:A:417:GLU:OE2	2.15	0.47
2:A:310:GLY:C	2:A:311:LYS:HE3	2.40	0.47
2:A:410:GLY:N	3:K:290:GLN:HG2	2.30	0.47
1:B:1:MET:HE2	1:B:1:MET:CA	2.35	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:A:413:MET:HA	2:A:413:MET:HE3	1.96	0.47
3:K:47:ARG:HE	3:K:49:GLU:CD	2.08	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:260:PHE:O	1:B:262:ARG:HD3	2.13	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: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
3:K:321:GLN:C	3:K:324:LEU:HD23	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:GLU:H	1:B:343:GLU:CD	2.23	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
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:147:MET:HB3	1:B:147:MET:HE3	1.73	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: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:191:LYS:HZ2	3:K:191:LYS:CB	2.28	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:250:LEU:C	1:B:253:LEU:HG	2.40	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:318:LEU:HD13	2:A:319:TYR:C	2.40	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: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
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
2:A:338:LYS:HZ3	2:A:338:LYS:HA	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LYS:CD	2:A:101:ASN:HB2	2.19	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:255:PHE:C	2:A:259:LEU:HG	2.40	0.46
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
2:A:370:LYS:HD3	2:A:370:LYS:C	2.40	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
3:K:342:ASN:C	3:K:342:ASN:HD22	2.23	0.46
1:B:1:MET:HE1	1:B:49:VAL:HA	1.96	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: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:28:PHE:CZ	3:K:37:ALA:C	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LYS:NZ	1:B:157:GLU:HB3	2.31	0.46
1:B:193:VAL:HG13	1:B:194:GLU:CD	2.41	0.46
1:B:228:LEU:HD21	1:B:300:MET:HE1	1.98	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
1:B:410:GLU:CD	1:B:413:SER:HB2	2.41	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
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
3:K:184:MET:HE1	3:K:318:ARG:HB3	1.97	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:223:THR:HB	2:A:226:ASN:OD1	2.14	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: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:251:ASP:CG	2:A:254:GLU:HB3	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:236:HIS:ND1	3:K:267:ALA:HB3	2.31	0.45
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:108:GLU:CD	1:B:147:MET:HA	2.41	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:261:PRO:C	2:A:262:TYR:CD1	2.95	0.45
2:A:281:ALA:HB3	2:A:369:ALA:H	1.81	0.45
2:A:409:VAL:HG12	3:K:290:GLN:CA	2.43	0.45
3:K:59:ASP:C	3:K:61:SER:H	2.24	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:6:HIS:C	1:B:7:ILE:HD13	2.41	0.45
1:B:12:CYS:CB	1:B:138:SER:CB	2.93	0.45
1:B:214:THR:HB	1:B:275:SER:C	2.40	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:102:ASN:CG	2:A:105:ARG:HB3	2.41	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:O	3:K:204:VAL:HG23	2.17	0.45
1:B:123:GLU:OE2	1:B:123:GLU:HA	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ALA:CB	1:B:143:THR:CG2	2.94	0.45
1:B:99:ASN:HA	1:B:142:GLY:C	2.41	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
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
2:A:243:ARG:C	2:A:244:PHE:CD1	2.94	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:145:GLU:HG2	3:K:207:LYS:HZ1	1.81	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: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: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: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:162:GLU:CD	3:K:235:SER:OG	2.59	0.45
3:K:203:THR:HG22	3:K:204:VAL:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:311:TYR:CD2	3:K:321:GLN:CD	2.95	0.45
1:B:1:MET:HE2	1:B:49:VAL:CB	2.37	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:305:PRO:HB3	1:B:310:TYR:HH	1.82	0.45
1:B:331:LEU:O	1:B:334:GLN:HG2	2.16	0.45
2:A:3:GLU:HG2	2:A:50:ASN:C	2.41	0.45
2:A:4:CYS:HG	2:A:135:PHE:HA	1.82	0.45
2:A:24:TYR:HA	2:A:27:GLU:CG	2.47	0.45
2:A:36:MET:HG3	2:A:38:SER:C	2.41	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
3:K:145:GLU:OE2	3:K:207:LYS:NZ	2.49	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
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:121:ARG:HE	1:B:121:ARG:N	2.15	0.44
1:B:228:LEU:HD21	1:B:300:MET:HE2	1.98	0.44
1:B:322:SER:OG	2:A:221:ARG:HB2	2.16	0.44
2:A:5:ILE:HG22	2:A:6:SER:N	2.31	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
3:K:28:PHE:CG	3:K:33:ARG:NH2	2.85	0.44
1:B:21:TRP:HH2	1:B:50:TYR:OH	1.98	0.44
1:B:73:MET:HE2	1:B:90:PHE:HZ	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:VAL:C	1:B:116:VAL:HG22	2.42	0.44
1:B:166:THR:HG22	1:B:167:PHE:N	2.32	0.44
2:A:154:MET:CA	2:A:154:MET:CE	2.95	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:68:LEU:HD23	1:B:68:LEU:C	2.43	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
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
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:156:ARG:CG	1:B:164:MET:HE1	2.48	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:318:ARG:HH21	1:B:357:PRO:C	2.26	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:B:406:MET:HE2	1:B:406:MET:HB3	1.78	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
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
1:B:330:MET:HE2	1:B:330:MET:HB3	1.56	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:147:MET:C	1:B:151:LEU:HD23	2.43	0.44
1:B:164:MET:HB2	1:B:164:MET:HE3	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:176:GLN:HB3	2:A:207:GLU:CD	2.43	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
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:111:GLY:C	2:A:114:ILE:HG22	2.43	0.43
2:A:135:PHE:CD1	2:A:135:PHE:C	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
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:363:MET:HE2	1:B:363:MET:N	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:K:48:LYS:HE3	3:K:70:MET:HG3	2.00	0.43
3:K:70:MET:HE1	3:K:85:VAL:CG2	2.48	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:86:ARG:HB3	1:B:88:ASP:CG	2.44	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:124:LYS:HZ3	2:A:125:LEU:HB2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:MET:SD	1:B:299:MET:HE3	2.59	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
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
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
2:A:46:ASP:CG	2:A:49:PHE:H	2.27	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:139:LEU:HD12	1:B:139:LEU:C	2.44	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:242:LEU:HD13	2:A:242:LEU:C	2.43	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:132:GLY:C	1:B:133:PHE:CD1	2.97	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:280:GLN:CD	1:B:281:TYR:CE1	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:158:GLU:C	1:B:159:TYR:CD1	2.96	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
2:A:248:LEU:HD23	2:A:249:ASN:C	2.44	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
1:B:134:GLN:C	1:B:135:LEU:HD22	2.44	0.42
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:361:LEU:HD21	1:B:364:SER:HG	1.84	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:210:TYR:C	2:A:213:CYS:HG	2.25	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:135:ILE:HD12	3:K:135:ILE:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:THR:CG2	1:B:188:SER:CA	2.95	0.42
1:B:179:VAL:C	1:B:182:PRO:HD2	2.44	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:342:GLN:O	2:A:342:GLN:HG3	2.19	0.42
2:A:343:PHE:HE1	2:A:349:THR:C	2.28	0.42
2:A:347:CYS:SG	2:A:349:THR:CG2	3.07	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
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
1:B:293:MET:HB3	1:B:293:MET:HE2	1.72	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: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
3:K:288:ILE:O	3:K:289:ASN:C	2.62	0.42
1:B:36:TYR:CE1	1:B:38:GLY:N	2.84	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:214:THR:C	1:B:276:ARG:HB3	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:267:MET:CE	1:B:367:PHE:HE1	2.30	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
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:1:MET:CE	1:B:49:VAL:CB	2.95	0.42
1:B:73:MET:HE2	1:B:90:PHE:CZ	2.53	0.42
1:B:103:LYS:HG2	1:B:401:GLU:CD	2.45	0.42
1:B:181:GLU:OE2	4:B:501:G2P:H5'1	2.20	0.42
1:B:182:PRO:C	1:B:385:PHE:CZ	2.98	0.42
1:B:187:LEU:HD22	1:B:187:LEU:N	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:269:GLY:CA	1:B:299:MET:HE1	2.50	0.42
2:A:11:GLN:NE2	4:A:501:G2P:H3A2	2.32	0.42
2:A:69:ASP:CG	2:A:71:GLU:HG2	2.45	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:287:SER:HB3	2:A:290:GLU:CD	2.45	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
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
1:B:166:THR:C	1:B:167:PHE:CD1	2.98	0.42
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: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
3:K:204:VAL:HB	3:K:209:GLU:CD	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:26:ARG:HD2	3:K:29:ASN:CG	2.44	0.42
3:K:28:PHE:CZ	3:K:38:HIS:C	2.98	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: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: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
3:K:26:ARG:HD3	3:K:108:GLY:C	2.45	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:155:ILE:C	1:B:158:GLU:HG3	2.44	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:203:MET:HE3	2:A:203:MET:HB3	1.85	0.41
2:A:250:VAL:HG22	2:A:254:GLU:OE1	2.20	0.41
2:A:296:PHE:N	2:A:296:PHE:CD2	2.85	0.41
2:A:389:ALA:N	2:A:425:MET:CE	2.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:125:LEU:HD12	2:A:128:GLN:CD	2.46	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
1:B:53:GLU:CD	1:B:59:TYR:CE2	2.99	0.41
1:B:186:THR:CG2	1:B:187:LEU:N	2.82	0.41
1:B:207:LEU:CG	1:B:208:TYR:N	2.83	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
3:K:162:GLU:HG3	3:K:235:SER:CB	2.29	0.41
3:K:227:LEU:CG	3:K:228:MET:CE	2.97	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
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:116:ASP:C	2:A:119:LEU:HG	2.45	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
2:A:395:PHE:C	2:A:395:PHE:CD2	2.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:377:LEU:C	1:B:380:ARG:HG3	2.44	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:48:LYS:HZ2	3:K:71:VAL:N	2.18	0.41
3:K:54:THR:C	3:K:56:GLY:H	2.28	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:68:LEU:C	1:B:68:LEU:CD2	2.94	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
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: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
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:CE2	1:B:369:GLY:C	2.99	0.41
1:B:266:PHE:HE1	1:B:312:THR:HG23	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:262:TYR:CD2	2:A:265:ILE:HG12	2.54	0.41
2:A:278:ALA:C	2:A:282:TYR:CE2	2.99	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:343:PHE:CE1	2:A:349:THR:C	2.98	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
3:K:228:MET:CA	3:K:228:MET:CE	2.96	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: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
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
2:A:352:LYS:CG	2:A:353:VAL:N	2.83	0.41
2:A:413:MET:HB3	2:A:417:GLU:CD	2.46	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:272:ILE:CG1	3:K:273:GLY:N	2.82	0.41
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:SER:C	1:B:429:THR:HB	2.46	0.40
1:B:381:ILE:HG23	1:B:384:GLN:CD	2.45	0.40
1:B:390:ARG:CZ	1:B:390:ARG:CA	2.96	0.40
2:A:84:ARG:HD2	2:A:84:ARG:C	2.45	0.40
2:A:111:GLY:HA2	2:A:114:ILE:CG2	2.51	0.40
2:A:154:MET:HA	2:A:154:MET:CE	2.36	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:245:GLN:H	1:B:245:GLN:CD	2.28	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:49:PHE:CZ	2:A:54:SER:C	2.99	0.40
2:A:68:VAL:O	2:A:68:VAL:HG23	2.21	0.40
2:A:248:LEU:C	2:A:248:LEU:CD2	2.95	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:200:TYR:CD1	1:B:268:PRO:HD3	2.56	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
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:112:LEU:CD2	1:B:112:LEU:C	2.95	0.40
1:B:150:LEU:C	1:B:150:LEU:CD1	2.95	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:5:ILE:HG23	2:A:65:ALA:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:369:LEU:N	3:K:369:LEU:CD2	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	427/429 (100%)	426 (100%)	1 (0%)	0	100	100
2	A	436/438 (100%)	434 (100%)	2 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	301 (82%)	68 (18%)	1	11
2	A	369/369 (100%)	307 (83%)	62 (17%)	2	13
3	K	292/343 (85%)	257 (88%)	35 (12%)	5	21
All	All	1030/1081 (95%)	865 (84%)	165 (16%)	4	14

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	GLU
1	B	8	GLN
1	B	14	ASN
1	B	19	LYS
1	B	21	TRP
1	B	22	GLU
1	B	31	ASP
1	B	37	HIS
1	B	42	LEU
1	B	43	GLN
1	B	44	LEU
1	B	45	GLU
1	B	73	MET
1	B	83	GLN
1	B	88	ASP
1	B	94	GLN
1	B	101	TRP

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Mol	Chain	Res	Type
1	B	103	LYS
1	B	114	ASP
1	B	122	LYS
1	B	134	GLN
1	B	135	LEU
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	191	GLN
1	B	197	ASP
1	B	208	TYR
1	B	213	ARG
1	B	216	LYS
1	B	217	LEU
1	B	222	TYR
1	B	227	HIS
1	B	228	LEU
1	B	242	PHE
1	B	252	LYS
1	B	260	PHE
1	B	263	LEU
1	B	265	PHE
1	B	266	PHE
1	B	273	LEU
1	B	276	ARG
1	B	291	GLN
1	B	292	GLN
1	B	297	LYS
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	363	MET

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Mol	Chain	Res	Type
1	B	375	GLN
1	B	376	GLU
1	B	377	LEU
1	B	383	GLU
1	B	390	ARG
1	B	414	ASN
1	B	415	MET
1	B	421	GLU
1	B	423	GLN
2	A	7	ILE
2	A	15	GLN
2	A	18	ASN
2	A	22	GLU
2	A	25	CYS
2	A	40	LYS
2	A	46	ASP
2	A	53	PHE
2	A	64	ARG
2	A	84	ARG
2	A	85	GLN
2	A	86	LEU
2	A	87	PHE
2	A	91	GLN
2	A	96	LYS
2	A	105	ARG
2	A	117	LEU
2	A	120	ASP
2	A	124	LYS
2	A	128	GLN
2	A	136	LEU
2	A	154	MET
2	A	155	GLU
2	A	156	ARG
2	A	163	LYS
2	A	164	LYS
2	A	181	VAL
2	A	210	TYR
2	A	211	ASP
2	A	214	ARG
2	A	215	ARG
2	A	218	ASP
2	A	220	GLU

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Mol	Chain	Res	Type
2	A	221	ARG
2	A	242	LEU
2	A	243	ARG
2	A	254	GLU
2	A	264	ARG
2	A	267	PHE
2	A	285	GLN
2	A	297	GLU
2	A	302	MET
2	A	308	ARG
2	A	311	LYS
2	A	313	MET
2	A	318	LEU
2	A	326	LYS
2	A	338	LYS
2	A	339	ARG
2	A	343	PHE
2	A	346	TRP
2	A	351	PHE
2	A	352	LYS
2	A	386	GLU
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	26	ARG
3	K	28	PHE
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	97	TYR
3	K	171	LEU

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Mol	Chain	Res	Type
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	215	GLU
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 (52) 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
1	B	131	GLN
1	B	137	HIS
1	B	226	ASN
1	B	245	GLN
1	B	279	GLN
1	B	280	GLN
1	B	291	GLN
1	B	292	GLN
1	B	329	GLN
1	B	334	GLN
1	B	335	ASN

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Mol	Chain	Res	Type
1	B	375	GLN
1	B	414	ASN
1	B	424	GLN
2	A	8	HIS
2	A	15	GLN
2	A	31	GLN
2	A	61	HIS
2	A	85	GLN
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
2	A	393	HIS
3	K	141	HIS
3	K	142	GLN
3	K	173	ASN
3	K	190	ASN
3	K	212	GLN
3	K	287	ASN
3	K	289	ASN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	MZK	K	501	-	23,23,23	1.39	1 (4%)	34,34,34	1.09	4 (11%)
4	G2P	A	501	5	30,34,34	0.71	0	46,54,54	0.46	0
4	G2P	B	501	5	30,34,34	0.87	2 (6%)	46,54,54	0.78	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MZK	K	501	-	-	0/10/19/19	0/3/3/3
4	G2P	A	501	5	-	7/19/38/38	0/3/3/3
4	G2P	B	501	5	-	4/19/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	501	MZK	C7-N1	3.72	1.39	1.35
4	B	501	G2P	PA-O1A	-2.37	1.50	1.56
4	B	501	G2P	PB-O1B	-2.31	1.50	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	G2P	O1B-PB-C3A	3.10	119.55	106.73
4	B	501	G2P	O1A-PA-C3A	2.86	118.59	106.73
6	K	501	MZK	C14-C13-C16	2.59	124.12	119.96
6	K	501	MZK	C2-C1-C3	2.55	121.19	118.54
6	K	501	MZK	C5-C1-C3	2.27	120.89	118.18
6	K	501	MZK	C10-C6-C9	2.01	124.72	121.25

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
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

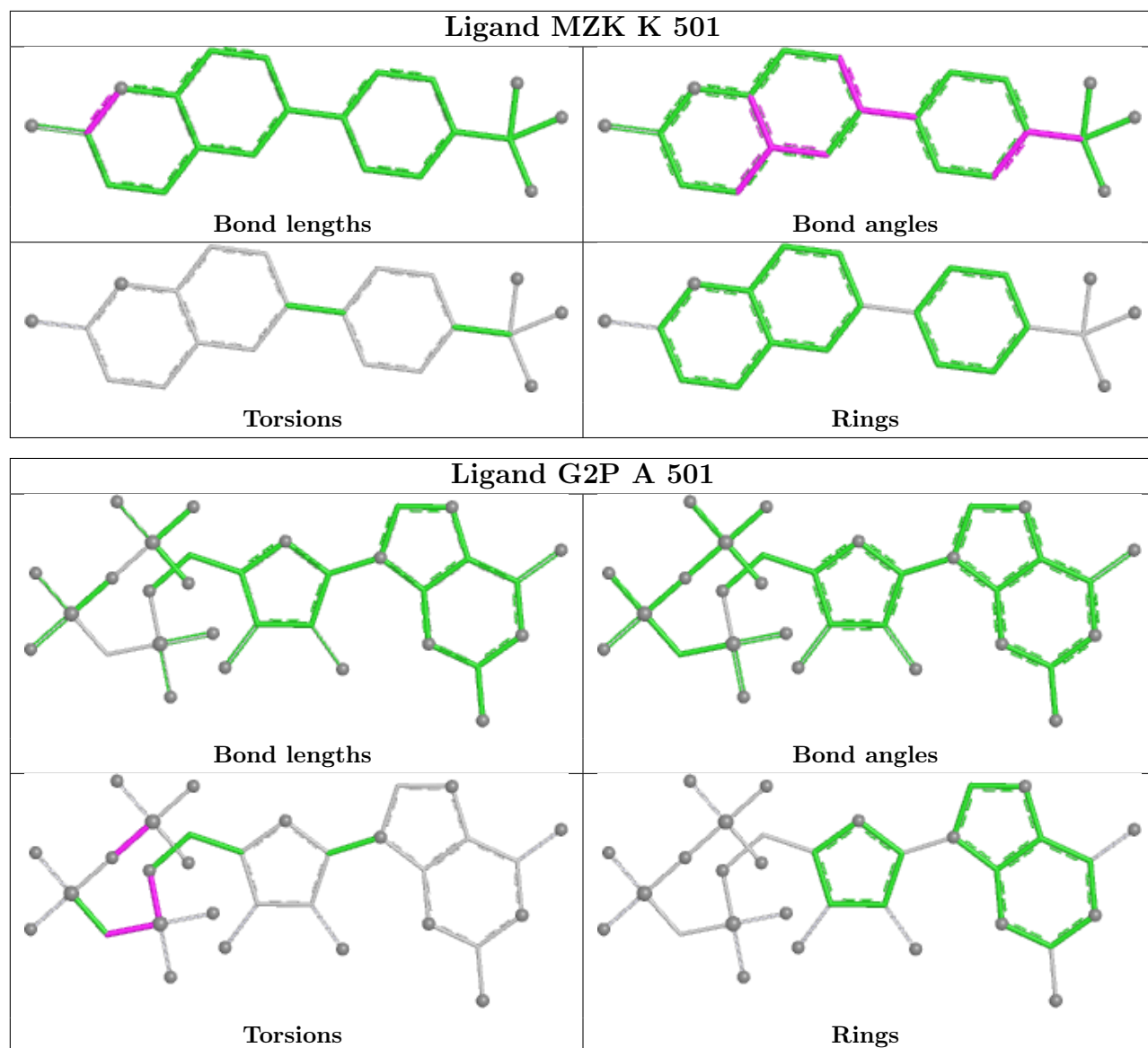
There are no ring outliers.

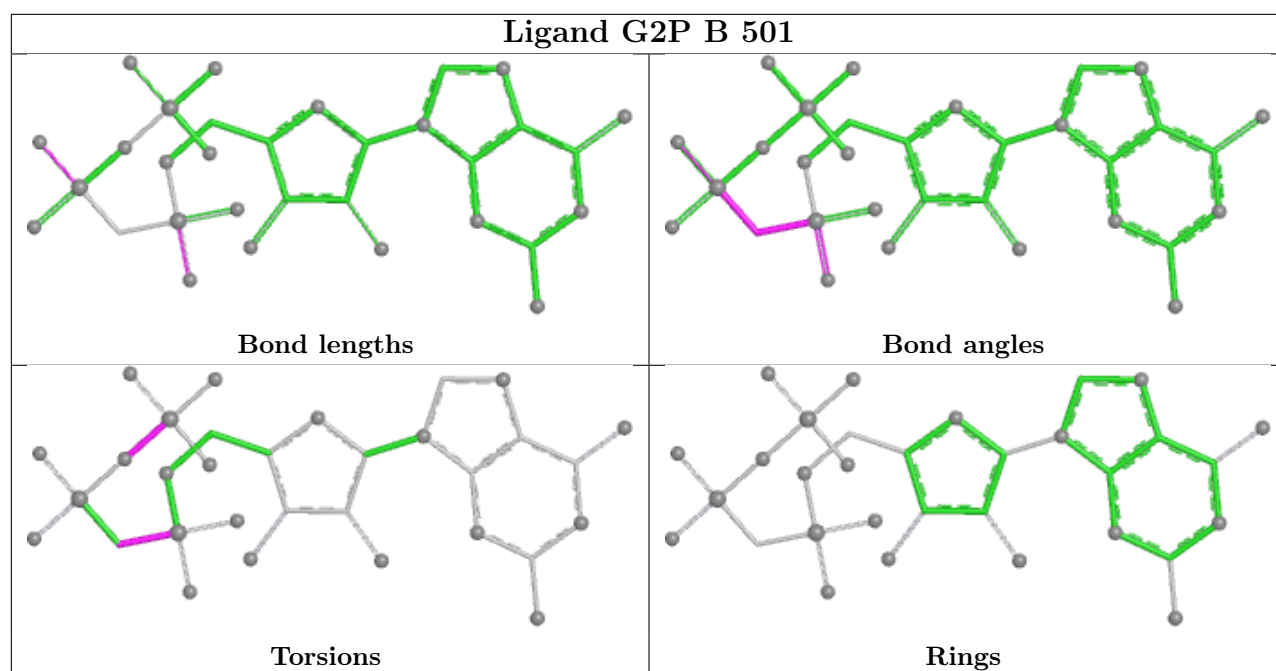
2 monomers are involved in 50 short contacts:

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

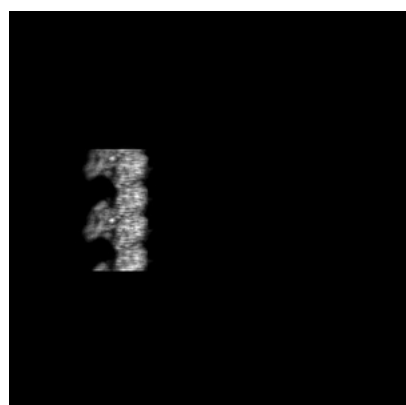
6 Map visualisation [i](#)

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.

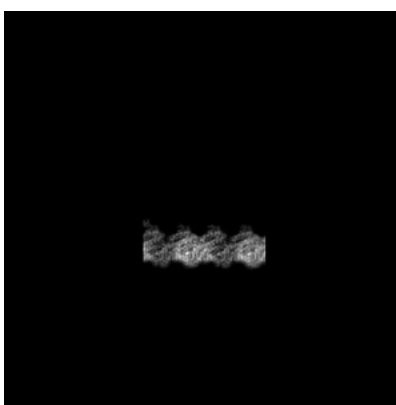
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

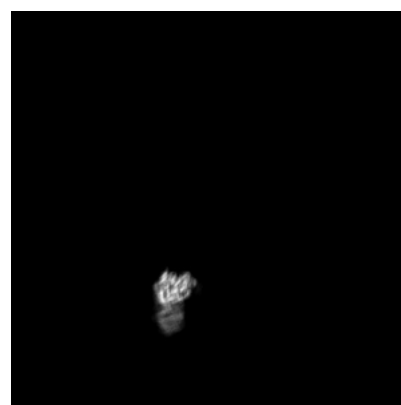
6.1.1 Primary map



X



Y

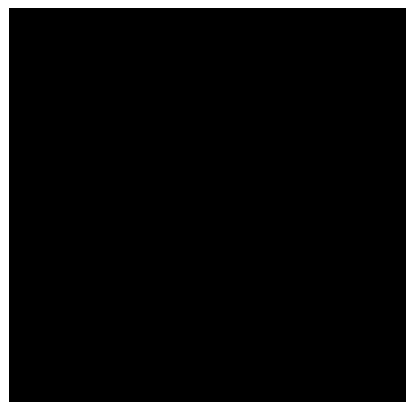


Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

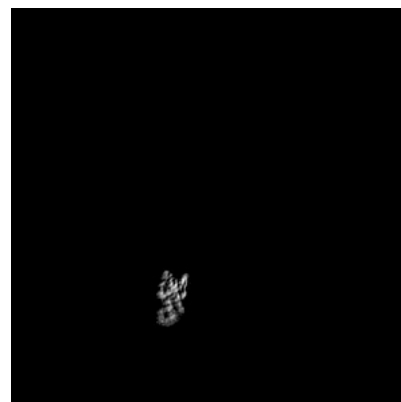
6.2.1 Primary map



X Index: 255



Y Index: 255



Z Index: 255

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

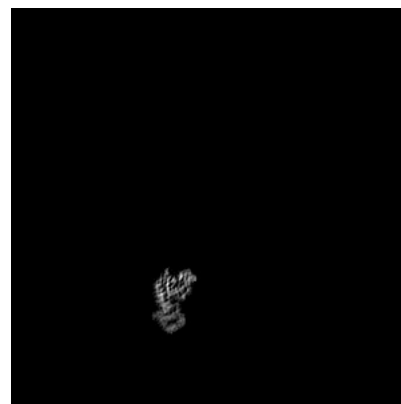
6.3.1 Primary map



X Index: 200



Y Index: 162



Z Index: 233

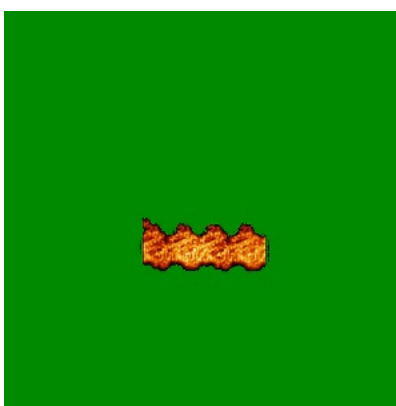
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X



Y

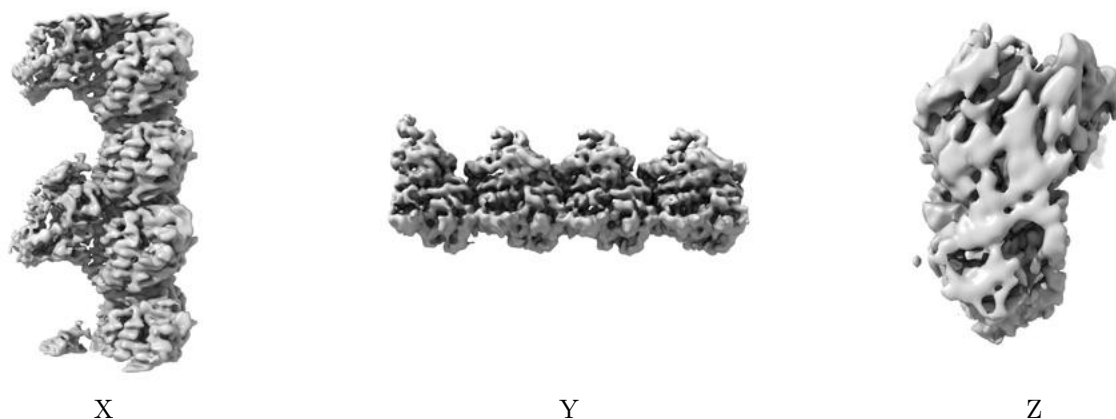


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

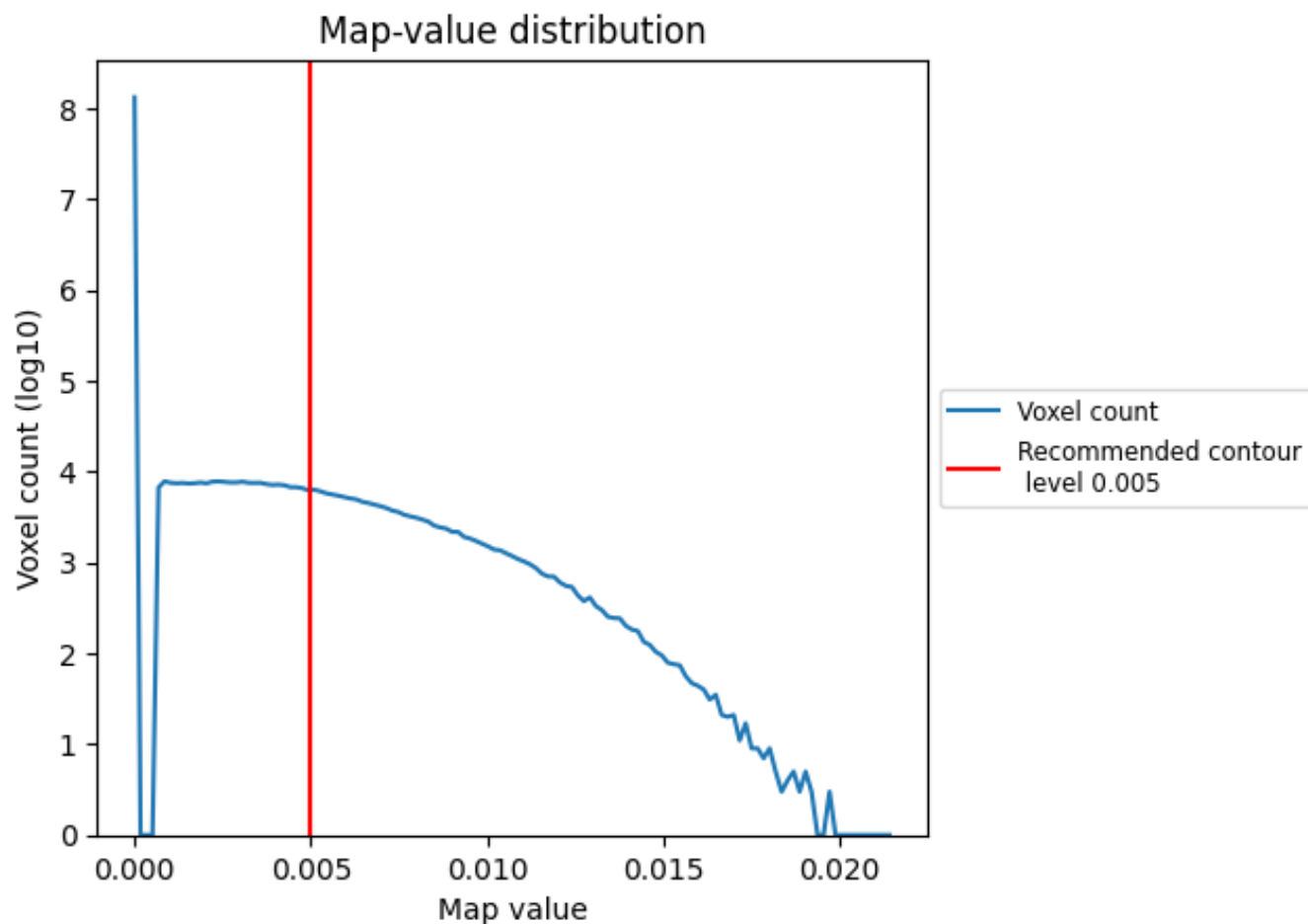
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

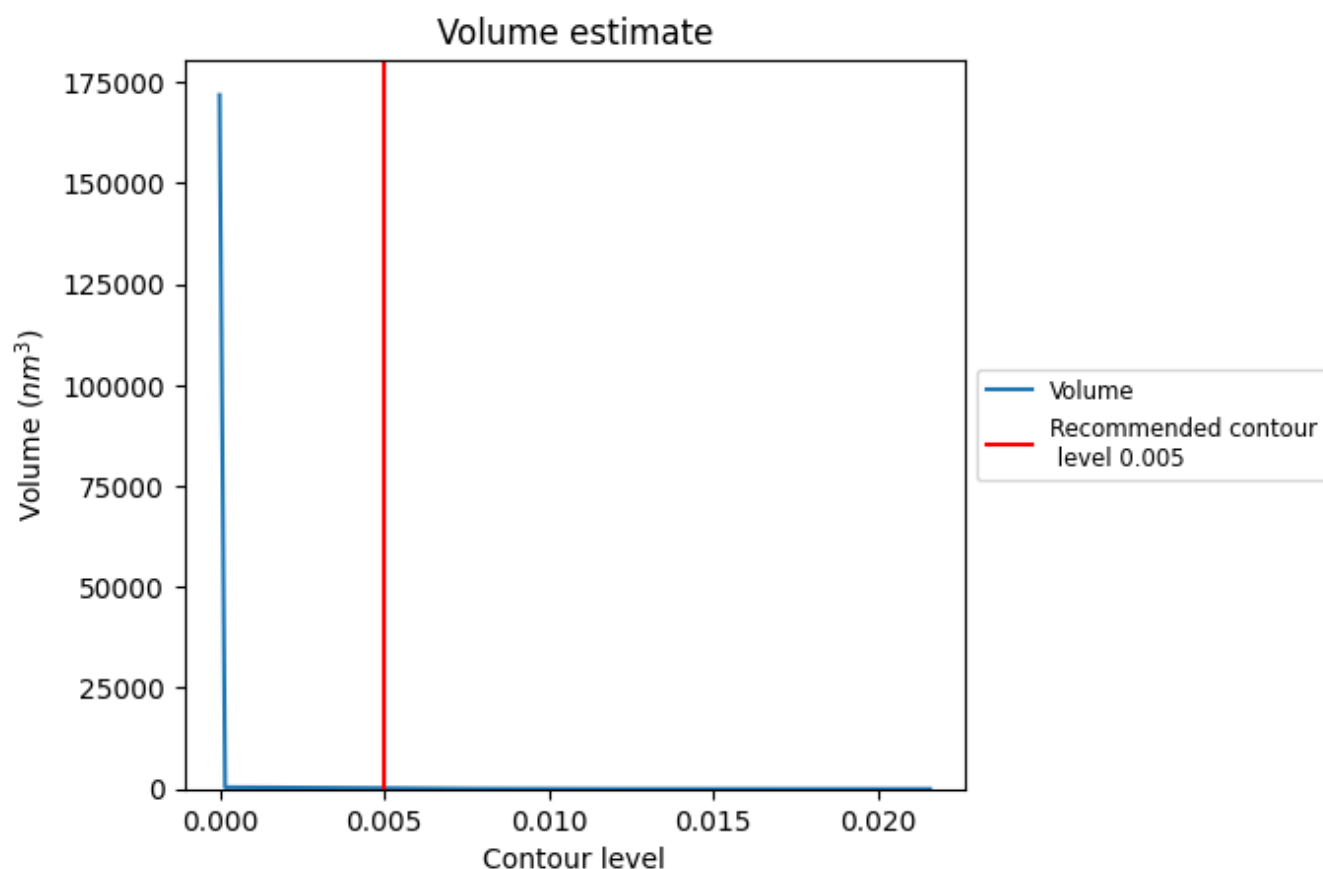
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

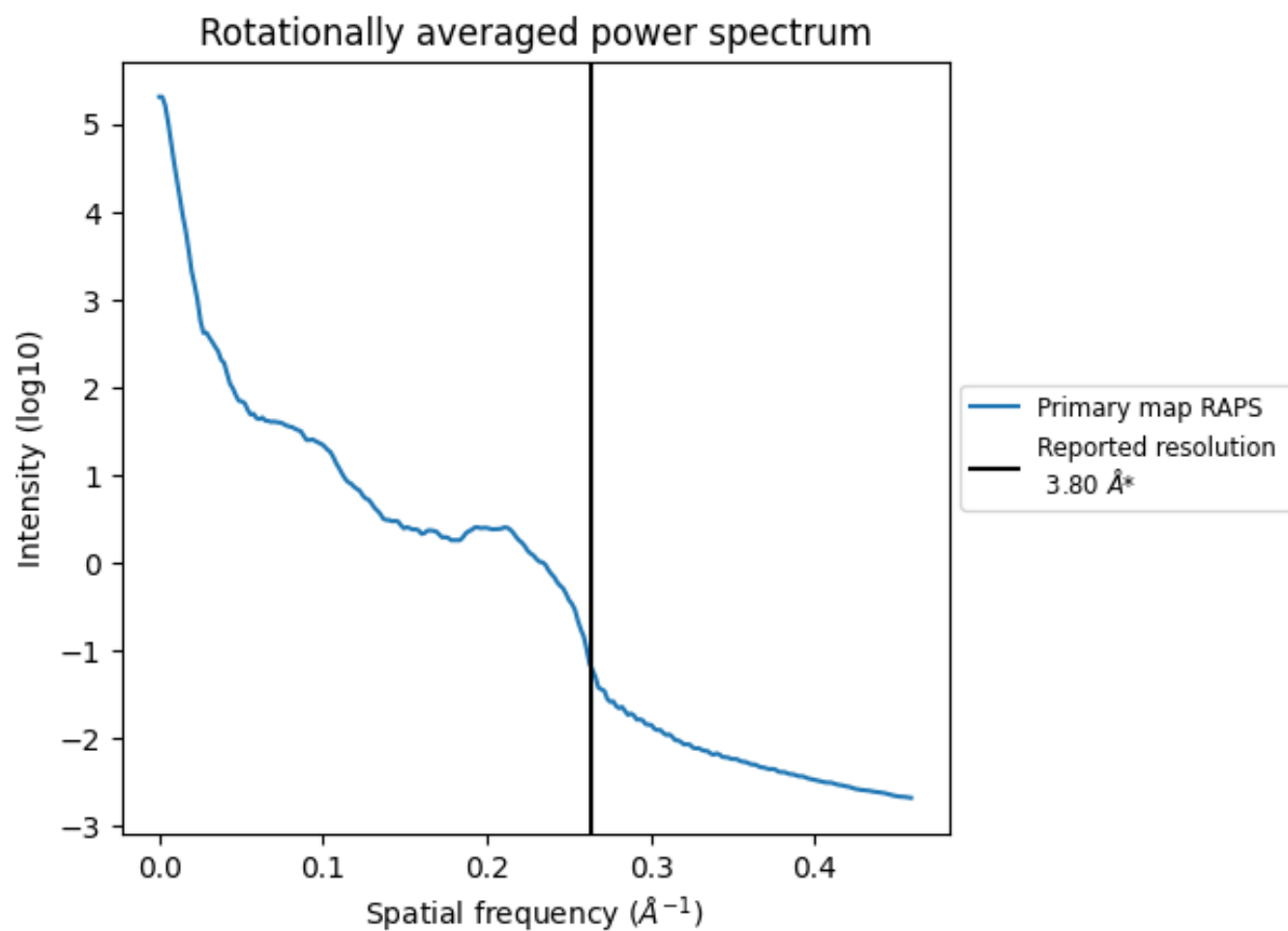
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm^3 ; this corresponds to an approximate mass of 152 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

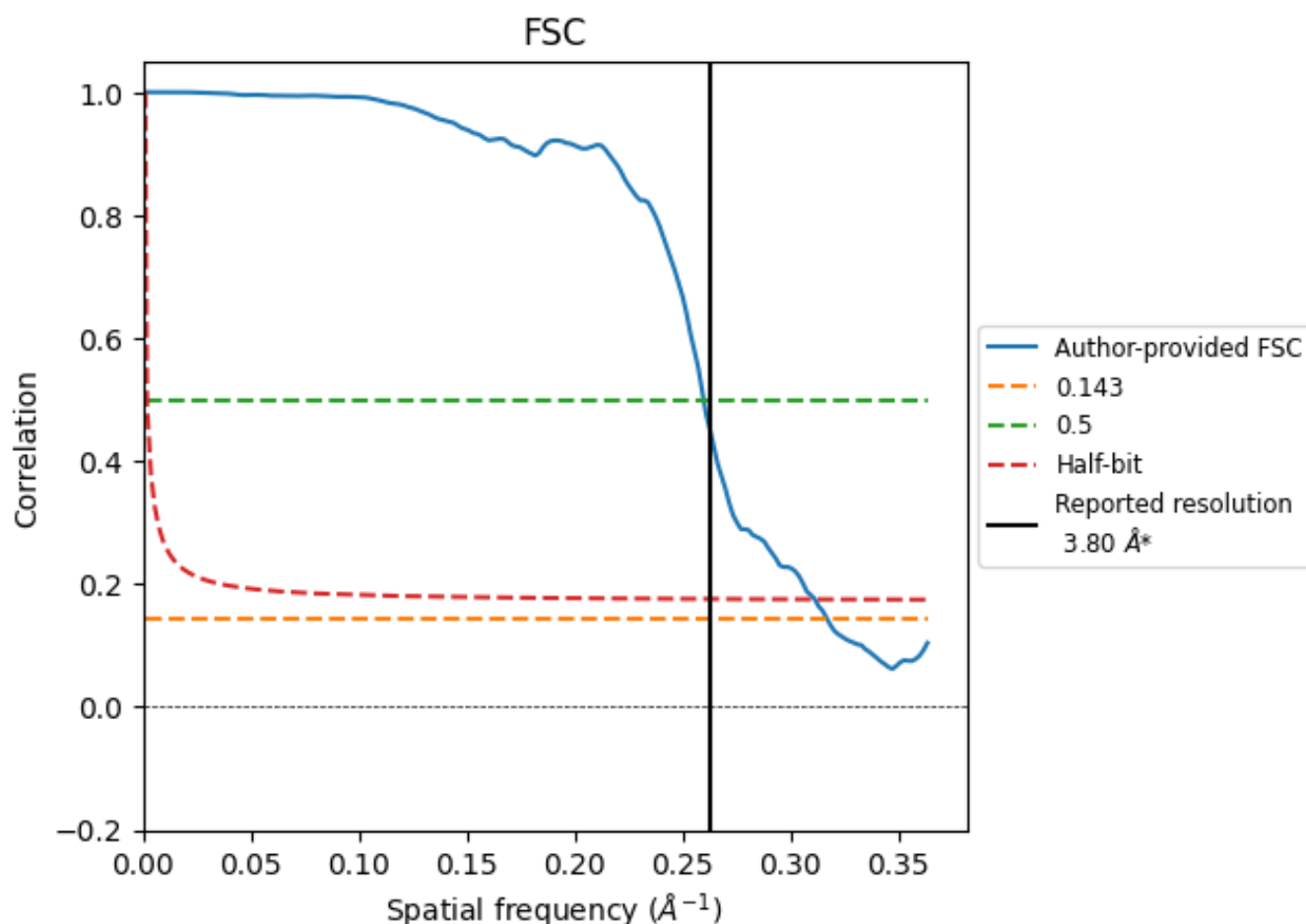


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

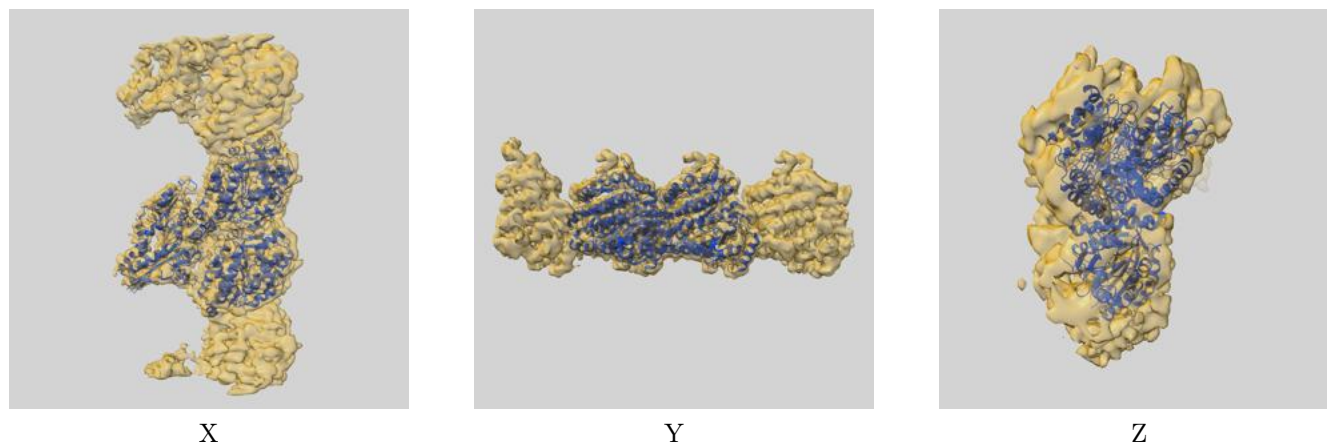
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.80	-
Author-provided FSC curve	3.16	3.85	3.21
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

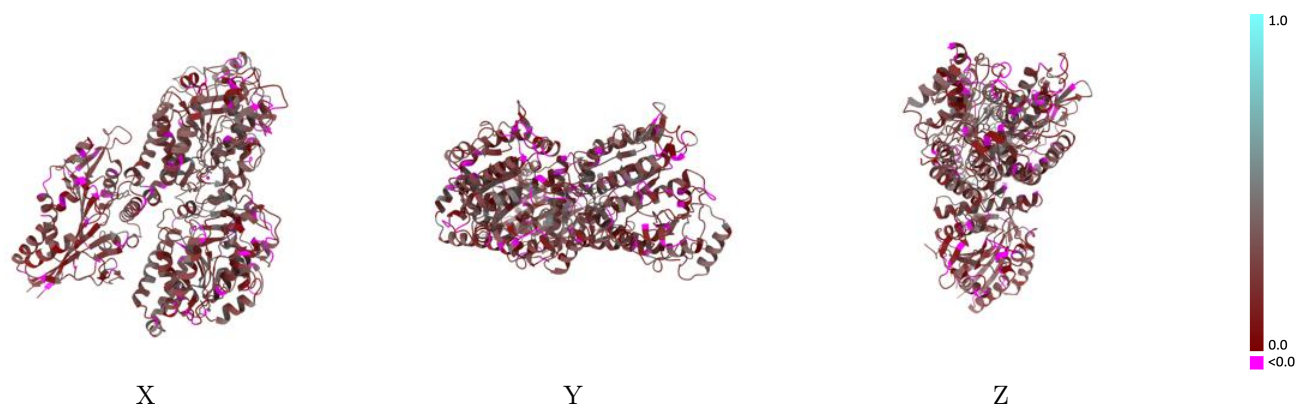
This section contains information regarding the fit between EMDB map EMD-10421 and PDB model 6TA3. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



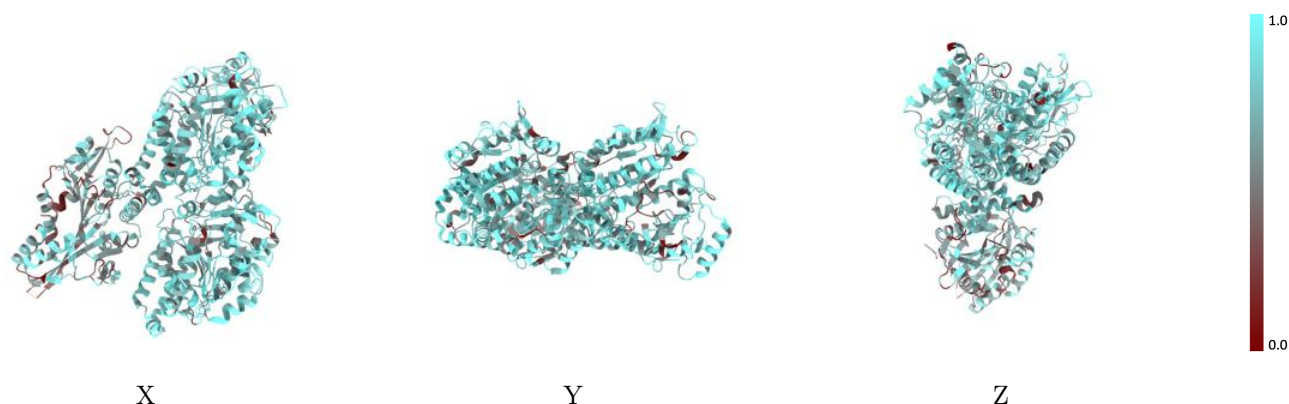
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



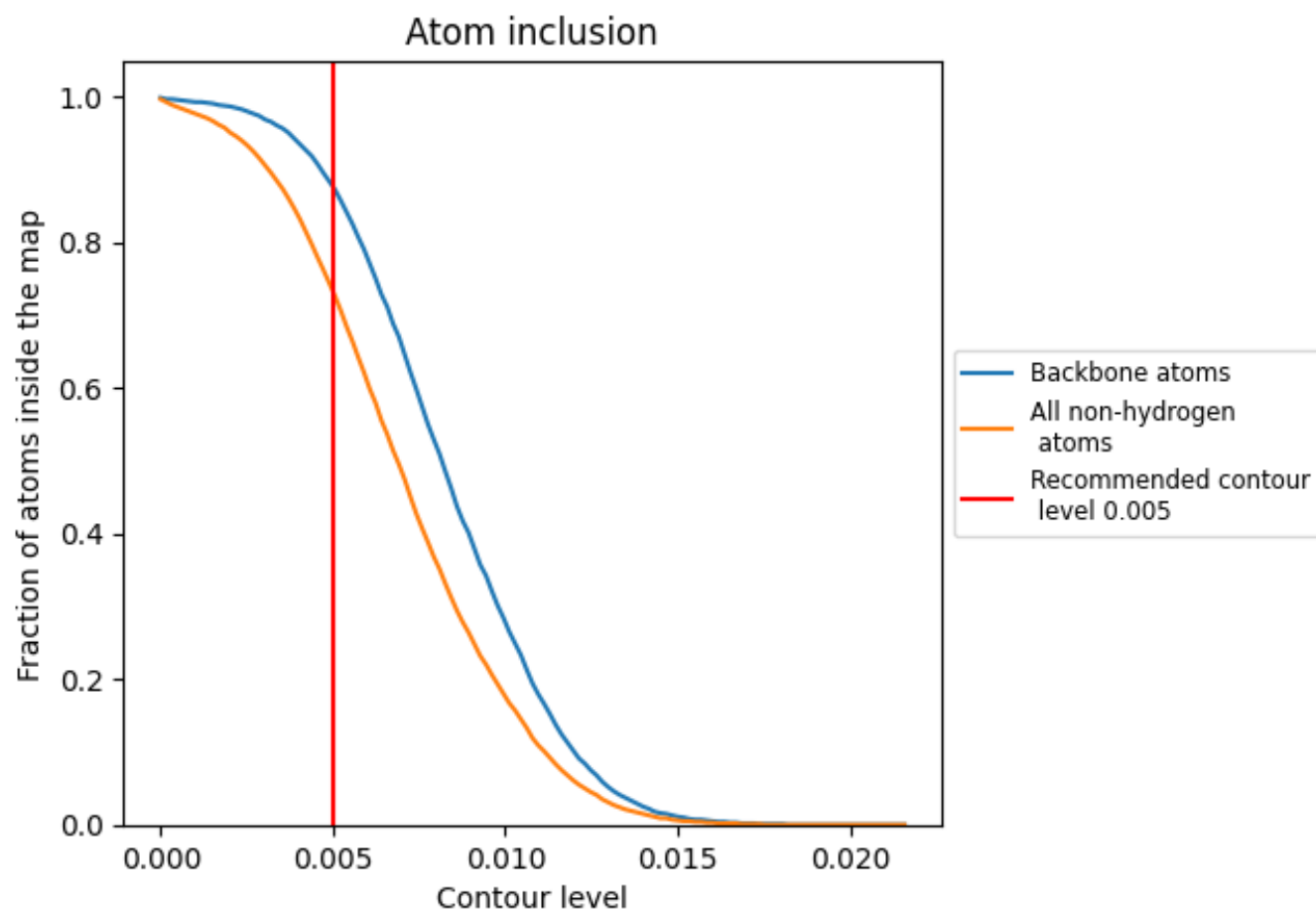
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7330	0.2150
A	0.7770	0.2380
B	0.7850	0.2220
K	0.6060	0.1780

