



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:47 PM BST

PDB ID : 3IXW
EMDB ID: : EMD-5101
Title : Scorpion Hemocyanin activated state pseudo atomic model built based on cryo-EM density map
Authors : Cong, Y.; Zhang, Q.; Woolford, D.; Schweikardt, T.; Khant, H.; Ludtke, S.; Chiu, W.; Decker, H.
Deposited on : 2009-02-13
Resolution : 8.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

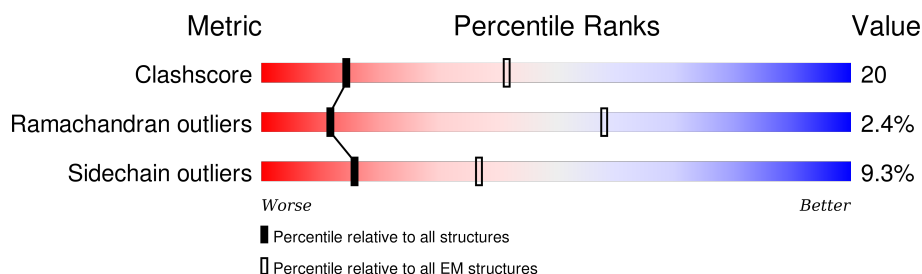
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	626	54% 36% 8% .
1	C	626	59% 33% 7% .
1	D	626	58% 34% 8% .
1	E	626	58% 34% 6% .
1	F	626	58% 32% 8% .
1	G	626	59% 33% 7% .
1	H	626	60% 32% 7% .
1	I	626	58% 34% 8% .
1	J	626	57% 35% 7% .

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Mol	Chain	Length	Quality of chain
1	K	626	<div><div></div><div>58%34%7%</div></div>
1	L	626	<div><div></div><div>59%33%8%</div></div>
1	M	626	<div><div></div><div>55%36%8%</div></div>

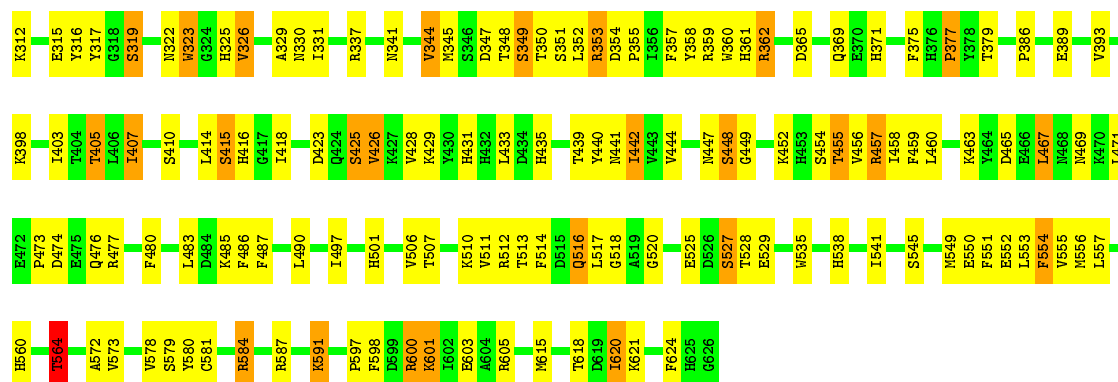
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 74208 atoms, of which 13476 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.

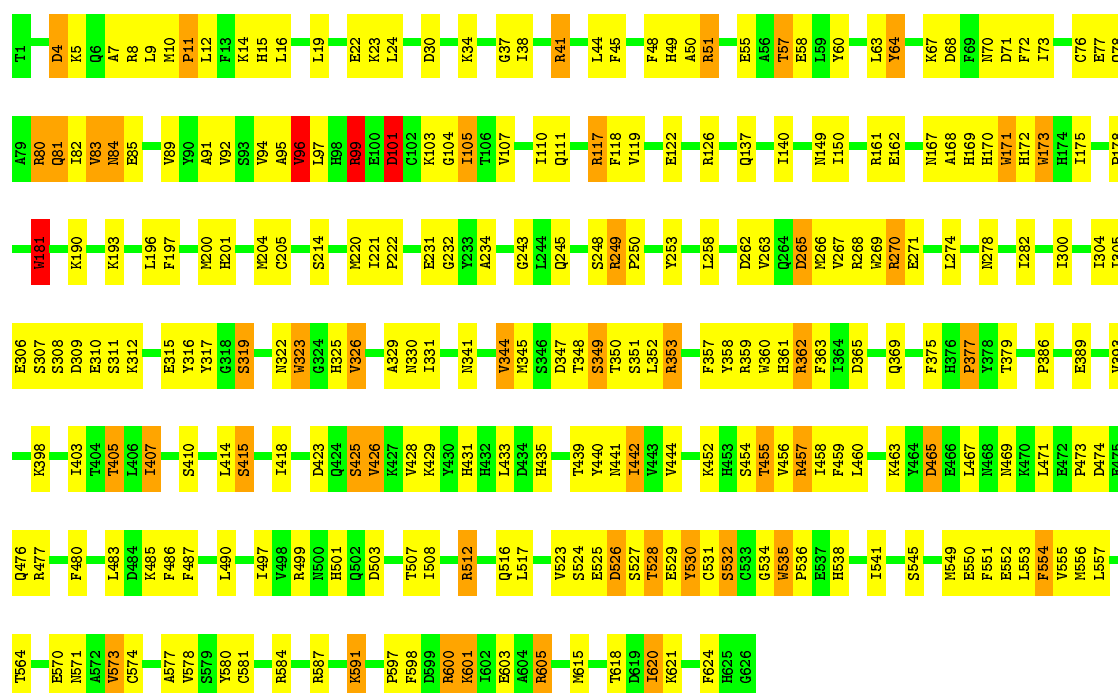
- Molecule 1 is a protein called Hemocyanin AA6 chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	C	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	D	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	E	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	F	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	G	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	H	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	I	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	J	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	K	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	L	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	M	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		



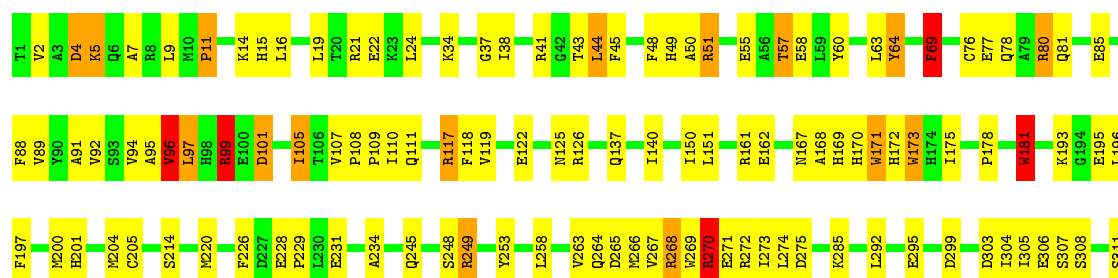
• Molecule 1: Hemocyanin AA6 chain

Chain D: 58% 34% 8%

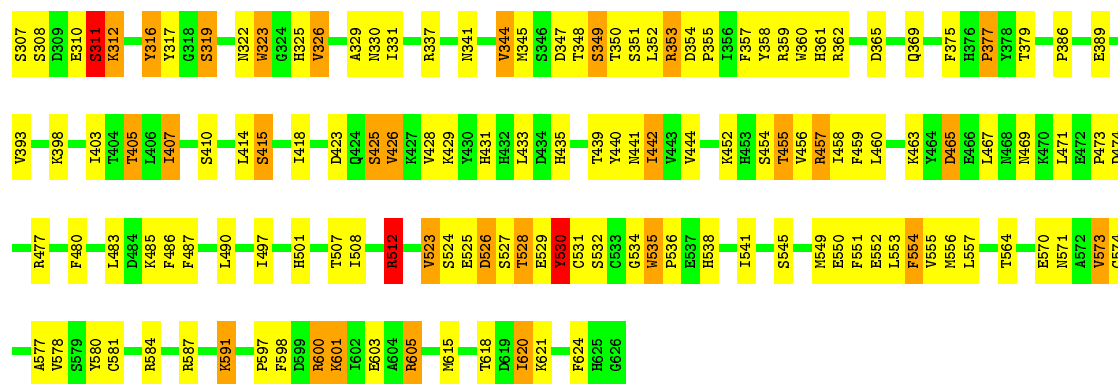


• Molecule 1: Hemocyanin AA6 chain

Chain E: 58% 34% 6%

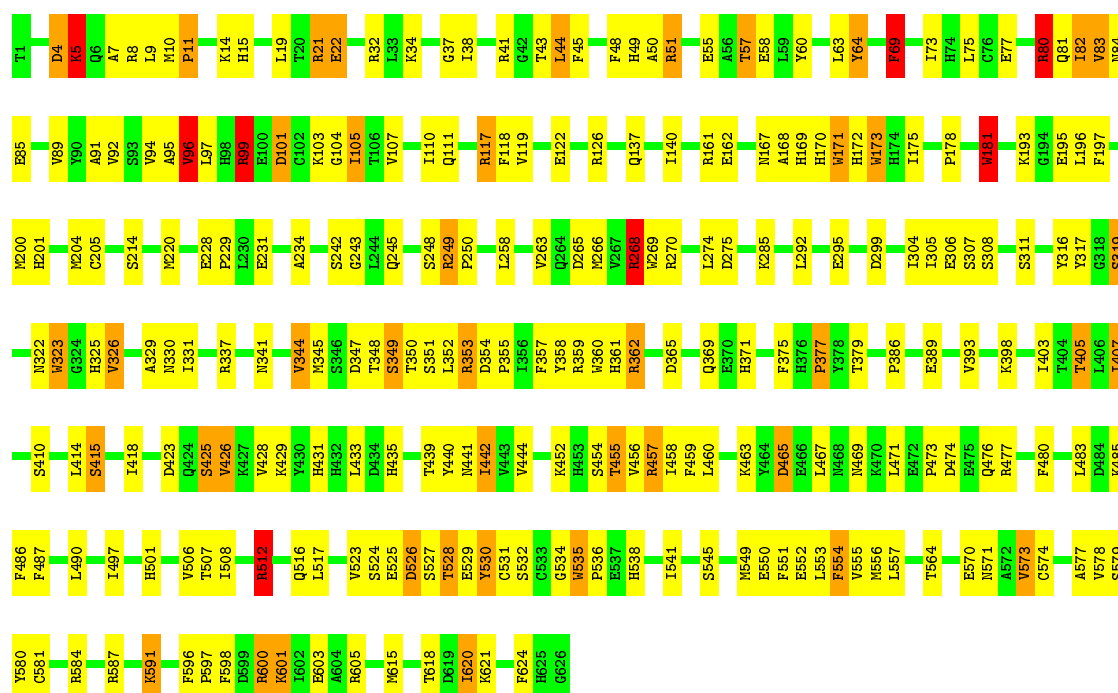






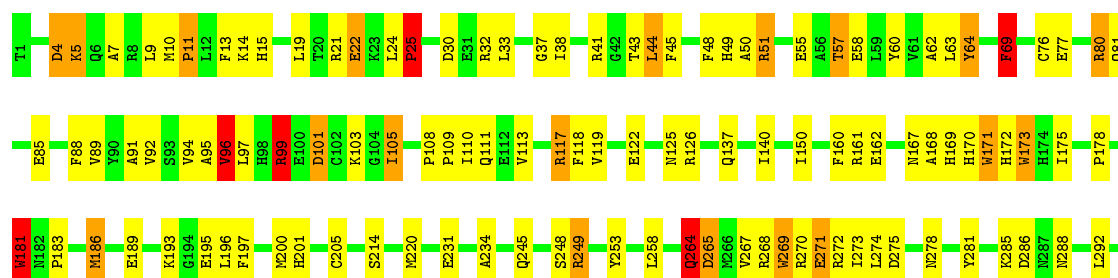
• Molecule 1: Hemocyanin AA6 chain

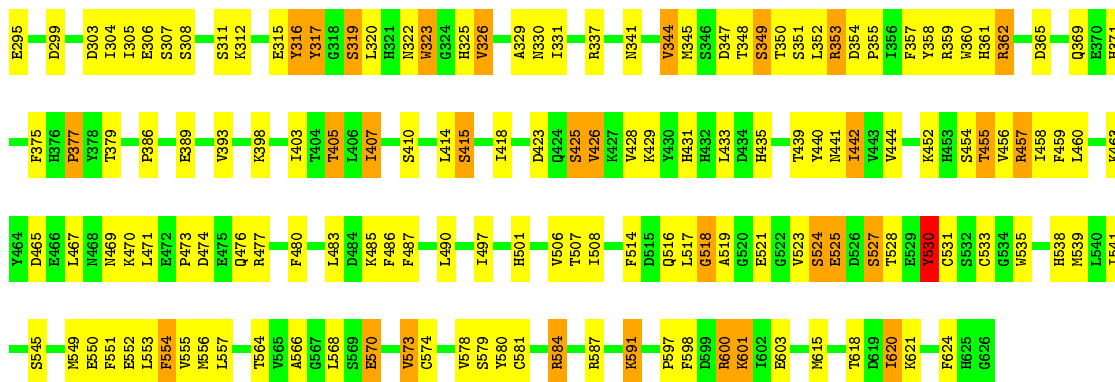
Chain H: 60% 32% 7% •



• Molecule 1: Hemocyanin AA6 chain

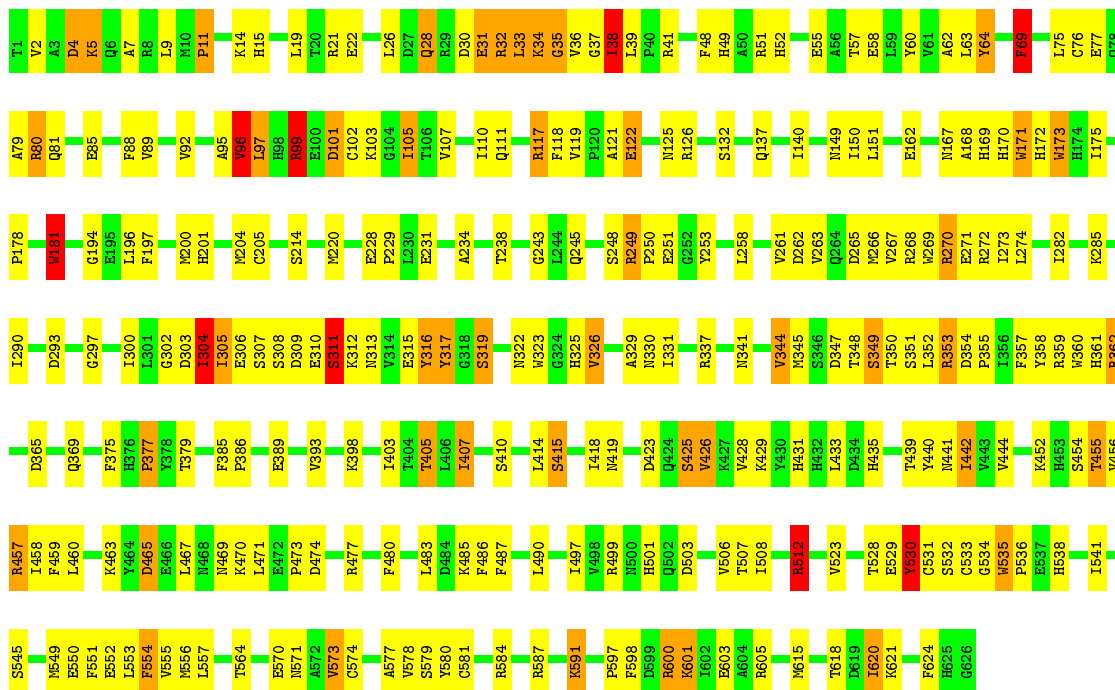
Chain I: 58% 34% 8% •





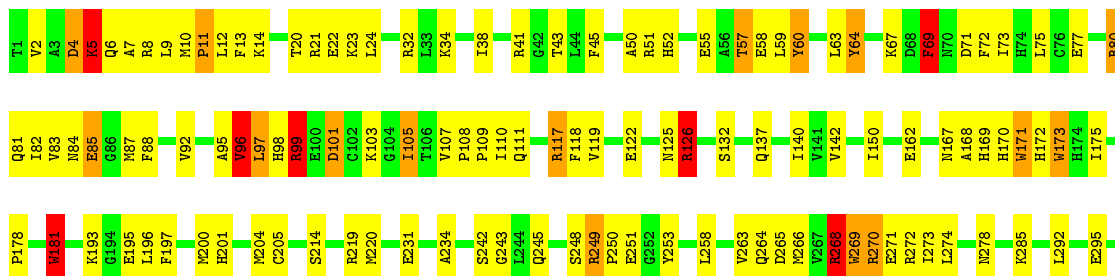
• Molecule 1: Hemocyanin AA6 chain

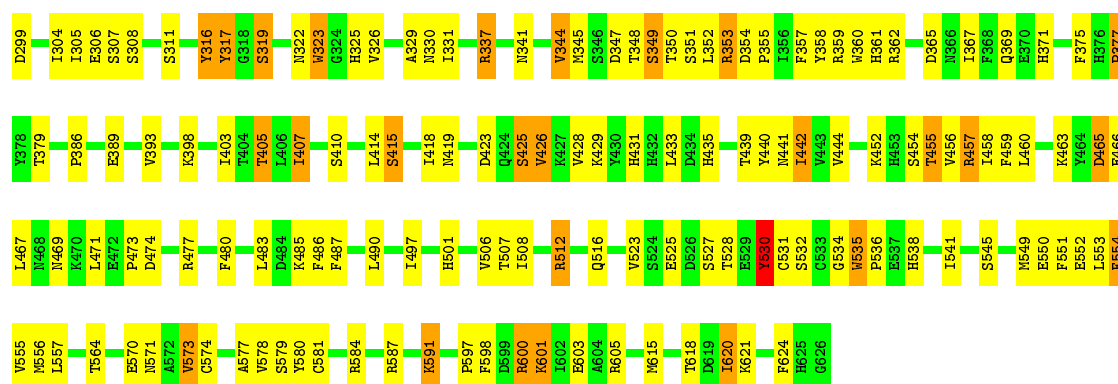
Chain J: 57% 35% 7% .



• Molecule 1: Hemocyanin AA6 chain

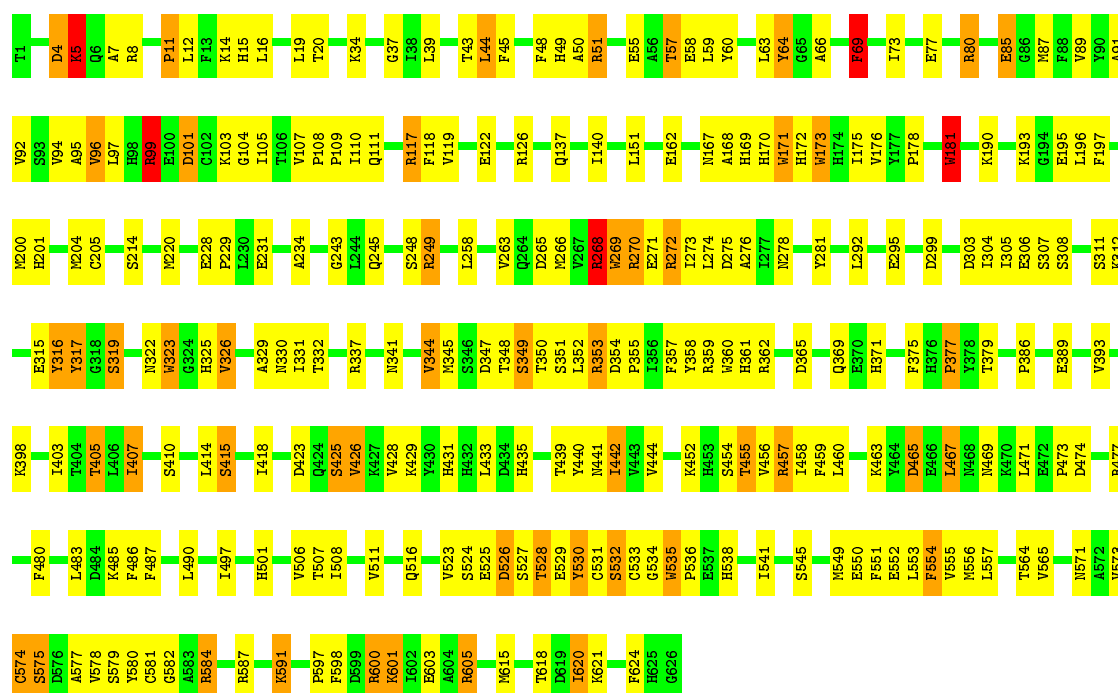
Chain K: 58% 34% 7% .





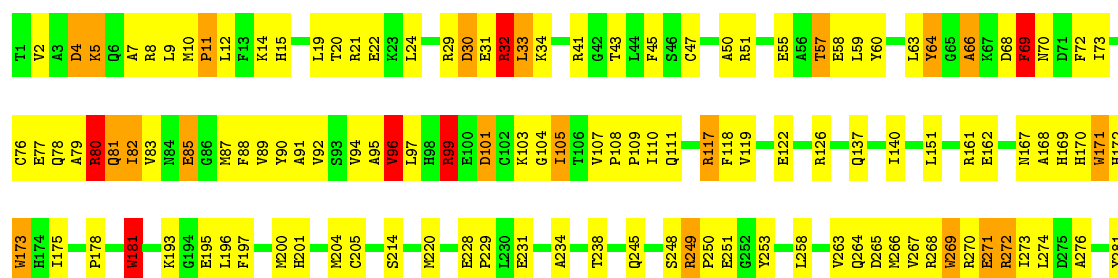
• Molecule 1: Hemocyanin AA6 chain

Chain L: 59% 33% 8% •



• Molecule 1: Hemocyanin AA6 chain

Chain M: 55% 36% 8% •



I541	D465	B376	L292
S545	E466	P377	E295
M549	L467	Y378	
E550	N468	T379	D299
F551	K470	P386	
E552	L471	E389	I304
L553	E472		I305
F554	P473	V393	E306
V555	D474		S307
M556		K398	S308
L557	R477		
	F480	I403	S311
T564		T404	
E570	L483	T405	E315
N571	D484	L406	Y316
A572	K485	I407	Y317
V573	F486		G318
C574	F487	S410	S319
A577	L490	L414	N322
V578		S415	N323
S579	K494		G324
Y580	N495	I418	H325
C581	T496		Y326
	I497	D423	
R584	V498	Q424	A329
	R499	S425	N330
	N500	V426	I331
R587	H501	K427	
K591	H502	V428	R337
	D503	K429	
		Y430	N341
P597	V506	H431	
F598	T507	H432	Y344
F599	I508	L433	K345
R600		D434	S346
K601	R512	H435	D347
L602			T348
E603	Q516	T439	S349
A604	L517	Y440	T350
R605		N441	S351
		I442	L352
M615	V523	V443	R353
	S524	V444	
	E525	E445	F357
T618	D526		Y358
D619	S527	K452	R359
I620	T528	H453	I360
K621	E529	S454	H361
	Y530	T455	R362
F624	C531	V456	
H625	S532	R457	D365
G626	C533	I458	
	Q534	F459	Q369
	H535	L460	E370
	F536		H371
	E537	K463	
	H538	Y464	F375

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C	Depositor
Number of images	13400	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	each micrograph	Depositor
Microscope	JEM3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	18	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	50000	Depositor
Image detector	Kodak SO163 film	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.55	11/5191 (0.2%)	1.55	54/7033 (0.8%)
1	C	1.54	8/5190 (0.2%)	1.48	38/7030 (0.5%)
1	D	0.73	1/5191 (0.0%)	1.39	46/7033 (0.7%)
1	E	1.55	9/5191 (0.2%)	1.49	44/7033 (0.6%)
1	F	1.54	8/5191 (0.2%)	1.50	46/7033 (0.7%)
1	G	1.52	8/5191 (0.2%)	1.40	47/7033 (0.7%)
1	H	1.53	9/5191 (0.2%)	1.51	49/7033 (0.7%)
1	I	1.54	8/5190 (0.2%)	1.51	46/7030 (0.7%)
1	J	1.53	8/5191 (0.2%)	1.38	40/7033 (0.6%)
1	K	1.51	8/5191 (0.2%)	1.39	42/7033 (0.6%)
1	L	1.53	9/5191 (0.2%)	1.49	43/7033 (0.6%)
1	M	1.52	8/5191 (0.2%)	1.40	47/7033 (0.7%)
All	All	1.48	95/62290 (0.2%)	1.46	542/84390 (0.6%)

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	A	0	20
1	C	0	15
1	D	0	13
1	E	0	15
1	F	0	16
1	G	0	16
1	H	0	16
1	I	0	15
1	J	0	14
1	K	0	18
1	L	0	18
1	M	0	19
All	All	0	195

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	5	LYS	CE-NZ	50.53	2.75	1.49
1	G	5	LYS	CE-NZ	50.45	2.75	1.49
1	H	5	LYS	CE-NZ	50.33	2.74	1.49
1	L	5	LYS	CE-NZ	50.29	2.74	1.49
1	I	5	LYS	CE-NZ	50.17	2.74	1.49
1	E	5	LYS	CE-NZ	47.09	2.66	1.49
1	A	5	LYS	CE-NZ	47.06	2.66	1.49
1	J	5	LYS	CE-NZ	47.05	2.66	1.49
1	C	5	LYS	CE-NZ	47.05	2.66	1.49
1	F	5	LYS	CE-NZ	47.02	2.66	1.49
1	M	5	LYS	CE-NZ	47.01	2.66	1.49
1	J	69	PHE	CG-CD2	40.64	1.99	1.38
1	E	69	PHE	CG-CD2	40.59	1.99	1.38
1	F	69	PHE	CG-CD2	40.58	1.99	1.38
1	C	69	PHE	CG-CD2	40.55	1.99	1.38
1	A	69	PHE	CG-CD2	40.51	1.99	1.38
1	M	69	PHE	CG-CD2	40.11	1.99	1.38
1	C	69	PHE	CG-CD1	40.09	1.98	1.38
1	A	69	PHE	CG-CD1	40.08	1.98	1.38
1	J	69	PHE	CG-CD1	40.06	1.98	1.38
1	E	69	PHE	CG-CD1	40.06	1.98	1.38
1	F	69	PHE	CG-CD1	40.03	1.98	1.38
1	I	69	PHE	CG-CD2	39.30	1.97	1.38
1	G	69	PHE	CG-CD2	39.07	1.97	1.38
1	L	69	PHE	CG-CD2	39.01	1.97	1.38
1	K	69	PHE	CG-CD1	39.00	1.97	1.38
1	H	69	PHE	CG-CD2	38.93	1.97	1.38
1	L	69	PHE	CG-CD1	38.89	1.97	1.38
1	K	69	PHE	CG-CD2	38.84	1.97	1.38
1	H	69	PHE	CG-CD1	38.84	1.97	1.38
1	G	69	PHE	CG-CD1	38.69	1.96	1.38
1	I	69	PHE	CG-CD1	38.68	1.96	1.38
1	M	69	PHE	CG-CD1	38.63	1.96	1.38
1	M	69	PHE	CE1-CZ	33.79	2.01	1.37
1	M	69	PHE	CE2-CZ	33.17	2.00	1.37
1	E	69	PHE	CE2-CZ	32.79	1.99	1.37
1	J	69	PHE	CE2-CZ	32.77	1.99	1.37
1	A	69	PHE	CE2-CZ	32.70	1.99	1.37
1	C	69	PHE	CE2-CZ	32.70	1.99	1.37
1	F	69	PHE	CE2-CZ	32.66	1.99	1.37
1	J	69	PHE	CE1-CZ	32.19	1.98	1.37
1	A	69	PHE	CE1-CZ	32.19	1.98	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	69	PHE	CE1-CZ	32.18	1.98	1.37
1	F	69	PHE	CE1-CZ	32.17	1.98	1.37
1	C	69	PHE	CE1-CZ	32.15	1.98	1.37
1	I	69	PHE	CE2-CZ	31.50	1.97	1.37
1	G	69	PHE	CE2-CZ	31.38	1.97	1.37
1	L	69	PHE	CE2-CZ	31.36	1.97	1.37
1	H	69	PHE	CE2-CZ	31.33	1.96	1.37
1	L	69	PHE	CE1-CZ	31.29	1.96	1.37
1	I	69	PHE	CE1-CZ	31.22	1.96	1.37
1	H	69	PHE	CE1-CZ	31.21	1.96	1.37
1	G	69	PHE	CE1-CZ	31.13	1.96	1.37
1	K	69	PHE	CE2-CZ	30.91	1.96	1.37
1	K	69	PHE	CE1-CZ	30.29	1.95	1.37
1	A	69	PHE	CD1-CE1	30.06	1.99	1.39
1	C	69	PHE	CD1-CE1	30.05	1.99	1.39
1	F	69	PHE	CD1-CE1	30.04	1.99	1.39
1	E	69	PHE	CD1-CE1	30.02	1.99	1.39
1	J	69	PHE	CD1-CE1	29.95	1.99	1.39
1	A	69	PHE	CD2-CE2	29.74	1.98	1.39
1	F	69	PHE	CD2-CE2	29.70	1.98	1.39
1	C	69	PHE	CD2-CE2	29.65	1.98	1.39
1	E	69	PHE	CD2-CE2	29.63	1.98	1.39
1	J	69	PHE	CD2-CE2	29.62	1.98	1.39
1	M	69	PHE	CD1-CE1	28.87	1.97	1.39
1	L	69	PHE	CD1-CE1	28.82	1.96	1.39
1	I	69	PHE	CD1-CE1	28.80	1.96	1.39
1	K	69	PHE	CD1-CE1	28.80	1.96	1.39
1	M	69	PHE	CD2-CE2	28.77	1.96	1.39
1	I	69	PHE	CD2-CE2	28.76	1.96	1.39
1	H	69	PHE	CD1-CE1	28.73	1.96	1.39
1	G	69	PHE	CD1-CE1	28.63	1.96	1.39
1	H	69	PHE	CD2-CE2	28.55	1.96	1.39
1	G	69	PHE	CD2-CE2	28.52	1.96	1.39
1	L	69	PHE	CD2-CE2	28.47	1.96	1.39
1	K	69	PHE	CD2-CE2	28.24	1.95	1.39
1	I	44	LEU	C-N	16.37	1.71	1.34
1	L	44	LEU	C-N	16.37	1.71	1.34
1	H	44	LEU	C-N	16.36	1.71	1.34
1	A	44	LEU	C-N	16.35	1.71	1.34
1	C	44	LEU	C-N	16.33	1.71	1.34
1	F	44	LEU	C-N	16.32	1.71	1.34
1	E	44	LEU	C-N	16.32	1.71	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	537	GLU	C-N	9.74	1.56	1.34
1	A	24	LEU	CB-CG	8.07	1.75	1.52
1	J	536	PRO	C-N	8.06	1.52	1.34
1	A	536	PRO	C-N	8.01	1.52	1.34
1	E	536	PRO	C-N	7.91	1.52	1.34
1	A	24	LEU	CA-CB	7.89	1.71	1.53
1	K	536	PRO	C-N	7.82	1.52	1.34
1	D	536	PRO	C-N	7.20	1.50	1.34
1	H	536	PRO	C-N	6.99	1.50	1.34
1	G	536	PRO	C-N	6.99	1.50	1.34
1	L	536	PRO	C-N	6.75	1.49	1.34

All (542) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	44	LEU	O-C-N	-41.48	56.33	122.70
1	A	44	LEU	O-C-N	-41.46	56.37	122.70
1	F	44	LEU	O-C-N	-41.45	56.38	122.70
1	C	44	LEU	O-C-N	-41.43	56.41	122.70
1	I	44	LEU	O-C-N	-41.43	56.41	122.70
1	H	44	LEU	O-C-N	-41.42	56.43	122.70
1	E	44	LEU	O-C-N	-41.40	56.46	122.70
1	A	44	LEU	CA-C-N	18.92	158.82	117.20
1	C	44	LEU	CA-C-N	18.91	158.81	117.20
1	E	44	LEU	CA-C-N	18.91	158.79	117.20
1	H	44	LEU	CA-C-N	18.88	158.74	117.20
1	L	44	LEU	CA-C-N	18.88	158.73	117.20
1	F	44	LEU	CA-C-N	18.88	158.72	117.20
1	I	44	LEU	CA-C-N	18.87	158.71	117.20
1	C	44	LEU	C-N-CA	14.27	157.36	121.70
1	H	44	LEU	C-N-CA	14.26	157.35	121.70
1	A	44	LEU	C-N-CA	14.26	157.34	121.70
1	F	44	LEU	C-N-CA	14.25	157.32	121.70
1	I	44	LEU	C-N-CA	14.24	157.31	121.70
1	E	44	LEU	C-N-CA	14.24	157.30	121.70
1	L	44	LEU	C-N-CA	14.22	157.24	121.70
1	A	24	LEU	CD1-CG-CD2	-12.59	72.74	110.50
1	F	5	LYS	CD-CE-NZ	12.17	139.69	111.70
1	J	5	LYS	CD-CE-NZ	12.15	139.66	111.70
1	M	5	LYS	CD-CE-NZ	12.15	139.64	111.70
1	E	5	LYS	CD-CE-NZ	12.14	139.62	111.70
1	C	5	LYS	CD-CE-NZ	12.13	139.61	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	LYS	CD-CE-NZ	12.13	139.59	111.70
1	K	5	LYS	CD-CE-NZ	12.09	139.51	111.70
1	L	272	ARG	NE-CZ-NH2	12.01	126.31	120.30
1	A	362	ARG	NE-CZ-NH2	-11.99	114.30	120.30
1	J	362	ARG	NE-CZ-NH2	-11.99	114.31	120.30
1	D	362	ARG	NE-CZ-NH2	-11.97	114.32	120.30
1	H	362	ARG	NE-CZ-NH2	-11.93	114.34	120.30
1	K	362	ARG	NE-CZ-NH2	-11.91	114.35	120.30
1	E	362	ARG	NE-CZ-NH2	-11.91	114.35	120.30
1	F	362	ARG	NE-CZ-NH2	-11.91	114.35	120.30
1	M	362	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	I	362	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	H	5	LYS	CD-CE-NZ	11.81	138.86	111.70
1	G	362	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	C	362	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	L	362	ARG	NE-CZ-NH2	-11.75	114.43	120.30
1	L	5	LYS	CD-CE-NZ	11.55	138.27	111.70
1	G	5	LYS	CD-CE-NZ	11.54	138.25	111.70
1	I	5	LYS	CD-CE-NZ	11.52	138.19	111.70
1	H	80	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	A	268	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	K	126	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	A	24	LEU	CA-CB-CG	9.96	138.21	115.30
1	A	24	LEU	CB-CG-CD2	9.92	127.86	111.00
1	D	81	GLN	N-CA-CB	-9.91	92.77	110.60
1	M	535	TRP	CD1-CG-CD2	8.81	113.35	106.30
1	A	24	LEU	CB-CG-CD1	8.78	125.92	111.00
1	L	535	TRP	CD1-CG-CD2	8.74	113.29	106.30
1	D	535	TRP	CD1-CG-CD2	8.74	113.29	106.30
1	H	535	TRP	CD1-CG-CD2	8.71	113.27	106.30
1	K	535	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	J	535	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	A	535	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	L	532	SER	N-CA-CB	-8.64	97.53	110.50
1	E	535	TRP	CD1-CG-CD2	8.64	113.21	106.30
1	G	535	TRP	CD1-CG-CD2	8.63	113.20	106.30
1	F	535	TRP	CD1-CG-CD2	8.53	113.12	106.30
1	A	268	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	J	181	TRP	CD1-CG-CD2	8.51	113.11	106.30
1	A	24	LEU	N-CA-CB	8.50	127.41	110.40
1	H	181	TRP	CD1-CG-CD2	8.49	113.09	106.30
1	E	181	TRP	CD1-CG-CD2	8.48	113.09	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	181	TRP	CD1-CG-CD2	8.47	113.08	106.30
1	C	181	TRP	CD1-CG-CD2	8.46	113.07	106.30
1	I	181	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	F	181	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	D	181	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	K	181	TRP	CD1-CG-CD2	8.43	113.05	106.30
1	L	181	TRP	CD1-CG-CD2	8.39	113.01	106.30
1	A	181	TRP	CD1-CG-CD2	8.36	112.99	106.30
1	A	126	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	G	181	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	D	173	TRP	CD1-CG-CD2	8.29	112.94	106.30
1	L	173	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	F	173	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	C	173	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	A	173	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	G	173	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	K	173	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	E	173	TRP	CD1-CG-CD2	8.22	112.87	106.30
1	M	173	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	H	173	TRP	CD1-CG-CD2	8.17	112.83	106.30
1	I	173	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	J	173	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	L	269	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	J	360	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	F	360	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	J	269	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	I	360	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	G	360	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	L	360	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	H	360	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	M	360	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	E	360	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	D	527	SER	O-C-N	-8.00	109.91	122.70
1	K	360	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	D	360	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	A	360	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	L	269	TRP	CE2-CD2-CG	-7.94	100.95	107.30
1	H	269	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	C	535	TRP	CD1-CG-CD2	7.92	112.64	106.30
1	H	181	TRP	CE2-CD2-CG	-7.92	100.97	107.30
1	M	527	SER	O-C-N	-7.92	110.03	122.70
1	I	269	TRP	CD1-CG-CD2	7.92	112.63	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	360	TRP	CD1-CG-CD2	7.91	112.63	106.30
1	M	181	TRP	CE2-CD2-CG	-7.91	100.97	107.30
1	C	181	TRP	CE2-CD2-CG	-7.91	100.97	107.30
1	F	360	TRP	CE2-CD2-CG	-7.89	100.99	107.30
1	M	535	TRP	CE2-CD2-CG	-7.89	100.99	107.30
1	G	360	TRP	CE2-CD2-CG	-7.88	101.00	107.30
1	I	360	TRP	CE2-CD2-CG	-7.88	101.00	107.30
1	L	181	TRP	CE2-CD2-CG	-7.87	101.01	107.30
1	I	535	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	M	126	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	E	360	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	A	269	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	L	535	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	K	269	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	J	269	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	M	360	TRP	CE2-CD2-CG	-7.84	101.02	107.30
1	D	126	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	D	535	TRP	CE2-CD2-CG	-7.83	101.03	107.30
1	F	126	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	J	360	TRP	CE2-CD2-CG	-7.83	101.03	107.30
1	J	181	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	E	126	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	D	181	TRP	CE2-CD2-CG	-7.82	101.05	107.30
1	E	535	TRP	CE2-CD2-CG	-7.82	101.05	107.30
1	H	535	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	F	181	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	F	269	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	E	181	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	K	181	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	L	360	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	I	181	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	535	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	J	535	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	F	535	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	H	360	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	D	360	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	A	360	TRP	CE2-CD2-CG	-7.78	101.08	107.30
1	C	360	TRP	CE2-CD2-CG	-7.77	101.08	107.30
1	G	535	TRP	CE2-CD2-CG	-7.77	101.08	107.30
1	D	81	GLN	CB-CA-C	7.77	125.94	110.40
1	H	512	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	I	126	ARG	NE-CZ-NH2	-7.76	116.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	360	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	G	269	TRP	CD1-CG-CD2	7.76	112.50	106.30
1	G	181	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	A	173	TRP	CE2-CD2-CG	-7.74	101.11	107.30
1	E	173	TRP	CE2-CD2-CG	-7.73	101.12	107.30
1	A	181	TRP	CE2-CD2-CG	-7.73	101.12	107.30
1	G	527	SER	O-C-N	-7.71	110.36	122.70
1	H	126	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	M	269	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	C	173	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	K	535	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	D	269	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	F	173	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	K	173	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	H	269	TRP	CE2-CD2-CG	-7.68	101.15	107.30
1	E	269	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	M	171	TRP	CE2-CD2-CG	-7.68	101.16	107.30
1	H	527	SER	O-C-N	-7.67	110.42	122.70
1	D	173	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	E	171	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	J	173	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	L	173	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	A	171	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	H	173	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	I	173	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	E	362	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	C	269	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	G	171	TRP	CE2-CD2-CG	-7.63	101.19	107.30
1	G	173	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	M	173	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	C	126	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	F	171	TRP	CE2-CD2-CG	-7.62	101.21	107.30
1	M	526	ASP	CA-C-N	7.62	133.96	117.20
1	H	171	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	D	526	ASP	CA-C-N	7.61	133.93	117.20
1	I	171	TRP	CE2-CD2-CG	-7.61	101.22	107.30
1	K	171	TRP	CE2-CD2-CG	-7.61	101.22	107.30
1	H	526	ASP	CA-C-N	7.60	133.93	117.20
1	G	526	ASP	CA-C-N	7.60	133.91	117.20
1	J	171	TRP	CE2-CD2-CG	-7.59	101.22	107.30
1	J	126	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	L	171	TRP	CE2-CD2-CG	-7.58	101.23	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	526	ASP	CA-C-N	7.57	133.86	117.20
1	K	269	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	A	269	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	J	362	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	D	171	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	F	269	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	L	362	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	C	171	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	A	270	ARG	NE-CZ-NH2	7.55	124.08	120.30
1	J	249	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	E	269	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	M	362	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	H	362	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	D	362	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	F	362	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	362	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	C	269	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	G	269	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	K	362	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	I	269	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	I	362	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	A	25	PRO	N-CA-C	-7.44	92.76	112.10
1	C	362	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	M	269	TRP	CE2-CD2-CG	-7.41	101.38	107.30
1	G	323	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	K	323	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	C	323	TRP	CD1-CG-CD2	7.38	112.21	106.30
1	H	323	TRP	CD1-CG-CD2	7.38	112.20	106.30
1	C	535	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	A	323	TRP	CD1-CG-CD2	7.37	112.20	106.30
1	G	362	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	D	269	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	F	323	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	J	323	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	D	323	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	M	171	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	I	323	TRP	CD1-CG-CD2	7.34	112.17	106.30
1	K	323	TRP	CE2-CD2-CG	-7.33	101.43	107.30
1	A	171	TRP	CD1-CG-CD2	7.33	112.17	106.30
1	D	323	TRP	CD1-CG-CD2	7.33	112.17	106.30
1	M	323	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	I	535	TRP	CE2-CD2-CG	-7.31	101.45	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	323	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	L	323	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	L	323	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	E	323	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	C	323	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	F	323	TRP	CE2-CD2-CG	-7.28	101.48	107.30
1	H	323	TRP	CE2-CD2-CG	-7.27	101.48	107.30
1	A	323	TRP	CE2-CD2-CG	-7.27	101.49	107.30
1	H	171	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	G	171	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	G	323	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	J	323	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	I	323	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	E	171	TRP	CD1-CG-CD2	7.24	112.09	106.30
1	K	171	TRP	CD1-CG-CD2	7.24	112.09	106.30
1	I	171	TRP	CD1-CG-CD2	7.23	112.09	106.30
1	J	171	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	L	171	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	F	171	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	K	126	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	K	60	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	D	171	TRP	CD1-CG-CD2	7.21	112.06	106.30
1	M	512	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	C	171	TRP	CD1-CG-CD2	7.13	112.00	106.30
1	E	323	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	L	249	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	I	519	ALA	CA-C-N	7.00	130.21	116.20
1	H	21	ARG	O-C-N	-6.99	111.52	122.70
1	G	605	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	I	530	TYR	CA-CB-CG	-6.92	100.24	113.40
1	G	457	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	G	249	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	H	249	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	L	457	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	E	249	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	K	457	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	D	249	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	C	457	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	F	532	SER	N-CA-CB	-6.83	100.25	110.50
1	E	457	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	249	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	A	457	ARG	NE-CZ-NH1	6.81	123.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	457	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	F	457	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	34	LYS	N-CA-C	6.79	129.33	111.00
1	D	457	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	K	249	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	G	80	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	E	512	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	H	457	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	J	457	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	D	83	VAL	N-CA-C	6.71	129.11	111.00
1	M	457	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	A	80	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	I	249	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	F	80	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	L	80	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	E	80	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	M	171	TRP	CG-CD2-CE3	6.64	139.88	133.90
1	G	171	TRP	CG-CD2-CE3	6.64	139.87	133.90
1	I	171	TRP	CG-CD2-CE3	6.62	139.86	133.90
1	H	171	TRP	CG-CD2-CE3	6.62	139.85	133.90
1	K	171	TRP	CG-CD2-CE3	6.60	139.84	133.90
1	A	171	TRP	CG-CD2-CE3	6.58	139.82	133.90
1	L	171	TRP	CG-CD2-CE3	6.58	139.82	133.90
1	E	171	TRP	CG-CD2-CE3	6.57	139.81	133.90
1	D	171	TRP	CG-CD2-CE3	6.57	139.81	133.90
1	J	171	TRP	CG-CD2-CE3	6.55	139.80	133.90
1	I	80	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	C	80	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	G	337	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	F	171	TRP	CG-CD2-CE3	6.54	139.79	133.90
1	A	24	LEU	N-CA-C	-6.54	93.35	111.00
1	C	171	TRP	CG-CD2-CE3	6.53	139.78	133.90
1	D	80	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	E	270	ARG	NE-CZ-NH2	6.49	123.55	120.30
1	K	80	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	F	34	LYS	N-CA-C	6.46	128.44	111.00
1	M	80	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	512	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	J	80	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	M	80	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	G	512	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	G	605	ARG	NE-CZ-NH1	6.29	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	117	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	M	337	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	F	249	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	I	117	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	M	69	PHE	CB-CG-CD1	-6.21	116.45	120.80
1	M	249	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	J	117	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	M	117	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	E	117	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	F	117	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	C	268	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	135	PRO	N-CA-C	6.16	128.11	112.10
1	D	527	SER	CA-C-N	6.15	130.73	117.20
1	D	587	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	M	527	SER	CA-C-N	6.09	130.60	117.20
1	L	117	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	C	117	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	L	268	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	H	587	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	L	587	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	I	587	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	K	117	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	M	69	PHE	CA-CB-CG	-6.02	99.45	113.90
1	M	587	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	D	44	LEU	N-CA-C	6.00	127.20	111.00
1	H	117	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	G	587	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	C	249	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	E	587	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	F	587	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	K	587	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	A	587	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	G	126	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	J	312	LYS	CA-CB-CG	-5.94	100.33	113.40
1	H	83	VAL	N-CA-C	5.93	127.01	111.00
1	J	587	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	A	22	GLU	CB-CA-C	5.92	122.24	110.40
1	D	117	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	G	527	SER	CA-C-N	5.91	130.20	117.20
1	H	337	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	J	51	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	M	51	ARG	NE-CZ-NH1	5.82	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	527	SER	CA-C-N	5.82	130.00	117.20
1	E	126	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	K	51	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	M	32	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	M	306	GLU	CA-C-N	5.76	129.87	117.20
1	K	306	GLU	CA-C-N	5.75	129.85	117.20
1	M	126	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	I	126	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	I	25	PRO	N-CA-C	5.73	127.00	112.10
1	A	306	GLU	CA-C-N	5.73	129.80	117.20
1	L	306	GLU	CA-C-N	5.73	129.80	117.20
1	F	306	GLU	CA-C-N	5.72	129.79	117.20
1	I	306	GLU	CA-C-N	5.72	129.79	117.20
1	C	306	GLU	CA-C-N	5.72	129.78	117.20
1	G	312	LYS	CA-C-N	5.72	129.78	117.20
1	F	126	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	51	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	E	306	GLU	CA-C-N	5.69	129.72	117.20
1	H	126	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	E	51	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	51	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	51	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	I	51	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	H	306	GLU	CA-C-N	5.66	129.66	117.20
1	L	51	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	F	531	CYS	C-N-CA	5.61	135.73	121.70
1	D	306	GLU	CA-C-N	5.61	129.54	117.20
1	C	605	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	G	51	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	126	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	F	51	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	G	311	SER	CA-C-N	-5.60	104.89	117.20
1	J	512	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	G	337	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	J	126	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	126	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	K	268	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	L	269	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	M	33	LEU	N-CA-C	5.53	125.94	111.00
1	H	51	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	J	38	ILE	CA-CB-CG1	5.50	121.46	111.00
1	F	20	THR	CA-CB-CG2	5.46	120.05	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	292	LEU	CA-C-N	-5.46	105.18	117.20
1	K	530	TYR	N-CA-C	5.45	125.73	111.00
1	C	527	SER	CB-CA-C	-5.43	99.78	110.10
1	I	530	TYR	N-CA-C	5.43	125.67	111.00
1	C	564	THR	CA-CB-CG2	5.43	120.00	112.40
1	G	126	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	J	360	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	I	360	TRP	CG-CD2-CE3	5.41	138.76	133.90
1	D	605	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	J	269	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	H	82	ILE	O-C-N	-5.38	114.10	122.70
1	J	35	GLY	O-C-N	-5.37	114.11	122.70
1	M	30	ASP	CB-CA-C	5.36	121.12	110.40
1	G	360	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	M	535	TRP	CG-CD1-NE1	-5.35	104.75	110.10
1	F	605	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	M	360	TRP	CG-CD2-CE3	5.35	138.71	133.90
1	A	360	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	E	527	SER	O-C-N	-5.34	114.16	122.70
1	L	360	TRP	CG-CD2-CE3	5.34	138.70	133.90
1	L	535	TRP	CG-CD1-NE1	-5.34	104.76	110.10
1	I	530	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	D	535	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	G	535	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	K	360	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	K	535	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	A	535	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	H	360	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	H	535	TRP	CG-CD1-NE1	-5.31	104.79	110.10
1	M	535	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	E	360	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	M	151	LEU	CA-CB-CG	5.31	127.50	115.30
1	H	323	TRP	CB-CG-CD1	-5.29	120.12	127.00
1	G	323	TRP	CB-CG-CD1	-5.29	120.13	127.00
1	I	521	GLU	N-CA-C	5.29	125.28	111.00
1	H	181	TRP	CG-CD2-CE3	5.28	138.65	133.90
1	E	323	TRP	CB-CG-CD1	-5.28	120.14	127.00
1	E	535	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	M	527	SER	N-CA-C	5.27	125.23	111.00
1	F	360	TRP	CG-CD2-CE3	5.26	138.64	133.90
1	L	535	TRP	CG-CD2-CE3	5.26	138.63	133.90
1	D	360	TRP	CG-CD2-CE3	5.26	138.63	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	323	TRP	CB-CG-CD1	-5.26	120.16	127.00
1	C	323	TRP	CB-CG-CD1	-5.25	120.17	127.00
1	D	527	SER	N-CA-C	5.25	125.18	111.00
1	G	535	TRP	CG-CD2-CE3	5.25	138.63	133.90
1	H	527	SER	N-CA-C	5.25	125.18	111.00
1	H	535	TRP	CG-CD2-CE3	5.25	138.63	133.90
1	I	265	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	535	TRP	CG-CD2-CE3	5.25	138.62	133.90
1	I	22	GLU	O-C-N	-5.25	114.30	122.70
1	F	323	TRP	CB-CG-CD1	-5.25	120.18	127.00
1	A	527	SER	N-CA-C	5.25	125.17	111.00
1	H	80	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	E	535	TRP	CG-CD2-CE3	5.24	138.62	133.90
1	F	605	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	360	TRP	CG-CD2-CE3	5.24	138.61	133.90
1	D	311	SER	CA-C-N	-5.23	105.69	117.20
1	K	69	PHE	CA-CB-CG	-5.23	101.34	113.90
1	L	181	TRP	CG-CD2-CE3	5.23	138.61	133.90
1	A	323	TRP	CB-CG-CD1	-5.23	120.20	127.00
1	M	181	TRP	CG-CD2-CE3	5.23	138.60	133.90
1	G	527	SER	N-CA-C	5.23	125.11	111.00
1	M	323	TRP	CB-CG-CD1	-5.22	120.21	127.00
1	J	535	TRP	CG-CD2-CE3	5.22	138.60	133.90
1	L	323	TRP	CB-CG-CD1	-5.22	120.22	127.00
1	M	295	GLU	CA-CB-CG	5.22	124.88	113.40
1	J	535	TRP	CG-CD1-NE1	-5.21	104.89	110.10
1	K	323	TRP	CB-CG-CD1	-5.21	120.22	127.00
1	I	264	GLN	CA-CB-CG	5.21	124.86	113.40
1	E	295	GLU	CA-CB-CG	5.21	124.86	113.40
1	H	295	GLU	CA-CB-CG	5.20	124.85	113.40
1	I	295	GLU	CA-CB-CG	5.20	124.83	113.40
1	J	323	TRP	CB-CG-CD1	-5.20	120.24	127.00
1	D	323	TRP	CB-CG-CD1	-5.19	120.25	127.00
1	E	181	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	K	535	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	A	295	GLU	CA-CB-CG	5.18	124.79	113.40
1	G	312	LYS	CA-C-O	-5.18	109.22	120.10
1	K	82	ILE	O-C-N	-5.18	114.41	122.70
1	L	39	LEU	N-CA-C	-5.18	97.01	111.00
1	A	126	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	J	181	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	K	295	GLU	CA-CB-CG	5.17	124.78	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	295	GLU	CA-CB-CG	5.17	124.78	113.40
1	F	535	TRP	CG-CD2-CE3	5.17	138.56	133.90
1	C	181	TRP	CG-CD2-CE3	5.17	138.55	133.90
1	E	457	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	F	295	GLU	CA-CB-CG	5.16	124.76	113.40
1	L	295	GLU	CA-CB-CG	5.16	124.76	113.40
1	K	337	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	I	181	TRP	CG-CD2-CE3	5.16	138.54	133.90
1	G	457	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	181	TRP	CG-CD2-CE3	5.15	138.53	133.90
1	K	527	SER	N-CA-C	5.15	124.90	111.00
1	A	323	TRP	CG-CD2-CE3	5.14	138.53	133.90
1	J	323	TRP	CG-CD2-CE3	5.14	138.53	133.90
1	A	535	TRP	CG-CD2-CE3	5.14	138.52	133.90
1	F	535	TRP	CG-CD1-NE1	-5.14	104.96	110.10
1	J	33	LEU	N-CA-C	5.13	124.85	111.00
1	C	295	GLU	CA-CB-CG	5.12	124.67	113.40
1	C	323	TRP	CG-CD2-CE3	5.12	138.51	133.90
1	F	181	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	K	323	TRP	CG-CD2-CE3	5.12	138.51	133.90
1	L	457	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	L	126	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	181	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	D	323	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	I	323	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	K	181	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	I	337	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	L	526	ASP	CA-C-N	5.08	128.37	117.20
1	A	530	TYR	N-CA-C	5.07	124.69	111.00
1	K	181	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	F	181	TRP	CG-CD2-CE3	5.07	138.46	133.90
1	G	323	TRP	CG-CD2-CE3	5.06	138.45	133.90
1	E	181	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	G	181	TRP	CG-CD2-CE3	5.05	138.45	133.90
1	I	181	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	D	101	ASP	CB-CG-OD2	5.04	122.84	118.30
1	H	181	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	H	323	TRP	CG-CD2-CE3	5.04	138.44	133.90
1	F	323	TRP	CG-CD2-CE3	5.04	138.44	133.90
1	H	269	TRP	CG-CD2-CE3	5.04	138.44	133.90
1	J	181	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	A	25	PRO	C-N-CA	-5.04	109.11	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	311	SER	N-CA-C	5.03	124.58	111.00
1	D	265	ASP	CB-CG-OD2	5.02	122.82	118.30
1	E	268	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	F	457	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	M	323	TRP	CG-CD2-CE3	5.02	138.41	133.90
1	D	457	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	E	323	TRP	CG-CD2-CE3	5.01	138.41	133.90
1	L	323	TRP	CG-CD2-CE3	5.01	138.41	133.90
1	D	181	TRP	CG-CD1-NE1	-5.01	105.09	110.10
1	E	499	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	F	101	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (195) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain
1	A	127	ALA	Peptide
1	A	22	GLU	Peptide
1	A	23	LYS	Peptide
1	A	24	LEU	Peptide
1	A	253	TYR	Sidechain
1	A	270	ARG	Sidechain
1	A	272	ARG	Sidechain
1	A	316	TYR	Sidechain
1	A	317	TYR	Sidechain
1	A	359	ARG	Sidechain
1	A	43	THR	Peptide
1	A	440	TYR	Sidechain
1	A	457	ARG	Sidechain
1	A	523	VAL	Peptide
1	A	530	TYR	Sidechain
1	A	600	ARG	Sidechain
1	A	69	PHE	Sidechain
1	A	96	VAL	Peptide
1	A	99	ARG	Peptide
1	C	253	TYR	Sidechain
1	C	270	ARG	Sidechain
1	C	316	TYR	Sidechain
1	C	317	TYR	Sidechain
1	C	337	ARG	Sidechain
1	C	359	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	43	THR	Peptide
1	C	440	TYR	Sidechain
1	C	457	ARG	Sidechain
1	C	518	GLY	Mainchain
1	C	600	ARG	Sidechain
1	C	64	TYR	Sidechain
1	C	69	PHE	Sidechain
1	C	96	VAL	Peptide
1	C	99	ARG	Peptide
1	D	270	ARG	Sidechain
1	D	316	TYR	Sidechain
1	D	317	TYR	Sidechain
1	D	359	ARG	Sidechain
1	D	440	TYR	Sidechain
1	D	457	ARG	Sidechain
1	D	523	VAL	Peptide
1	D	530	TYR	Sidechain
1	D	600	ARG	Sidechain
1	D	64	TYR	Sidechain
1	D	84	ASN	Peptide
1	D	96	VAL	Peptide
1	D	99	ARG	Peptide
1	E	253	TYR	Sidechain
1	E	270	ARG	Sidechain
1	E	316	TYR	Sidechain
1	E	317	TYR	Sidechain
1	E	359	ARG	Sidechain
1	E	43	THR	Peptide
1	E	440	TYR	Sidechain
1	E	457	ARG	Sidechain
1	E	523	VAL	Peptide
1	E	530	TYR	Sidechain
1	E	600	ARG	Sidechain
1	E	64	TYR	Sidechain
1	E	69	PHE	Sidechain
1	E	96	VAL	Peptide
1	E	99	ARG	Peptide
1	F	23	LYS	Peptide
1	F	270	ARG	Sidechain
1	F	316	TYR	Sidechain
1	F	317	TYR	Sidechain
1	F	359	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	43	THR	Peptide
1	F	440	TYR	Sidechain
1	F	457	ARG	Sidechain
1	F	512	ARG	Sidechain
1	F	523	VAL	Peptide
1	F	530	TYR	Sidechain
1	F	600	ARG	Sidechain
1	F	64	TYR	Sidechain
1	F	69	PHE	Sidechain
1	F	96	VAL	Peptide
1	F	99	ARG	Peptide
1	G	253	TYR	Sidechain
1	G	270	ARG	Sidechain
1	G	272	ARG	Sidechain
1	G	316	TYR	Sidechain
1	G	317	TYR	Sidechain
1	G	359	ARG	Sidechain
1	G	43	THR	Peptide
1	G	440	TYR	Sidechain
1	G	457	ARG	Sidechain
1	G	523	VAL	Peptide
1	G	530	TYR	Sidechain
1	G	600	ARG	Sidechain
1	G	64	TYR	Sidechain
1	G	69	PHE	Sidechain
1	G	96	VAL	Peptide
1	G	99	ARG	Peptide
1	H	268	ARG	Sidechain
1	H	316	TYR	Sidechain
1	H	317	TYR	Sidechain
1	H	359	ARG	Sidechain
1	H	43	THR	Peptide
1	H	440	TYR	Sidechain
1	H	457	ARG	Sidechain
1	H	523	VAL	Peptide
1	H	530	TYR	Sidechain
1	H	600	ARG	Sidechain
1	H	64	TYR	Sidechain
1	H	69	PHE	Sidechain
1	H	80	ARG	Sidechain
1	H	84	ASN	Peptide
1	H	96	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	H	99	ARG	Peptide
1	I	253	TYR	Sidechain
1	I	281	TYR	Sidechain
1	I	316	TYR	Sidechain
1	I	317	TYR	Sidechain
1	I	359	ARG	Sidechain
1	I	43	THR	Peptide
1	I	440	TYR	Sidechain
1	I	457	ARG	Sidechain
1	I	518	GLY	Mainchain
1	I	530	TYR	Sidechain
1	I	600	ARG	Sidechain
1	I	64	TYR	Sidechain
1	I	69	PHE	Sidechain
1	I	96	VAL	Peptide
1	I	99	ARG	Peptide
1	J	270	ARG	Sidechain
1	J	31	GLU	Peptide
1	J	316	TYR	Sidechain
1	J	317	TYR	Sidechain
1	J	359	ARG	Sidechain
1	J	440	TYR	Sidechain
1	J	457	ARG	Sidechain
1	J	49	HIS	Sidechain
1	J	530	TYR	Sidechain
1	J	600	ARG	Sidechain
1	J	64	TYR	Sidechain
1	J	69	PHE	Sidechain
1	J	96	VAL	Peptide
1	J	99	ARG	Peptide
1	K	126	ARG	Sidechain
1	K	253	TYR	Sidechain
1	K	270	ARG	Sidechain
1	K	316	TYR	Sidechain
1	K	317	TYR	Sidechain
1	K	337	ARG	Sidechain
1	K	359	ARG	Sidechain
1	K	43	THR	Peptide
1	K	440	TYR	Sidechain
1	K	457	ARG	Sidechain
1	K	523	VAL	Peptide
1	K	530	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	K	600	ARG	Sidechain
1	K	605	ARG	Sidechain
1	K	64	TYR	Sidechain
1	K	69	PHE	Sidechain
1	K	96	VAL	Peptide
1	K	99	ARG	Peptide
1	L	268	ARG	Sidechain
1	L	270	ARG	Sidechain
1	L	316	TYR	Sidechain
1	L	317	TYR	Sidechain
1	L	337	ARG	Sidechain
1	L	359	ARG	Sidechain
1	L	43	THR	Peptide
1	L	440	TYR	Sidechain
1	L	457	ARG	Sidechain
1	L	523	VAL	Peptide
1	L	530	TYR	Sidechain
1	L	575	SER	Peptide
1	L	600	ARG	Sidechain
1	L	605	ARG	Sidechain
1	L	64	TYR	Sidechain
1	L	69	PHE	Sidechain
1	L	96	VAL	Peptide
1	L	99	ARG	Peptide
1	M	272	ARG	Sidechain
1	M	31	GLU	Peptide
1	M	316	TYR	Sidechain
1	M	317	TYR	Sidechain
1	M	32	ARG	Sidechain
1	M	337	ARG	Sidechain
1	M	359	ARG	Sidechain
1	M	43	THR	Peptide
1	M	440	TYR	Sidechain
1	M	457	ARG	Sidechain
1	M	523	VAL	Peptide
1	M	530	TYR	Sidechain
1	M	600	ARG	Sidechain
1	M	64	TYR	Sidechain
1	M	66	ALA	Mainchain
1	M	69	PHE	Sidechain
1	M	80	ARG	Sidechain
1	M	96	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	M	99	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5061	1123	4864	260	0
1	C	5061	1123	4863	199	0
1	D	5061	1123	4865	181	0
1	E	5061	1123	4864	190	0
1	F	5061	1123	4864	193	0
1	G	5061	1123	4865	214	0
1	H	5061	1123	4864	205	0
1	I	5061	1123	4863	207	0
1	J	5061	1123	4865	242	0
1	K	5061	1123	4865	225	0
1	L	5061	1123	4864	210	0
1	M	5061	1123	4865	230	0
All	All	60732	13476	58371	2404	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 20.

All (2404) 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)
1:A:24:LEU:CB	1:A:24:LEU:CG	1.76	1.56
1:K:69:PHE:CZ	1:K:69:PHE:CE1	1.94	1.55
1:G:69:PHE:CD2	1:G:69:PHE:CE2	1.96	1.54
1:G:69:PHE:CE1	1:G:69:PHE:CD1	1.96	1.54
1:H:69:PHE:CD2	1:H:69:PHE:CE2	1.96	1.53
1:K:69:PHE:CG	1:K:69:PHE:CD2	1.97	1.53
1:H:69:PHE:CE1	1:H:69:PHE:CD1	1.96	1.53
1:H:69:PHE:CZ	1:H:69:PHE:CE2	1.96	1.53
1:H:69:PHE:CD2	1:H:69:PHE:CG	1.97	1.53
1:H:69:PHE:CE1	1:H:69:PHE:CZ	1.96	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:69:PHE:CE2	1:K:69:PHE:CD2	1.95	1.52
1:L:69:PHE:CE2	1:L:69:PHE:CZ	1.96	1.52
1:H:69:PHE:CG	1:H:69:PHE:CD1	1.97	1.52
1:E:69:PHE:CZ	1:E:69:PHE:CE1	1.98	1.52
1:L:69:PHE:CG	1:L:69:PHE:CD1	1.97	1.52
1:M:69:PHE:CG	1:M:69:PHE:CD1	1.96	1.52
1:C:69:PHE:CE2	1:C:69:PHE:CD2	1.98	1.52
1:E:69:PHE:CG	1:E:69:PHE:CD1	1.98	1.51
1:M:69:PHE:CE1	1:M:69:PHE:CD1	1.97	1.51
1:J:69:PHE:CD1	1:J:69:PHE:CG	1.98	1.51
1:C:69:PHE:CG	1:C:69:PHE:CD1	1.98	1.51
1:G:69:PHE:CD1	1:G:69:PHE:CG	1.96	1.51
1:E:69:PHE:CG	1:E:69:PHE:CD2	1.99	1.51
1:C:69:PHE:CE1	1:C:69:PHE:CD1	1.99	1.51
1:J:69:PHE:CZ	1:J:69:PHE:CE2	1.99	1.51
1:A:69:PHE:CE2	1:A:69:PHE:CD2	1.98	1.51
1:K:69:PHE:CD1	1:K:69:PHE:CE1	1.96	1.51
1:J:69:PHE:CE2	1:J:69:PHE:CD2	1.98	1.51
1:A:69:PHE:CG	1:A:69:PHE:CD1	1.98	1.51
1:A:69:PHE:CZ	1:A:69:PHE:CE2	1.99	1.51
1:E:69:PHE:CE2	1:E:69:PHE:CD2	1.98	1.50
1:C:69:PHE:CZ	1:C:69:PHE:CE2	1.99	1.50
1:I:69:PHE:CD1	1:I:69:PHE:CG	1.96	1.50
1:K:69:PHE:CE2	1:K:69:PHE:CZ	1.96	1.50
1:M:69:PHE:CD2	1:M:69:PHE:CE2	1.96	1.50
1:J:69:PHE:CD1	1:J:69:PHE:CE1	1.99	1.50
1:A:69:PHE:CE1	1:A:69:PHE:CD1	1.99	1.50
1:G:69:PHE:CE1	1:G:69:PHE:CZ	1.96	1.50
1:L:69:PHE:CE2	1:L:69:PHE:CD2	1.96	1.50
1:E:69:PHE:CZ	1:E:69:PHE:CE2	1.99	1.50
1:I:69:PHE:CE1	1:I:69:PHE:CZ	1.96	1.50
1:F:69:PHE:CD2	1:F:69:PHE:CE2	1.98	1.50
1:L:69:PHE:CD1	1:L:69:PHE:CE1	1.96	1.50
1:E:69:PHE:CD1	1:E:69:PHE:CE1	1.99	1.50
1:I:69:PHE:CD1	1:I:69:PHE:CE1	1.96	1.50
1:M:69:PHE:CD2	1:M:69:PHE:CG	1.98	1.50
1:G:69:PHE:CZ	1:G:69:PHE:CE2	1.97	1.49
1:I:69:PHE:CD2	1:I:69:PHE:CE2	1.96	1.49
1:A:79:ALA:HB3	1:A:88:PHE:CE1	1.45	1.49
1:L:69:PHE:CG	1:L:69:PHE:CD2	1.97	1.49
1:I:69:PHE:CZ	1:I:69:PHE:CE2	1.97	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:PHE:CE1	1:F:69:PHE:CD1	1.99	1.49
1:K:69:PHE:CD1	1:K:69:PHE:CG	1.97	1.49
1:L:69:PHE:CZ	1:L:69:PHE:CE1	1.96	1.49
1:M:69:PHE:CE2	1:M:69:PHE:CZ	2.00	1.49
1:A:69:PHE:CG	1:A:69:PHE:CD2	1.99	1.49
1:A:69:PHE:CZ	1:A:69:PHE:CE1	1.98	1.49
1:F:69:PHE:CD1	1:F:69:PHE:CG	1.98	1.48
1:F:69:PHE:CE1	1:F:69:PHE:CZ	1.98	1.48
1:C:69:PHE:CD2	1:C:69:PHE:CG	1.99	1.48
1:I:69:PHE:CG	1:I:69:PHE:CD2	1.97	1.48
1:F:69:PHE:CD2	1:F:69:PHE:CG	1.99	1.48
1:F:69:PHE:CE2	1:F:69:PHE:CZ	1.99	1.48
1:L:104:GLY:CA	1:L:525:GLU:HB3	1.39	1.48
1:G:69:PHE:CD2	1:G:69:PHE:CG	1.97	1.48
1:J:69:PHE:CZ	1:J:69:PHE:CE1	1.98	1.48
1:C:69:PHE:CZ	1:C:69:PHE:CE1	1.98	1.48
1:J:69:PHE:CG	1:J:69:PHE:CD2	1.99	1.47
1:D:104:GLY:CA	1:D:525:GLU:HB3	1.41	1.46
1:M:104:GLY:CA	1:M:525:GLU:HB3	1.41	1.46
1:M:69:PHE:CE1	1:M:69:PHE:CZ	2.01	1.46
1:H:104:GLY:CA	1:H:525:GLU:HB3	1.41	1.46
1:G:104:GLY:CA	1:G:525:GLU:HB3	1.43	1.43
1:K:175:ILE:CG2	1:K:528:THR:HG21	1.47	1.42
1:E:175:ILE:CG2	1:E:528:THR:HG21	1.47	1.42
1:J:175:ILE:CG2	1:J:528:THR:HG21	1.48	1.41
1:L:63:LEU:CD2	1:L:91:ALA:HB1	1.47	1.39
1:C:151:LEU:CD1	1:G:467:LEU:HD11	1.54	1.37
1:F:104:GLY:CA	1:F:525:GLU:HB3	1.54	1.35
1:H:467:LEU:CD1	1:J:151:LEU:HD13	1.55	1.35
1:C:151:LEU:HD13	1:G:467:LEU:CD1	1.56	1.33
1:H:467:LEU:HD11	1:J:151:LEU:CD1	1.57	1.32
1:H:467:LEU:CD1	1:J:151:LEU:HA	1.59	1.30
1:K:8:ARG:NE	1:K:73:ILE:HG21	1.48	1.26
1:E:175:ILE:HG23	1:E:528:THR:HG21	1.25	1.19
1:D:104:GLY:HA2	1:D:525:GLU:HB3	1.20	1.19
1:M:104:GLY:HA2	1:M:525:GLU:HB3	1.19	1.18
1:L:104:GLY:CA	1:L:525:GLU:CB	2.23	1.16
1:G:104:GLY:HA2	1:G:525:GLU:HB3	1.22	1.16
1:M:104:GLY:CA	1:M:525:GLU:CB	2.25	1.15
1:C:151:LEU:HA	1:G:467:LEU:CD1	1.75	1.15
1:G:63:LEU:CD2	1:G:91:ALA:HB1	1.75	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:104:GLY:HA2	1:L:525:GLU:HB3	1.20	1.15
1:E:97:LEU:HD11	1:E:528:THR:HB	1.19	1.15
1:A:66:ALA:CB	1:A:99:ARG:HH21	1.60	1.14
1:A:104:GLY:HA2	1:A:525:GLU:CB	1.76	1.14
1:J:175:ILE:HG23	1:J:528:THR:HG21	1.26	1.13
1:D:104:GLY:CA	1:D:525:GLU:CB	2.25	1.13
1:A:72:PHE:CZ	1:A:96:VAL:HB	1.83	1.13
1:J:175:ILE:HG21	1:J:528:THR:HG21	1.24	1.13
1:F:104:GLY:HA3	1:F:525:GLU:HB3	1.21	1.13
1:H:104:GLY:CA	1:H:525:GLU:CB	2.25	1.12
1:H:104:GLY:HA2	1:H:525:GLU:HB3	1.20	1.12
1:J:97:LEU:HD11	1:J:528:THR:HB	1.20	1.12
1:G:104:GLY:CA	1:G:525:GLU:CB	2.27	1.12
1:J:290:ILE:CD1	1:J:300:ILE:HD12	1.80	1.11
1:K:175:ILE:HG23	1:K:528:THR:HG21	1.25	1.11
1:K:175:ILE:HG21	1:K:528:THR:HG21	1.25	1.11
1:E:175:ILE:HG21	1:E:528:THR:HG21	1.24	1.10
1:A:72:PHE:HZ	1:A:96:VAL:HB	1.12	1.10
1:K:97:LEU:HD11	1:K:528:THR:HB	1.19	1.10
1:J:204:MET:HG2	1:J:535:TRP:CH2	1.86	1.10
1:E:204:MET:HG2	1:E:535:TRP:CH2	1.87	1.10
1:K:204:MET:HG2	1:K:535:TRP:CH2	1.87	1.10
1:M:204:MET:HG2	1:M:535:TRP:CH2	1.87	1.10
1:A:204:MET:HG2	1:A:535:TRP:CH2	1.87	1.09
1:K:59:LEU:HD11	1:K:87:MET:CE	1.83	1.09
1:H:104:GLY:HA3	1:H:525:GLU:HB3	1.09	1.08
1:G:104:GLY:HA3	1:G:525:GLU:HB3	1.10	1.08
1:E:175:ILE:CG2	1:E:528:THR:CG2	2.32	1.08
1:I:272:ARG:HB3	1:I:316:TYR:CZ	1.88	1.08
1:H:467:LEU:HD13	1:J:151:LEU:HA	1.31	1.08
1:L:63:LEU:HD23	1:L:91:ALA:HB1	1.25	1.08
1:A:104:GLY:CA	1:A:525:GLU:HB3	1.84	1.08
1:J:132:SER:HB2	1:K:419:ASN:ND2	1.69	1.08
1:L:204:MET:HG2	1:L:535:TRP:CH2	1.89	1.08
1:G:204:MET:HG2	1:G:535:TRP:CH2	1.88	1.08
1:H:467:LEU:CD1	1:J:151:LEU:CA	2.32	1.07
1:G:24:LEU:HD13	1:G:81:GLN:NE2	1.68	1.07
1:A:24:LEU:CB	1:A:24:LEU:HG	1.84	1.07
1:J:5:LYS:NZ	1:J:69:PHE:CZ	2.23	1.07
1:J:175:ILE:CG2	1:J:528:THR:CG2	2.33	1.07
1:E:5:LYS:NZ	1:E:69:PHE:CZ	2.23	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:175:ILE:CG2	1:K:528:THR:CG2	2.32	1.07
1:D:204:MET:HG2	1:D:535:TRP:CH2	1.88	1.07
1:C:5:LYS:NZ	1:C:69:PHE:CG	2.23	1.07
1:K:59:LEU:HD11	1:K:87:MET:HE3	1.08	1.07
1:D:9:LEU:HD21	1:D:72:PHE:CZ	1.90	1.07
1:H:5:LYS:NZ	1:H:69:PHE:CZ	2.23	1.07
1:J:5:LYS:NZ	1:J:69:PHE:CG	2.23	1.07
1:E:5:LYS:NZ	1:E:69:PHE:CE1	2.23	1.06
1:E:5:LYS:NZ	1:E:69:PHE:CE2	2.23	1.06
1:E:5:LYS:NZ	1:E:69:PHE:CD1	2.24	1.06
1:C:5:LYS:NZ	1:C:69:PHE:CE1	2.23	1.06
1:J:5:LYS:NZ	1:J:69:PHE:CD1	2.24	1.06
1:A:72:PHE:CE2	1:A:96:VAL:HG23	1.89	1.06
1:F:5:LYS:NZ	1:F:69:PHE:CZ	2.23	1.06
1:F:104:GLY:HA2	1:F:525:GLU:HB3	1.27	1.06
1:H:204:MET:HG2	1:H:535:TRP:CH2	1.89	1.06
1:K:5:LYS:NZ	1:K:69:PHE:CG	2.24	1.06
1:G:5:LYS:NZ	1:G:69:PHE:CZ	2.23	1.06
1:C:5:LYS:NZ	1:C:69:PHE:CD1	2.24	1.06
1:I:5:LYS:NZ	1:I:69:PHE:CZ	2.23	1.06
1:F:5:LYS:NZ	1:F:69:PHE:CD1	2.24	1.06
1:M:64:TYR:OH	1:M:94:VAL:HG12	1.54	1.06
1:K:5:LYS:NZ	1:K:69:PHE:CE1	2.24	1.06
1:M:5:LYS:NZ	1:M:69:PHE:CE2	2.24	1.06
1:C:5:LYS:NZ	1:C:69:PHE:CZ	2.23	1.06
1:A:5:LYS:NZ	1:A:69:PHE:CZ	2.23	1.06
1:A:5:LYS:NZ	1:A:69:PHE:CE2	2.23	1.06
1:G:5:LYS:NZ	1:G:69:PHE:CE1	2.24	1.06
1:H:5:LYS:NZ	1:H:69:PHE:CG	2.24	1.06
1:H:5:LYS:NZ	1:H:69:PHE:CE1	2.24	1.06
1:A:5:LYS:NZ	1:A:69:PHE:CG	2.23	1.06
1:I:5:LYS:NZ	1:I:69:PHE:CE1	2.24	1.06
1:H:5:LYS:NZ	1:H:69:PHE:CE2	2.24	1.06
1:E:5:LYS:NZ	1:E:69:PHE:CG	2.23	1.06
1:J:5:LYS:NZ	1:J:69:PHE:CE2	2.23	1.06
1:F:5:LYS:NZ	1:F:69:PHE:CE1	2.23	1.06
1:K:5:LYS:NZ	1:K:69:PHE:CD1	2.24	1.05
1:K:5:LYS:NZ	1:K:69:PHE:CE2	2.24	1.05
1:C:5:LYS:NZ	1:C:69:PHE:CD2	2.24	1.05
1:C:5:LYS:NZ	1:C:69:PHE:CE2	2.23	1.05
1:I:5:LYS:NZ	1:I:69:PHE:CD2	2.24	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:5:LYS:NZ	1:I:69:PHE:CE2	2.24	1.05
1:I:5:LYS:NZ	1:I:69:PHE:CG	2.24	1.05
1:F:5:LYS:NZ	1:F:69:PHE:CD2	2.24	1.05
1:D:104:GLY:HA3	1:D:525:GLU:HB3	1.09	1.05
1:M:104:GLY:HA3	1:M:525:GLU:HB3	1.10	1.05
1:K:5:LYS:NZ	1:K:69:PHE:CZ	2.24	1.05
1:G:5:LYS:NZ	1:G:69:PHE:CG	2.24	1.05
1:L:5:LYS:NZ	1:L:69:PHE:CE2	2.24	1.05
1:M:5:LYS:NZ	1:M:69:PHE:CZ	2.23	1.05
1:J:5:LYS:NZ	1:J:69:PHE:CD2	2.24	1.05
1:I:5:LYS:NZ	1:I:69:PHE:CD1	2.24	1.05
1:K:5:LYS:NZ	1:K:69:PHE:CD2	2.25	1.05
1:G:5:LYS:NZ	1:G:69:PHE:CD1	2.24	1.05
1:H:5:LYS:NZ	1:H:69:PHE:CD2	2.24	1.05
1:L:5:LYS:NZ	1:L:69:PHE:CD1	2.24	1.05
1:L:5:LYS:NZ	1:L:69:PHE:CE1	2.24	1.05
1:L:5:LYS:NZ	1:L:69:PHE:CZ	2.24	1.05
1:E:5:LYS:NZ	1:E:69:PHE:CD2	2.24	1.05
1:A:5:LYS:NZ	1:A:69:PHE:CE1	2.23	1.05
1:A:5:LYS:NZ	1:A:69:PHE:CD1	2.24	1.05
1:A:76:CYS:HA	1:A:88:PHE:CZ	1.91	1.05
1:G:5:LYS:NZ	1:G:69:PHE:CE2	2.24	1.05
1:M:5:LYS:NZ	1:M:69:PHE:CD1	2.25	1.05
1:A:5:LYS:NZ	1:A:69:PHE:CD2	2.24	1.05
1:F:5:LYS:NZ	1:F:69:PHE:CE2	2.23	1.05
1:L:5:LYS:NZ	1:L:69:PHE:CG	2.23	1.05
1:J:5:LYS:NZ	1:J:69:PHE:CE1	2.23	1.05
1:G:5:LYS:NZ	1:G:69:PHE:CD2	2.24	1.04
1:M:5:LYS:NZ	1:M:69:PHE:CG	2.25	1.04
1:A:79:ALA:CB	1:A:88:PHE:CE1	2.39	1.04
1:L:104:GLY:HA3	1:L:525:GLU:CB	1.83	1.04
1:H:5:LYS:NZ	1:H:69:PHE:CD1	2.24	1.04
1:M:5:LYS:NZ	1:M:69:PHE:CE1	2.25	1.04
1:M:9:LEU:CD1	1:M:73:ILE:HD11	1.85	1.04
1:F:5:LYS:NZ	1:F:69:PHE:CG	2.23	1.04
1:D:104:GLY:HA3	1:D:525:GLU:CB	1.86	1.04
1:L:63:LEU:CD2	1:L:91:ALA:CB	2.35	1.04
1:A:72:PHE:CE2	1:A:96:VAL:CG2	2.40	1.04
1:D:9:LEU:HD11	1:D:72:PHE:CE2	1.92	1.04
1:L:5:LYS:NZ	1:L:69:PHE:CD2	2.25	1.03
1:M:9:LEU:HD11	1:M:73:ILE:HD11	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:5:LYS:NZ	1:M:69:PHE:CD2	2.25	1.03
1:A:66:ALA:HB1	1:A:99:ARG:HH21	1.20	1.03
1:H:104:GLY:HA3	1:H:525:GLU:CB	1.87	1.02
1:K:24:LEU:HD13	1:K:81:GLN:NE2	1.74	1.02
1:G:64:TYR:OH	1:G:94:VAL:HG12	1.57	1.02
1:A:104:GLY:HA2	1:A:525:GLU:HB3	1.04	1.02
1:M:104:GLY:HA2	1:M:525:GLU:CB	1.90	1.01
1:I:10:MET:HE1	1:I:517:LEU:O	1.60	1.01
1:D:9:LEU:HD11	1:D:72:PHE:HE2	1.24	1.00
1:F:104:GLY:CA	1:F:525:GLU:CB	2.37	1.00
1:D:9:LEU:CD1	1:D:72:PHE:HE2	1.74	1.00
1:L:104:GLY:HA3	1:L:525:GLU:HB3	1.06	1.00
1:M:104:GLY:HA3	1:M:525:GLU:CB	1.86	1.00
1:J:290:ILE:HD12	1:J:300:ILE:HD12	1.43	1.00
1:G:104:GLY:HA3	1:G:525:GLU:CB	1.87	1.00
1:G:63:LEU:HD22	1:G:91:ALA:HB1	1.41	1.00
1:M:79:ALA:HB3	1:M:88:PHE:CE1	1.96	0.99
1:H:104:GLY:HA2	1:H:525:GLU:CB	1.92	0.99
1:J:175:ILE:HG21	1:J:528:THR:CG2	1.92	0.99
1:F:172:HIS:CD2	1:F:532:SER:HB3	1.98	0.98
1:E:175:ILE:HG21	1:E:528:THR:CG2	1.92	0.98
1:E:97:LEU:CD1	1:E:528:THR:HB	1.95	0.97
1:K:97:LEU:CD1	1:K:528:THR:HB	1.95	0.96
1:C:278:ASN:HB3	1:F:315:GLU:HG3	1.48	0.96
1:L:104:GLY:HA2	1:L:525:GLU:CB	1.90	0.96
1:K:175:ILE:HG21	1:K:528:THR:CG2	1.93	0.96
1:J:97:LEU:CD1	1:J:528:THR:HB	1.95	0.95
1:H:103:LYS:HG2	1:H:525:GLU:O	1.64	0.95
1:K:97:LEU:HD11	1:K:528:THR:CB	1.96	0.95
1:D:104:GLY:HA2	1:D:525:GLU:CB	1.91	0.95
1:E:97:LEU:HD11	1:E:528:THR:CB	1.96	0.95
1:A:24:LEU:HD11	1:A:27:ASP:HA	1.47	0.95
1:I:272:ARG:HD3	1:I:316:TYR:CD1	2.02	0.94
1:C:448:SER:HA	1:I:286:ASP:HB3	1.49	0.94
1:K:59:LEU:CD1	1:K:87:MET:HE3	1.97	0.94
1:J:97:LEU:HD11	1:J:528:THR:CB	1.97	0.94
1:H:467:LEU:HD11	1:J:151:LEU:HA	1.45	0.94
1:J:63:LEU:HA	1:J:75:LEU:HD21	1.49	0.94
1:G:104:GLY:HA2	1:G:525:GLU:CB	1.93	0.94
1:L:8:ARG:CZ	1:L:73:ILE:HG21	1.99	0.94
1:D:103:LYS:HG2	1:D:525:GLU:O	1.66	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:8:ARG:CZ	1:K:73:ILE:HG21	1.99	0.93
1:M:9:LEU:CD1	1:M:73:ILE:CD1	2.46	0.93
1:H:274:LEU:HB2	1:K:268:ARG:HH12	1.31	0.93
1:J:238:THR:HG21	1:K:243:GLY:O	1.69	0.93
1:G:103:LYS:HG2	1:G:525:GLU:O	1.68	0.92
1:L:19:LEU:HB3	1:L:80:ARG:CD	1.98	0.92
1:H:467:LEU:HD12	1:J:150:ILE:C	1.90	0.92
1:A:72:PHE:HE2	1:A:96:VAL:CG2	1.81	0.92
1:I:272:ARG:HD3	1:I:316:TYR:CE1	2.04	0.91
1:F:104:GLY:HA3	1:F:525:GLU:CB	1.98	0.91
1:G:32:ARG:NH2	1:G:75:LEU:HD22	1.85	0.91
1:M:103:LYS:HG2	1:M:525:GLU:O	1.69	0.91
1:M:5:LYS:CE	1:M:69:PHE:CE2	2.54	0.91
1:I:10:MET:SD	1:I:517:LEU:CB	2.59	0.91
1:A:79:ALA:CB	1:A:88:PHE:HE1	1.79	0.91
1:M:5:LYS:CE	1:M:69:PHE:CE1	2.54	0.90
1:H:8:ARG:CZ	1:H:73:ILE:HG21	2.02	0.90
1:M:5:LYS:CE	1:M:69:PHE:CD2	2.55	0.90
1:H:467:LEU:CG	1:J:151:LEU:HD13	2.01	0.90
1:M:5:LYS:CE	1:M:69:PHE:CZ	2.55	0.89
1:A:24:LEU:HD13	1:A:81:GLN:NE2	1.87	0.89
1:D:24:LEU:HB2	1:D:81:GLN:HB3	1.54	0.89
1:J:107:VAL:HG21	1:J:528:THR:OG1	1.73	0.89
1:M:5:LYS:CE	1:M:69:PHE:CD1	2.56	0.89
1:K:107:VAL:HG21	1:K:528:THR:OG1	1.73	0.89
1:K:50:ALA:HB2	1:K:323:TRP:CH2	2.07	0.89
1:M:5:LYS:CE	1:M:69:PHE:CG	2.55	0.89
1:D:8:ARG:CZ	1:D:73:ILE:HG21	2.02	0.89
1:K:5:LYS:CE	1:K:69:PHE:CD2	2.56	0.88
1:H:5:LYS:CE	1:H:69:PHE:CD2	2.57	0.88
1:K:24:LEU:HD13	1:K:81:GLN:HE21	1.37	0.88
1:K:5:LYS:CE	1:K:69:PHE:CD1	2.56	0.88
1:F:5:LYS:CE	1:F:69:PHE:CD1	2.57	0.88
1:C:5:LYS:CE	1:C:69:PHE:CD1	2.57	0.88
1:I:5:LYS:CE	1:I:69:PHE:CD1	2.57	0.88
1:G:5:LYS:CE	1:G:69:PHE:CD1	2.57	0.88
1:G:24:LEU:HD13	1:G:81:GLN:HE22	1.39	0.88
1:G:5:LYS:CE	1:G:69:PHE:CD2	2.57	0.88
1:L:5:LYS:CE	1:L:69:PHE:CG	2.57	0.88
1:E:5:LYS:CE	1:E:69:PHE:CD2	2.57	0.88
1:C:5:LYS:CE	1:C:69:PHE:CD2	2.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:LYS:CE	1:J:69:PHE:CD2	2.56	0.88
1:A:76:CYS:HA	1:A:88:PHE:HZ	1.33	0.88
1:L:63:LEU:HD22	1:L:91:ALA:HB1	1.52	0.88
1:J:290:ILE:HD12	1:J:300:ILE:CD1	2.03	0.88
1:K:5:LYS:CE	1:K:69:PHE:CG	2.56	0.87
1:H:5:LYS:CE	1:H:69:PHE:CG	2.57	0.87
1:L:5:LYS:CE	1:L:69:PHE:CD1	2.57	0.87
1:M:9:LEU:HD11	1:M:73:ILE:CD1	2.03	0.87
1:I:5:LYS:CE	1:I:69:PHE:CD2	2.56	0.87
1:L:5:LYS:CE	1:L:69:PHE:CD2	2.57	0.87
1:J:5:LYS:CE	1:J:69:PHE:CD1	2.57	0.87
1:G:63:LEU:CD2	1:G:91:ALA:CB	2.52	0.87
1:H:5:LYS:CE	1:H:69:PHE:CE2	2.57	0.87
1:C:5:LYS:CE	1:C:69:PHE:CG	2.58	0.87
1:A:5:LYS:CE	1:A:69:PHE:CG	2.58	0.87
1:H:5:LYS:CE	1:H:69:PHE:CD1	2.57	0.87
1:E:5:LYS:CE	1:E:69:PHE:CG	2.58	0.87
1:J:5:LYS:CE	1:J:69:PHE:CG	2.58	0.87
1:E:5:LYS:CE	1:E:69:PHE:CE2	2.58	0.87
1:M:5:LYS:HE2	1:M:69:PHE:CD2	2.10	0.87
1:F:5:LYS:CE	1:F:69:PHE:CD2	2.56	0.87
1:F:5:LYS:CE	1:F:69:PHE:CE1	2.58	0.87
1:C:5:LYS:CE	1:C:69:PHE:CE1	2.58	0.87
1:C:5:LYS:CE	1:C:69:PHE:CE2	2.58	0.87
1:A:5:LYS:CE	1:A:69:PHE:CE2	2.58	0.87
1:A:5:LYS:CE	1:A:69:PHE:CD1	2.57	0.87
1:F:104:GLY:HA2	1:F:525:GLU:CB	2.00	0.87
1:A:5:LYS:CE	1:A:69:PHE:CE1	2.58	0.87
1:F:5:LYS:CE	1:F:69:PHE:CE2	2.57	0.87
1:I:272:ARG:HB3	1:I:316:TYR:CE2	2.10	0.87
1:L:5:LYS:CE	1:L:69:PHE:CE2	2.57	0.87
1:A:5:LYS:CE	1:A:69:PHE:CD2	2.57	0.87
1:I:5:LYS:CE	1:I:69:PHE:CE2	2.57	0.87
1:H:467:LEU:HD12	1:J:151:LEU:N	1.90	0.87
1:E:5:LYS:CE	1:E:69:PHE:CD1	2.57	0.87
1:E:5:LYS:CE	1:E:69:PHE:CE1	2.58	0.87
1:J:5:LYS:CE	1:J:69:PHE:CE2	2.58	0.87
1:K:59:LEU:CD1	1:K:87:MET:CE	2.51	0.87
1:G:5:LYS:CE	1:G:69:PHE:CE2	2.57	0.86
1:L:5:LYS:CE	1:L:69:PHE:CE1	2.59	0.86
1:I:10:MET:SD	1:I:517:LEU:HB3	2.14	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:LEU:HB3	1:H:80:ARG:HD3	1.56	0.86
1:K:5:LYS:CE	1:K:69:PHE:CE2	2.58	0.86
1:H:5:LYS:CE	1:H:69:PHE:CE1	2.58	0.86
1:E:107:VAL:HG21	1:E:528:THR:OG1	1.75	0.86
1:C:151:LEU:HA	1:G:467:LEU:HD13	1.54	0.86
1:L:19:LEU:HB3	1:L:80:ARG:HD2	1.56	0.86
1:K:5:LYS:CE	1:K:69:PHE:CZ	2.59	0.86
1:J:5:LYS:CE	1:J:69:PHE:CE1	2.58	0.86
1:I:5:LYS:CE	1:I:69:PHE:CG	2.58	0.86
1:G:5:LYS:CE	1:G:69:PHE:CE1	2.58	0.86
1:G:5:LYS:CE	1:G:69:PHE:CG	2.58	0.86
1:H:8:ARG:NH2	1:H:73:ILE:HG13	1.90	0.86
1:F:5:LYS:CE	1:F:69:PHE:CG	2.58	0.86
1:K:5:LYS:CE	1:K:69:PHE:CE1	2.58	0.86
1:G:32:ARG:HH21	1:G:75:LEU:HD13	1.41	0.86
1:L:172:HIS:CD2	1:L:532:SER:HB3	2.09	0.86
1:A:24:LEU:HD23	1:A:82:ILE:HG22	1.56	0.86
1:H:243:GLY:N	1:I:125:ASN:ND2	2.24	0.86
1:I:5:LYS:CE	1:I:69:PHE:CE1	2.58	0.86
1:A:66:ALA:CB	1:A:99:ARG:NH2	2.38	0.86
1:A:5:LYS:CE	1:A:69:PHE:CZ	2.59	0.85
1:D:9:LEU:CG	1:D:72:PHE:HE2	1.88	0.85
1:C:5:LYS:CE	1:C:69:PHE:CZ	2.59	0.85
1:G:5:LYS:CE	1:G:69:PHE:CZ	2.59	0.85
1:F:5:LYS:CE	1:F:69:PHE:CZ	2.59	0.85
1:E:5:LYS:CE	1:E:69:PHE:CZ	2.59	0.85
1:I:5:LYS:CE	1:I:69:PHE:CZ	2.59	0.85
1:L:5:LYS:CE	1:L:69:PHE:CZ	2.59	0.85
1:L:64:TYR:OH	1:L:94:VAL:HG12	1.75	0.85
1:F:5:LYS:HE2	1:F:69:PHE:CD2	2.12	0.85
1:C:14:LYS:HE2	1:C:514:PHE:CZ	2.11	0.85
1:H:5:LYS:CE	1:H:69:PHE:CZ	2.59	0.85
1:J:5:LYS:HE2	1:J:69:PHE:CD2	2.12	0.85
1:F:103:LYS:HG2	1:F:525:GLU:O	1.77	0.85
1:J:5:LYS:CE	1:J:69:PHE:CZ	2.59	0.84
1:E:5:LYS:HE2	1:E:69:PHE:CD2	2.12	0.84
1:C:5:LYS:HE2	1:C:69:PHE:CD2	2.12	0.84
1:A:204:MET:HG2	1:A:535:TRP:CZ3	2.12	0.84
1:H:467:LEU:HG	1:J:149:ASN:OD1	1.77	0.84
1:A:5:LYS:HE2	1:A:69:PHE:CD2	2.12	0.83
1:H:467:LEU:HD11	1:J:151:LEU:HD13	0.87	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:63:LEU:CD2	1:M:91:ALA:HB1	2.07	0.83
1:H:275:ASP:OD1	1:K:316:TYR:HE1	1.61	0.83
1:E:204:MET:HG2	1:E:535:TRP:CZ3	2.13	0.83
1:M:204:MET:HG2	1:M:535:TRP:CZ3	2.12	0.83
1:K:57:THR:HA	1:K:60:TYR:HD2	1.43	0.83
1:J:204:MET:HG2	1:J:535:TRP:CZ3	2.13	0.82
1:K:204:MET:HG2	1:K:535:TRP:CZ3	2.13	0.82
1:I:268:ARG:HH12	1:J:274:LEU:HB2	1.42	0.82
1:L:5:LYS:HE3	1:L:69:PHE:CG	2.15	0.82
1:A:72:PHE:CZ	1:A:96:VAL:CB	2.62	0.82
1:C:151:LEU:HA	1:G:467:LEU:HD11	1.61	0.81
1:H:467:LEU:HD11	1:J:151:LEU:CA	2.04	0.81
1:A:66:ALA:HB3	1:A:99:ARG:HH21	1.45	0.81
1:E:97:LEU:CD1	1:E:528:THR:CB	2.57	0.81
1:G:5:LYS:HE2	1:G:69:PHE:CD2	2.15	0.81
1:L:204:MET:HG2	1:L:535:TRP:CZ3	2.15	0.81
1:D:9:LEU:CD2	1:D:72:PHE:CZ	2.63	0.81
1:D:204:MET:HG2	1:D:535:TRP:CZ3	2.14	0.81
1:H:204:MET:HG2	1:H:535:TRP:CZ3	2.14	0.81
1:G:204:MET:HG2	1:G:535:TRP:CZ3	2.15	0.81
1:A:24:LEU:CD1	1:A:27:ASP:HA	2.09	0.81
1:I:10:MET:SD	1:I:517:LEU:HB2	2.20	0.81
1:L:8:ARG:HH21	1:L:73:ILE:HG13	1.45	0.81
1:M:5:LYS:HE3	1:M:69:PHE:CD1	2.14	0.81
1:J:268:ARG:HH22	1:L:274:LEU:HD12	1.46	0.81
1:D:78:GLN:O	1:D:81:GLN:HB2	1.81	0.81
1:I:5:LYS:HE2	1:I:69:PHE:CD2	2.16	0.80
1:J:132:SER:CB	1:K:419:ASN:HD22	1.95	0.80
1:J:132:SER:CB	1:K:419:ASN:ND2	2.43	0.80
1:F:5:LYS:HE3	1:F:69:PHE:CD1	2.17	0.80
1:A:5:LYS:HE3	1:A:69:PHE:CD1	2.17	0.80
1:M:22:GLU:HB2	1:M:81:GLN:HB3	1.61	0.80
1:F:529:GLU:HG3	1:F:574:CYS:SG	2.21	0.80
1:K:97:LEU:CD1	1:K:528:THR:CB	2.57	0.80
1:G:50:ALA:HB2	1:G:323:TRP:CH2	2.17	0.80
1:L:8:ARG:NH2	1:L:73:ILE:HG13	1.97	0.80
1:K:5:LYS:HE2	1:K:69:PHE:CD2	2.16	0.79
1:J:5:LYS:HE3	1:J:69:PHE:CD1	2.17	0.79
1:C:151:LEU:CA	1:G:467:LEU:CD1	2.58	0.79
1:D:9:LEU:HD21	1:D:72:PHE:CE2	2.17	0.79
1:E:5:LYS:HE3	1:E:69:PHE:CD1	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:272:ARG:HH11	1:I:316:TYR:HA	1.47	0.79
1:H:8:ARG:HH21	1:H:73:ILE:HG13	1.44	0.79
1:L:508:ILE:HD11	1:L:531:CYS:HA	1.63	0.79
1:D:9:LEU:CG	1:D:72:PHE:CE2	2.65	0.79
1:H:5:LYS:HE2	1:H:69:PHE:CD2	2.17	0.79
1:D:8:ARG:NE	1:D:73:ILE:HG13	1.97	0.79
1:M:63:LEU:HD22	1:M:91:ALA:HB1	1.65	0.79
1:M:5:LYS:HZ2	1:M:72:PHE:HD2	1.28	0.79
1:A:66:ALA:HB3	1:A:99:ARG:NH2	1.97	0.78
1:C:151:LEU:HD13	1:G:467:LEU:HD11	0.82	0.78
1:A:129:LYS:HZ1	1:C:243:GLY:HA3	1.47	0.78
1:L:5:LYS:HE2	1:L:69:PHE:CE2	2.19	0.78
1:G:63:LEU:HD23	1:G:91:ALA:HB1	1.66	0.78
1:M:8:ARG:NE	1:M:73:ILE:HG21	1.98	0.78
1:C:5:LYS:HE3	1:C:69:PHE:CD1	2.17	0.78
1:I:273:ILE:HG12	1:I:317:TYR:HD1	1.48	0.78
1:K:10:MET:HG2	1:K:108:PRO:HG3	1.65	0.78
1:L:19:LEU:HD22	1:L:80:ARG:HH11	1.47	0.78
1:L:104:GLY:HA2	1:L:525:GLU:CA	2.14	0.77
1:M:9:LEU:HD12	1:M:73:ILE:HD11	1.66	0.77
1:M:9:LEU:HD12	1:M:73:ILE:CD1	2.14	0.77
1:G:50:ALA:HB2	1:G:323:TRP:HH2	1.49	0.77
1:A:129:LYS:NZ	1:C:243:GLY:HA3	1.99	0.77
1:H:467:LEU:CD1	1:J:151:LEU:N	2.46	0.77
1:K:32:ARG:HH21	1:K:75:LEU:HD13	1.50	0.77
1:K:274:LEU:HD12	1:M:268:ARG:HH22	1.50	0.77
1:A:268:ARG:HH12	1:G:274:LEU:HB2	1.49	0.77
1:G:5:LYS:HE3	1:G:69:PHE:CD1	2.20	0.76
1:H:242:SER:C	1:I:125:ASN:HD21	1.88	0.76
1:G:194:GLY:HA3	1:G:302:GLY:HA3	1.67	0.76
1:L:63:LEU:HD21	1:L:91:ALA:HB1	1.65	0.76
1:G:24:LEU:HB2	1:G:81:GLN:NE2	2.00	0.76
1:D:12:LEU:HD13	1:D:76:CYS:SG	2.25	0.76
1:F:17:THR:HG23	1:F:85:GLU:HG3	1.67	0.76
1:J:97:LEU:CD1	1:J:528:THR:CB	2.58	0.76
1:J:290:ILE:HD11	1:J:300:ILE:HD12	1.68	0.76
1:J:132:SER:HB2	1:K:419:ASN:HD22	1.47	0.76
1:J:32:ARG:HB3	1:J:62:ALA:HB1	1.66	0.76
1:A:24:LEU:HD13	1:A:81:GLN:HE21	1.51	0.75
1:A:72:PHE:HE2	1:A:96:VAL:HG21	1.49	0.75
1:G:304:ILE:HD11	1:G:312:LYS:HB2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:VAL:HG22	1:E:105:ILE:HG21	1.69	0.75
1:M:104:GLY:HA2	1:M:525:GLU:CA	2.16	0.74
1:A:20:THR:OG1	1:A:85:GLU:HB3	1.87	0.74
1:A:204:MET:HG2	1:A:535:TRP:HH2	1.50	0.74
1:D:104:GLY:HA2	1:D:525:GLU:CA	2.17	0.74
1:K:2:VAL:O	1:K:5:LYS:HB3	1.88	0.74
1:M:69:PHE:CE1	1:M:72:PHE:CD2	2.76	0.74
1:A:76:CYS:O	1:A:88:PHE:HE2	1.70	0.74
1:C:315:GLU:HG3	1:D:278:ASN:HB3	1.70	0.74
1:G:204:MET:HG2	1:G:535:TRP:HH2	1.51	0.74
1:E:204:MET:HG2	1:E:535:TRP:HH2	1.50	0.73
1:M:79:ALA:CB	1:M:88:PHE:CE1	2.70	0.73
1:K:5:LYS:HE3	1:K:69:PHE:CD1	2.22	0.73
1:A:80:ARG:HB2	1:A:88:PHE:CE2	2.23	0.73
1:A:76:CYS:O	1:A:88:PHE:CE2	2.41	0.73
1:I:272:ARG:CB	1:I:316:TYR:CZ	2.70	0.73
1:A:129:LYS:NZ	1:C:243:GLY:CA	2.52	0.73
1:E:512:ARG:HB2	1:E:531:CYS:SG	2.28	0.73
1:G:104:GLY:HA2	1:G:525:GLU:CA	2.17	0.73
1:G:24:LEU:CD1	1:G:81:GLN:NE2	2.48	0.73
1:A:249:ARG:HE	1:A:331:ILE:HG21	1.53	0.73
1:D:315:GLU:HG3	1:F:278:ASN:HB3	1.69	0.73
1:H:104:GLY:HA2	1:H:525:GLU:CA	2.18	0.73
1:D:30:ASP:OD1	1:D:78:GLN:NE2	2.21	0.73
1:I:9:LEU:HD22	1:I:105:ILE:HD11	1.71	0.73
1:I:5:LYS:HE3	1:I:69:PHE:CD1	2.23	0.72
1:L:63:LEU:HD21	1:L:91:ALA:CB	2.19	0.72
1:J:204:MET:HG2	1:J:535:TRP:HH2	1.50	0.72
1:L:103:LYS:HG2	1:L:525:GLU:O	1.88	0.72
1:K:5:LYS:HE3	1:K:69:PHE:CG	2.23	0.72
1:A:128:ASN:ND2	1:A:414:LEU:HD12	2.04	0.72
1:C:448:SER:HA	1:I:286:ASP:CB	2.18	0.71
1:H:5:LYS:HE3	1:H:69:PHE:CD1	2.23	0.71
1:I:249:ARG:HE	1:I:331:ILE:HG21	1.56	0.71
1:K:8:ARG:CD	1:K:73:ILE:HG21	2.19	0.71
1:H:5:LYS:HE3	1:H:69:PHE:CG	2.24	0.71
1:M:204:MET:HG2	1:M:535:TRP:HH2	1.51	0.71
1:F:24:LEU:HD11	1:F:29:ARG:HG3	1.72	0.71
1:K:249:ARG:HE	1:K:331:ILE:HG21	1.56	0.71
1:A:24:LEU:HD22	1:A:81:GLN:HE21	1.56	0.71
1:D:204:MET:HG2	1:D:535:TRP:HH2	1.51	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:467:LEU:CD1	1:J:150:ILE:C	2.59	0.71
1:J:194:GLY:HA3	1:J:302:GLY:HA3	1.73	0.71
1:H:204:MET:HG2	1:H:535:TRP:HH2	1.52	0.70
1:G:249:ARG:HE	1:G:331:ILE:HG21	1.56	0.70
1:A:129:LYS:HZ2	1:C:243:GLY:CA	2.04	0.70
1:E:249:ARG:HE	1:E:331:ILE:HG21	1.56	0.70
1:F:249:ARG:HE	1:F:331:ILE:HG21	1.55	0.70
1:C:249:ARG:HE	1:C:331:ILE:HG21	1.55	0.70
1:I:5:LYS:HE3	1:I:69:PHE:CG	2.26	0.70
1:H:467:LEU:CD1	1:J:150:ILE:O	2.39	0.70
1:M:33:LEU:HA	1:M:58:GLU:OE2	1.90	0.70
1:M:249:ARG:HE	1:M:331:ILE:HG21	1.57	0.70
1:C:63:LEU:CD2	1:C:91:ALA:HB1	2.22	0.70
1:F:511:VAL:HA	1:F:531:CYS:HB2	1.72	0.70
1:E:63:LEU:CD2	1:E:91:ALA:HB1	2.22	0.70
1:J:304:ILE:HG12	1:J:313:ASN:H	1.57	0.70
1:D:249:ARG:HE	1:D:331:ILE:HG21	1.56	0.70
1:M:5:LYS:HE3	1:M:69:PHE:CG	2.27	0.70
1:J:375:PHE:HB2	1:J:600:ARG:HD3	1.74	0.70
1:D:63:LEU:CD2	1:D:91:ALA:HB1	2.22	0.70
1:H:375:PHE:HB2	1:H:600:ARG:HD3	1.74	0.70
1:L:64:TYR:OH	1:L:94:VAL:CG1	2.40	0.70
1:G:307:SER:H	1:G:319:SER:HB3	1.56	0.70
1:E:21:ARG:HD3	1:E:41:ARG:CD	2.22	0.70
1:I:63:LEU:CD2	1:I:91:ALA:HB1	2.22	0.70
1:K:8:ARG:CZ	1:K:73:ILE:CG2	2.69	0.69
1:J:26:LEU:HB3	1:J:28:GLN:HG3	1.74	0.69
1:C:21:ARG:HD3	1:C:41:ARG:CD	2.22	0.69
1:L:249:ARG:HE	1:L:331:ILE:HG21	1.57	0.69
1:J:307:SER:H	1:J:319:SER:HB3	1.56	0.69
1:A:274:LEU:HD12	1:E:268:ARG:HH22	1.56	0.69
1:H:21:ARG:HD3	1:H:41:ARG:CD	2.22	0.69
1:D:19:LEU:HD22	1:D:80:ARG:HD3	1.74	0.69
1:A:24:LEU:CD1	1:A:81:GLN:NE2	2.55	0.69
1:A:24:LEU:HD23	1:A:82:ILE:CG2	2.21	0.69
1:G:194:GLY:CA	1:G:302:GLY:HA3	2.21	0.69
1:M:21:ARG:HD3	1:M:41:ARG:CD	2.22	0.69
1:H:169:HIS:HE1	1:H:581:CYS:SG	2.16	0.69
1:L:344:VAL:HB	1:L:350:THR:HB	1.75	0.69
1:A:175:ILE:HG21	1:A:528:THR:HG21	1.75	0.69
1:I:169:HIS:HE1	1:I:581:CYS:SG	2.16	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:VAL:HB	1:A:350:THR:HB	1.75	0.69
1:I:10:MET:CE	1:I:517:LEU:O	2.39	0.69
1:G:375:PHE:HB2	1:G:600:ARG:HD3	1.74	0.69
1:K:375:PHE:HB2	1:K:600:ARG:HD3	1.74	0.69
1:E:169:HIS:HE1	1:E:581:CYS:SG	2.16	0.69
1:A:375:PHE:HB2	1:A:600:ARG:HD3	1.74	0.69
1:G:32:ARG:NH2	1:G:75:LEU:HD13	2.07	0.69
1:H:96:VAL:HG22	1:H:105:ILE:HG21	1.75	0.69
1:K:344:VAL:HB	1:K:350:THR:HB	1.75	0.69
1:I:21:ARG:HD3	1:I:41:ARG:CD	2.22	0.69
1:H:344:VAL:HB	1:H:350:THR:HB	1.75	0.69
1:K:204:MET:HG2	1:K:535:TRP:HH2	1.50	0.69
1:F:63:LEU:CD2	1:F:91:ALA:HB1	2.22	0.69
1:J:21:ARG:HD3	1:J:41:ARG:CD	2.22	0.69
1:J:122:GLU:HG2	1:K:242:SER:OG	1.92	0.69
1:M:96:VAL:HG22	1:M:105:ILE:HG21	1.75	0.68
1:F:169:HIS:HE1	1:F:581:CYS:SG	2.16	0.68
1:I:96:VAL:HG22	1:I:105:ILE:HG21	1.76	0.68
1:G:169:HIS:HE1	1:G:581:CYS:SG	2.16	0.68
1:G:344:VAL:HB	1:G:350:THR:HB	1.75	0.68
1:I:375:PHE:HB2	1:I:600:ARG:HD3	1.74	0.68
1:A:129:LYS:HZ2	1:C:243:GLY:HA2	1.56	0.68
1:H:63:LEU:CD2	1:H:91:ALA:HB1	2.22	0.68
1:D:169:HIS:HE1	1:D:581:CYS:SG	2.16	0.68
1:C:375:PHE:HB2	1:C:600:ARG:HD3	1.74	0.68
1:C:169:HIS:HE1	1:C:581:CYS:SG	2.16	0.68
1:E:375:PHE:HB2	1:E:600:ARG:HD3	1.74	0.68
1:M:375:PHE:HB2	1:M:600:ARG:HD3	1.74	0.68
1:J:169:HIS:HE1	1:J:581:CYS:SG	2.16	0.68
1:G:96:VAL:HG22	1:G:105:ILE:HG21	1.75	0.68
1:D:96:VAL:HG22	1:D:105:ILE:HG21	1.75	0.68
1:J:308:SER:O	1:J:311:SER:HB2	1.93	0.68
1:K:169:HIS:HE1	1:K:581:CYS:SG	2.16	0.68
1:A:24:LEU:HD12	1:A:26:LEU:O	1.94	0.68
1:H:249:ARG:HE	1:H:331:ILE:HG21	1.57	0.68
1:E:344:VAL:HB	1:E:350:THR:HB	1.75	0.68
1:K:512:ARG:HB2	1:K:531:CYS:SG	2.34	0.68
1:D:300:ILE:HG22	1:D:312:LYS:HE2	1.76	0.68
1:F:375:PHE:HB2	1:F:600:ARG:HD3	1.74	0.68
1:L:169:HIS:HE1	1:L:581:CYS:SG	2.16	0.68
1:D:344:VAL:HB	1:D:350:THR:HB	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD11	1:A:87:MET:HE3	1.74	0.68
1:J:512:ARG:HB2	1:J:531:CYS:SG	2.34	0.68
1:A:24:LEU:HA	1:A:81:GLN:NE2	2.08	0.68
1:L:103:LYS:CG	1:L:525:GLU:O	2.42	0.68
1:H:467:LEU:HD13	1:J:150:ILE:O	1.94	0.68
1:F:344:VAL:HB	1:F:350:THR:HB	1.75	0.68
1:M:169:HIS:HE1	1:M:581:CYS:SG	2.16	0.68
1:L:63:LEU:HD23	1:L:91:ALA:CB	2.12	0.67
1:M:79:ALA:HB3	1:M:88:PHE:CZ	2.29	0.67
1:F:125:ASN:ND2	1:G:242:SER:O	2.28	0.67
1:L:375:PHE:HB2	1:L:600:ARG:HD3	1.74	0.67
1:C:344:VAL:HB	1:C:350:THR:HB	1.75	0.67
1:A:169:HIS:HE1	1:A:581:CYS:SG	2.16	0.67
1:K:5:LYS:HA	1:K:69:PHE:CE2	2.29	0.67
1:A:80:ARG:HB2	1:A:88:PHE:CD2	2.29	0.67
1:D:375:PHE:HB2	1:D:600:ARG:HD3	1.74	0.67
1:L:162:GLU:HG2	1:L:353:ARG:HB3	1.77	0.67
1:J:249:ARG:HE	1:J:331:ILE:HG21	1.58	0.67
1:J:162:GLU:HG2	1:J:353:ARG:HB3	1.76	0.67
1:M:405:THR:HA	1:M:435:HIS:HA	1.77	0.67
1:M:442:ILE:HG23	1:M:497:ILE:HB	1.75	0.67
1:J:5:LYS:HE3	1:J:69:PHE:CG	2.29	0.67
1:G:24:LEU:CD1	1:G:81:GLN:HE22	2.07	0.67
1:F:97:LEU:CD1	1:F:528:THR:OG1	2.43	0.67
1:G:405:THR:HA	1:G:435:HIS:HA	1.76	0.67
1:I:19:LEU:HD13	1:I:80:ARG:HH11	1.60	0.67
1:J:344:VAL:HB	1:J:350:THR:HB	1.75	0.67
1:M:344:VAL:HB	1:M:350:THR:HB	1.75	0.67
1:F:405:THR:HA	1:F:435:HIS:HA	1.76	0.67
1:G:5:LYS:HE3	1:G:69:PHE:CG	2.30	0.67
1:C:151:LEU:HD13	1:G:467:LEU:CG	2.23	0.67
1:I:264:GLN:HE22	1:J:270:ARG:HH12	1.43	0.67
1:M:19:LEU:O	1:M:81:GLN:HA	1.93	0.67
1:F:96:VAL:HG22	1:F:105:ILE:HG21	1.75	0.67
1:I:344:VAL:HB	1:I:350:THR:HB	1.75	0.67
1:J:405:THR:HA	1:J:435:HIS:HA	1.77	0.67
1:I:405:THR:HA	1:I:435:HIS:HA	1.77	0.67
1:A:512:ARG:HB2	1:A:531:CYS:SG	2.35	0.67
1:H:405:THR:HA	1:H:435:HIS:HA	1.77	0.67
1:E:19:LEU:HD13	1:E:80:ARG:HH11	1.60	0.67
1:C:162:GLU:HG2	1:C:353:ARG:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:LYS:HE3	1:F:69:PHE:CG	2.29	0.67
1:H:467:LEU:CG	1:J:149:ASN:OD1	2.43	0.67
1:L:5:LYS:HE2	1:L:69:PHE:CD2	2.30	0.67
1:E:5:LYS:HE3	1:E:69:PHE:CG	2.30	0.67
1:A:5:LYS:HE3	1:A:69:PHE:CG	2.29	0.67
1:L:204:MET:HG2	1:L:535:TRP:HH2	1.52	0.67
1:C:96:VAL:HG22	1:C:105:ILE:HG21	1.75	0.67
1:D:162:GLU:HG2	1:D:353:ARG:HB3	1.77	0.67
1:A:19:LEU:HD13	1:A:80:ARG:HH11	1.59	0.66
1:J:19:LEU:HD13	1:J:80:ARG:HH11	1.60	0.66
1:C:405:THR:HA	1:C:435:HIS:HA	1.77	0.66
1:H:467:LEU:HD11	1:J:151:LEU:CG	2.22	0.66
1:G:162:GLU:HG2	1:G:353:ARG:HB3	1.77	0.66
1:H:162:GLU:HG2	1:H:353:ARG:HB3	1.76	0.66
1:I:162:GLU:HG2	1:I:353:ARG:HB3	1.77	0.66
1:K:8:ARG:NH2	1:K:73:ILE:HB	2.10	0.66
1:A:24:LEU:CD1	1:A:81:GLN:HE21	2.07	0.66
1:F:162:GLU:HG2	1:F:353:ARG:HB3	1.76	0.66
1:G:512:ARG:HB2	1:G:531:CYS:SG	2.35	0.66
1:D:22:GLU:HB2	1:D:80:ARG:O	1.96	0.66
1:C:5:LYS:HE3	1:C:69:PHE:CG	2.29	0.66
1:E:162:GLU:HG2	1:E:353:ARG:HB3	1.77	0.66
1:F:268:ARG:HD2	1:F:272:ARG:HE	1.61	0.66
1:G:24:LEU:HB2	1:G:81:GLN:HE21	1.58	0.66
1:M:162:GLU:HG2	1:M:353:ARG:HB3	1.77	0.66
1:L:405:THR:HA	1:L:435:HIS:HA	1.77	0.66
1:M:69:PHE:O	1:M:72:PHE:HB3	1.94	0.66
1:G:64:TYR:HH	1:G:181:TRP:HZ3	1.44	0.66
1:K:22:GLU:HB2	1:K:81:GLN:HA	1.78	0.65
1:A:162:GLU:HG2	1:A:353:ARG:HB3	1.77	0.65
1:F:169:HIS:CE1	1:F:533:CYS:SG	2.89	0.65
1:H:405:THR:HG23	1:H:624:PHE:HA	1.78	0.65
1:K:162:GLU:HG2	1:K:353:ARG:HB3	1.77	0.65
1:E:405:THR:HA	1:E:435:HIS:HA	1.77	0.65
1:I:405:THR:HG23	1:I:624:PHE:HA	1.78	0.65
1:H:205:CYS:HG	1:H:358:TYR:HD1	1.45	0.65
1:I:278:ASN:HB3	1:L:315:GLU:HG3	1.79	0.65
1:D:8:ARG:CZ	1:D:73:ILE:HG13	2.26	0.65
1:D:405:THR:HA	1:D:435:HIS:HA	1.77	0.65
1:D:9:LEU:CD2	1:D:72:PHE:CE2	2.80	0.65
1:L:405:THR:HG23	1:L:624:PHE:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:ARG:HH21	1:F:75:LEU:HD13	1.61	0.65
1:A:59:LEU:HD21	1:A:87:MET:CE	2.27	0.65
1:C:19:LEU:HD13	1:C:80:ARG:HH11	1.60	0.65
1:E:175:ILE:HG23	1:E:528:THR:CG2	2.14	0.65
1:G:405:THR:HG23	1:G:624:PHE:HA	1.78	0.65
1:L:564:THR:HG22	1:L:565:VAL:O	1.97	0.65
1:A:405:THR:HA	1:A:435:HIS:HA	1.77	0.65
1:M:30:ASP:HB2	1:M:33:LEU:HB2	1.79	0.65
1:E:19:LEU:HD13	1:E:80:ARG:NH1	2.12	0.65
1:G:64:TYR:OH	1:G:94:VAL:CG1	2.39	0.65
1:J:405:THR:HG23	1:J:624:PHE:HA	1.78	0.65
1:K:405:THR:HA	1:K:435:HIS:HA	1.77	0.65
1:D:405:THR:HG23	1:D:624:PHE:HA	1.79	0.64
1:E:270:ARG:NH1	1:G:264:GLN:OE1	2.30	0.64
1:M:273:ILE:HG12	1:M:317:TYR:HD1	1.63	0.64
1:J:245:GLN:HG2	1:K:245:GLN:HG2	1.79	0.64
1:K:57:THR:HA	1:K:60:TYR:CD2	2.30	0.64
1:C:21:ARG:HD3	1:C:41:ARG:HD2	1.80	0.64
1:H:21:ARG:HD3	1:H:41:ARG:HD2	1.80	0.64
1:A:24:LEU:CG	1:A:81:GLN:HE21	2.10	0.64
1:M:405:THR:HG23	1:M:624:PHE:HA	1.78	0.64
1:F:405:THR:HG23	1:F:624:PHE:HA	1.79	0.64
1:K:405:THR:HG23	1:K:624:PHE:HA	1.78	0.64
1:J:19:LEU:HD13	1:J:80:ARG:NH1	2.12	0.64
1:F:32:ARG:NH2	1:F:75:LEU:HD13	2.11	0.64
1:A:19:LEU:HD13	1:A:80:ARG:NH1	2.12	0.64
1:L:19:LEU:HB3	1:L:80:ARG:HD3	1.75	0.64
1:A:405:THR:HG23	1:A:624:PHE:HA	1.78	0.64
1:C:150:ILE:C	1:G:467:LEU:HD12	2.18	0.64
1:H:467:LEU:HD21	1:J:151:LEU:CD1	2.28	0.64
1:D:9:LEU:CD2	1:D:72:PHE:HZ	2.09	0.64
1:H:242:SER:C	1:I:125:ASN:ND2	2.52	0.64
1:I:5:LYS:HE2	1:I:69:PHE:CE2	2.33	0.64
1:F:104:GLY:HA2	1:F:525:GLU:CA	2.28	0.64
1:F:97:LEU:HD11	1:F:528:THR:HB	1.80	0.64
1:I:19:LEU:HD13	1:I:80:ARG:NH1	2.12	0.64
1:E:405:THR:HG23	1:E:624:PHE:HA	1.79	0.64
1:M:512:ARG:HB2	1:M:531:CYS:SG	2.37	0.64
1:C:268:ARG:NE	1:C:272:ARG:HH21	1.96	0.64
1:C:416:HIS:CE1	1:C:514:PHE:CB	2.81	0.63
1:C:405:THR:HG23	1:C:624:PHE:HA	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD13	1:C:80:ARG:NH1	2.12	0.63
1:K:5:LYS:HE2	1:K:69:PHE:CE2	2.33	0.63
1:K:32:ARG:NH2	1:K:75:LEU:HD13	2.12	0.63
1:J:175:ILE:HG23	1:J:528:THR:CG2	2.15	0.63
1:G:59:LEU:HD11	1:G:87:MET:HE1	1.81	0.63
1:A:76:CYS:CA	1:A:88:PHE:HZ	2.10	0.63
1:I:442:ILE:HG23	1:I:497:ILE:HB	1.81	0.63
1:A:270:ARG:O	1:A:274:LEU:HG	1.99	0.63
1:D:107:VAL:HG21	1:D:528:THR:OG1	1.98	0.63
1:J:442:ILE:HG23	1:J:497:ILE:HB	1.81	0.63
1:H:377:PRO:HG3	1:H:601:LYS:HB3	1.81	0.63
1:H:5:LYS:HE2	1:H:69:PHE:CE2	2.32	0.63
1:I:13:PHE:HD2	1:I:113:VAL:HG11	1.63	0.63
1:F:97:LEU:HG	1:F:528:THR:OG1	1.99	0.63
1:M:63:LEU:CD2	1:M:91:ALA:CB	2.77	0.63
1:F:97:LEU:HD23	1:F:527:SER:HB2	1.81	0.63
1:I:21:ARG:HD3	1:I:41:ARG:HD2	1.80	0.63
1:C:270:ARG:HH12	1:F:264:GLN:NE2	1.97	0.63
1:A:104:GLY:CA	1:A:525:GLU:CB	2.59	0.63
1:M:21:ARG:HD3	1:M:41:ARG:HD2	1.80	0.63
1:D:8:ARG:HE	1:D:73:ILE:HG13	1.62	0.63
1:E:21:ARG:HD3	1:E:41:ARG:HD2	1.80	0.63
1:I:377:PRO:HG3	1:I:601:LYS:HB3	1.81	0.63
1:C:377:PRO:HG3	1:C:601:LYS:HB3	1.81	0.63
1:A:377:PRO:HG3	1:A:601:LYS:HB3	1.81	0.62
1:M:107:VAL:HG21	1:M:528:THR:OG1	1.98	0.62
1:K:377:PRO:HG3	1:K:601:LYS:HB3	1.81	0.62
1:A:24:LEU:CD2	1:A:81:GLN:HE21	2.12	0.62
1:K:8:ARG:O	1:K:12:LEU:HG	1.99	0.62
1:H:107:VAL:HG21	1:H:528:THR:OG1	1.99	0.62
1:C:442:ILE:HG23	1:C:497:ILE:HB	1.81	0.62
1:L:329:ALA:HB2	1:L:345:MET:HB3	1.82	0.62
1:C:525:GLU:HA	1:C:572:ALA:HB1	1.79	0.62
1:M:20:THR:HA	1:M:80:ARG:O	1.99	0.62
1:I:273:ILE:HA	1:I:317:TYR:HE1	1.62	0.62
1:A:268:ARG:NE	1:A:272:ARG:HH21	1.98	0.62
1:C:63:LEU:HD23	1:C:91:ALA:HB1	1.81	0.62
1:H:329:ALA:HB2	1:H:345:MET:HB3	1.82	0.62
1:M:377:PRO:HG3	1:M:601:LYS:HB3	1.81	0.62
1:C:416:HIS:HE1	1:C:514:PHE:HB3	1.63	0.62
1:F:329:ALA:HB2	1:F:345:MET:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:ALA:HB2	1:D:345:MET:HB3	1.81	0.62
1:L:377:PRO:HG3	1:L:601:LYS:HB3	1.81	0.62
1:F:442:ILE:HG23	1:F:497:ILE:HB	1.81	0.62
1:E:377:PRO:HG3	1:E:601:LYS:HB3	1.81	0.62
1:I:63:LEU:HD23	1:I:91:ALA:HB1	1.81	0.62
1:H:63:LEU:HD23	1:H:91:ALA:HB1	1.81	0.62
1:D:4:ASP:HA	1:D:7:ALA:HB3	1.82	0.62
1:M:205:CYS:HG	1:M:358:TYR:HD1	1.46	0.62
1:G:377:PRO:HG3	1:G:601:LYS:HB3	1.81	0.62
1:J:205:CYS:HG	1:J:358:TYR:HD1	1.48	0.62
1:G:442:ILE:HG23	1:G:497:ILE:HB	1.81	0.62
1:I:329:ALA:HB2	1:I:345:MET:HB3	1.82	0.61
1:J:110:ILE:HD11	1:J:168:ALA:HA	1.82	0.61
1:F:110:ILE:HD11	1:F:168:ALA:HA	1.82	0.61
1:M:329:ALA:HB2	1:M:345:MET:HB3	1.82	0.61
1:G:329:ALA:HB2	1:G:345:MET:HB3	1.81	0.61
1:A:329:ALA:HB2	1:A:345:MET:HB3	1.82	0.61
1:H:442:ILE:HG23	1:H:497:ILE:HB	1.81	0.61
1:M:59:LEU:HD11	1:M:87:MET:HE1	1.81	0.61
1:H:32:ARG:NH2	1:H:75:LEU:HD22	2.15	0.61
1:J:329:ALA:HB2	1:J:345:MET:HB3	1.81	0.61
1:M:19:LEU:HB2	1:M:80:ARG:HD2	1.81	0.61
1:F:377:PRO:HG3	1:F:601:LYS:HB3	1.81	0.61
1:J:407:ILE:HD11	1:J:431:HIS:HD2	1.65	0.61
1:J:21:ARG:HD3	1:J:41:ARG:HD2	1.80	0.61
1:G:107:VAL:HG21	1:G:528:THR:OG1	1.99	0.61
1:D:442:ILE:HG23	1:D:497:ILE:HB	1.81	0.61
1:E:110:ILE:HD11	1:E:168:ALA:HA	1.82	0.61
1:M:5:LYS:HE2	1:M:69:PHE:CE2	2.35	0.61
1:E:63:LEU:HD23	1:E:91:ALA:HB1	1.81	0.61
1:K:442:ILE:HG23	1:K:497:ILE:HB	1.81	0.61
1:A:407:ILE:HD11	1:A:431:HIS:HD2	1.65	0.61
1:L:110:ILE:HD11	1:L:168:ALA:HA	1.82	0.61
1:M:110:ILE:HD11	1:M:168:ALA:HA	1.82	0.61
1:F:407:ILE:HD11	1:F:431:HIS:HD2	1.66	0.61
1:D:23:LYS:O	1:D:81:GLN:HB3	1.99	0.61
1:L:442:ILE:HG23	1:L:497:ILE:HB	1.81	0.61
1:H:110:ILE:HD11	1:H:168:ALA:HA	1.82	0.61
1:D:103:LYS:HD2	1:D:526:ASP:OD1	2.01	0.61
1:H:103:LYS:HD2	1:H:526:ASP:OD1	2.01	0.61
1:D:9:LEU:HG	1:D:72:PHE:CE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:ARG:HA	1:H:83:VAL:HG22	1.83	0.61
1:E:442:ILE:HG23	1:E:497:ILE:HB	1.81	0.61
1:D:307:SER:H	1:D:319:SER:HB3	1.64	0.61
1:D:377:PRO:HG3	1:D:601:LYS:HB3	1.81	0.61
1:G:110:ILE:HD11	1:G:168:ALA:HA	1.82	0.61
1:C:416:HIS:CE1	1:C:514:PHE:HB2	2.36	0.61
1:F:63:LEU:HD23	1:F:91:ALA:HB1	1.81	0.61
1:D:205:CYS:HG	1:D:358:TYR:HD1	1.49	0.61
1:J:377:PRO:HG3	1:J:601:LYS:HB3	1.81	0.61
1:E:329:ALA:HB2	1:E:345:MET:HB3	1.81	0.61
1:D:512:ARG:HB2	1:D:531:CYS:SG	2.41	0.61
1:K:110:ILE:HD11	1:K:168:ALA:HA	1.83	0.61
1:C:407:ILE:HD11	1:C:431:HIS:HD2	1.66	0.61
1:D:407:ILE:HD11	1:D:431:HIS:HD2	1.66	0.61
1:A:77:GLU:HA	1:A:80:ARG:NH2	2.16	0.60
1:K:268:ARG:NE	1:K:272:ARG:HH21	1.98	0.60
1:M:407:ILE:HD11	1:M:431:HIS:HD2	1.65	0.60
1:A:64:TYR:OH	1:A:94:VAL:HG12	2.01	0.60
1:L:268:ARG:CZ	1:L:272:ARG:HH21	2.15	0.60
1:A:442:ILE:HG23	1:A:497:ILE:HB	1.81	0.60
1:L:407:ILE:HD11	1:L:431:HIS:HD2	1.66	0.60
1:I:110:ILE:HD11	1:I:168:ALA:HA	1.82	0.60
1:A:24:LEU:HG	1:A:24:LEU:HB3	1.80	0.60
1:E:275:ASP:N	1:G:268:ARG:HH12	1.97	0.60
1:A:205:CYS:HG	1:A:358:TYR:HD1	1.47	0.60
1:C:329:ALA:HB2	1:C:345:MET:HB3	1.81	0.60
1:A:110:ILE:HD11	1:A:168:ALA:HA	1.83	0.60
1:K:10:MET:HG2	1:K:108:PRO:CG	2.32	0.60
1:L:273:ILE:HG12	1:L:317:TYR:HD1	1.66	0.60
1:G:407:ILE:HD11	1:G:431:HIS:HD2	1.66	0.60
1:I:407:ILE:HD11	1:I:431:HIS:HD2	1.66	0.60
1:D:110:ILE:HD11	1:D:168:ALA:HA	1.82	0.60
1:E:407:ILE:HD11	1:E:431:HIS:HD2	1.66	0.60
1:K:278:ASN:HB3	1:M:315:GLU:HG3	1.83	0.60
1:K:59:LEU:HD13	1:K:87:MET:SD	2.41	0.60
1:D:63:LEU:HD23	1:D:91:ALA:HB1	1.81	0.60
1:L:272:ARG:HB3	1:L:316:TYR:CE2	2.36	0.60
1:I:4:ASP:HA	1:I:7:ALA:HB3	1.84	0.60
1:C:89:VAL:HA	1:C:92:VAL:HG22	1.84	0.60
1:I:307:SER:H	1:I:319:SER:HB3	1.67	0.60
1:L:89:VAL:HA	1:L:92:VAL:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:LYS:HD2	1:G:526:ASP:OD1	2.02	0.60
1:H:407:ILE:HD11	1:H:431:HIS:HD2	1.65	0.60
1:I:76:CYS:HA	1:I:88:PHE:HZ	1.67	0.60
1:G:554:PHE:HE1	1:G:615:MET:HB3	1.67	0.60
1:E:307:SER:H	1:E:319:SER:HB3	1.67	0.60
1:F:97:LEU:HD11	1:F:528:THR:CB	2.31	0.60
1:J:270:ARG:O	1:J:274:LEU:HG	2.02	0.60
1:L:554:PHE:HE1	1:L:615:MET:HB3	1.67	0.60
1:C:110:ILE:HD11	1:C:168:ALA:HA	1.83	0.60
1:F:307:SER:H	1:F:319:SER:HB3	1.67	0.60
1:I:273:ILE:HA	1:I:317:TYR:CE1	2.36	0.60
1:I:89:VAL:HA	1:I:92:VAL:HG22	1.84	0.60
1:K:329:ALA:HB2	1:K:345:MET:HB3	1.82	0.60
1:D:89:VAL:HA	1:D:92:VAL:HG22	1.84	0.60
1:E:89:VAL:HA	1:E:92:VAL:HG22	1.84	0.60
1:A:76:CYS:HA	1:A:88:PHE:CE2	2.37	0.59
1:I:10:MET:CE	1:I:517:LEU:C	2.70	0.59
1:H:89:VAL:HA	1:H:92:VAL:HG22	1.84	0.59
1:C:76:CYS:HA	1:C:88:PHE:HZ	1.67	0.59
1:M:72:PHE:CZ	1:M:96:VAL:CG2	2.85	0.59
1:I:10:MET:HE1	1:I:517:LEU:C	2.21	0.59
1:A:307:SER:H	1:A:319:SER:HB3	1.67	0.59
1:H:554:PHE:HE1	1:H:615:MET:HB3	1.67	0.59
1:I:10:MET:HB3	1:I:514:PHE:CE1	2.37	0.59
1:A:64:TYR:HH	1:A:181:TRP:HZ3	1.49	0.59
1:M:554:PHE:HE1	1:M:615:MET:HB3	1.67	0.59
1:E:554:PHE:HE1	1:E:615:MET:HB3	1.67	0.59
1:I:554:PHE:HE1	1:I:615:MET:HB3	1.67	0.59
1:F:89:VAL:HA	1:F:92:VAL:HG22	1.84	0.59
1:G:89:VAL:HA	1:G:92:VAL:HG22	1.84	0.59
1:K:407:ILE:HD11	1:K:431:HIS:HD2	1.66	0.59
1:G:205:CYS:HG	1:G:358:TYR:HD1	1.50	0.59
1:I:205:CYS:HG	1:I:358:TYR:HD1	1.50	0.59
1:C:416:HIS:CE1	1:C:514:PHE:HB3	2.38	0.59
1:D:554:PHE:HE1	1:D:615:MET:HB3	1.67	0.59
1:H:307:SER:H	1:H:319:SER:HB3	1.67	0.59
1:M:307:SER:H	1:M:319:SER:HB3	1.67	0.59
1:J:76:CYS:HA	1:J:88:PHE:HZ	1.67	0.59
1:F:5:LYS:HE2	1:F:69:PHE:CE2	2.38	0.59
1:M:103:LYS:HD2	1:M:526:ASP:OD1	2.03	0.59
1:F:175:ILE:HG21	1:F:528:THR:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:554:PHE:HE1	1:J:615:MET:HB3	1.67	0.59
1:M:64:TYR:HH	1:M:94:VAL:HG12	1.68	0.59
1:D:8:ARG:NH2	1:D:73:ILE:HG13	2.17	0.59
1:E:205:CYS:HG	1:E:358:TYR:HD1	1.50	0.59
1:G:5:LYS:HE2	1:G:69:PHE:CE2	2.37	0.59
1:J:307:SER:N	1:J:319:SER:HB3	2.17	0.59
1:L:169:HIS:CE1	1:L:533:CYS:SG	2.96	0.59
1:A:304:ILE:HA	1:A:311:SER:OG	2.03	0.59
1:E:5:LYS:NZ	1:E:5:LYS:CE	2.66	0.58
1:L:8:ARG:NH2	1:L:73:ILE:CG1	2.65	0.58
1:M:304:ILE:HA	1:M:311:SER:OG	2.03	0.58
1:C:304:ILE:HA	1:C:311:SER:OG	2.03	0.58
1:F:554:PHE:HE1	1:F:615:MET:HB3	1.67	0.58
1:K:307:SER:H	1:K:319:SER:HB3	1.67	0.58
1:L:304:ILE:HA	1:L:311:SER:OG	2.03	0.58
1:C:5:LYS:NZ	1:C:5:LYS:CE	2.66	0.58
1:J:5:LYS:NZ	1:J:5:LYS:CE	2.66	0.58
1:M:24:LEU:HD22	1:M:82:ILE:HG21	1.84	0.58
1:J:529:GLU:HG3	1:J:574:CYS:SG	2.42	0.58
1:M:29:ARG:HG3	1:M:78:GLN:HE22	1.69	0.58
1:M:5:LYS:NZ	1:M:5:LYS:CE	2.66	0.58
1:A:69:PHE:HE1	1:A:96:VAL:CG2	2.16	0.58
1:A:79:ALA:HB3	1:A:88:PHE:HE1	0.89	0.58
1:K:32:ARG:NH2	1:K:75:LEU:HD22	2.18	0.58
1:J:125:ASN:ND2	1:K:242:SER:O	2.37	0.58
1:A:508:ILE:HD11	1:A:531:CYS:HA	1.84	0.58
1:H:304:ILE:HA	1:H:311:SER:OG	2.03	0.58
1:I:272:ARG:CD	1:I:316:TYR:CE1	2.84	0.58
1:A:554:PHE:HE1	1:A:615:MET:HB3	1.67	0.58
1:J:89:VAL:HA	1:J:92:VAL:HG22	1.84	0.58
1:K:304:ILE:HA	1:K:311:SER:OG	2.03	0.58
1:L:307:SER:H	1:L:319:SER:HB3	1.67	0.58
1:A:5:LYS:CE	1:A:5:LYS:NZ	2.66	0.58
1:G:32:ARG:CZ	1:G:75:LEU:HD22	2.33	0.58
1:M:89:VAL:HA	1:M:92:VAL:HG22	1.84	0.58
1:C:307:SER:H	1:C:319:SER:HB3	1.67	0.58
1:A:214:SER:HA	1:A:549:MET:SD	2.44	0.58
1:K:214:SER:HA	1:K:549:MET:SD	2.44	0.58
1:L:214:SER:HA	1:L:549:MET:SD	2.44	0.58
1:H:512:ARG:HB2	1:H:531:CYS:SG	2.43	0.58
1:K:97:LEU:HG	1:K:528:THR:OG1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:467:LEU:HD11	1:J:151:LEU:CB	2.33	0.58
1:A:59:LEU:CD1	1:A:87:MET:SD	2.91	0.58
1:A:119:VAL:HG11	1:A:428:VAL:HG11	1.85	0.58
1:E:214:SER:HA	1:E:549:MET:SD	2.44	0.58
1:I:304:ILE:HA	1:I:311:SER:OG	2.03	0.58
1:E:76:CYS:HA	1:E:88:PHE:HZ	1.67	0.58
1:K:24:LEU:CD1	1:K:81:GLN:NE2	2.58	0.58
1:D:8:ARG:NH1	1:D:73:ILE:HG21	2.18	0.58
1:I:271:GLU:HA	1:L:268:ARG:NH1	2.18	0.58
1:C:77:GLU:HA	1:C:80:ARG:NH2	2.19	0.58
1:C:214:SER:HA	1:C:549:MET:SD	2.44	0.58
1:F:304:ILE:HA	1:F:311:SER:OG	2.03	0.58
1:K:77:GLU:HA	1:K:80:ARG:NH2	2.19	0.58
1:F:5:LYS:CE	1:F:5:LYS:NZ	2.66	0.58
1:H:270:ARG:O	1:H:274:LEU:HG	2.04	0.58
1:K:554:PHE:HE1	1:K:615:MET:HB3	1.68	0.58
1:G:214:SER:HA	1:G:549:MET:SD	2.44	0.58
1:E:304:ILE:HA	1:E:311:SER:OG	2.03	0.58
1:F:76:CYS:HA	1:F:88:PHE:HZ	1.67	0.58
1:G:77:GLU:HA	1:G:80:ARG:NH2	2.19	0.58
1:I:214:SER:HA	1:I:549:MET:SD	2.44	0.58
1:A:5:LYS:HE2	1:A:69:PHE:CE2	2.38	0.57
1:L:77:GLU:HA	1:L:80:ARG:NH2	2.19	0.57
1:L:529:GLU:HB2	1:L:574:CYS:HB3	1.85	0.57
1:J:77:GLU:HA	1:J:80:ARG:NH2	2.19	0.57
1:D:24:LEU:HB2	1:D:81:GLN:CB	2.31	0.57
1:H:243:GLY:CA	1:I:125:ASN:ND2	2.67	0.57
1:A:59:LEU:HD13	1:A:87:MET:SD	2.44	0.57
1:M:59:LEU:CD1	1:M:87:MET:CE	2.82	0.57
1:C:554:PHE:HE1	1:C:615:MET:HB3	1.67	0.57
1:I:33:LEU:HG	1:I:58:GLU:HG2	1.85	0.57
1:A:128:ASN:OD1	1:A:426:VAL:HB	2.04	0.57
1:L:5:LYS:HE3	1:L:69:PHE:CD1	2.40	0.57
1:L:19:LEU:HD13	1:L:80:ARG:HD3	1.86	0.57
1:K:13:PHE:HD1	1:K:108:PRO:HG2	1.69	0.57
1:G:512:ARG:HH22	1:G:523:VAL:HG21	1.70	0.57
1:F:77:GLU:HA	1:F:80:ARG:NH2	2.19	0.57
1:F:97:LEU:HG	1:F:528:THR:H	1.70	0.57
1:G:529:GLU:HG3	1:G:574:CYS:SG	2.45	0.57
1:D:214:SER:HA	1:D:549:MET:SD	2.44	0.57
1:M:214:SER:HA	1:M:549:MET:SD	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:214:SER:HA	1:H:549:MET:SD	2.44	0.57
1:K:50:ALA:HB2	1:K:323:TRP:HH2	1.66	0.57
1:G:270:ARG:O	1:G:274:LEU:HG	2.05	0.57
1:E:77:GLU:HA	1:E:80:ARG:NH2	2.19	0.57
1:C:296:HIS:HE1	1:I:566:ALA:O	1.87	0.57
1:F:214:SER:HA	1:F:549:MET:SD	2.44	0.57
1:K:64:TYR:OH	1:K:181:TRP:HZ3	1.88	0.57
1:J:5:LYS:HE2	1:J:69:PHE:CE2	2.38	0.57
1:J:214:SER:HA	1:J:549:MET:SD	2.44	0.57
1:G:553:LEU:HB2	1:G:620:ILE:HD12	1.87	0.57
1:M:69:PHE:CE2	1:M:73:ILE:HG12	2.40	0.56
1:D:77:GLU:HA	1:D:80:ARG:NH2	2.19	0.56
1:A:79:ALA:HB3	1:A:88:PHE:CD1	2.29	0.56
1:D:553:LEU:HB2	1:D:620:ILE:HD12	1.87	0.56
1:M:444:VAL:HG11	1:M:490:LEU:HD23	1.87	0.56
1:J:553:LEU:HB2	1:J:620:ILE:HD12	1.87	0.56
1:D:9:LEU:CD1	1:D:72:PHE:CE2	2.61	0.56
1:I:77:GLU:HA	1:I:80:ARG:NH2	2.19	0.56
1:J:273:ILE:HG12	1:J:317:TYR:HD1	1.71	0.56
1:K:553:LEU:HB2	1:K:620:ILE:HD12	1.87	0.56
1:A:389:GLU:O	1:A:444:VAL:HA	2.05	0.56
1:F:4:ASP:HA	1:F:7:ALA:HB3	1.87	0.56
1:I:183:PRO:HB3	1:I:189:GLU:HB3	1.88	0.56
1:H:4:ASP:HA	1:H:7:ALA:HB3	1.87	0.56
1:J:306:GLU:N	1:J:307:SER:HA	2.20	0.56
1:H:389:GLU:O	1:H:444:VAL:HA	2.05	0.56
1:K:389:GLU:O	1:K:444:VAL:HA	2.05	0.56
1:A:553:LEU:HB2	1:A:620:ILE:HD12	1.87	0.56
1:C:172:HIS:HA	1:C:175:ILE:HG22	1.88	0.56
1:K:9:LEU:CD1	1:K:73:ILE:HD11	2.35	0.56
1:M:389:GLU:O	1:M:444:VAL:HA	2.05	0.56
1:C:553:LEU:HB2	1:C:620:ILE:HD12	1.87	0.56
1:L:389:GLU:O	1:L:444:VAL:HA	2.05	0.56
1:M:4:ASP:HA	1:M:7:ALA:HB3	1.87	0.56
1:C:389:GLU:O	1:C:444:VAL:HA	2.05	0.56
1:K:172:HIS:HA	1:K:175:ILE:HG22	1.88	0.56
1:J:238:THR:CG2	1:K:243:GLY:O	2.46	0.56
1:H:172:HIS:HA	1:H:175:ILE:HG22	1.88	0.56
1:E:553:LEU:HB2	1:E:620:ILE:HD12	1.87	0.56
1:F:389:GLU:O	1:F:444:VAL:HA	2.05	0.56
1:F:205:CYS:HG	1:F:358:TYR:HD1	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:ARG:NH1	1:F:271:GLU:HA	2.21	0.56
1:E:4:ASP:HA	1:E:7:ALA:HB3	1.87	0.56
1:J:389:GLU:O	1:J:444:VAL:HA	2.05	0.56
1:C:151:LEU:CA	1:G:467:LEU:HD11	2.31	0.56
1:A:172:HIS:HA	1:A:175:ILE:HG22	1.88	0.56
1:K:508:ILE:HD11	1:K:531:CYS:HA	1.87	0.56
1:L:410:SER:O	1:L:429:LYS:HA	2.06	0.56
1:F:22:GLU:HB2	1:F:81:GLN:HB3	1.87	0.56
1:H:410:SER:O	1:H:429:LYS:HA	2.06	0.56
1:C:5:LYS:HE2	1:C:69:PHE:CE2	2.38	0.56
1:G:172:HIS:HA	1:G:175:ILE:HG22	1.88	0.56
1:D:389:GLU:O	1:D:444:VAL:HA	2.05	0.56
1:D:410:SER:O	1:D:429:LYS:HA	2.06	0.56
1:K:8:ARG:HE	1:K:73:ILE:HG21	1.61	0.56
1:G:410:SER:O	1:G:429:LYS:HA	2.06	0.56
1:L:553:LEU:HB2	1:L:620:ILE:HD12	1.87	0.56
1:F:553:LEU:HB2	1:F:620:ILE:HD12	1.87	0.56
1:G:389:GLU:O	1:G:444:VAL:HA	2.05	0.56
1:K:268:ARG:CZ	1:K:272:ARG:HH21	2.19	0.56
1:L:19:LEU:CB	1:L:80:ARG:HD3	2.36	0.56
1:A:118:PHE:HA	1:A:353:ARG:HH12	1.71	0.56
1:M:95:ALA:HB1	1:M:99:ARG:HD2	1.88	0.56
1:K:96:VAL:HG22	1:K:105:ILE:HG21	1.88	0.56
1:H:553:LEU:HB2	1:H:620:ILE:HD12	1.87	0.56
1:E:172:HIS:HA	1:E:175:ILE:HG22	1.88	0.55
1:E:97:LEU:HG	1:E:528:THR:OG1	2.05	0.55
1:E:389:GLU:O	1:E:444:VAL:HA	2.05	0.55
1:A:410:SER:O	1:A:429:LYS:HA	2.06	0.55
1:M:172:HIS:HA	1:M:175:ILE:HG22	1.88	0.55
1:A:4:ASP:HA	1:A:7:ALA:HB3	1.87	0.55
1:K:410:SER:O	1:K:429:LYS:HA	2.06	0.55
1:J:167:ASN:HB3	1:J:349:SER:O	2.07	0.55
1:J:97:LEU:HG	1:J:528:THR:OG1	2.06	0.55
1:F:107:VAL:HG21	1:F:528:THR:OG1	2.05	0.55
1:C:14:LYS:HG3	1:C:514:PHE:CE2	2.41	0.55
1:C:274:LEU:HD12	1:F:268:ARG:NH2	2.22	0.55
1:D:95:ALA:HB1	1:D:99:ARG:HD2	1.88	0.55
1:E:95:ALA:HB1	1:E:99:ARG:HD2	1.88	0.55
1:C:95:ALA:HB1	1:C:99:ARG:HD2	1.88	0.55
1:H:167:ASN:HB3	1:H:349:SER:O	2.07	0.55
1:L:573:VAL:CG1	1:L:584:ARG:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:389:GLU:O	1:I:444:VAL:HA	2.05	0.55
1:L:5:LYS:HA	1:L:69:PHE:CE2	2.42	0.55
1:G:24:LEU:CB	1:G:81:GLN:NE2	2.70	0.55
1:A:59:LEU:HD21	1:A:87:MET:HE3	1.88	0.55
1:G:508:ILE:HD11	1:G:531:CYS:HA	1.88	0.55
1:E:226:PHE:CE1	1:E:270:ARG:NH2	2.75	0.55
1:C:560:HIS:O	1:C:564:THR:HB	2.05	0.55
1:F:167:ASN:HB3	1:F:349:SER:O	2.07	0.55
1:A:167:ASN:HB3	1:A:349:SER:O	2.07	0.55
1:E:263:VAL:O	1:E:266:MET:HB2	2.07	0.55
1:I:553:LEU:HB2	1:I:620:ILE:HD12	1.87	0.55
1:K:2:VAL:HG11	1:K:103:LYS:O	2.07	0.55
1:D:172:HIS:HA	1:D:175:ILE:HG22	1.88	0.55
1:A:127:ALA:HB2	1:A:142:VAL:HG21	1.86	0.55
1:F:410:SER:O	1:F:429:LYS:HA	2.06	0.55
1:C:167:ASN:HB3	1:C:349:SER:O	2.07	0.55
1:I:172:HIS:HA	1:I:175:ILE:HG22	1.88	0.55
1:M:69:PHE:CZ	1:M:72:PHE:HD2	2.25	0.55
1:C:4:ASP:HA	1:C:7:ALA:HB3	1.88	0.55
1:H:95:ALA:HB1	1:H:99:ARG:HD2	1.89	0.55
1:C:410:SER:O	1:C:429:LYS:HA	2.06	0.55
1:J:95:ALA:HB1	1:J:99:ARG:HD2	1.88	0.55
1:I:167:ASN:HB3	1:I:349:SER:O	2.07	0.55
1:J:172:HIS:HA	1:J:175:ILE:HG22	1.88	0.55
1:L:172:HIS:HA	1:L:175:ILE:HG22	1.88	0.55
1:F:95:ALA:HB1	1:F:99:ARG:HD2	1.88	0.55
1:I:410:SER:O	1:I:429:LYS:HA	2.06	0.55
1:H:508:ILE:HD11	1:H:531:CYS:HA	1.89	0.55
1:F:234:ALA:HA	1:F:248:SER:HB2	1.89	0.55
1:M:410:SER:O	1:M:429:LYS:HA	2.06	0.55
1:L:50:ALA:HB2	1:L:323:TRP:HH2	1.72	0.55
1:M:553:LEU:HB2	1:M:620:ILE:HD12	1.87	0.55
1:H:234:ALA:HA	1:H:248:SER:HB2	1.89	0.55
1:K:167:ASN:HB3	1:K:349:SER:O	2.07	0.55
1:K:234:ALA:HA	1:K:248:SER:HB2	1.89	0.55
1:F:172:HIS:HA	1:F:175:ILE:HG22	1.88	0.55
1:J:4:ASP:HA	1:J:7:ALA:HB3	1.88	0.55
1:L:234:ALA:HA	1:L:248:SER:HB2	1.89	0.55
1:I:234:ALA:HA	1:I:248:SER:HB2	1.89	0.55
1:E:234:ALA:HA	1:E:248:SER:HB2	1.89	0.54
1:G:234:ALA:HA	1:G:248:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:456:VAL:HG22	1:L:557:LEU:HG	1.90	0.54
1:I:10:MET:HE3	1:I:518:GLY:HA2	1.89	0.54
1:K:205:CYS:HG	1:K:358:TYR:HD1	1.54	0.54
1:A:234:ALA:HA	1:A:248:SER:HB2	1.89	0.54
1:K:4:ASP:HA	1:K:7:ALA:HB3	1.88	0.54
1:J:245:GLN:CG	1:K:245:GLN:HG2	2.36	0.54
1:L:167:ASN:HB3	1:L:349:SER:O	2.07	0.54
1:K:456:VAL:HG22	1:K:557:LEU:HG	1.89	0.54
1:I:173:TRP:HZ2	1:I:196:LEU:HG	1.73	0.54
1:M:167:ASN:HB3	1:M:349:SER:O	2.07	0.54
1:F:173:TRP:HZ2	1:F:196:LEU:HG	1.73	0.54
1:C:173:TRP:HZ2	1:C:196:LEU:HG	1.73	0.54
1:E:167:ASN:HB3	1:E:349:SER:O	2.07	0.54
1:G:307:SER:N	1:G:319:SER:HB3	2.22	0.54
1:L:322:ASN:O	1:L:325:HIS:HB2	2.08	0.54
1:G:167:ASN:HB3	1:G:349:SER:O	2.07	0.54
1:F:50:ALA:HB2	1:F:323:TRP:HH2	1.73	0.54
1:J:322:ASN:O	1:J:325:HIS:HB2	2.08	0.54
1:J:48:PHE:HB3	1:J:326:VAL:HG22	1.89	0.54
1:D:234:ALA:HA	1:D:248:SER:HB2	1.89	0.54
1:K:95:ALA:HB1	1:K:99:ARG:HD2	1.89	0.54
1:I:456:VAL:HG22	1:I:557:LEU:HG	1.90	0.54
1:E:5:LYS:HE2	1:E:69:PHE:CE2	2.38	0.54
1:L:511:VAL:HA	1:L:531:CYS:HB2	1.89	0.54
1:A:322:ASN:O	1:A:325:HIS:HB2	2.08	0.54
1:E:456:VAL:HG22	1:E:557:LEU:HG	1.89	0.54
1:H:322:ASN:O	1:H:325:HIS:HB2	2.08	0.54
1:H:50:ALA:HB2	1:H:323:TRP:HH2	1.73	0.54
1:D:167:ASN:HB3	1:D:349:SER:O	2.07	0.54
1:F:270:ARG:O	1:F:274:LEU:HG	2.08	0.54
1:I:322:ASN:O	1:I:325:HIS:HB2	2.08	0.54
1:K:322:ASN:O	1:K:325:HIS:HB2	2.08	0.54
1:M:72:PHE:HZ	1:M:96:VAL:HB	1.72	0.54
1:K:175:ILE:HG23	1:K:528:THR:CG2	2.15	0.54
1:M:82:ILE:HG23	1:M:83:VAL:HG13	1.88	0.54
1:I:50:ALA:HB2	1:I:323:TRP:HH2	1.72	0.54
1:H:268:ARG:NH1	1:M:274:LEU:HB2	2.23	0.54
1:J:410:SER:O	1:J:429:LYS:HA	2.06	0.54
1:E:410:SER:O	1:E:429:LYS:HA	2.06	0.54
1:L:176:VAL:HG11	1:L:529:GLU:HB3	1.89	0.54
1:J:173:TRP:HZ2	1:J:196:LEU:HG	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:234:ALA:HA	1:M:248:SER:HB2	1.89	0.54
1:G:173:TRP:HZ2	1:G:196:LEU:HG	1.73	0.54
1:L:173:TRP:HZ2	1:L:196:LEU:HG	1.73	0.54
1:A:456:VAL:HG22	1:A:557:LEU:HG	1.89	0.54
1:C:234:ALA:HA	1:C:248:SER:HB2	1.89	0.54
1:A:173:TRP:HZ2	1:A:196:LEU:HG	1.73	0.54
1:H:77:GLU:HA	1:H:80:ARG:NH2	2.23	0.54
1:D:249:ARG:HG2	1:D:250:PRO:O	2.07	0.54
1:A:107:VAL:HG21	1:A:528:THR:OG1	2.08	0.54
1:A:50:ALA:HB2	1:A:323:TRP:HH2	1.72	0.54
1:J:263:VAL:O	1:J:266:MET:HB2	2.08	0.54
1:E:97:LEU:CD1	1:E:528:THR:OG1	2.56	0.54
1:A:59:LEU:HD21	1:A:87:MET:HE2	1.90	0.54
1:D:529:GLU:HG3	1:D:574:CYS:SG	2.48	0.54
1:E:50:ALA:HB2	1:E:323:TRP:HH2	1.72	0.54
1:D:48:PHE:CB	1:D:326:VAL:HG22	2.38	0.54
1:I:48:PHE:CB	1:I:326:VAL:HG22	2.38	0.54
1:F:322:ASN:O	1:F:325:HIS:HB2	2.08	0.54
1:F:172:HIS:HD2	1:F:532:SER:HB3	1.70	0.53
1:H:529:GLU:HG3	1:H:574:CYS:SG	2.48	0.53
1:L:444:VAL:HG11	1:L:490:LEU:HD23	1.90	0.53
1:A:136:ASP:O	1:A:423:ASP:HB3	2.08	0.53
1:I:95:ALA:HB1	1:I:99:ARG:HD2	1.88	0.53
1:C:50:ALA:HB2	1:C:323:TRP:HH2	1.72	0.53
1:M:69:PHE:CE2	1:M:73:ILE:CG1	2.90	0.53
1:K:59:LEU:CD1	1:K:87:MET:SD	2.96	0.53
1:C:274:LEU:HB2	1:F:268:ARG:HH22	1.74	0.53
1:C:444:VAL:HG11	1:C:490:LEU:HD23	1.91	0.53
1:E:529:GLU:HG3	1:E:574:CYS:SG	2.48	0.53
1:M:456:VAL:HG22	1:M:557:LEU:HG	1.90	0.53
1:G:456:VAL:HG22	1:G:557:LEU:HG	1.89	0.53
1:J:456:VAL:HG22	1:J:557:LEU:HG	1.89	0.53
1:E:322:ASN:O	1:E:325:HIS:HB2	2.08	0.53
1:C:38:ILE:HD13	1:D:605:ARG:HH12	1.73	0.53
1:J:121:ALA:HB1	1:K:243:GLY:HA3	1.90	0.53
1:E:118:PHE:HA	1:E:353:ARG:HH12	1.74	0.53
1:J:444:VAL:HG11	1:J:490:LEU:HD23	1.91	0.53
1:I:444:VAL:HG11	1:I:490:LEU:HD23	1.91	0.53
1:K:21:ARG:HD3	1:K:41:ARG:HD2	1.89	0.53
1:D:173:TRP:HZ2	1:D:196:LEU:HG	1.73	0.53
1:D:456:VAL:HG22	1:D:557:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ASN:O	1:C:325:HIS:HB2	2.08	0.53
1:A:69:PHE:CE1	1:A:96:VAL:CG2	2.92	0.53
1:K:270:ARG:O	1:K:274:LEU:HG	2.09	0.53
1:F:444:VAL:HG11	1:F:490:LEU:HD23	1.91	0.53
1:A:76:CYS:CA	1:A:88:PHE:CZ	2.79	0.53
1:A:268:ARG:HD2	1:A:272:ARG:HE	1.73	0.53
1:J:573:VAL:HG22	1:J:574:CYS:H	1.74	0.53
1:F:117:ARG:HB2	1:F:350:THR:HG23	1.91	0.53
1:M:269:TRP:O	1:M:273:ILE:HG13	2.08	0.53
1:A:444:VAL:HG11	1:A:490:LEU:HD23	1.91	0.53
1:D:50:ALA:HB2	1:D:323:TRP:HH2	1.72	0.53
1:A:84:ASN:HD22	1:A:84:ASN:N	2.07	0.53
1:G:95:ALA:HB1	1:G:99:ARG:HD2	1.88	0.53
1:G:322:ASN:O	1:G:325:HIS:HB2	2.08	0.53
1:L:465:ASP:HB3	1:L:467:LEU:H	1.74	0.53
1:M:72:PHE:CE2	1:M:96:VAL:CG2	2.91	0.53
1:K:97:LEU:CD1	1:K:528:THR:OG1	2.56	0.53
1:H:8:ARG:NH2	1:H:73:ILE:CG1	2.66	0.53
1:C:270:ARG:O	1:C:274:LEU:HG	2.08	0.53
1:K:444:VAL:HG11	1:K:490:LEU:HD23	1.91	0.53
1:A:48:PHE:CB	1:A:326:VAL:HG22	2.38	0.53
1:C:48:PHE:CB	1:C:326:VAL:HG22	2.38	0.53
1:D:322:ASN:O	1:D:325:HIS:HB2	2.08	0.53
1:M:9:LEU:HD12	1:M:73:ILE:HD12	1.89	0.53
1:C:14:LYS:HG3	1:C:514:PHE:CZ	2.44	0.53
1:I:268:ARG:NH1	1:J:271:GLU:HA	2.24	0.53
1:D:118:PHE:HA	1:D:353:ARG:HH12	1.74	0.53
1:G:118:PHE:HA	1:G:353:ARG:HH12	1.74	0.53
1:D:444:VAL:HG11	1:D:490:LEU:HD23	1.91	0.53
1:F:573:VAL:HG22	1:F:574:CYS:H	1.74	0.53
1:J:30:ASP:O	1:J:33:LEU:N	2.42	0.53
1:C:118:PHE:HA	1:C:353:ARG:HH12	1.74	0.53
1:H:118:PHE:HA	1:H:353:ARG:HH12	1.74	0.53
1:K:173:TRP:HZ2	1:K:196:LEU:HG	1.73	0.53
1:E:173:TRP:HZ2	1:E:196:LEU:HG	1.73	0.53
1:L:460:LEU:HA	1:L:552:GLU:O	2.09	0.53
1:A:23:LYS:O	1:A:25:PRO:HD3	2.09	0.53
1:J:118:PHE:HA	1:J:353:ARG:HH12	1.74	0.53
1:I:117:ARG:HB2	1:I:350:THR:HG23	1.91	0.53
1:F:118:PHE:HA	1:F:353:ARG:HH12	1.74	0.53
1:H:444:VAL:HG11	1:H:490:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:VAL:HG11	1:E:490:LEU:HD23	1.90	0.53
1:L:48:PHE:CB	1:L:326:VAL:HG22	2.38	0.53
1:C:456:VAL:HG22	1:C:557:LEU:HG	1.89	0.53
1:F:456:VAL:HG22	1:F:557:LEU:HG	1.89	0.53
1:H:456:VAL:HG22	1:H:557:LEU:HG	1.89	0.53
1:D:117:ARG:HB2	1:D:350:THR:HG23	1.91	0.53
1:M:117:ARG:HB2	1:M:350:THR:HG23	1.91	0.53
1:M:508:ILE:HD11	1:M:531:CYS:HA	1.90	0.53
1:G:444:VAL:HG11	1:G:490:LEU:HD23	1.91	0.53
1:F:456:VAL:O	1:F:485:LYS:HA	2.10	0.53
1:C:460:LEU:HA	1:C:552:GLU:O	2.09	0.53
1:E:48:PHE:CB	1:E:326:VAL:HG22	2.38	0.53
1:J:117:ARG:HB2	1:J:350:THR:HG23	1.91	0.52
1:E:270:ARG:O	1:E:274:LEU:HG	2.10	0.52
1:L:95:ALA:HB1	1:L:99:ARG:HD2	1.91	0.52
1:D:270:ARG:O	1:D:274:LEU:HG	2.09	0.52
1:F:337:ARG:HA	1:G:151:LEU:HD23	1.91	0.52
1:H:64:TYR:OH	1:H:94:VAL:HG12	2.09	0.52
1:F:460:LEU:HA	1:F:552:GLU:O	2.09	0.52
1:K:573:VAL:HG22	1:K:574:CYS:H	1.74	0.52
1:C:510:LYS:HE2	1:C:511:VAL:O	2.08	0.52
1:M:460:LEU:HA	1:M:552:GLU:O	2.09	0.52
1:L:172:HIS:HD2	1:L:532:SER:O	1.93	0.52
1:L:118:PHE:HA	1:L:353:ARG:HH12	1.74	0.52
1:M:456:VAL:O	1:M:485:LYS:HA	2.10	0.52
1:J:456:VAL:O	1:J:485:LYS:HA	2.10	0.52
1:M:433:LEU:O	1:M:538:HIS:HB2	2.10	0.52
1:H:173:TRP:HZ2	1:H:196:LEU:HG	1.73	0.52
1:H:460:LEU:HA	1:H:552:GLU:O	2.09	0.52
1:A:89:VAL:HA	1:A:92:VAL:HG22	1.91	0.52
1:D:23:LYS:O	1:D:81:GLN:CB	2.56	0.52
1:G:117:ARG:HB2	1:G:350:THR:HG23	1.91	0.52
1:C:117:ARG:HB2	1:C:350:THR:HG23	1.91	0.52
1:D:456:VAL:O	1:D:485:LYS:HA	2.10	0.52
1:H:456:VAL:O	1:H:485:LYS:HA	2.10	0.52
1:E:433:LEU:O	1:E:538:HIS:HB2	2.10	0.52
1:M:322:ASN:O	1:M:325:HIS:HB2	2.08	0.52
1:A:433:LEU:O	1:A:538:HIS:HB2	2.10	0.52
1:F:48:PHE:CB	1:F:326:VAL:HG22	2.38	0.52
1:M:173:TRP:HZ2	1:M:196:LEU:HG	1.73	0.52
1:C:433:LEU:O	1:C:538:HIS:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:LEU:O	1:D:538:HIS:HB2	2.10	0.52
1:E:107:VAL:HG21	1:E:528:THR:HG1	1.72	0.52
1:G:23:LYS:O	1:G:81:GLN:CD	2.48	0.52
1:I:13:PHE:HB2	1:I:514:PHE:HZ	1.74	0.52
1:A:59:LEU:HD11	1:A:87:MET:CE	2.40	0.52
1:I:30:ASP:HB3	1:I:33:LEU:HD13	1.90	0.52
1:C:64:TYR:OH	1:C:94:VAL:HG12	2.09	0.52
1:M:60:TYR:HH	1:M:90:TYR:HD2	1.54	0.52
1:K:117:ARG:HB2	1:K:350:THR:HG23	1.91	0.52
1:J:459:PHE:O	1:J:553:LEU:HA	2.10	0.52
1:C:473:PRO:O	1:C:477:ARG:HG3	2.10	0.52
1:I:64:TYR:OH	1:I:94:VAL:HG12	2.09	0.52
1:M:178:PRO:HG2	1:M:181:TRP:HB2	1.92	0.52
1:G:460:LEU:HA	1:G:552:GLU:O	2.09	0.52
1:I:38:ILE:HD12	1:J:605:ARG:HH22	1.75	0.52
1:H:48:PHE:CB	1:H:326:VAL:HG22	2.38	0.52
1:J:460:LEU:HA	1:J:552:GLU:O	2.09	0.52
1:E:178:PRO:HG2	1:E:181:TRP:HB2	1.92	0.52
1:L:433:LEU:O	1:L:538:HIS:HB2	2.09	0.52
1:F:433:LEU:O	1:F:538:HIS:HB2	2.10	0.52
1:I:178:PRO:HG2	1:I:181:TRP:HB2	1.92	0.52
1:M:72:PHE:CZ	1:M:96:VAL:HG23	2.45	0.52
1:M:253:TYR:HD2	1:M:331:ILE:HG13	1.75	0.52
1:L:117:ARG:HB2	1:L:350:THR:HG23	1.91	0.52
1:J:508:ILE:HD11	1:J:531:CYS:HA	1.91	0.52
1:I:118:PHE:HA	1:I:353:ARG:HH12	1.74	0.52
1:M:118:PHE:HA	1:M:353:ARG:HH12	1.74	0.52
1:A:178:PRO:HG2	1:A:181:TRP:HB2	1.91	0.52
1:F:459:PHE:O	1:F:553:LEU:HA	2.10	0.52
1:L:456:VAL:O	1:L:485:LYS:HA	2.10	0.52
1:D:170:HIS:CG	1:D:352:LEU:HD11	2.45	0.52
1:F:178:PRO:HG2	1:F:181:TRP:HB2	1.92	0.52
1:G:433:LEU:O	1:G:538:HIS:HB2	2.10	0.52
1:A:170:HIS:CG	1:A:352:LEU:HD11	2.45	0.52
1:H:170:HIS:CG	1:H:352:LEU:HD11	2.45	0.52
1:I:433:LEU:O	1:I:538:HIS:HB2	2.09	0.52
1:A:473:PRO:O	1:A:477:ARG:HG3	2.10	0.52
1:G:64:TYR:OH	1:G:181:TRP:HZ3	1.92	0.52
1:I:268:ARG:HH11	1:J:271:GLU:HA	1.74	0.52
1:H:573:VAL:HG22	1:H:574:CYS:H	1.74	0.52
1:K:456:VAL:O	1:K:485:LYS:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:573:VAL:HG22	1:E:574:CYS:H	1.74	0.52
1:C:456:VAL:O	1:C:485:LYS:HA	2.10	0.52
1:K:263:VAL:O	1:K:266:MET:HB2	2.09	0.52
1:J:473:PRO:O	1:J:477:ARG:HG3	2.10	0.52
1:J:178:PRO:HG2	1:J:181:TRP:HB2	1.92	0.52
1:M:69:PHE:CZ	1:M:72:PHE:CD2	2.98	0.52
1:J:97:LEU:CG	1:J:528:THR:HB	2.40	0.52
1:C:151:LEU:N	1:G:467:LEU:HD12	2.25	0.52
1:C:14:LYS:HE2	1:C:514:PHE:CE1	2.44	0.52
1:D:573:VAL:HG22	1:D:574:CYS:H	1.74	0.52
1:E:459:PHE:O	1:E:553:LEU:HA	2.10	0.52
1:M:66:ALA:HB3	1:M:99:ARG:HH21	1.74	0.52
1:A:456:VAL:O	1:A:485:LYS:HA	2.10	0.52
1:G:456:VAL:O	1:G:485:LYS:HA	2.09	0.52
1:I:473:PRO:O	1:I:477:ARG:HG3	2.10	0.52
1:K:460:LEU:HA	1:K:552:GLU:O	2.09	0.52
1:F:170:HIS:CG	1:F:352:LEU:HD11	2.45	0.52
1:M:170:HIS:CG	1:M:352:LEU:HD11	2.45	0.52
1:H:433:LEU:O	1:H:538:HIS:HB2	2.10	0.52
1:E:64:TYR:OH	1:E:94:VAL:HG12	2.09	0.52
1:G:473:PRO:O	1:G:477:ARG:HG3	2.10	0.52
1:E:97:LEU:CG	1:E:528:THR:HB	2.40	0.52
1:J:107:VAL:HG21	1:J:528:THR:HG1	1.71	0.52
1:A:104:GLY:HA2	1:A:525:GLU:HB2	1.85	0.52
1:C:278:ASN:O	1:F:315:GLU:OE2	2.28	0.52
1:L:8:ARG:NE	1:L:73:ILE:HG21	2.24	0.52
1:M:573:VAL:HG22	1:M:574:CYS:H	1.74	0.52
1:M:59:LEU:HD13	1:M:87:MET:CE	2.39	0.52
1:I:456:VAL:O	1:I:485:LYS:HA	2.10	0.52
1:E:170:HIS:CG	1:E:352:LEU:HD11	2.45	0.52
1:D:473:PRO:O	1:D:477:ARG:HG3	2.10	0.52
1:L:170:HIS:CG	1:L:352:LEU:HD11	2.45	0.52
1:F:263:VAL:O	1:F:266:MET:HB2	2.09	0.52
1:F:64:TYR:OH	1:F:94:VAL:HG12	2.09	0.52
1:J:419:ASN:HD22	1:K:132:SER:HB2	1.74	0.52
1:A:460:LEU:HA	1:A:552:GLU:O	2.09	0.52
1:C:205:CYS:HG	1:C:358:TYR:HD1	1.57	0.52
1:J:433:LEU:O	1:J:538:HIS:HB2	2.10	0.52
1:K:459:PHE:O	1:K:553:LEU:HA	2.10	0.51
1:A:137:GLN:HA	1:A:423:ASP:HA	1.92	0.51
1:D:178:PRO:HG2	1:D:181:TRP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:HA	1:A:133:ASN:HB2	1.91	0.51
1:I:573:VAL:HG22	1:I:574:CYS:H	1.74	0.51
1:G:170:HIS:CG	1:G:352:LEU:HD11	2.45	0.51
1:I:11:PRO:HA	1:I:14:LYS:HE3	1.92	0.51
1:H:178:PRO:HG2	1:H:181:TRP:HB2	1.92	0.51
1:A:573:VAL:HG22	1:A:574:CYS:H	1.74	0.51
1:I:455:THR:HA	1:I:486:PHE:O	2.11	0.51
1:A:24:LEU:HB2	1:A:24:LEU:CG	2.18	0.51
1:J:97:LEU:CD1	1:J:528:THR:OG1	2.58	0.51
1:G:178:PRO:HG2	1:G:181:TRP:HB2	1.92	0.51
1:F:508:ILE:HG12	1:F:531:CYS:O	2.10	0.51
1:H:117:ARG:HB2	1:H:350:THR:HG23	1.91	0.51
1:H:459:PHE:O	1:H:553:LEU:HA	2.10	0.51
1:L:205:CYS:HG	1:L:358:TYR:HD1	1.57	0.51
1:K:473:PRO:O	1:K:477:ARG:HG3	2.10	0.51
1:E:455:THR:HA	1:E:486:PHE:O	2.11	0.51
1:F:455:THR:HA	1:F:486:PHE:O	2.11	0.51
1:L:270:ARG:O	1:L:274:LEU:HG	2.11	0.51
1:G:459:PHE:O	1:G:553:LEU:HA	2.10	0.51
1:A:459:PHE:O	1:A:553:LEU:HA	2.10	0.51
1:I:459:PHE:O	1:I:553:LEU:HA	2.10	0.51
1:M:459:PHE:O	1:M:553:LEU:HA	2.10	0.51
1:E:460:LEU:HA	1:E:552:GLU:O	2.09	0.51
1:K:433:LEU:O	1:K:538:HIS:HB2	2.10	0.51
1:M:455:THR:HA	1:M:486:PHE:O	2.11	0.51
1:D:64:TYR:OH	1:D:94:VAL:HG12	2.09	0.51
1:M:63:LEU:HD23	1:M:91:ALA:HB1	1.89	0.51
1:C:528:THR:OG1	1:C:584:ARG:HB3	2.11	0.51
1:I:170:HIS:CG	1:I:352:LEU:HD11	2.45	0.51
1:M:473:PRO:O	1:M:477:ARG:HG3	2.10	0.51
1:C:170:HIS:CG	1:C:352:LEU:HD11	2.45	0.51
1:K:249:ARG:NE	1:K:331:ILE:HG21	2.25	0.51
1:G:573:VAL:HG22	1:G:574:CYS:H	1.74	0.51
1:I:271:GLU:HB3	1:L:268:ARG:HD3	1.93	0.51
1:H:407:ILE:HD11	1:H:431:HIS:CD2	2.46	0.51
1:K:178:PRO:HG2	1:K:181:TRP:HB2	1.92	0.51
1:D:459:PHE:O	1:D:553:LEU:HA	2.10	0.51
1:J:38:ILE:HD12	1:L:605:ARG:NH1	2.25	0.51
1:L:55:GLU:O	1:L:58:GLU:HB3	2.11	0.51
1:A:55:GLU:O	1:A:58:GLU:HB3	2.11	0.51
1:H:473:PRO:O	1:H:477:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:132:SER:HB3	1:K:419:ASN:HD22	1.74	0.51
1:E:9:LEU:HD22	1:E:105:ILE:HD11	1.91	0.51
1:E:249:ARG:NE	1:E:331:ILE:HG21	2.25	0.51
1:M:55:GLU:O	1:M:58:GLU:HB3	2.11	0.51
1:J:303:ASP:HB2	1:J:310:GLU:HB3	1.93	0.51
1:K:118:PHE:HA	1:K:353:ARG:HH12	1.74	0.51
1:L:455:THR:HA	1:L:486:PHE:O	2.11	0.51
1:K:455:THR:HA	1:K:486:PHE:O	2.11	0.51
1:A:455:THR:HA	1:A:486:PHE:O	2.11	0.51
1:K:9:LEU:HD12	1:K:73:ILE:HD11	1.92	0.51
1:H:275:ASP:OD1	1:K:316:TYR:CE1	2.52	0.51
1:K:170:HIS:CG	1:K:352:LEU:HD11	2.45	0.51
1:D:460:LEU:HA	1:D:552:GLU:O	2.09	0.51
1:E:473:PRO:O	1:E:477:ARG:HG3	2.10	0.51
1:H:455:THR:HA	1:H:486:PHE:O	2.11	0.51
1:E:55:GLU:O	1:E:58:GLU:HB3	2.11	0.51
1:C:178:PRO:HG2	1:C:181:TRP:HB2	1.92	0.51
1:H:55:GLU:O	1:H:58:GLU:HB3	2.11	0.51
1:M:407:ILE:HD11	1:M:431:HIS:CD2	2.46	0.51
1:C:459:PHE:O	1:C:553:LEU:HA	2.10	0.51
1:J:36:VAL:HG23	1:J:55:GLU:HB3	1.91	0.51
1:J:55:GLU:HG2	1:L:605:ARG:HH22	1.75	0.51
1:E:117:ARG:HB2	1:E:350:THR:HG23	1.91	0.51
1:C:55:GLU:O	1:C:58:GLU:HB3	2.11	0.51
1:F:11:PRO:HA	1:F:14:LYS:HE3	1.92	0.51
1:F:473:PRO:O	1:F:477:ARG:HG3	2.10	0.51
1:H:5:LYS:NZ	1:H:5:LYS:CE	2.74	0.51
1:K:97:LEU:CG	1:K:528:THR:HB	2.40	0.51
1:L:459:PHE:O	1:L:553:LEU:HA	2.10	0.51
1:E:456:VAL:O	1:E:485:LYS:HA	2.10	0.51
1:A:123:THR:HG21	1:A:144:ALA:HA	1.93	0.51
1:I:5:LYS:CE	1:I:5:LYS:NZ	2.74	0.50
1:L:103:LYS:HD2	1:L:526:ASP:OD1	2.11	0.50
1:C:150:ILE:O	1:G:467:LEU:CD1	2.59	0.50
1:F:477:ARG:HG2	1:F:598:PHE:HB3	1.93	0.50
1:I:467:LEU:HD22	1:I:470:LYS:HE3	1.94	0.50
1:K:126:ARG:HD3	1:K:142:VAL:HG11	1.93	0.50
1:G:455:THR:HA	1:G:486:PHE:O	2.11	0.50
1:J:170:HIS:CG	1:J:352:LEU:HD11	2.45	0.50
1:G:5:LYS:NZ	1:G:5:LYS:CE	2.75	0.50
1:L:5:LYS:CE	1:L:5:LYS:NZ	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:ASN:ND2	1:G:242:SER:C	2.65	0.50
1:C:268:ARG:HD2	1:C:272:ARG:HE	1.76	0.50
1:D:48:PHE:HB3	1:D:326:VAL:HG22	1.94	0.50
1:C:477:ARG:HG2	1:C:598:PHE:HB3	1.94	0.50
1:I:460:LEU:HA	1:I:552:GLU:O	2.09	0.50
1:L:477:ARG:HG2	1:L:598:PHE:HB3	1.94	0.50
1:G:32:ARG:HH22	1:G:75:LEU:HD22	1.70	0.50
1:J:19:LEU:HB3	1:J:80:ARG:HD2	1.94	0.50
1:M:477:ARG:HG2	1:M:598:PHE:HB3	1.94	0.50
1:L:473:PRO:O	1:L:477:ARG:HG3	2.10	0.50
1:L:178:PRO:HG2	1:L:181:TRP:HB2	1.92	0.50
1:J:107:VAL:CG2	1:J:528:THR:OG1	2.54	0.50
1:C:275:ASP:HB2	1:F:268:ARG:HH11	1.77	0.50
1:D:68:ASP:CG	1:D:70:ASN:HB2	2.31	0.50
1:H:268:ARG:HH12	1:M:274:LEU:HB2	1.77	0.50
1:K:477:ARG:HG2	1:K:598:PHE:HB3	1.94	0.50
1:C:455:THR:HA	1:C:486:PHE:O	2.11	0.50
1:G:55:GLU:O	1:G:58:GLU:HB3	2.11	0.50
1:A:24:LEU:HD12	1:A:26:LEU:C	2.31	0.50
1:D:263:VAL:O	1:D:266:MET:HB2	2.10	0.50
1:E:477:ARG:HG2	1:E:598:PHE:HB3	1.94	0.50
1:D:455:THR:HA	1:D:486:PHE:O	2.11	0.50
1:D:9:LEU:HD21	1:D:72:PHE:HZ	1.59	0.50
1:L:12:LEU:HD22	1:L:80:ARG:NH1	2.26	0.50
1:M:20:THR:OG1	1:M:85:GLU:HB3	2.12	0.50
1:A:407:ILE:HD11	1:A:431:HIS:CD2	2.46	0.50
1:J:477:ARG:HA	1:J:480:PHE:HD2	1.77	0.50
1:H:477:ARG:HA	1:H:480:PHE:HD2	1.77	0.50
1:K:55:GLU:O	1:K:58:GLU:HB3	2.11	0.50
1:F:55:GLU:O	1:F:58:GLU:HB3	2.11	0.50
1:I:264:GLN:NE2	1:J:270:ARG:HH12	2.08	0.50
1:E:508:ILE:HD11	1:E:531:CYS:HA	1.94	0.50
1:G:249:ARG:HG2	1:G:250:PRO:O	2.11	0.50
1:D:477:ARG:HG2	1:D:598:PHE:HB3	1.94	0.50
1:M:272:ARG:HH11	1:M:316:TYR:HA	1.76	0.50
1:A:19:LEU:HB3	1:A:80:ARG:HD2	1.93	0.50
1:J:249:ARG:NE	1:J:331:ILE:HG21	2.26	0.50
1:F:407:ILE:HD11	1:F:431:HIS:CD2	2.46	0.50
1:E:407:ILE:HD11	1:E:431:HIS:CD2	2.46	0.50
1:A:477:ARG:HG2	1:A:598:PHE:HB3	1.94	0.50
1:D:477:ARG:HA	1:D:480:PHE:HD2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:ARG:HA	1:E:480:PHE:HD2	1.77	0.50
1:J:293:ASP:HB3	1:J:297:GLY:H	1.76	0.50
1:J:315:GLU:HG3	1:L:278:ASN:HB3	1.93	0.50
1:K:5:LYS:CE	1:K:5:LYS:NZ	2.75	0.50
1:M:72:PHE:CE2	1:M:96:VAL:HG23	2.46	0.50
1:M:77:GLU:HA	1:M:80:ARG:HH22	1.75	0.50
1:C:19:LEU:HB3	1:C:80:ARG:HD2	1.93	0.50
1:K:477:ARG:HA	1:K:480:PHE:HD2	1.77	0.50
1:L:243:GLY:O	1:M:238:THR:HG21	2.11	0.50
1:J:39:LEU:HD13	1:J:52:HIS:NE2	2.27	0.50
1:I:19:LEU:HB3	1:I:80:ARG:HD2	1.93	0.49
1:I:48:PHE:HB3	1:I:326:VAL:HG22	1.94	0.49
1:E:48:PHE:HB3	1:E:326:VAL:HG22	1.94	0.49
1:M:477:ARG:HA	1:M:480:PHE:HD2	1.77	0.49
1:H:467:LEU:HA	1:J:150:ILE:O	2.11	0.49
1:H:465:ASP:HB3	1:H:467:LEU:H	1.77	0.49
1:F:97:LEU:CG	1:F:528:THR:OG1	2.60	0.49
1:D:249:ARG:NE	1:D:331:ILE:HG21	2.25	0.49
1:L:66:ALA:HB3	1:L:99:ARG:HH21	1.76	0.49
1:C:477:ARG:HA	1:C:480:PHE:HD2	1.77	0.49
1:I:477:ARG:HA	1:I:480:PHE:HD2	1.77	0.49
1:D:55:GLU:O	1:D:58:GLU:HB3	2.11	0.49
1:J:455:THR:HA	1:J:486:PHE:O	2.11	0.49
1:A:2:VAL:HA	1:A:5:LYS:HB3	1.94	0.49
1:L:407:ILE:HD11	1:L:431:HIS:CD2	2.46	0.49
1:D:68:ASP:HA	1:D:101:ASP:OD2	2.12	0.49
1:A:24:LEU:CA	1:A:81:GLN:NE2	2.73	0.49
1:C:150:ILE:O	1:G:467:LEU:HD12	2.12	0.49
1:I:272:ARG:NH1	1:I:316:TYR:HA	2.22	0.49
1:L:172:HIS:NE2	1:L:532:SER:HB3	2.27	0.49
1:C:14:LYS:HE2	1:C:514:PHE:HZ	1.67	0.49
1:I:269:TRP:O	1:I:273:ILE:HG13	2.12	0.49
1:J:305:ILE:C	1:J:307:SER:HA	2.33	0.49
1:A:59:LEU:HD11	1:A:87:MET:SD	2.52	0.49
1:E:226:PHE:HE1	1:E:270:ARG:CZ	2.26	0.49
1:D:38:ILE:HD12	1:F:605:ARG:HH21	1.78	0.49
1:A:72:PHE:CE2	1:A:96:VAL:CB	2.89	0.49
1:M:79:ALA:HB3	1:M:88:PHE:HE1	1.68	0.49
1:H:249:ARG:NE	1:H:331:ILE:HG21	2.25	0.49
1:D:407:ILE:HD11	1:D:431:HIS:CD2	2.46	0.49
1:G:477:ARG:HA	1:G:480:PHE:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:477:ARG:HA	1:L:480:PHE:HD2	1.77	0.49
1:C:10:MET:HB3	1:C:514:PHE:CE2	2.48	0.49
1:F:249:ARG:NE	1:F:331:ILE:HG21	2.25	0.49
1:G:306:GLU:N	1:G:307:SER:HA	2.28	0.49
1:H:249:ARG:HG2	1:H:250:PRO:O	2.13	0.49
1:G:477:ARG:HG2	1:G:598:PHE:HB3	1.93	0.49
1:L:414:LEU:HB2	1:L:426:VAL:HG23	1.95	0.49
1:A:48:PHE:HB3	1:A:326:VAL:HG22	1.93	0.49
1:C:48:PHE:HB3	1:C:326:VAL:HG22	1.94	0.49
1:A:477:ARG:HA	1:A:480:PHE:HD2	1.77	0.49
1:D:454:SER:O	1:D:487:PHE:HA	2.13	0.49
1:C:463:LYS:HD3	1:C:550:GLU:HG2	1.95	0.49
1:M:454:SER:O	1:M:487:PHE:HA	2.13	0.49
1:F:463:LYS:HD3	1:F:550:GLU:HG2	1.95	0.49
1:J:119:VAL:HG11	1:J:428:VAL:HG11	1.95	0.49
1:D:119:VAL:HG11	1:D:428:VAL:HG11	1.95	0.49
1:K:12:LEU:HD13	1:K:80:ARG:NH2	2.27	0.49
1:K:59:LEU:HD13	1:K:87:MET:CE	2.42	0.49
1:K:407:ILE:HD11	1:K:431:HIS:CD2	2.46	0.49
1:L:573:VAL:HG12	1:L:584:ARG:HB2	1.95	0.49
1:I:527:SER:HA	1:I:584:ARG:HB3	1.94	0.49
1:F:119:VAL:HG11	1:F:428:VAL:HG11	1.95	0.49
1:A:38:ILE:HG12	1:G:605:ARG:HH22	1.78	0.49
1:E:151:LEU:HA	1:F:467:LEU:HD22	1.95	0.49
1:E:2:VAL:HA	1:E:5:LYS:HB3	1.95	0.49
1:G:465:ASP:HB3	1:G:467:LEU:H	1.78	0.49
1:J:407:ILE:HD11	1:J:431:HIS:CD2	2.46	0.49
1:G:407:ILE:HD11	1:G:431:HIS:CD2	2.46	0.49
1:D:268:ARG:HH11	1:F:271:GLU:HA	1.77	0.49
1:E:22:GLU:HB2	1:E:81:GLN:HB3	1.95	0.49
1:E:463:LYS:HD3	1:E:550:GLU:HG2	1.95	0.49
1:L:454:SER:O	1:L:487:PHE:HA	2.13	0.49
1:E:454:SER:O	1:E:487:PHE:HA	2.13	0.49
1:J:22:GLU:HB2	1:J:81:GLN:HB3	1.95	0.49
1:A:454:SER:O	1:A:487:PHE:HA	2.13	0.49
1:L:48:PHE:HB3	1:L:326:VAL:HG22	1.93	0.48
1:I:38:ILE:HD11	1:I:55:GLU:HG2	1.94	0.48
1:M:119:VAL:HG11	1:M:428:VAL:HG11	1.95	0.48
1:H:454:SER:O	1:H:487:PHE:HA	2.13	0.48
1:E:414:LEU:HB2	1:E:426:VAL:HG23	1.95	0.48
1:M:2:VAL:HA	1:M:5:LYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD22	1:A:87:MET:HG2	1.95	0.48
1:E:19:LEU:HB3	1:E:80:ARG:HD2	1.94	0.48
1:H:32:ARG:HH22	1:H:75:LEU:HD22	1.78	0.48
1:C:407:ILE:HD11	1:C:431:HIS:CD2	2.46	0.48
1:F:477:ARG:HA	1:F:480:PHE:HD2	1.77	0.48
1:H:119:VAL:HG11	1:H:428:VAL:HG11	1.95	0.48
1:C:414:LEU:HB2	1:C:426:VAL:HG23	1.95	0.48
1:F:36:VAL:HG11	1:F:59:LEU:HD11	1.94	0.48
1:M:463:LYS:HD3	1:M:550:GLU:HG2	1.95	0.48
1:G:463:LYS:HD3	1:G:550:GLU:HG2	1.95	0.48
1:J:414:LEU:HB2	1:J:426:VAL:HG23	1.95	0.48
1:D:232:GLY:HA3	1:E:338:PHE:HZ	1.78	0.48
1:C:151:LEU:HD12	1:G:467:LEU:HD11	1.76	0.48
1:M:249:ARG:HG2	1:M:250:PRO:O	2.13	0.48
1:I:275:ASP:HA	1:I:278:ASN:ND2	2.28	0.48
1:E:267:VAL:HA	1:E:270:ARG:HH21	1.79	0.48
1:H:48:PHE:HB3	1:H:326:VAL:HG22	1.94	0.48
1:I:477:ARG:HG2	1:I:598:PHE:HB3	1.94	0.48
1:F:414:LEU:HB2	1:F:426:VAL:HG23	1.95	0.48
1:M:10:MET:SD	1:M:517:LEU:HB3	2.54	0.48
1:K:119:VAL:HG11	1:K:428:VAL:HG11	1.95	0.48
1:I:119:VAL:HG11	1:I:428:VAL:HG11	1.95	0.48
1:K:271:GLU:HA	1:M:268:ARG:HH11	1.77	0.48
1:M:245:GLN:O	1:M:341:ASN:HB2	2.14	0.48
1:K:45:PHE:HE1	1:K:52:HIS:HB3	1.78	0.48
1:A:463:LYS:HD3	1:A:550:GLU:HG2	1.95	0.48
1:H:463:LYS:HD3	1:H:550:GLU:HG2	1.95	0.48
1:A:24:LEU:CD2	1:A:81:GLN:HB2	2.44	0.48
1:C:2:VAL:HA	1:C:5:LYS:HB3	1.94	0.48
1:J:2:VAL:HA	1:J:5:LYS:HB3	1.95	0.48
1:C:169:HIS:CE1	1:C:581:CYS:SG	3.04	0.48
1:C:275:ASP:OD1	1:F:316:TYR:CE1	2.66	0.48
1:F:48:PHE:HB3	1:F:326:VAL:HG22	1.94	0.48
1:I:463:LYS:HD3	1:I:550:GLU:HG2	1.95	0.48
1:K:463:LYS:HD3	1:K:550:GLU:HG2	1.95	0.48
1:F:2:VAL:HA	1:F:5:LYS:HB3	1.95	0.48
1:H:467:LEU:HD12	1:J:150:ILE:O	2.06	0.48
1:A:66:ALA:HB1	1:A:99:ARG:NH2	2.06	0.48
1:G:249:ARG:NE	1:G:331:ILE:HG21	2.25	0.48
1:E:169:HIS:CE1	1:E:581:CYS:SG	3.04	0.48
1:J:477:ARG:HG2	1:J:598:PHE:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:477:ARG:HG2	1:H:598:PHE:HB3	1.94	0.48
1:D:365:ASP:O	1:D:369:GLN:HG2	2.14	0.48
1:A:365:ASP:O	1:A:369:GLN:HG2	2.14	0.48
1:H:365:ASP:O	1:H:369:GLN:HG2	2.14	0.48
1:H:195:GLU:H	1:H:299:ASP:HA	1.79	0.48
1:K:23:LYS:O	1:K:81:GLN:HB3	2.14	0.48
1:A:249:ARG:NE	1:A:331:ILE:HG21	2.24	0.48
1:I:169:HIS:CE1	1:I:581:CYS:SG	3.04	0.48
1:I:407:ILE:HD11	1:I:431:HIS:CD2	2.46	0.48
1:C:195:GLU:H	1:C:299:ASP:HA	1.79	0.48
1:E:195:GLU:H	1:E:299:ASP:HA	1.79	0.48
1:F:454:SER:O	1:F:487:PHE:HA	2.13	0.48
1:H:414:LEU:HB2	1:H:426:VAL:HG23	1.95	0.48
1:L:463:LYS:HD3	1:L:550:GLU:HG2	1.95	0.48
1:G:365:ASP:O	1:G:369:GLN:HG2	2.14	0.48
1:A:24:LEU:CB	1:A:81:GLN:NE2	2.76	0.48
1:D:169:HIS:CE1	1:D:581:CYS:SG	3.04	0.48
1:J:549:MET:HB3	1:J:551:PHE:HE1	1.79	0.48
1:A:263:VAL:O	1:A:266:MET:HB2	2.14	0.48
1:I:463:LYS:HG3	1:I:471:LEU:HD21	1.96	0.48
1:G:179:ALA:O	1:G:308:SER:HA	2.13	0.48
1:K:454:SER:O	1:K:487:PHE:HA	2.13	0.48
1:G:195:GLU:HB2	1:G:298:THR:HB	1.94	0.48
1:I:22:GLU:HB2	1:I:81:GLN:HB3	1.95	0.48
1:E:119:VAL:HG11	1:E:428:VAL:HG11	1.95	0.48
1:L:103:LYS:HG3	1:L:525:GLU:O	2.13	0.48
1:G:24:LEU:HD13	1:G:81:GLN:HE21	1.67	0.48
1:G:60:TYR:HH	1:G:90:TYR:HE2	1.53	0.48
1:L:249:ARG:NE	1:L:331:ILE:HG21	2.26	0.48
1:J:169:HIS:CE1	1:J:581:CYS:SG	3.04	0.48
1:K:549:MET:HB3	1:K:551:PHE:HE1	1.79	0.48
1:C:463:LYS:HG3	1:C:471:LEU:HD21	1.96	0.48
1:J:34:LYS:HD2	1:J:35:GLY:N	2.28	0.48
1:C:454:SER:O	1:C:487:PHE:HA	2.13	0.48
1:I:414:LEU:HB2	1:I:426:VAL:HG23	1.95	0.48
1:M:365:ASP:O	1:M:369:GLN:HG2	2.14	0.48
1:M:195:GLU:H	1:M:299:ASP:HA	1.79	0.48
1:J:365:ASP:O	1:J:369:GLN:HG2	2.14	0.48
1:A:76:CYS:SG	1:A:92:VAL:HG21	2.54	0.48
1:M:22:GLU:HB2	1:M:81:GLN:CB	2.41	0.48
1:C:249:ARG:NE	1:C:331:ILE:HG21	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:CD2	1:A:367:ILE:HG23	2.44	0.48
1:G:512:ARG:NH2	1:G:523:VAL:HG21	2.29	0.48
1:H:549:MET:HB3	1:H:551:PHE:HE1	1.79	0.48
1:L:463:LYS:HG3	1:L:471:LEU:HD21	1.96	0.48
1:M:414:LEU:HB2	1:M:426:VAL:HG23	1.95	0.48
1:L:365:ASP:O	1:L:369:GLN:HG2	2.14	0.48
1:L:195:GLU:H	1:L:299:ASP:HA	1.79	0.48
1:A:467:LEU:HG	1:D:150:ILE:O	2.14	0.48
1:C:22:GLU:HB2	1:C:81:GLN:HB3	1.95	0.48
1:I:365:ASP:O	1:I:369:GLN:HG2	2.14	0.48
1:A:22:GLU:HB3	1:A:24:LEU:N	2.29	0.47
1:A:24:LEU:CD1	1:A:27:ASP:CA	2.87	0.47
1:M:72:PHE:CZ	1:M:96:VAL:HB	2.49	0.47
1:F:38:ILE:HD13	1:F:38:ILE:H	1.79	0.47
1:J:454:SER:O	1:J:487:PHE:HA	2.13	0.47
1:J:102:CYS:O	1:J:105:ILE:HG22	2.14	0.47
1:I:268:ARG:NH1	1:J:274:LEU:HB2	2.18	0.47
1:L:529:GLU:HA	1:L:533:CYS:HB3	1.96	0.47
1:L:549:MET:HB3	1:L:551:PHE:HE1	1.79	0.47
1:I:549:MET:HB3	1:I:551:PHE:HE1	1.79	0.47
1:H:463:LYS:HG3	1:H:471:LEU:HD21	1.96	0.47
1:F:108:PRO:HA	1:F:109:PRO:HD3	1.81	0.47
1:D:414:LEU:HB2	1:D:426:VAL:HG23	1.95	0.47
1:A:549:MET:HB3	1:A:551:PHE:HE1	1.79	0.47
1:F:463:LYS:HG3	1:F:471:LEU:HD21	1.96	0.47
1:G:463:LYS:HG3	1:G:471:LEU:HD21	1.96	0.47
1:L:119:VAL:HG11	1:L:428:VAL:HG11	1.95	0.47
1:D:463:LYS:HD3	1:D:550:GLU:HG2	1.95	0.47
1:I:454:SER:O	1:I:487:PHE:HA	2.13	0.47
1:J:463:LYS:HD3	1:J:550:GLU:HG2	1.95	0.47
1:E:365:ASP:O	1:E:369:GLN:HG2	2.14	0.47
1:C:119:VAL:HG11	1:C:428:VAL:HG11	1.95	0.47
1:C:365:ASP:O	1:C:369:GLN:HG2	2.14	0.47
1:F:549:MET:HB3	1:F:551:PHE:HE1	1.79	0.47
1:K:195:GLU:H	1:K:299:ASP:HA	1.79	0.47
1:L:4:ASP:HA	1:L:7:ALA:HB3	1.95	0.47
1:G:454:SER:O	1:G:487:PHE:HA	2.13	0.47
1:H:467:LEU:HB3	1:J:149:ASN:OD1	2.15	0.47
1:G:304:ILE:HA	1:G:311:SER:OG	2.14	0.47
1:A:512:ARG:HH22	1:A:523:VAL:HG21	1.80	0.47
1:I:24:LEU:HD12	1:I:81:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:414:LEU:HB2	1:K:426:VAL:HG23	1.95	0.47
1:H:19:LEU:HD22	1:H:80:ARG:HH11	1.79	0.47
1:C:38:ILE:HD13	1:D:605:ARG:NH1	2.30	0.47
1:M:463:LYS:HG3	1:M:471:LEU:HD21	1.96	0.47
1:G:414:LEU:HB2	1:G:426:VAL:HG23	1.95	0.47
1:K:467:LEU:HD22	1:L:151:LEU:HA	1.97	0.47
1:G:39:LEU:HD21	1:G:45:PHE:HB2	1.97	0.47
1:M:64:TYR:OH	1:M:94:VAL:CG1	2.45	0.47
1:J:63:LEU:HA	1:J:75:LEU:CD2	2.33	0.47
1:J:267:VAL:O	1:J:271:GLU:HG2	2.15	0.47
1:M:249:ARG:NE	1:M:331:ILE:HG21	2.26	0.47
1:C:549:MET:HB3	1:C:551:PHE:HE1	1.79	0.47
1:G:549:MET:HB3	1:G:551:PHE:HE1	1.79	0.47
1:I:57:THR:HA	1:I:60:TYR:CD2	2.50	0.47
1:A:150:ILE:O	1:D:467:LEU:HG	2.15	0.47
1:K:365:ASP:O	1:K:369:GLN:HG2	2.14	0.47
1:H:38:ILE:HD12	1:M:605:ARG:NH2	2.30	0.47
1:A:258:LEU:HD22	1:A:330:ASN:HD21	1.80	0.47
1:G:119:VAL:HG11	1:G:428:VAL:HG11	1.95	0.47
1:I:32:ARG:NH2	1:I:62:ALA:HA	2.30	0.47
1:H:258:LEU:HD22	1:H:330:ASN:HD21	1.80	0.47
1:M:19:LEU:HD13	1:M:80:ARG:HH11	1.80	0.47
1:F:249:ARG:HG2	1:F:250:PRO:O	2.15	0.47
1:E:463:LYS:HG3	1:E:471:LEU:HD21	1.96	0.47
1:C:587:ARG:NH2	1:I:568:LEU:HB2	2.30	0.47
1:F:365:ASP:O	1:F:369:GLN:HG2	2.14	0.47
1:A:278:ASN:HB3	1:E:315:GLU:HG3	1.96	0.47
1:L:107:VAL:HG21	1:L:528:THR:OG1	2.15	0.47
1:M:30:ASP:HB3	1:M:32:ARG:HB2	1.95	0.47
1:A:463:LYS:HG3	1:A:471:LEU:HD21	1.96	0.47
1:D:463:LYS:HG3	1:D:471:LEU:HD21	1.96	0.47
1:E:467:LEU:HD22	1:F:151:LEU:HA	1.97	0.47
1:K:268:ARG:HD2	1:K:272:ARG:HE	1.79	0.47
1:M:20:THR:HG23	1:M:83:VAL:O	2.15	0.47
1:A:169:HIS:CE1	1:A:581:CYS:SG	3.04	0.47
1:C:275:ASP:N	1:F:268:ARG:HH12	2.12	0.47
1:M:549:MET:HB3	1:M:551:PHE:HE1	1.79	0.47
1:J:463:LYS:HG3	1:J:471:LEU:HD21	1.96	0.47
1:K:273:ILE:HG12	1:K:317:TYR:HD1	1.80	0.47
1:I:200:MET:SD	1:I:580:TYR:HB3	2.55	0.47
1:I:193:LYS:NZ	1:I:308:SER:OG	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:MET:SD	1:E:580:TYR:HB3	2.55	0.47
1:D:403:ILE:HG21	1:D:541:ILE:HG21	1.97	0.47
1:G:169:HIS:CE1	1:G:581:CYS:SG	3.04	0.46
1:I:525:GLU:HB2	1:I:570:GLU:HG2	1.97	0.46
1:C:149:ASN:OD1	1:G:467:LEU:HG	2.15	0.46
1:M:24:LEU:HD22	1:M:82:ILE:CG2	2.45	0.46
1:E:549:MET:HB3	1:E:551:PHE:HE1	1.79	0.46
1:D:549:MET:HB3	1:D:551:PHE:HE1	1.79	0.46
1:I:528:THR:O	1:I:574:CYS:HB2	2.15	0.46
1:I:103:LYS:NZ	1:I:525:GLU:O	2.49	0.46
1:M:258:LEU:HD22	1:M:330:ASN:HD21	1.80	0.46
1:E:108:PRO:HA	1:E:109:PRO:HD3	1.81	0.46
1:G:23:LYS:O	1:G:81:GLN:NE2	2.48	0.46
1:L:258:LEU:HD22	1:L:330:ASN:HD21	1.80	0.46
1:J:200:MET:SD	1:J:580:TYR:HB3	2.55	0.46
1:F:195:GLU:H	1:F:299:ASP:HA	1.79	0.46
1:L:200:MET:SD	1:L:580:TYR:HB3	2.55	0.46
1:E:226:PHE:HE1	1:E:270:ARG:NH2	2.12	0.46
1:I:195:GLU:H	1:I:299:ASP:HA	1.79	0.46
1:M:50:ALA:HB2	1:M:323:TRP:HH2	1.80	0.46
1:F:13:PHE:CD2	1:F:16:LEU:HD22	2.51	0.46
1:D:200:MET:SD	1:D:580:TYR:HB3	2.55	0.46
1:A:195:GLU:H	1:A:299:ASP:HA	1.79	0.46
1:K:274:LEU:CD2	1:K:367:ILE:HG23	2.45	0.46
1:K:249:ARG:HG2	1:K:250:PRO:O	2.15	0.46
1:I:274:LEU:HB2	1:L:268:ARG:HH12	1.79	0.46
1:J:465:ASP:HB3	1:J:467:LEU:H	1.79	0.46
1:E:193:LYS:NZ	1:E:308:SER:OG	2.48	0.46
1:F:200:MET:SD	1:F:580:TYR:HB3	2.56	0.46
1:I:5:LYS:HG3	1:I:69:PHE:CZ	2.49	0.46
1:D:268:ARG:HH12	1:F:274:LEU:HB2	1.80	0.46
1:G:258:LEU:HD22	1:G:330:ASN:HD21	1.80	0.46
1:K:107:VAL:CG2	1:K:528:THR:OG1	2.55	0.46
1:G:32:ARG:NH2	1:G:75:LEU:CD2	2.68	0.46
1:A:120:PRO:O	1:A:123:THR:HG22	2.16	0.46
1:A:63:LEU:HA	1:A:75:LEU:HD21	1.98	0.46
1:C:258:LEU:HD22	1:C:330:ASN:HD21	1.80	0.46
1:D:258:LEU:HD22	1:D:330:ASN:HD21	1.80	0.46
1:G:24:LEU:HD11	1:G:78:GLN:HE21	1.80	0.46
1:H:169:HIS:CE1	1:H:581:CYS:SG	3.04	0.46
1:K:463:LYS:HG3	1:K:471:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:MET:SD	1:C:580:TYR:HB3	2.55	0.46
1:K:506:VAL:HG12	1:K:579:SER:HB2	1.98	0.46
1:M:386:PRO:O	1:M:452:LYS:NZ	2.49	0.46
1:A:386:PRO:O	1:A:452:LYS:NZ	2.49	0.46
1:M:200:MET:SD	1:M:580:TYR:HB3	2.56	0.46
1:I:272:ARG:CG	1:I:316:TYR:CE1	2.98	0.46
1:I:531:CYS:HB2	1:I:574:CYS:SG	2.56	0.46
1:A:245:GLN:O	1:A:341:ASN:HB2	2.16	0.46
1:A:80:ARG:CB	1:A:88:PHE:CD2	2.98	0.46
1:M:529:GLU:HG3	1:M:574:CYS:SG	2.55	0.46
1:A:465:ASP:HB3	1:A:467:LEU:H	1.80	0.46
1:C:108:PRO:HA	1:C:109:PRO:HD3	1.81	0.46
1:A:171:TRP:HA	1:A:348:THR:HG23	1.98	0.46
1:M:556:MET:SD	1:M:597:PRO:HG3	2.56	0.46
1:I:245:GLN:O	1:I:341:ASN:HB2	2.16	0.46
1:D:10:MET:SD	1:D:517:LEU:HB3	2.56	0.46
1:L:193:LYS:NZ	1:L:308:SER:OG	2.48	0.46
1:D:245:GLN:O	1:D:341:ASN:HB2	2.16	0.46
1:H:200:MET:SD	1:H:580:TYR:HB3	2.56	0.46
1:L:243:GLY:C	1:M:238:THR:HG21	2.36	0.45
1:L:245:GLN:O	1:L:341:ASN:HB2	2.16	0.45
1:C:556:MET:SD	1:C:597:PRO:HG3	2.56	0.45
1:K:219:ARG:HD2	1:K:466:GLU:OE2	2.16	0.45
1:L:556:MET:SD	1:L:597:PRO:HG3	2.56	0.45
1:E:258:LEU:HD22	1:E:330:ASN:HD21	1.80	0.45
1:A:24:LEU:H	1:A:81:GLN:HB3	1.80	0.45
1:I:13:PHE:HB2	1:I:514:PHE:CZ	2.50	0.45
1:M:19:LEU:HD22	1:M:80:ARG:NH1	2.31	0.45
1:L:268:ARG:NH2	1:L:272:ARG:HH21	2.15	0.45
1:A:273:ILE:HG12	1:A:317:TYR:HD1	1.81	0.45
1:H:556:MET:SD	1:H:597:PRO:HG3	2.57	0.45
1:L:386:PRO:O	1:L:452:LYS:NZ	2.49	0.45
1:G:171:TRP:HA	1:G:348:THR:HG23	1.99	0.45
1:H:245:GLN:O	1:H:341:ASN:HB2	2.16	0.45
1:H:171:TRP:HA	1:H:348:THR:HG23	1.98	0.45
1:C:171:TRP:HA	1:C:348:THR:HG23	1.99	0.45
1:K:258:LEU:HD22	1:K:330:ASN:HD21	1.80	0.45
1:G:200:MET:SD	1:G:580:TYR:HB3	2.55	0.45
1:K:5:LYS:HB2	1:K:5:LYS:HE2	1.36	0.45
1:H:9:LEU:HD11	1:H:69:PHE:HZ	1.81	0.45
1:M:5:LYS:NZ	1:M:69:PHE:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:99:ARG:HH12	1:K:101:ASP:CG	2.19	0.45
1:F:258:LEU:HD22	1:F:330:ASN:HD21	1.80	0.45
1:F:171:TRP:HA	1:F:348:THR:HG23	1.98	0.45
1:J:556:MET:SD	1:J:597:PRO:HG3	2.56	0.45
1:K:200:MET:SD	1:K:580:TYR:HB3	2.56	0.45
1:L:59:LEU:HD11	1:L:87:MET:HE1	1.97	0.45
1:A:200:MET:SD	1:A:580:TYR:HB3	2.55	0.45
1:K:9:LEU:HD11	1:K:73:ILE:HD11	1.99	0.45
1:C:11:PRO:HA	1:C:14:LYS:HE3	1.99	0.45
1:L:549:MET:O	1:L:621:LYS:HA	2.17	0.45
1:H:549:MET:O	1:H:621:LYS:HA	2.17	0.45
1:A:127:ALA:HB2	1:A:142:VAL:CG2	2.45	0.45
1:A:266:MET:SD	1:A:323:TRP:HB3	2.56	0.45
1:J:55:GLU:O	1:J:58:GLU:HB3	2.16	0.45
1:I:258:LEU:HD22	1:I:330:ASN:HD21	1.80	0.45
1:A:556:MET:SD	1:A:597:PRO:HG3	2.57	0.45
1:E:556:MET:SD	1:E:597:PRO:HG3	2.56	0.45
1:K:20:THR:HG23	1:K:83:VAL:O	2.16	0.45
1:A:128:ASN:HD22	1:A:414:LEU:HD12	1.79	0.45
1:M:169:HIS:CE1	1:M:581:CYS:SG	3.04	0.45
1:J:249:ARG:HG2	1:J:250:PRO:O	2.17	0.45
1:I:271:GLU:HA	1:L:268:ARG:HH12	1.81	0.45
1:I:275:ASP:HA	1:I:278:ASN:HD22	1.82	0.45
1:J:245:GLN:O	1:J:341:ASN:HB2	2.16	0.45
1:K:393:VAL:HB	1:K:618:THR:OG1	2.17	0.45
1:F:273:ILE:HG12	1:F:317:TYR:HD1	1.82	0.45
1:F:556:MET:SD	1:F:597:PRO:HG3	2.56	0.45
1:H:11:PRO:HA	1:H:14:LYS:HE3	1.99	0.45
1:K:556:MET:SD	1:K:597:PRO:HG3	2.57	0.45
1:J:258:LEU:HD22	1:J:330:ASN:HD21	1.80	0.45
1:E:171:TRP:HA	1:E:348:THR:HG23	1.99	0.45
1:D:171:TRP:HA	1:D:348:THR:HG23	1.99	0.45
1:A:24:LEU:CD2	1:A:82:ILE:CG2	2.92	0.45
1:J:290:ILE:HD12	1:J:300:ILE:HD13	1.95	0.45
1:L:8:ARG:NH2	1:L:73:ILE:CB	2.80	0.45
1:H:8:ARG:NH1	1:H:73:ILE:HG21	2.30	0.45
1:G:59:LEU:HD11	1:G:87:MET:CE	2.45	0.45
1:I:549:MET:O	1:I:621:LYS:HA	2.16	0.45
1:M:549:MET:O	1:M:621:LYS:HA	2.17	0.45
1:H:362:ARG:HA	1:H:362:ARG:HD3	1.84	0.45
1:G:245:GLN:O	1:G:341:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:MET:SD	1:D:597:PRO:HG3	2.56	0.45
1:J:171:TRP:HA	1:J:348:THR:HG23	1.99	0.45
1:J:354:ASP:HA	1:J:355:PRO:HD3	1.85	0.45
1:K:5:LYS:NZ	1:K:72:PHE:HD2	2.15	0.45
1:L:169:HIS:CE1	1:L:581:CYS:SG	3.04	0.45
1:K:549:MET:O	1:K:621:LYS:HA	2.17	0.45
1:E:549:MET:O	1:E:621:LYS:HA	2.16	0.45
1:M:228:GLU:HA	1:M:229:PRO:HD3	1.88	0.45
1:D:393:VAL:HB	1:D:618:THR:OG1	2.17	0.45
1:J:393:VAL:HB	1:J:618:THR:OG1	2.17	0.45
1:C:245:GLN:O	1:C:341:ASN:HB2	2.17	0.45
1:E:393:VAL:HB	1:E:618:THR:OG1	2.17	0.45
1:C:354:ASP:HA	1:C:355:PRO:HD3	1.85	0.45
1:J:9:LEU:HD22	1:J:105:ILE:HD11	1.99	0.45
1:H:270:ARG:NH1	1:K:264:GLN:OE1	2.49	0.45
1:H:243:GLY:N	1:I:125:ASN:HD21	2.00	0.45
1:G:549:MET:O	1:G:621:LYS:HA	2.17	0.45
1:D:549:MET:O	1:D:621:LYS:HA	2.17	0.45
1:J:549:MET:O	1:J:621:LYS:HA	2.17	0.45
1:G:11:PRO:HA	1:G:14:LYS:HE3	1.99	0.45
1:C:228:GLU:HA	1:C:229:PRO:HD3	1.88	0.45
1:A:393:VAL:HB	1:A:618:THR:OG1	2.17	0.45
1:I:270:ARG:HD3	1:I:320:LEU:HD21	1.98	0.45
1:K:193:LYS:NZ	1:K:308:SER:OG	2.48	0.45
1:H:386:PRO:O	1:H:452:LYS:NZ	2.49	0.45
1:E:245:GLN:O	1:E:341:ASN:HB2	2.16	0.45
1:K:108:PRO:HA	1:K:109:PRO:HD3	1.81	0.45
1:M:250:PRO:HB2	1:M:253:TYR:CE1	2.52	0.45
1:A:528:THR:O	1:A:532:SER:HB3	2.16	0.45
1:J:467:LEU:HD22	1:J:470:LYS:HE3	1.98	0.45
1:H:10:MET:SD	1:H:517:LEU:HB3	2.57	0.45
1:M:171:TRP:HA	1:M:348:THR:HG23	1.99	0.45
1:M:263:VAL:O	1:M:266:MET:HB2	2.17	0.45
1:I:171:TRP:HA	1:I:348:THR:HG23	1.99	0.45
1:G:304:ILE:HA	1:G:311:SER:CB	2.47	0.45
1:E:268:ARG:O	1:E:272:ARG:HG3	2.17	0.45
1:K:403:ILE:HG21	1:K:541:ILE:HG21	1.99	0.45
1:E:273:ILE:HG12	1:E:317:TYR:HD1	1.81	0.45
1:I:556:MET:SD	1:I:597:PRO:HG3	2.56	0.45
1:H:393:VAL:HB	1:H:618:THR:OG1	2.17	0.45
1:K:171:TRP:HA	1:K:348:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PHE:HZ	1:A:89:VAL:HG23	1.82	0.44
1:H:467:LEU:CD2	1:J:151:LEU:HD13	2.45	0.44
1:H:8:ARG:CZ	1:H:73:ILE:HG13	2.46	0.44
1:I:249:ARG:NE	1:I:331:ILE:HG21	2.25	0.44
1:F:253:TYR:OH	1:G:250:PRO:HG3	2.17	0.44
1:A:205:CYS:SG	1:A:358:TYR:HD1	2.40	0.44
1:A:38:ILE:HD13	1:G:605:ARG:HH12	1.82	0.44
1:A:316:TYR:HE1	1:G:275:ASP:OD1	1.99	0.44
1:K:354:ASP:HA	1:K:355:PRO:HD3	1.85	0.44
1:M:393:VAL:HB	1:M:618:THR:OG1	2.17	0.44
1:I:403:ILE:HG21	1:I:541:ILE:HG21	1.99	0.44
1:F:386:PRO:O	1:F:452:LYS:NZ	2.49	0.44
1:F:403:ILE:HG21	1:F:541:ILE:HG21	1.99	0.44
1:A:22:GLU:HB3	1:A:24:LEU:H	1.82	0.44
1:E:107:VAL:CG2	1:E:528:THR:OG1	2.56	0.44
1:G:29:ARG:HB3	1:G:78:GLN:HE22	1.82	0.44
1:D:270:ARG:HD3	1:D:363:PHE:CZ	2.52	0.44
1:F:245:GLN:O	1:F:341:ASN:HB2	2.16	0.44
1:H:605:ARG:NH2	1:K:38:ILE:HD12	2.32	0.44
1:D:386:PRO:O	1:D:452:LYS:NZ	2.49	0.44
1:L:20:THR:OG1	1:L:85:GLU:HB3	2.18	0.44
1:M:445:GLU:OE2	1:M:494:LYS:NZ	2.50	0.44
1:I:273:ILE:HG12	1:I:317:TYR:CD1	2.40	0.44
1:E:512:ARG:CB	1:E:531:CYS:SG	3.02	0.44
1:L:231:GLU:O	1:L:249:ARG:HD2	2.17	0.44
1:E:205:CYS:SG	1:E:358:TYR:HD1	2.40	0.44
1:K:386:PRO:O	1:K:452:LYS:NZ	2.49	0.44
1:L:354:ASP:HA	1:L:355:PRO:HD3	1.85	0.44
1:L:393:VAL:HB	1:L:618:THR:OG1	2.17	0.44
1:G:393:VAL:HB	1:G:618:THR:OG1	2.17	0.44
1:I:386:PRO:O	1:I:452:LYS:NZ	2.49	0.44
1:L:162:GLU:HG2	1:L:353:ARG:CB	2.47	0.44
1:I:205:CYS:SG	1:I:358:TYR:HD1	2.40	0.44
1:F:549:MET:O	1:F:621:LYS:HA	2.16	0.44
1:L:11:PRO:HA	1:L:14:LYS:HE3	1.99	0.44
1:F:458:ILE:HG23	1:F:555:VAL:HG22	2.00	0.44
1:M:403:ILE:HG21	1:M:541:ILE:HG21	1.99	0.44
1:G:403:ILE:HG21	1:G:541:ILE:HG21	1.99	0.44
1:K:11:PRO:HA	1:K:14:LYS:HE3	1.99	0.44
1:J:11:PRO:HA	1:J:14:LYS:HE3	1.99	0.44
1:L:403:ILE:HG21	1:L:541:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:97:LEU:CG	1:K:528:THR:CB	2.96	0.44
1:E:96:VAL:HG22	1:E:105:ILE:CG2	2.45	0.44
1:C:231:GLU:O	1:C:249:ARG:HD2	2.18	0.44
1:K:169:HIS:CE1	1:K:581:CYS:SG	3.04	0.44
1:C:162:GLU:HG2	1:C:353:ARG:CB	2.47	0.44
1:A:549:MET:O	1:A:621:LYS:HA	2.17	0.44
1:F:267:VAL:O	1:F:271:GLU:HG2	2.17	0.44
1:L:99:ARG:HH12	1:L:101:ASP:CG	2.21	0.44
1:M:11:PRO:HA	1:M:14:LYS:HE3	1.99	0.44
1:A:193:LYS:NZ	1:A:308:SER:OG	2.48	0.44
1:M:467:LEU:HD22	1:M:470:LYS:HE3	1.98	0.44
1:G:556:MET:SD	1:G:597:PRO:HG3	2.57	0.44
1:D:243:GLY:CA	1:E:125:ASN:ND2	2.80	0.44
1:C:403:ILE:HG21	1:C:541:ILE:HG21	1.99	0.44
1:A:59:LEU:CD2	1:A:87:MET:CE	2.96	0.44
1:H:458:ILE:HG23	1:H:555:VAL:HG22	2.00	0.44
1:K:64:TYR:OH	1:K:98:HIS:HB2	2.18	0.44
1:C:205:CYS:SG	1:C:358:TYR:HD1	2.40	0.44
1:L:205:CYS:SG	1:L:358:TYR:HD1	2.41	0.44
1:I:393:VAL:HB	1:I:618:THR:OG1	2.17	0.44
1:E:403:ILE:HG21	1:E:541:ILE:HG21	1.99	0.44
1:E:11:PRO:HA	1:E:14:LYS:HE3	1.99	0.44
1:M:5:LYS:HG3	1:M:69:PHE:CZ	2.53	0.44
1:L:8:ARG:CZ	1:L:73:ILE:HG13	2.45	0.44
1:J:512:ARG:HH22	1:J:523:VAL:HG21	1.82	0.44
1:F:162:GLU:HG2	1:F:353:ARG:CB	2.47	0.44
1:K:245:GLN:O	1:K:341:ASN:HB2	2.16	0.44
1:G:59:LEU:CD1	1:G:87:MET:CE	2.95	0.44
1:L:458:ILE:HG23	1:L:555:VAL:HG22	2.00	0.44
1:A:50:ALA:HB2	1:A:323:TRP:CH2	2.53	0.44
1:C:447:ASN:HB2	1:I:288:ASN:HD21	1.81	0.44
1:L:171:TRP:HA	1:L:348:THR:HG23	1.99	0.44
1:M:47:CYS:HB2	1:M:346:SER:O	2.17	0.44
1:M:231:GLU:O	1:M:249:ARG:HD2	2.18	0.44
1:C:467:LEU:HD11	1:G:149:ASN:OD1	2.18	0.44
1:A:103:LYS:HD2	1:A:526:ASP:OD1	2.18	0.44
1:A:10:MET:SD	1:A:517:LEU:HB3	2.58	0.44
1:M:506:VAL:HG12	1:M:579:SER:HB2	1.99	0.44
1:F:97:LEU:CD2	1:F:528:THR:H	2.30	0.44
1:H:205:CYS:SG	1:H:358:TYR:HD1	2.41	0.44
1:E:458:ILE:HG23	1:E:555:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ILE:HG23	1:A:555:VAL:HG22	2.00	0.44
1:C:393:VAL:HB	1:C:618:THR:OG1	2.17	0.44
1:J:386:PRO:O	1:J:452:LYS:NZ	2.49	0.44
1:A:403:ILE:HG21	1:A:541:ILE:HG21	1.99	0.44
1:L:108:PRO:HA	1:L:109:PRO:HD3	1.81	0.44
1:H:263:VAL:O	1:H:266:MET:HB2	2.17	0.44
1:D:310:GLU:O	1:D:312:LYS:NZ	2.51	0.43
1:J:205:CYS:SG	1:J:358:TYR:HD1	2.40	0.43
1:K:205:CYS:SG	1:K:358:TYR:HD1	2.41	0.43
1:A:11:PRO:HA	1:A:14:LYS:HE3	1.99	0.43
1:G:386:PRO:O	1:G:452:LYS:NZ	2.49	0.43
1:A:197:PHE:O	1:A:201:HIS:ND1	2.51	0.43
1:M:197:PHE:O	1:M:201:HIS:ND1	2.51	0.43
1:K:197:PHE:O	1:K:201:HIS:ND1	2.51	0.43
1:H:534:GLY:HA2	1:H:577:ALA:CB	2.48	0.43
1:F:393:VAL:HB	1:F:618:THR:OG1	2.17	0.43
1:D:11:PRO:HA	1:D:14:LYS:HE3	1.99	0.43
1:D:250:PRO:HG2	1:D:253:TYR:CZ	2.53	0.43
1:D:282:ILE:HD11	1:D:300:ILE:HD12	1.99	0.43
1:M:205:CYS:SG	1:M:358:TYR:HD1	2.40	0.43
1:C:549:MET:O	1:C:621:LYS:HA	2.17	0.43
1:A:34:LYS:NZ	1:A:58:GLU:OE1	2.48	0.43
1:G:354:ASP:HA	1:G:355:PRO:HD3	1.85	0.43
1:L:197:PHE:O	1:L:201:HIS:ND1	2.51	0.43
1:G:63:LEU:HD23	1:G:91:ALA:CB	2.38	0.43
1:G:458:ILE:HG23	1:G:555:VAL:HG22	2.00	0.43
1:G:205:CYS:SG	1:G:358:TYR:HD1	2.40	0.43
1:F:205:CYS:SG	1:F:358:TYR:HD1	2.41	0.43
1:E:386:PRO:O	1:E:452:LYS:NZ	2.49	0.43
1:I:49:HIS:CE1	1:I:51:ARG:HG2	2.54	0.43
1:L:49:HIS:CE1	1:L:51:ARG:HG2	2.54	0.43
1:C:197:PHE:O	1:C:201:HIS:ND1	2.51	0.43
1:C:513:THR:HG23	1:C:516:GLN:H	1.82	0.43
1:G:197:PHE:O	1:G:201:HIS:ND1	2.51	0.43
1:M:72:PHE:CE2	1:M:96:VAL:HG21	2.54	0.43
1:J:33:LEU:HD21	1:J:79:ALA:HB1	2.00	0.43
1:D:5:LYS:HE3	1:D:105:ILE:HG13	2.00	0.43
1:D:197:PHE:O	1:D:201:HIS:ND1	2.51	0.43
1:I:197:PHE:O	1:I:201:HIS:ND1	2.51	0.43
1:F:49:HIS:CE1	1:F:51:ARG:HG2	2.54	0.43
1:M:276:ALA:HB1	1:M:281:TYR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:PRO:HG2	1:C:253:TYR:CZ	2.54	0.43
1:M:108:PRO:HA	1:M:109:PRO:HD3	1.81	0.43
1:A:25:PRO:C	1:A:26:LEU:HG	2.38	0.43
1:H:467:LEU:HD21	1:J:151:LEU:HD12	1.99	0.43
1:C:375:PHE:CB	1:C:600:ARG:HD3	2.48	0.43
1:D:508:ILE:HD11	1:D:531:CYS:HA	2.00	0.43
1:A:266:MET:HE3	1:A:266:MET:HB3	1.86	0.43
1:L:107:VAL:HB	1:L:528:THR:HG23	1.99	0.43
1:H:193:LYS:NZ	1:H:308:SER:OG	2.48	0.43
1:M:458:ILE:HG23	1:M:555:VAL:HG22	2.00	0.43
1:J:403:ILE:HG21	1:J:541:ILE:HG21	1.99	0.43
1:K:20:THR:OG1	1:K:85:GLU:HB3	2.18	0.43
1:G:375:PHE:CB	1:G:600:ARG:HD3	2.48	0.43
1:C:525:GLU:CD	1:C:529:GLU:HA	2.39	0.43
1:D:205:CYS:SG	1:D:358:TYR:HD1	2.41	0.43
1:I:458:ILE:HG23	1:I:555:VAL:HG22	2.00	0.43
1:J:419:ASN:HD22	1:K:132:SER:CB	2.32	0.43
1:L:137:GLN:HA	1:L:423:ASP:HA	2.01	0.43
1:E:49:HIS:CE1	1:E:51:ARG:HG2	2.54	0.43
1:H:49:HIS:CE1	1:H:51:ARG:HG2	2.54	0.43
1:K:97:LEU:HG	1:K:528:THR:CB	2.49	0.43
1:E:97:LEU:CG	1:E:528:THR:CB	2.96	0.43
1:M:12:LEU:HD22	1:M:80:ARG:HH12	1.84	0.43
1:F:169:HIS:CE1	1:F:581:CYS:SG	3.04	0.43
1:K:269:TRP:O	1:K:273:ILE:HG13	2.18	0.43
1:I:103:LYS:NZ	1:I:524:SER:OG	2.46	0.43
1:H:393:VAL:HA	1:H:441:ASN:O	2.19	0.43
1:D:362:ARG:HA	1:D:362:ARG:HD3	1.84	0.43
1:D:458:ILE:HG23	1:D:555:VAL:HG22	2.00	0.43
1:G:221:ILE:HA	1:G:222:PRO:HD2	1.92	0.43
1:E:197:PHE:O	1:E:201:HIS:ND1	2.52	0.43
1:M:267:VAL:HG22	1:M:270:ARG:NH2	2.34	0.43
1:C:49:HIS:CE1	1:C:51:ARG:HG2	2.54	0.43
1:A:49:HIS:CE1	1:A:51:ARG:HG2	2.54	0.43
1:F:197:PHE:O	1:F:201:HIS:ND1	2.51	0.43
1:J:250:PRO:HB2	1:J:253:TYR:CE1	2.54	0.43
1:M:50:ALA:HB2	1:M:323:TRP:CH2	2.53	0.43
1:K:393:VAL:HA	1:K:441:ASN:O	2.19	0.43
1:F:393:VAL:HA	1:F:441:ASN:O	2.19	0.43
1:M:443:VAL:HA	1:M:495:ASN:O	2.19	0.43
1:C:263:VAL:O	1:C:266:MET:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:PHE:O	1:H:201:HIS:ND1	2.51	0.43
1:M:79:ALA:CB	1:M:88:PHE:HE1	2.26	0.43
1:L:19:LEU:HD13	1:L:80:ARG:CD	2.49	0.43
1:D:162:GLU:HG2	1:D:353:ARG:CB	2.47	0.43
1:J:76:CYS:HG	1:J:88:PHE:HE2	1.65	0.43
1:I:527:SER:HB3	1:I:573:VAL:HG21	2.01	0.43
1:I:393:VAL:HA	1:I:441:ASN:O	2.19	0.43
1:D:49:HIS:CE1	1:D:51:ARG:HG2	2.54	0.43
1:D:193:LYS:NZ	1:D:308:SER:OG	2.47	0.43
1:C:386:PRO:O	1:C:452:LYS:NZ	2.49	0.43
1:L:228:GLU:HA	1:L:229:PRO:HD3	1.88	0.43
1:M:76:CYS:O	1:M:80:ARG:NH2	2.49	0.42
1:I:271:GLU:HB3	1:L:268:ARG:HH11	1.84	0.42
1:A:393:VAL:HA	1:A:441:ASN:O	2.19	0.42
1:C:393:VAL:HA	1:C:441:ASN:O	2.19	0.42
1:K:458:ILE:HG23	1:K:555:VAL:HG22	2.00	0.42
1:A:354:ASP:HA	1:A:355:PRO:HD3	1.85	0.42
1:G:357:PHE:O	1:G:361:HIS:ND1	2.53	0.42
1:K:137:GLN:HA	1:K:423:ASP:HA	2.01	0.42
1:G:5:LYS:HG3	1:G:69:PHE:CZ	2.54	0.42
1:E:97:LEU:HG	1:E:528:THR:CB	2.49	0.42
1:A:529:GLU:O	1:A:531:CYS:N	2.52	0.42
1:G:529:GLU:O	1:G:531:CYS:N	2.51	0.42
1:C:458:ILE:HG23	1:C:555:VAL:HG22	2.00	0.42
1:A:316:TYR:CE1	1:G:275:ASP:OD1	2.72	0.42
1:A:591:LYS:HE3	1:A:591:LYS:HA	2.02	0.42
1:M:137:GLN:HA	1:M:423:ASP:HA	2.01	0.42
1:H:228:GLU:HA	1:H:229:PRO:HD3	1.88	0.42
1:L:263:VAL:O	1:L:266:MET:HB2	2.19	0.42
1:G:263:VAL:O	1:G:266:MET:HB2	2.19	0.42
1:J:228:GLU:HA	1:J:229:PRO:HD3	1.88	0.42
1:A:276:ALA:HB1	1:A:281:TYR:O	2.19	0.42
1:E:303:ASP:OD2	1:E:312:LYS:NZ	2.52	0.42
1:C:527:SER:HB3	1:C:573:VAL:HG23	2.00	0.42
1:D:8:ARG:HH21	1:D:73:ILE:HG13	1.83	0.42
1:D:231:GLU:O	1:D:249:ARG:HD2	2.19	0.42
1:J:393:VAL:HA	1:J:441:ASN:O	2.19	0.42
1:D:534:GLY:HA2	1:D:577:ALA:CB	2.49	0.42
1:J:197:PHE:O	1:J:201:HIS:ND1	2.51	0.42
1:D:137:GLN:HA	1:D:423:ASP:HA	2.01	0.42
1:C:357:PHE:O	1:C:361:HIS:ND1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:96:VAL:HG22	1:J:105:ILE:HG21	2.01	0.42
1:J:5:LYS:HG2	1:J:105:ILE:HB	2.01	0.42
1:H:467:LEU:CB	1:J:149:ASN:OD1	2.66	0.42
1:H:467:LEU:CD2	1:J:151:LEU:CD1	2.97	0.42
1:A:90:TYR:O	1:A:94:VAL:HG23	2.20	0.42
1:H:529:GLU:O	1:H:531:CYS:N	2.52	0.42
1:E:266:MET:HB3	1:E:266:MET:HE3	1.91	0.42
1:I:50:ALA:HB2	1:I:323:TRP:CH2	2.53	0.42
1:L:393:VAL:HA	1:L:441:ASN:O	2.19	0.42
1:J:591:LYS:HA	1:J:591:LYS:HE3	2.02	0.42
1:I:137:GLN:HA	1:I:423:ASP:HA	2.01	0.42
1:F:506:VAL:HG12	1:F:579:SER:HB2	2.01	0.42
1:J:137:GLN:HA	1:J:423:ASP:HA	2.01	0.42
1:A:79:ALA:CB	1:A:88:PHE:CD1	2.97	0.42
1:J:97:LEU:CG	1:J:528:THR:CB	2.97	0.42
1:K:24:LEU:HD13	1:K:81:GLN:HE22	1.70	0.42
1:L:19:LEU:CD1	1:L:80:ARG:HD3	2.49	0.42
1:K:231:GLU:O	1:K:249:ARG:HD2	2.19	0.42
1:J:303:ASP:C	1:J:311:SER:HA	2.39	0.42
1:C:275:ASP:OD1	1:F:316:TYR:HE1	2.03	0.42
1:D:529:GLU:O	1:D:531:CYS:N	2.52	0.42
1:G:393:VAL:HA	1:G:441:ASN:O	2.19	0.42
1:D:591:LYS:HE3	1:D:591:LYS:HA	2.02	0.42
1:G:303:ASP:HB2	1:G:310:GLU:HB2	2.01	0.42
1:F:357:PHE:O	1:F:361:HIS:ND1	2.53	0.42
1:M:193:LYS:NZ	1:M:308:SER:OG	2.48	0.42
1:M:357:PHE:O	1:M:361:HIS:ND1	2.52	0.42
1:G:34:LYS:HG3	1:G:35:GLY:H	1.85	0.42
1:A:9:LEU:HD22	1:A:105:ILE:HD11	2.02	0.42
1:A:108:PRO:HA	1:A:109:PRO:HD3	1.81	0.42
1:I:357:PHE:O	1:I:361:HIS:ND1	2.53	0.42
1:M:5:LYS:CD	1:M:69:PHE:CZ	3.02	0.42
1:J:282:ILE:HD12	1:J:304:ILE:HD12	2.01	0.42
1:J:162:GLU:HG2	1:J:353:ARG:CB	2.47	0.42
1:M:529:GLU:O	1:M:531:CYS:N	2.52	0.42
1:H:107:VAL:HG21	1:H:528:THR:HG1	1.85	0.42
1:A:467:LEU:HD23	1:D:149:ASN:OD1	2.19	0.42
1:K:465:ASP:HB3	1:K:467:LEU:H	1.84	0.42
1:D:393:VAL:HA	1:D:441:ASN:O	2.19	0.42
1:I:267:VAL:HG13	1:I:270:ARG:NH2	2.34	0.42
1:H:605:ARG:NH1	1:K:38:ILE:HB	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:591:LYS:HA	1:M:591:LYS:HE3	2.02	0.42
1:D:357:PHE:O	1:D:361:HIS:ND1	2.53	0.42
1:F:137:GLN:HA	1:F:423:ASP:HA	2.01	0.42
1:H:403:ILE:HG21	1:H:541:ILE:HG21	1.99	0.42
1:A:303:ASP:OD2	1:A:312:LYS:NZ	2.52	0.42
1:J:357:PHE:O	1:J:361:HIS:ND1	2.53	0.42
1:A:267:VAL:HG13	1:A:270:ARG:NH2	2.34	0.42
1:F:375:PHE:CB	1:F:600:ARG:HD3	2.47	0.42
1:E:50:ALA:HB2	1:E:323:TRP:CH2	2.53	0.42
1:M:393:VAL:HA	1:M:441:ASN:O	2.19	0.42
1:E:357:PHE:O	1:E:361:HIS:ND1	2.52	0.42
1:L:357:PHE:O	1:L:361:HIS:ND1	2.52	0.42
1:G:534:GLY:HA2	1:G:577:ALA:CB	2.49	0.42
1:K:8:ARG:NE	1:K:73:ILE:CG2	2.43	0.42
1:F:97:LEU:HD11	1:F:528:THR:OG1	2.18	0.42
1:I:162:GLU:HG2	1:I:353:ARG:CB	2.47	0.42
1:K:162:GLU:HG2	1:K:353:ARG:CB	2.47	0.42
1:E:76:CYS:HG	1:E:88:PHE:HE2	1.66	0.42
1:I:48:PHE:HB2	1:I:326:VAL:HG22	2.02	0.42
1:J:140:ILE:HB	1:J:426:VAL:HG12	2.02	0.42
1:D:232:GLY:HA3	1:E:338:PHE:CZ	2.55	0.42
1:H:140:ILE:HB	1:H:426:VAL:HG12	2.02	0.42
1:G:591:LYS:HA	1:G:591:LYS:HE3	2.01	0.42
1:M:362:ARG:HD3	1:M:362:ARG:HA	1.84	0.42
1:F:415:SER:OG	1:F:425:SER:HA	2.20	0.42
1:M:415:SER:OG	1:M:425:SER:HA	2.20	0.42
1:H:137:GLN:HA	1:H:423:ASP:HA	2.01	0.42
1:C:137:GLN:HA	1:C:423:ASP:HA	2.01	0.42
1:I:508:ILE:HD13	1:I:533:CYS:O	2.20	0.42
1:A:357:PHE:O	1:A:361:HIS:ND1	2.52	0.42
1:F:588:TYR:HA	1:F:589:PRO:HD3	1.91	0.42
1:J:534:GLY:HA2	1:J:577:ALA:CB	2.49	0.42
1:A:231:GLU:O	1:A:249:ARG:HD2	2.20	0.42
1:J:458:ILE:HG23	1:J:555:VAL:HG22	2.00	0.42
1:E:266:MET:SD	1:E:323:TRP:HB3	2.60	0.42
1:I:99:ARG:HH12	1:I:101:ASP:CG	2.24	0.42
1:C:48:PHE:HB2	1:C:326:VAL:HG22	2.02	0.42
1:C:591:LYS:HE3	1:C:591:LYS:HA	2.02	0.42
1:K:357:PHE:O	1:K:361:HIS:ND1	2.53	0.42
1:E:137:GLN:HA	1:E:423:ASP:HA	2.01	0.42
1:M:69:PHE:CE1	1:M:72:PHE:HD2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:ILE:HD11	1:D:312:LYS:HB2	2.01	0.42
1:M:107:VAL:HB	1:M:528:THR:HG23	2.02	0.42
1:L:269:TRP:O	1:L:273:ILE:HG13	2.19	0.42
1:D:50:ALA:HB2	1:D:323:TRP:CH2	2.53	0.42
1:D:605:ARG:HD3	1:D:605:ARG:HA	1.90	0.42
1:F:140:ILE:HB	1:F:426:VAL:HG12	2.02	0.42
1:E:393:VAL:HA	1:E:441:ASN:O	2.19	0.42
1:K:292:LEU:HB3	1:K:371:HIS:CE1	2.55	0.42
1:L:276:ALA:HB1	1:L:281:TYR:O	2.20	0.42
1:H:354:ASP:HA	1:H:355:PRO:HD3	1.85	0.42
1:J:234:ALA:HA	1:J:248:SER:HB2	2.01	0.42
1:F:193:LYS:NZ	1:F:308:SER:OG	2.48	0.42
1:F:221:ILE:HA	1:F:222:PRO:HD2	1.92	0.42
1:E:5:LYS:HG3	1:E:69:PHE:CZ	2.55	0.41
1:J:97:LEU:HG	1:J:528:THR:CB	2.49	0.41
1:C:416:HIS:ND1	1:C:514:PHE:HB2	2.35	0.41
1:J:529:GLU:O	1:J:531:CYS:N	2.53	0.41
1:E:529:GLU:HB2	1:E:533:CYS:HB2	2.01	0.41
1:A:84:ASN:ND2	1:A:84:ASN:N	2.68	0.41
1:F:48:PHE:HB2	1:F:326:VAL:HG22	2.02	0.41
1:I:140:ILE:HB	1:I:426:VAL:HG12	2.02	0.41
1:K:140:ILE:HB	1:K:426:VAL:HG12	2.02	0.41
1:E:354:ASP:HA	1:E:355:PRO:HD3	1.85	0.41
1:J:60:TYR:O	1:J:64:TYR:HD2	2.04	0.41
1:D:415:SER:OG	1:D:425:SER:HA	2.20	0.41
1:H:357:PHE:O	1:H:361:HIS:ND1	2.52	0.41
1:L:8:ARG:HH21	1:L:73:ILE:CG1	2.20	0.41
1:G:231:GLU:O	1:G:249:ARG:HD2	2.19	0.41
1:C:271:GLU:HB3	1:F:268:ARG:HD3	2.02	0.41
1:A:162:GLU:HG2	1:A:353:ARG:CB	2.47	0.41
1:M:140:ILE:HB	1:M:426:VAL:HG12	2.02	0.41
1:J:362:ARG:HD3	1:J:362:ARG:HA	1.84	0.41
1:F:591:LYS:HE3	1:F:591:LYS:HA	2.01	0.41
1:G:137:GLN:HA	1:G:423:ASP:HA	2.01	0.41
1:E:292:LEU:HB3	1:E:371:HIS:CE1	2.55	0.41
1:E:506:VAL:HG12	1:E:579:SER:HB2	2.02	0.41
1:E:97:LEU:HG	1:E:528:THR:H	1.86	0.41
1:I:271:GLU:HG3	1:L:268:ARG:HG3	2.02	0.41
1:F:76:CYS:HG	1:F:88:PHE:HE2	1.65	0.41
1:M:99:ARG:HH12	1:M:101:ASP:CG	2.24	0.41
1:E:57:THR:HA	1:E:60:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:ASP:HA	1:D:477:ARG:HE	1.86	0.41
1:I:591:LYS:HE3	1:I:591:LYS:HA	2.01	0.41
1:C:292:LEU:HB3	1:C:371:HIS:CE1	2.56	0.41
1:A:415:SER:OG	1:A:425:SER:HA	2.20	0.41
1:F:276:ALA:HB1	1:F:281:TYR:O	2.20	0.41
1:E:228:GLU:HA	1:E:229:PRO:HD3	1.88	0.41
1:I:231:GLU:O	1:I:249:ARG:HD2	2.19	0.41
1:E:231:GLU:O	1:E:249:ARG:HD2	2.19	0.41
1:D:161:ARG:HB3	1:D:353:ARG:HA	2.03	0.41
1:M:59:LEU:CD1	1:M:87:MET:HE3	2.50	0.41
1:L:48:PHE:HB2	1:L:326:VAL:HG22	2.02	0.41
1:D:270:ARG:HD3	1:D:363:PHE:HZ	1.85	0.41
1:G:474:ASP:HA	1:G:477:ARG:HE	1.85	0.41
1:M:474:ASP:HA	1:M:477:ARG:HE	1.86	0.41
1:L:140:ILE:HB	1:L:426:VAL:HG12	2.02	0.41
1:A:588:TYR:HA	1:A:589:PRO:HD3	1.92	0.41
1:A:292:LEU:HB3	1:A:371:HIS:CE1	2.55	0.41
1:K:24:LEU:CD1	1:K:81:GLN:HE21	2.20	0.41
1:L:12:LEU:HD22	1:L:80:ARG:CZ	2.51	0.41
1:L:332:THR:OG1	1:M:250:PRO:HG2	2.21	0.41
1:E:375:PHE:CB	1:E:600:ARG:HD3	2.48	0.41
1:M:375:PHE:CB	1:M:600:ARG:HD3	2.48	0.41
1:M:442:ILE:O	1:M:496:THR:HA	2.21	0.41
1:E:161:ARG:HB3	1:E:353:ARG:HA	2.03	0.41
1:L:272:ARG:NH1	1:L:315:GLU:O	2.53	0.41
1:M:59:LEU:HD11	1:M:87:MET:CE	2.44	0.41
1:I:474:ASP:HA	1:I:477:ARG:HE	1.86	0.41
1:E:474:ASP:HA	1:E:477:ARG:HE	1.85	0.41
1:H:591:LYS:HA	1:H:591:LYS:HE3	2.02	0.41
1:I:506:VAL:HG12	1:I:579:SER:HB2	2.02	0.41
1:A:499:ARG:NH1	1:A:503:ASP:O	2.53	0.41
1:D:57:THR:HA	1:D:60:TYR:CD2	2.56	0.41
1:C:193:LYS:NZ	1:C:308:SER:OG	2.48	0.41
1:D:221:ILE:HA	1:D:222:PRO:HD2	1.92	0.41
1:J:415:SER:OG	1:J:425:SER:HA	2.20	0.41
1:M:534:GLY:HA2	1:M:577:ALA:CB	2.51	0.41
1:A:24:LEU:CG	1:A:27:ASP:N	2.83	0.41
1:K:80:ARG:HA	1:K:83:VAL:HG22	2.02	0.41
1:G:161:ARG:HB3	1:G:353:ARG:HA	2.03	0.41
1:A:161:ARG:HB3	1:A:353:ARG:HA	2.03	0.41
1:G:99:ARG:HH12	1:G:101:ASP:CG	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:THR:HA	1:F:60:TYR:CD2	2.56	0.41
1:F:474:ASP:HA	1:F:477:ARG:HE	1.86	0.41
1:D:465:ASP:HB3	1:D:467:LEU:H	1.85	0.41
1:E:591:LYS:HE3	1:E:591:LYS:HA	2.02	0.41
1:I:108:PRO:HA	1:I:109:PRO:HD3	1.81	0.41
1:G:415:SER:OG	1:G:425:SER:HA	2.20	0.41
1:I:354:ASP:HA	1:I:355:PRO:HD3	1.85	0.41
1:K:9:LEU:HD11	1:K:69:PHE:CZ	2.56	0.41
1:D:9:LEU:HG	1:D:72:PHE:HE2	1.68	0.41
1:K:22:GLU:O	1:K:81:GLN:O	2.38	0.41
1:M:161:ARG:HB3	1:M:353:ARG:HA	2.03	0.41
1:K:6:GLN:NE2	1:K:105:ILE:HA	2.35	0.41
1:E:99:ARG:HH12	1:E:101:ASP:CG	2.24	0.41
1:J:48:PHE:CB	1:J:326:VAL:HG22	2.50	0.41
1:D:266:MET:SD	1:D:323:TRP:HB3	2.60	0.41
1:E:60:TYR:O	1:E:64:TYR:HD2	2.04	0.41
1:I:24:LEU:HG	1:I:25:PRO:HD2	2.02	0.41
1:L:591:LYS:HA	1:L:591:LYS:HE3	2.02	0.41
1:I:292:LEU:HB3	1:I:371:HIS:CE1	2.56	0.41
1:M:499:ARG:NH1	1:M:503:ASP:O	2.53	0.41
1:H:415:SER:OG	1:H:425:SER:HA	2.20	0.41
1:I:415:SER:OG	1:I:425:SER:HA	2.20	0.41
1:K:88:PHE:O	1:K:92:VAL:HG22	2.20	0.41
1:K:415:SER:OG	1:K:425:SER:HA	2.20	0.41
1:J:5:LYS:HG3	1:J:69:PHE:CZ	2.55	0.41
1:F:5:LYS:HG3	1:F:69:PHE:CZ	2.55	0.41
1:F:231:GLU:O	1:F:249:ARG:HD2	2.20	0.41
1:H:162:GLU:HG2	1:H:353:ARG:CB	2.47	0.41
1:I:161:ARG:HB3	1:I:353:ARG:HA	2.03	0.41
1:C:275:ASP:HB2	1:F:268:ARG:NH1	2.36	0.41
1:D:107:VAL:HB	1:D:528:THR:HG23	2.03	0.41
1:J:99:ARG:HH12	1:J:101:ASP:CG	2.24	0.41
1:H:50:ALA:HB2	1:H:323:TRP:CH2	2.53	0.41
1:C:474:ASP:HA	1:C:477:ARG:HE	1.86	0.41
1:E:140:ILE:HB	1:E:426:VAL:HG12	2.02	0.41
1:D:140:ILE:HB	1:D:426:VAL:HG12	2.02	0.41
1:K:591:LYS:HA	1:K:591:LYS:HE3	2.02	0.41
1:L:506:VAL:HG12	1:L:579:SER:HB2	2.02	0.41
1:E:534:GLY:HA2	1:E:577:ALA:CB	2.50	0.41
1:L:415:SER:OG	1:L:425:SER:HA	2.20	0.41
1:L:534:GLY:HA2	1:L:577:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:243:GLY:HA2	1:K:125:ASN:HB2	2.02	0.41
1:G:21:ARG:HD3	1:G:41:ARG:HD3	2.02	0.41
1:D:499:ARG:NH1	1:D:503:ASP:O	2.53	0.41
1:L:303:ASP:OD2	1:L:312:LYS:NZ	2.52	0.41
1:H:292:LEU:HB3	1:H:371:HIS:CE1	2.56	0.41
1:A:24:LEU:CG	1:A:81:GLN:NE2	2.79	0.41
1:A:24:LEU:CD2	1:A:82:ILE:HG22	2.40	0.41
1:K:5:LYS:HA	1:K:69:PHE:HE2	1.83	0.41
1:C:5:LYS:HG3	1:C:69:PHE:CZ	2.56	0.41
1:A:5:LYS:HG3	1:A:69:PHE:CZ	2.55	0.41
1:L:104:GLY:HA2	1:L:525:GLU:C	2.42	0.41
1:I:272:ARG:HB3	1:I:316:TYR:CE1	2.50	0.41
1:L:60:TYR:O	1:L:64:TYR:HD2	2.04	0.41
1:M:82:ILE:HG23	1:M:83:VAL:N	2.36	0.41
1:A:512:ARG:CB	1:A:531:CYS:SG	3.08	0.41
1:G:107:VAL:HB	1:G:528:THR:HG23	2.03	0.41
1:C:99:ARG:HH12	1:C:101:ASP:CG	2.24	0.41
1:H:268:ARG:HH11	1:M:271:GLU:HA	1.85	0.41
1:D:48:PHE:HB2	1:D:326:VAL:HG22	2.02	0.41
1:E:48:PHE:HB2	1:E:326:VAL:HG22	2.02	0.41
1:C:511:VAL:HG22	1:C:512:ARG:H	1.86	0.41
1:C:473:PRO:HA	1:C:476:GLN:HB2	2.03	0.41
1:A:474:ASP:HA	1:A:477:ARG:HE	1.86	0.41
1:A:596:PHE:HA	1:A:597:PRO:C	2.41	0.41
1:E:596:PHE:HA	1:E:597:PRO:C	2.41	0.41
1:J:385:PHE:HA	1:J:386:PRO:HD3	1.90	0.41
1:J:499:ARG:NH1	1:J:503:ASP:O	2.53	0.41
1:L:575:SER:HA	1:L:582:GLY:O	2.21	0.41
1:F:362:ARG:HD3	1:F:362:ARG:HA	1.84	0.41
1:C:506:VAL:HG12	1:C:579:SER:HB2	2.02	0.41
1:D:67:LYS:HB3	1:D:71:ASP:HB2	2.02	0.41
1:K:534:GLY:HA2	1:K:577:ALA:CB	2.50	0.41
1:G:60:TYR:O	1:G:64:TYR:HD2	2.04	0.41
1:G:555:VAL:O	1:G:615:MET:HA	2.21	0.41
1:C:76:CYS:HG	1:C:88:PHE:HE2	1.64	0.41
1:D:68:ASP:C	1:D:70:ASN:N	2.75	0.41
1:F:99:ARG:HH12	1:F:101:ASP:CG	2.24	0.41
1:K:474:ASP:HA	1:K:477:ARG:HE	1.86	0.41
1:H:474:ASP:HA	1:H:477:ARG:HE	1.85	0.41
1:H:596:PHE:HA	1:H:597:PRO:C	2.41	0.41
1:I:150:ILE:O	1:M:467:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:303:ASP:OD2	1:I:312:LYS:NZ	2.52	0.41
1:F:292:LEU:HB3	1:F:371:HIS:CE1	2.55	0.41
1:G:272:ARG:HD3	1:G:316:TYR:CE1	2.56	0.41
1:C:415:SER:OG	1:C:425:SER:HA	2.20	0.41
1:M:292:LEU:HB3	1:M:371:HIS:CE1	2.55	0.41
1:H:57:THR:HA	1:H:60:TYR:CD2	2.56	0.41
1:J:261:VAL:HG12	1:J:262:ASP:O	2.21	0.41
1:K:2:VAL:C	1:K:5:LYS:HB3	2.41	0.40
1:F:69:PHE:CD1	1:F:102:CYS:SG	3.14	0.40
1:M:104:GLY:HA2	1:M:525:GLU:C	2.42	0.40
1:J:97:LEU:HG	1:J:528:THR:H	1.86	0.40
1:G:323:TRP:O	1:G:326:VAL:HG23	2.22	0.40
1:J:30:ASP:HB3	1:J:32:ARG:HB2	2.03	0.40
1:H:231:GLU:O	1:H:249:ARG:HD2	2.21	0.40
1:J:530:TYR:CD2	1:J:531:CYS:SG	3.14	0.40
1:F:161:ARG:HB3	1:F:353:ARG:HA	2.02	0.40
1:G:530:TYR:CD2	1:G:531:CYS:SG	3.12	0.40
1:E:274:LEU:HB2	1:G:268:ARG:NH1	2.37	0.40
1:H:175:ILE:HG21	1:H:528:THR:HG21	2.02	0.40
1:H:555:VAL:O	1:H:615:MET:HA	2.21	0.40
1:I:555:VAL:O	1:I:615:MET:HA	2.21	0.40
1:H:99:ARG:HH12	1:H:101:ASP:CG	2.24	0.40
1:D:267:VAL:HG13	1:D:270:ARG:NH2	2.36	0.40
1:H:473:PRO:HA	1:H:476:GLN:HB2	2.03	0.40
1:E:473:PRO:HA	1:E:476:GLN:HB2	2.03	0.40
1:L:474:ASP:HA	1:L:477:ARG:HE	1.86	0.40
1:C:140:ILE:HB	1:C:426:VAL:HG12	2.02	0.40
1:I:186:MET:SD	1:I:186:MET:N	2.94	0.40
1:C:57:THR:HA	1:C:60:TYR:CD2	2.56	0.40
1:C:303:ASP:OD2	1:C:312:LYS:NZ	2.52	0.40
1:L:292:LEU:HB3	1:L:371:HIS:CE1	2.55	0.40
1:A:57:THR:HA	1:A:60:TYR:CD2	2.56	0.40
1:E:415:SER:OG	1:E:425:SER:HA	2.20	0.40
1:K:97:LEU:HD11	1:K:528:THR:CG2	2.51	0.40
1:G:63:LEU:HD22	1:G:91:ALA:CB	2.28	0.40
1:I:272:ARG:NH1	1:I:315:GLU:O	2.54	0.40
1:M:57:THR:HA	1:M:60:TYR:CD2	2.56	0.40
1:M:60:TYR:O	1:M:64:TYR:HD2	2.04	0.40
1:G:57:THR:HA	1:G:60:TYR:CD2	2.56	0.40
1:G:267:VAL:HG13	1:G:270:ARG:NH2	2.36	0.40
1:A:140:ILE:HB	1:A:426:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:555:VAL:O	1:E:615:MET:HA	2.21	0.40
1:A:555:VAL:O	1:A:615:MET:HA	2.21	0.40
1:D:99:ARG:HH12	1:D:101:ASP:CG	2.24	0.40
1:D:172:HIS:CD2	1:D:532:SER:HG	2.39	0.40
1:A:48:PHE:HB2	1:A:326:VAL:HG22	2.02	0.40
1:K:150:ILE:O	1:L:467:LEU:HD22	2.21	0.40
1:A:473:PRO:HA	1:A:476:GLN:HB2	2.03	0.40
1:G:140:ILE:HB	1:G:426:VAL:HG12	2.02	0.40
1:C:24:LEU:HD11	1:C:78:GLN:HE21	1.87	0.40
1:C:517:LEU:HA	1:C:520:GLY:N	2.36	0.40
1:L:19:LEU:HD22	1:L:80:ARG:NH1	2.25	0.40
1:L:57:THR:HA	1:L:60:TYR:CD2	2.56	0.40
1:M:12:LEU:HD13	1:M:80:ARG:NH2	2.37	0.40
1:E:16:LEU:HD12	1:E:19:LEU:HD12	2.04	0.40
1:J:555:VAL:O	1:J:615:MET:HA	2.21	0.40
1:G:80:ARG:HA	1:G:83:VAL:HG22	2.03	0.40
1:I:60:TYR:O	1:I:64:TYR:HD2	2.04	0.40
1:J:474:ASP:HA	1:J:477:ARG:HE	1.86	0.40
1:D:473:PRO:HA	1:D:476:GLN:HB2	2.03	0.40
1:F:60:TYR:O	1:F:64:TYR:HD2	2.03	0.40
1:M:323:TRP:O	1:M:326:VAL:HG23	2.22	0.40
1:D:190:LYS:HD3	1:D:190:LYS:HA	1.88	0.40
1:C:362:ARG:HA	1:C:362:ARG:HD3	1.84	0.40
1:J:272:ARG:HB3	1:J:316:TYR:CE2	2.57	0.40
1:J:337:ARG:NH2	1:K:251:GLU:OE1	2.55	0.40
1:A:69:PHE:CE1	1:A:96:VAL:HG23	2.57	0.40
1:F:107:VAL:HG21	1:F:528:THR:HG1	1.85	0.40
1:D:16:LEU:HD12	1:D:19:LEU:HD12	2.04	0.40
1:H:161:ARG:HB3	1:H:353:ARG:HA	2.03	0.40
1:E:162:GLU:HG2	1:E:353:ARG:CB	2.47	0.40
1:E:99:ARG:O	1:E:99:ARG:NH1	2.55	0.40
1:L:323:TRP:O	1:L:326:VAL:HG23	2.22	0.40
1:H:323:TRP:O	1:H:326:VAL:HG23	2.22	0.40
1:F:269:TRP:O	1:F:273:ILE:HG13	2.21	0.40
1:E:24:LEU:HD11	1:E:78:GLN:HE21	1.86	0.40
1:E:499:ARG:NH1	1:E:503:ASP:O	2.53	0.40
1:L:5:LYS:CD	1:L:69:PHE:CE1	3.04	0.40
1:L:16:LEU:HD12	1:L:19:LEU:HD12	2.04	0.40
1:L:531:CYS:SG	1:L:532:SER:N	2.95	0.40
1:F:529:GLU:HA	1:F:533:CYS:HB2	2.03	0.40
1:J:231:GLU:O	1:J:249:ARG:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ARG:HB3	1:C:353:ARG:HA	2.03	0.40
1:G:530:TYR:HD2	1:G:531:CYS:HG	1.62	0.40
1:H:107:VAL:HB	1:H:528:THR:HG23	2.04	0.40
1:G:175:ILE:HG21	1:G:528:THR:HG21	2.02	0.40
1:L:555:VAL:O	1:L:615:MET:HA	2.21	0.40
1:C:555:VAL:O	1:C:615:MET:HA	2.21	0.40
1:F:99:ARG:NH1	1:F:99:ARG:O	2.55	0.40
1:A:323:TRP:O	1:A:326:VAL:HG23	2.22	0.40
1:D:323:TRP:O	1:D:326:VAL:HG23	2.22	0.40
1:I:473:PRO:HA	1:I:476:GLN:HB2	2.03	0.40
1:L:190:LYS:HD3	1:L:190:LYS:HA	1.88	0.40
1:I:362:ARG:HA	1:I:362:ARG:HD3	1.84	0.40
1:H:506:VAL:HG12	1:H:579:SER:HB2	2.03	0.40
1:K:67:LYS:HB3	1:K:71:ASP:HB3	2.03	0.40
1:J:506:VAL:HG12	1:J:579:SER:HB2	2.04	0.40
1:I:160:PHE:HD1	1:I:539:MET:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	624/626 (100%)	527 (84%)	77 (12%)	20 (3%)	5	41
1	C	622/626 (99%)	526 (85%)	84 (14%)	12 (2%)	10	52
1	D	624/626 (100%)	526 (84%)	82 (13%)	16 (3%)	7	45
1	E	624/626 (100%)	529 (85%)	81 (13%)	14 (2%)	8	49
1	F	624/626 (100%)	529 (85%)	77 (12%)	18 (3%)	6	43
1	G	624/626 (100%)	532 (85%)	76 (12%)	16 (3%)	7	45
1	H	624/626 (100%)	528 (85%)	78 (12%)	18 (3%)	6	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	622/626 (99%)	529 (85%)	79 (13%)	14 (2%)	8	48
1	J	624/626 (100%)	533 (85%)	75 (12%)	16 (3%)	7	45
1	K	624/626 (100%)	532 (85%)	81 (13%)	11 (2%)	11	53
1	L	624/626 (100%)	531 (85%)	81 (13%)	12 (2%)	10	52
1	M	624/626 (100%)	526 (84%)	82 (13%)	16 (3%)	7	45
All	All	7484/7512 (100%)	6348 (85%)	953 (13%)	183 (2%)	12	47

All (183) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	351	SER
1	A	530	TYR
1	C	34	LYS
1	C	351	SER
1	D	34	LYS
1	D	45	PHE
1	D	351	SER
1	D	530	TYR
1	E	34	LYS
1	E	351	SER
1	F	34	LYS
1	F	351	SER
1	F	524	SER
1	G	34	LYS
1	G	351	SER
1	G	530	TYR
1	H	34	LYS
1	H	351	SER
1	H	530	TYR
1	I	25	PRO
1	I	285	LYS
1	I	351	SER
1	J	32	ARG
1	J	311	SER
1	J	351	SER
1	J	530	TYR
1	K	34	LYS
1	K	351	SER
1	K	530	TYR

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Mol	Chain	Res	Type
1	L	34	LYS
1	L	351	SER
1	L	574	CYS
1	M	34	LYS
1	M	351	SER
1	M	530	TYR
1	A	32	ARG
1	A	144	ALA
1	A	524	SER
1	A	573	VAL
1	C	448	SER
1	D	41	ARG
1	D	82	ILE
1	D	573	VAL
1	E	573	VAL
1	F	16	LEU
1	F	17	THR
1	F	20	THR
1	F	27	ASP
1	F	573	VAL
1	G	524	SER
1	G	573	VAL
1	H	524	SER
1	H	573	VAL
1	I	527	SER
1	I	573	VAL
1	J	573	VAL
1	K	525	GLU
1	K	573	VAL
1	M	45	PHE
1	M	81	GLN
1	M	524	SER
1	M	573	VAL
1	A	15	HIS
1	A	44	LEU
1	A	532	SER
1	C	15	HIS
1	C	44	LEU
1	D	15	HIS
1	E	15	HIS
1	E	44	LEU
1	F	15	HIS

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Mol	Chain	Res	Type
1	F	44	LEU
1	F	530	TYR
1	G	15	HIS
1	G	311	SER
1	H	15	HIS
1	H	44	LEU
1	I	44	LEU
1	I	525	GLU
1	J	15	HIS
1	J	28	GLN
1	J	31	GLU
1	L	15	HIS
1	L	44	LEU
1	M	15	HIS
1	A	31	GLU
1	A	181	TRP
1	A	344	VAL
1	A	571	ASN
1	C	181	TRP
1	C	344	VAL
1	C	415	SER
1	D	37	GLY
1	D	181	TRP
1	D	344	VAL
1	D	415	SER
1	D	524	SER
1	D	571	ASN
1	E	181	TRP
1	E	344	VAL
1	E	415	SER
1	E	571	ASN
1	F	181	TRP
1	F	344	VAL
1	F	415	SER
1	F	571	ASN
1	G	37	GLY
1	G	67	LYS
1	G	181	TRP
1	G	344	VAL
1	G	415	SER
1	G	571	ASN
1	H	22	GLU

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Mol	Chain	Res	Type
1	H	181	TRP
1	H	344	VAL
1	H	415	SER
1	H	571	ASN
1	I	37	GLY
1	I	344	VAL
1	I	415	SER
1	J	181	TRP
1	J	304	ILE
1	J	344	VAL
1	J	415	SER
1	J	571	ASN
1	K	181	TRP
1	K	344	VAL
1	K	415	SER
1	K	571	ASN
1	L	181	TRP
1	L	344	VAL
1	L	415	SER
1	L	524	SER
1	M	181	TRP
1	M	344	VAL
1	M	415	SER
1	M	571	ASN
1	A	415	SER
1	A	521	GLU
1	C	45	PHE
1	D	83	VAL
1	E	37	GLY
1	E	45	PHE
1	E	524	SER
1	F	45	PHE
1	G	82	ILE
1	H	45	PHE
1	H	81	GLN
1	I	45	PHE
1	I	181	TRP
1	I	523	VAL
1	J	37	GLY
1	L	37	GLY
1	L	45	PHE
1	M	69	PHE

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Mol	Chain	Res	Type
1	M	70	ASN
1	A	37	GLY
1	A	45	PHE
1	A	285	LYS
1	C	285	LYS
1	E	285	LYS
1	F	285	LYS
1	G	285	LYS
1	H	37	GLY
1	H	285	LYS
1	J	285	LYS
1	K	285	LYS
1	M	82	ILE
1	H	82	ILE
1	K	377	PRO
1	M	377	PRO
1	A	377	PRO
1	C	377	PRO
1	C	449	GLY
1	D	377	PRO
1	E	150	ILE
1	F	377	PRO
1	G	377	PRO
1	H	377	PRO
1	I	377	PRO
1	J	377	PRO
1	L	377	PRO

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	A	556/556 (100%)	496 (89%)	60 (11%)	8	35
1	C	556/556 (100%)	508 (91%)	48 (9%)	13	47
1	D	556/556 (100%)	503 (90%)	53 (10%)	11	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	556/556 (100%)	506 (91%)	50 (9%)	12	44
1	F	556/556 (100%)	505 (91%)	51 (9%)	11	43
1	G	556/556 (100%)	508 (91%)	48 (9%)	13	47
1	H	556/556 (100%)	505 (91%)	51 (9%)	11	43
1	I	556/556 (100%)	504 (91%)	52 (9%)	11	42
1	J	556/556 (100%)	503 (90%)	53 (10%)	11	41
1	K	556/556 (100%)	505 (91%)	51 (9%)	11	43
1	L	556/556 (100%)	504 (91%)	52 (9%)	11	42
1	M	556/556 (100%)	504 (91%)	52 (9%)	11	42
All	All	6672/6672 (100%)	6051 (91%)	621 (9%)	16	42

All (621) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	11	PRO
1	A	22	GLU
1	A	24	LEU
1	A	30	ASP
1	A	57	THR
1	A	78	GLN
1	A	84	ASN
1	A	85	GLU
1	A	96	VAL
1	A	97	LEU
1	A	99	ARG
1	A	100	GLU
1	A	101	ASP
1	A	105	ILE
1	A	111	GLN
1	A	122	GLU
1	A	134	HIS
1	A	142	VAL
1	A	220	MET
1	A	251	GLU
1	A	264	GLN
1	A	265	ASP
1	A	268	ARG
1	A	271	GLU

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Mol	Chain	Res	Type
1	A	305	ILE
1	A	319	SER
1	A	326	VAL
1	A	347	ASP
1	A	349	SER
1	A	353	ARG
1	A	379	THR
1	A	398	LYS
1	A	405	THR
1	A	407	ILE
1	A	414	LEU
1	A	418	ILE
1	A	425	SER
1	A	426	VAL
1	A	439	THR
1	A	442	ILE
1	A	455	THR
1	A	465	ASP
1	A	469	ASN
1	A	483	LEU
1	A	501	HIS
1	A	507	THR
1	A	512	ARG
1	A	516	GLN
1	A	528	THR
1	A	532	SER
1	A	545	SER
1	A	554	PHE
1	A	564	THR
1	A	570	GLU
1	A	578	VAL
1	A	584	ARG
1	A	591	LYS
1	A	601	LYS
1	A	620	ILE
1	C	4	ASP
1	C	11	PRO
1	C	57	THR
1	C	85	GLU
1	C	96	VAL
1	C	97	LEU
1	C	99	ARG

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Mol	Chain	Res	Type
1	C	101	ASP
1	C	105	ILE
1	C	111	GLN
1	C	122	GLU
1	C	220	MET
1	C	251	GLU
1	C	265	ASP
1	C	268	ARG
1	C	271	GLU
1	C	305	ILE
1	C	319	SER
1	C	326	VAL
1	C	347	ASP
1	C	349	SER
1	C	353	ARG
1	C	379	THR
1	C	398	LYS
1	C	405	THR
1	C	407	ILE
1	C	418	ILE
1	C	425	SER
1	C	426	VAL
1	C	439	THR
1	C	442	ILE
1	C	455	THR
1	C	465	ASP
1	C	467	LEU
1	C	469	ASN
1	C	483	LEU
1	C	501	HIS
1	C	507	THR
1	C	516	GLN
1	C	545	SER
1	C	554	PHE
1	C	564	THR
1	C	578	VAL
1	C	584	ARG
1	C	591	LYS
1	C	601	LYS
1	C	603	GLU
1	C	620	ILE
1	D	4	ASP

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Mol	Chain	Res	Type
1	D	11	PRO
1	D	41	ARG
1	D	57	THR
1	D	84	ASN
1	D	85	GLU
1	D	96	VAL
1	D	97	LEU
1	D	99	ARG
1	D	101	ASP
1	D	105	ILE
1	D	111	GLN
1	D	122	GLU
1	D	220	MET
1	D	262	ASP
1	D	265	ASP
1	D	271	GLU
1	D	305	ILE
1	D	309	ASP
1	D	319	SER
1	D	326	VAL
1	D	347	ASP
1	D	349	SER
1	D	353	ARG
1	D	379	THR
1	D	398	LYS
1	D	405	THR
1	D	407	ILE
1	D	418	ILE
1	D	425	SER
1	D	426	VAL
1	D	439	THR
1	D	442	ILE
1	D	455	THR
1	D	465	ASP
1	D	469	ASN
1	D	483	LEU
1	D	501	HIS
1	D	507	THR
1	D	512	ARG
1	D	516	GLN
1	D	528	THR
1	D	532	SER

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Mol	Chain	Res	Type
1	D	545	SER
1	D	554	PHE
1	D	564	THR
1	D	570	GLU
1	D	578	VAL
1	D	584	ARG
1	D	591	LYS
1	D	601	LYS
1	D	603	GLU
1	D	620	ILE
1	E	4	ASP
1	E	11	PRO
1	E	38	ILE
1	E	57	THR
1	E	85	GLU
1	E	96	VAL
1	E	97	LEU
1	E	99	ARG
1	E	101	ASP
1	E	105	ILE
1	E	111	GLN
1	E	122	GLU
1	E	220	MET
1	E	264	GLN
1	E	265	ASP
1	E	271	GLU
1	E	305	ILE
1	E	319	SER
1	E	326	VAL
1	E	347	ASP
1	E	349	SER
1	E	353	ARG
1	E	379	THR
1	E	398	LYS
1	E	405	THR
1	E	407	ILE
1	E	418	ILE
1	E	425	SER
1	E	426	VAL
1	E	439	THR
1	E	442	ILE
1	E	455	THR

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Mol	Chain	Res	Type
1	E	465	ASP
1	E	469	ASN
1	E	483	LEU
1	E	501	HIS
1	E	507	THR
1	E	512	ARG
1	E	516	GLN
1	E	532	SER
1	E	545	SER
1	E	554	PHE
1	E	564	THR
1	E	570	GLU
1	E	578	VAL
1	E	584	ARG
1	E	591	LYS
1	E	601	LYS
1	E	603	GLU
1	E	620	ILE
1	F	4	ASP
1	F	11	PRO
1	F	17	THR
1	F	20	THR
1	F	24	LEU
1	F	38	ILE
1	F	57	THR
1	F	85	GLU
1	F	96	VAL
1	F	97	LEU
1	F	99	ARG
1	F	101	ASP
1	F	105	ILE
1	F	111	GLN
1	F	122	GLU
1	F	220	MET
1	F	265	ASP
1	F	271	GLU
1	F	305	ILE
1	F	319	SER
1	F	326	VAL
1	F	347	ASP
1	F	349	SER
1	F	353	ARG

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Mol	Chain	Res	Type
1	F	379	THR
1	F	398	LYS
1	F	405	THR
1	F	407	ILE
1	F	418	ILE
1	F	425	SER
1	F	426	VAL
1	F	439	THR
1	F	442	ILE
1	F	455	THR
1	F	465	ASP
1	F	469	ASN
1	F	483	LEU
1	F	501	HIS
1	F	507	THR
1	F	528	THR
1	F	529	GLU
1	F	545	SER
1	F	554	PHE
1	F	564	THR
1	F	570	GLU
1	F	578	VAL
1	F	584	ARG
1	F	591	LYS
1	F	601	LYS
1	F	603	GLU
1	F	620	ILE
1	G	4	ASP
1	G	11	PRO
1	G	57	THR
1	G	85	GLU
1	G	96	VAL
1	G	97	LEU
1	G	99	ARG
1	G	101	ASP
1	G	105	ILE
1	G	111	GLN
1	G	122	GLU
1	G	220	MET
1	G	265	ASP
1	G	271	GLU
1	G	305	ILE

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Mol	Chain	Res	Type
1	G	319	SER
1	G	326	VAL
1	G	347	ASP
1	G	349	SER
1	G	353	ARG
1	G	379	THR
1	G	398	LYS
1	G	405	THR
1	G	407	ILE
1	G	418	ILE
1	G	425	SER
1	G	426	VAL
1	G	439	THR
1	G	442	ILE
1	G	455	THR
1	G	465	ASP
1	G	469	ASN
1	G	483	LEU
1	G	501	HIS
1	G	507	THR
1	G	512	ARG
1	G	528	THR
1	G	532	SER
1	G	545	SER
1	G	554	PHE
1	G	564	THR
1	G	570	GLU
1	G	578	VAL
1	G	584	ARG
1	G	591	LYS
1	G	601	LYS
1	G	603	GLU
1	G	620	ILE
1	H	4	ASP
1	H	5	LYS
1	H	11	PRO
1	H	22	GLU
1	H	57	THR
1	H	85	GLU
1	H	96	VAL
1	H	97	LEU
1	H	99	ARG

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Mol	Chain	Res	Type
1	H	101	ASP
1	H	105	ILE
1	H	111	GLN
1	H	122	GLU
1	H	220	MET
1	H	265	ASP
1	H	268	ARG
1	H	305	ILE
1	H	319	SER
1	H	326	VAL
1	H	347	ASP
1	H	349	SER
1	H	353	ARG
1	H	379	THR
1	H	398	LYS
1	H	405	THR
1	H	407	ILE
1	H	418	ILE
1	H	425	SER
1	H	426	VAL
1	H	439	THR
1	H	442	ILE
1	H	455	THR
1	H	465	ASP
1	H	469	ASN
1	H	483	LEU
1	H	501	HIS
1	H	507	THR
1	H	512	ARG
1	H	516	GLN
1	H	528	THR
1	H	532	SER
1	H	545	SER
1	H	554	PHE
1	H	564	THR
1	H	570	GLU
1	H	578	VAL
1	H	584	ARG
1	H	591	LYS
1	H	601	LYS
1	H	603	GLU
1	H	620	ILE

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Mol	Chain	Res	Type
1	I	4	ASP
1	I	11	PRO
1	I	15	HIS
1	I	25	PRO
1	I	57	THR
1	I	85	GLU
1	I	96	VAL
1	I	97	LEU
1	I	99	ARG
1	I	101	ASP
1	I	105	ILE
1	I	111	GLN
1	I	122	GLU
1	I	186	MET
1	I	220	MET
1	I	264	GLN
1	I	265	ASP
1	I	271	GLU
1	I	305	ILE
1	I	319	SER
1	I	326	VAL
1	I	347	ASP
1	I	349	SER
1	I	353	ARG
1	I	379	THR
1	I	398	LYS
1	I	405	THR
1	I	407	ILE
1	I	418	ILE
1	I	425	SER
1	I	426	VAL
1	I	439	THR
1	I	442	ILE
1	I	455	THR
1	I	465	ASP
1	I	469	ASN
1	I	483	LEU
1	I	501	HIS
1	I	507	THR
1	I	516	GLN
1	I	524	SER
1	I	530	TYR

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Mol	Chain	Res	Type
1	I	545	SER
1	I	554	PHE
1	I	564	THR
1	I	570	GLU
1	I	578	VAL
1	I	584	ARG
1	I	591	LYS
1	I	601	LYS
1	I	603	GLU
1	I	620	ILE
1	J	4	ASP
1	J	11	PRO
1	J	34	LYS
1	J	38	ILE
1	J	57	THR
1	J	85	GLU
1	J	96	VAL
1	J	97	LEU
1	J	99	ARG
1	J	101	ASP
1	J	103	LYS
1	J	105	ILE
1	J	111	GLN
1	J	122	GLU
1	J	220	MET
1	J	251	GLU
1	J	265	ASP
1	J	304	ILE
1	J	305	ILE
1	J	309	ASP
1	J	319	SER
1	J	326	VAL
1	J	347	ASP
1	J	349	SER
1	J	353	ARG
1	J	379	THR
1	J	398	LYS
1	J	405	THR
1	J	407	ILE
1	J	418	ILE
1	J	425	SER
1	J	426	VAL

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Mol	Chain	Res	Type
1	J	439	THR
1	J	442	ILE
1	J	455	THR
1	J	465	ASP
1	J	469	ASN
1	J	483	LEU
1	J	501	HIS
1	J	507	THR
1	J	512	ARG
1	J	532	SER
1	J	533	CYS
1	J	545	SER
1	J	554	PHE
1	J	564	THR
1	J	570	GLU
1	J	578	VAL
1	J	584	ARG
1	J	591	LYS
1	J	601	LYS
1	J	603	GLU
1	J	620	ILE
1	K	4	ASP
1	K	5	LYS
1	K	11	PRO
1	K	57	THR
1	K	63	LEU
1	K	84	ASN
1	K	85	GLU
1	K	96	VAL
1	K	97	LEU
1	K	99	ARG
1	K	101	ASP
1	K	105	ILE
1	K	111	GLN
1	K	122	GLU
1	K	220	MET
1	K	265	ASP
1	K	268	ARG
1	K	305	ILE
1	K	319	SER
1	K	326	VAL
1	K	347	ASP

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Mol	Chain	Res	Type
1	K	349	SER
1	K	353	ARG
1	K	379	THR
1	K	398	LYS
1	K	405	THR
1	K	407	ILE
1	K	418	ILE
1	K	425	SER
1	K	426	VAL
1	K	439	THR
1	K	442	ILE
1	K	455	THR
1	K	465	ASP
1	K	469	ASN
1	K	483	LEU
1	K	501	HIS
1	K	507	THR
1	K	512	ARG
1	K	516	GLN
1	K	532	SER
1	K	545	SER
1	K	554	PHE
1	K	564	THR
1	K	570	GLU
1	K	578	VAL
1	K	584	ARG
1	K	591	LYS
1	K	601	LYS
1	K	603	GLU
1	K	620	ILE
1	L	4	ASP
1	L	5	LYS
1	L	11	PRO
1	L	57	THR
1	L	85	GLU
1	L	96	VAL
1	L	97	LEU
1	L	99	ARG
1	L	101	ASP
1	L	105	ILE
1	L	111	GLN
1	L	122	GLU

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Mol	Chain	Res	Type
1	L	220	MET
1	L	265	ASP
1	L	268	ARG
1	L	271	GLU
1	L	275	ASP
1	L	305	ILE
1	L	319	SER
1	L	326	VAL
1	L	347	ASP
1	L	349	SER
1	L	353	ARG
1	L	379	THR
1	L	398	LYS
1	L	405	THR
1	L	407	ILE
1	L	418	ILE
1	L	425	SER
1	L	426	VAL
1	L	439	THR
1	L	442	ILE
1	L	455	THR
1	L	465	ASP
1	L	467	LEU
1	L	469	ASN
1	L	483	LEU
1	L	501	HIS
1	L	507	THR
1	L	516	GLN
1	L	527	SER
1	L	528	THR
1	L	530	TYR
1	L	545	SER
1	L	554	PHE
1	L	571	ASN
1	L	578	VAL
1	L	584	ARG
1	L	591	LYS
1	L	601	LYS
1	L	603	GLU
1	L	620	ILE
1	M	4	ASP
1	M	11	PRO

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Mol	Chain	Res	Type
1	M	57	THR
1	M	68	ASP
1	M	85	GLU
1	M	96	VAL
1	M	97	LEU
1	M	99	ARG
1	M	101	ASP
1	M	105	ILE
1	M	111	GLN
1	M	122	GLU
1	M	220	MET
1	M	251	GLU
1	M	264	GLN
1	M	265	ASP
1	M	271	GLU
1	M	305	ILE
1	M	319	SER
1	M	326	VAL
1	M	347	ASP
1	M	349	SER
1	M	353	ARG
1	M	379	THR
1	M	398	LYS
1	M	405	THR
1	M	407	ILE
1	M	418	ILE
1	M	425	SER
1	M	426	VAL
1	M	439	THR
1	M	442	ILE
1	M	455	THR
1	M	465	ASP
1	M	469	ASN
1	M	483	LEU
1	M	501	HIS
1	M	507	THR
1	M	512	ARG
1	M	516	GLN
1	M	528	THR
1	M	532	SER
1	M	545	SER
1	M	554	PHE

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Mol	Chain	Res	Type
1	M	564	THR
1	M	570	GLU
1	M	578	VAL
1	M	584	ARG
1	M	591	LYS
1	M	601	LYS
1	M	603	GLU
1	M	620	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	84	ASN
1	A	133	ASN
1	A	169	HIS
1	A	431	HIS
1	C	81	GLN
1	C	278	ASN
1	C	431	HIS
1	D	81	GLN
1	D	125	ASN
1	D	169	HIS
1	D	278	ASN
1	D	431	HIS
1	E	81	GLN
1	E	125	ASN
1	E	169	HIS
1	E	278	ASN
1	E	431	HIS
1	F	81	GLN
1	F	169	HIS
1	F	278	ASN
1	F	431	HIS
1	G	78	GLN
1	G	81	GLN
1	G	133	ASN
1	G	169	HIS
1	G	278	ASN
1	G	431	HIS
1	H	169	HIS
1	H	224	HIS

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Mol	Chain	Res	Type
1	H	278	ASN
1	H	431	HIS
1	I	81	GLN
1	I	125	ASN
1	I	278	ASN
1	I	288	ASN
1	I	431	HIS
1	J	81	GLN
1	J	125	ASN
1	J	169	HIS
1	J	278	ASN
1	J	419	ASN
1	J	431	HIS
1	K	81	GLN
1	K	125	ASN
1	K	169	HIS
1	K	278	ASN
1	K	419	ASN
1	K	431	HIS
1	L	81	GLN
1	L	133	ASN
1	L	169	HIS
1	L	172	HIS
1	L	278	ASN
1	L	431	HIS
1	M	81	GLN
1	M	169	HIS
1	M	278	ASN
1	M	431	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.