



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:23 am GMT

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 Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

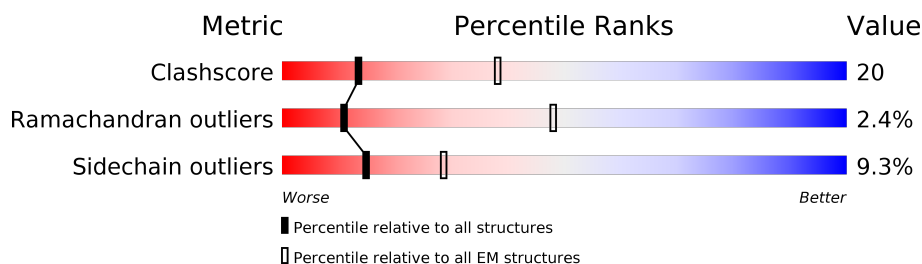
# 1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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.

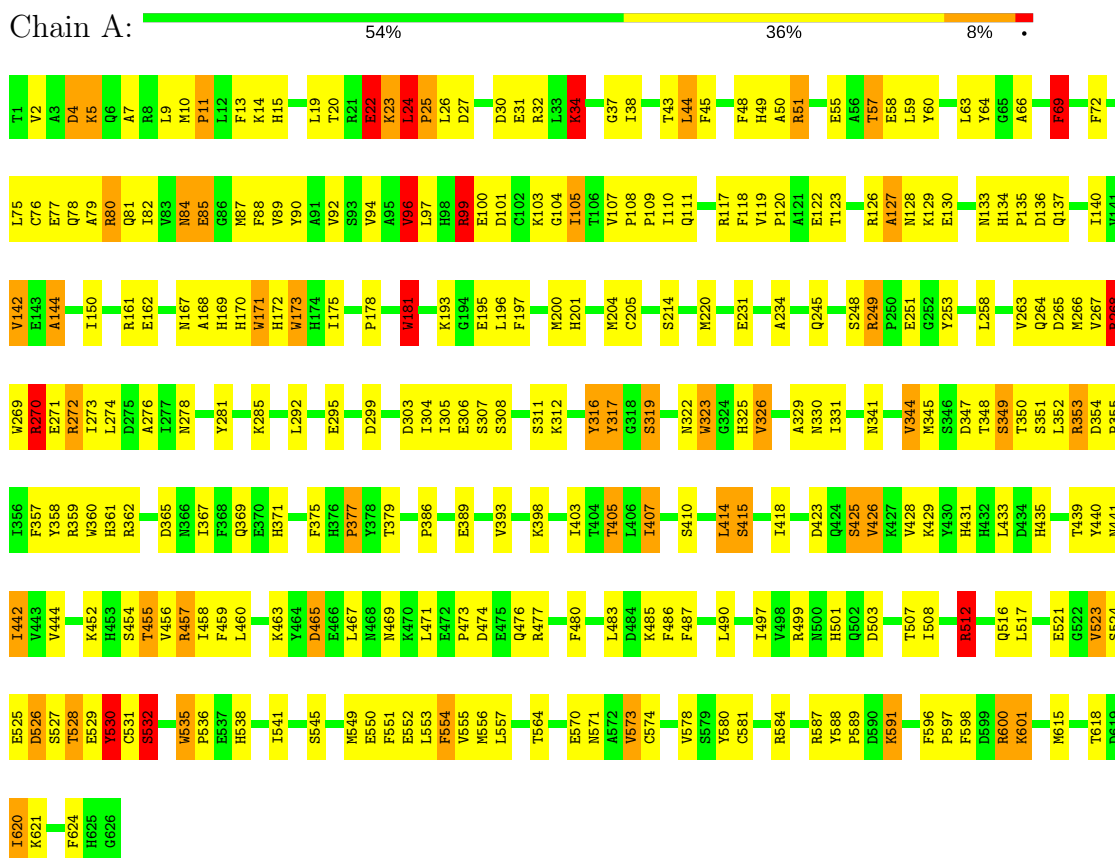
- Molecule 1 is a protein called Hemocyanin AA6 chain.

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		

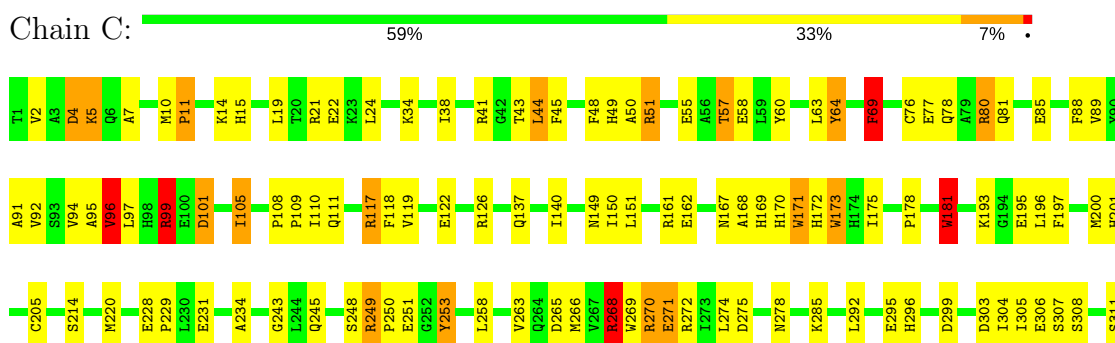
### 3 Residue-property plots

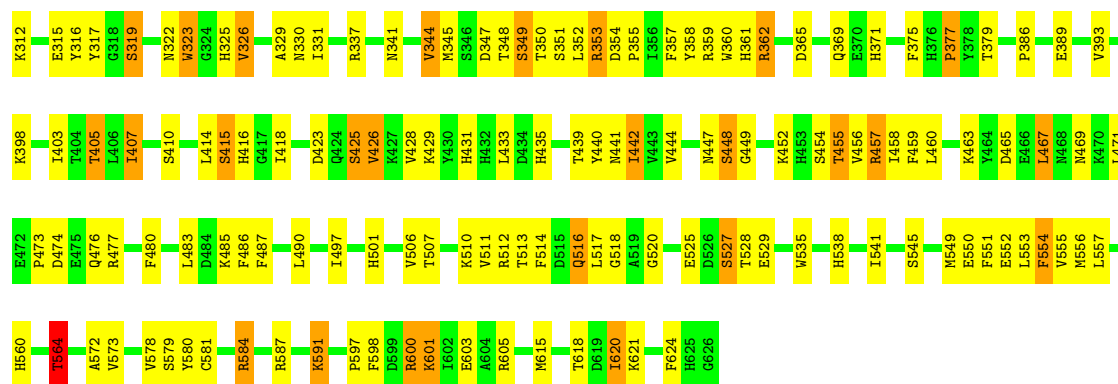
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

#### • Molecule 1: Hemocyanin AA6 chain



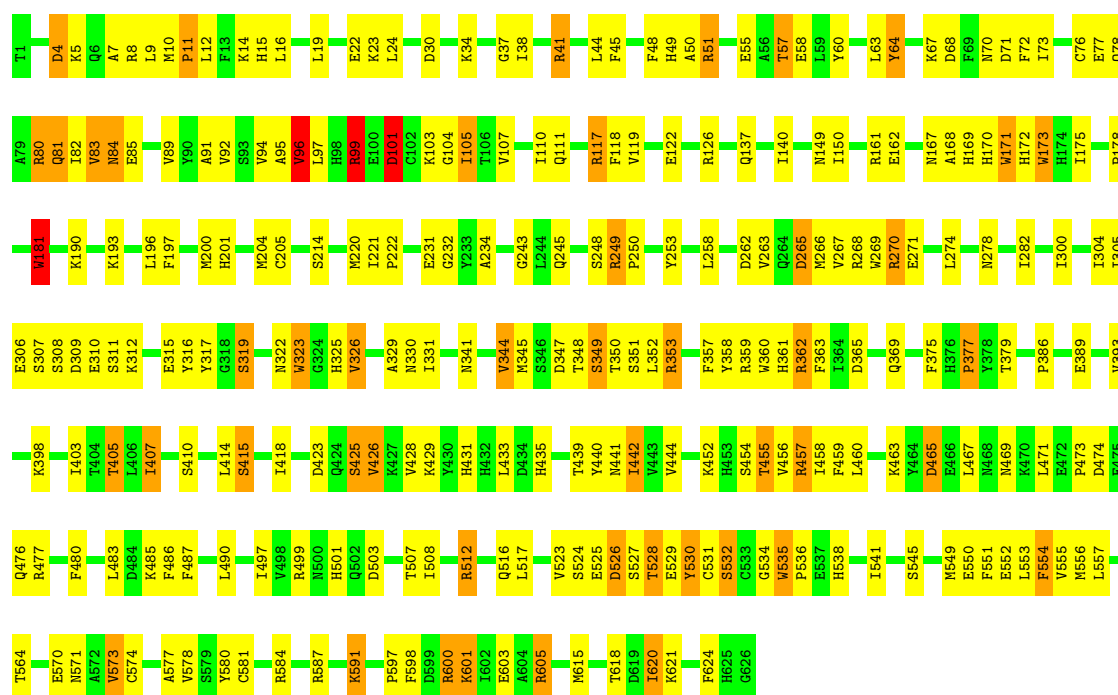
#### • Molecule 1: Hemocyanin AA6 chain





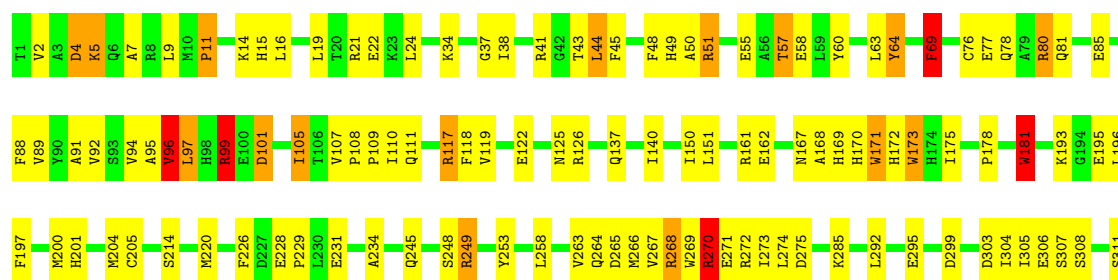
• Molecule 1: Hemocyanin AA6 chain

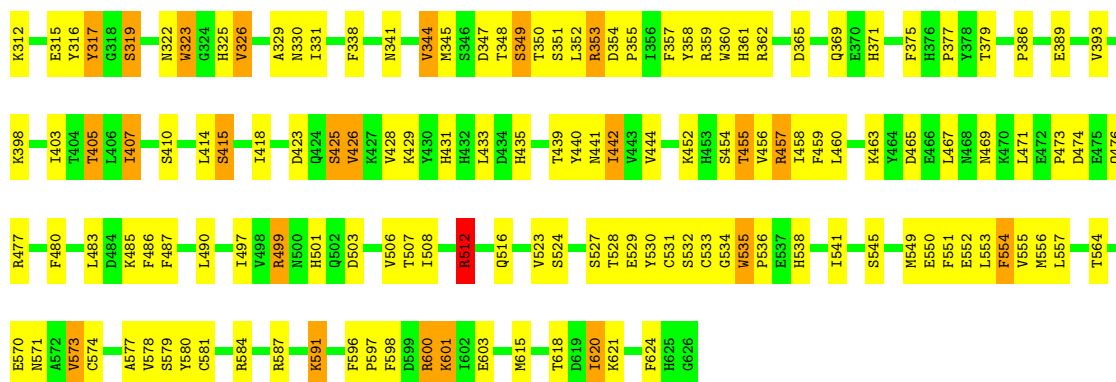
Chain D: 58% 34% 8% .



• Molecule 1: Hemocyanin AA6 chain

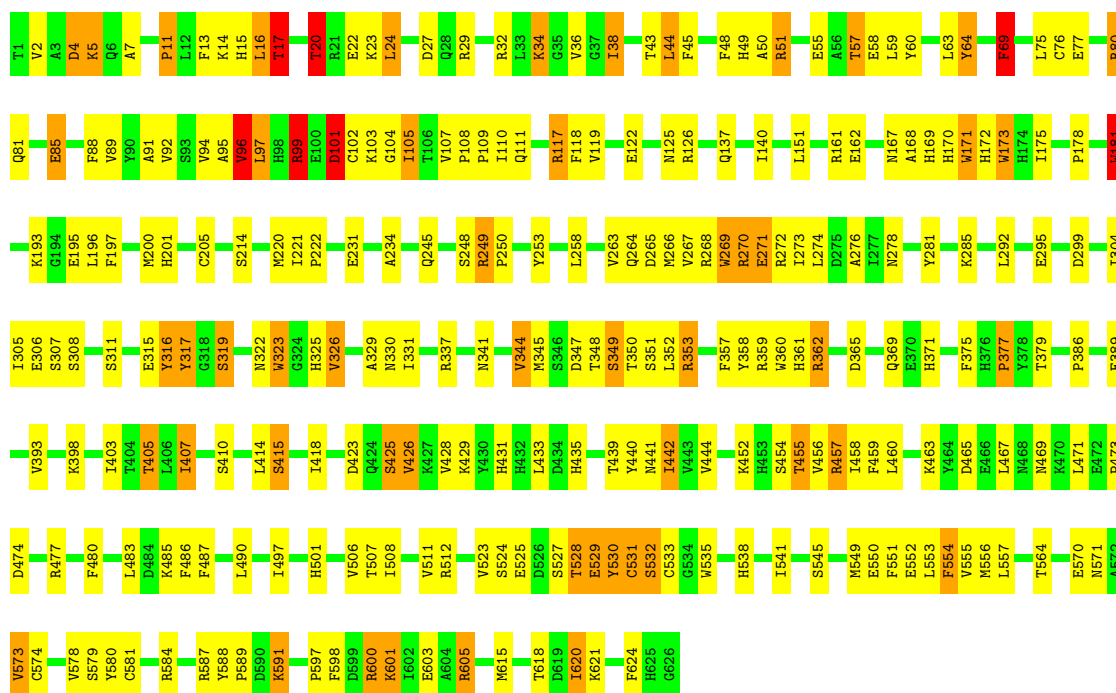
Chain E: 58% 34% 6% .





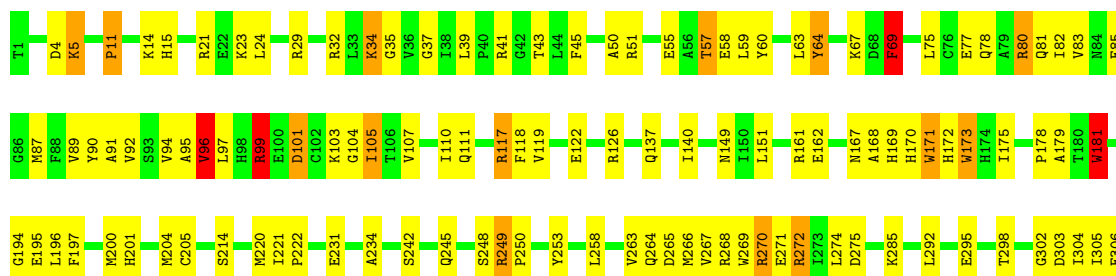
• Molecule 1: Hemocyanin AA6 chain

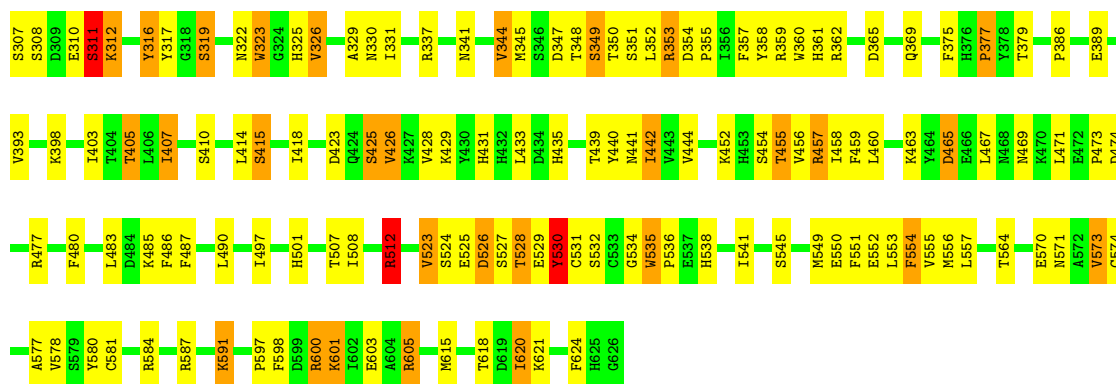
Chain F: 58% 32% 8% •



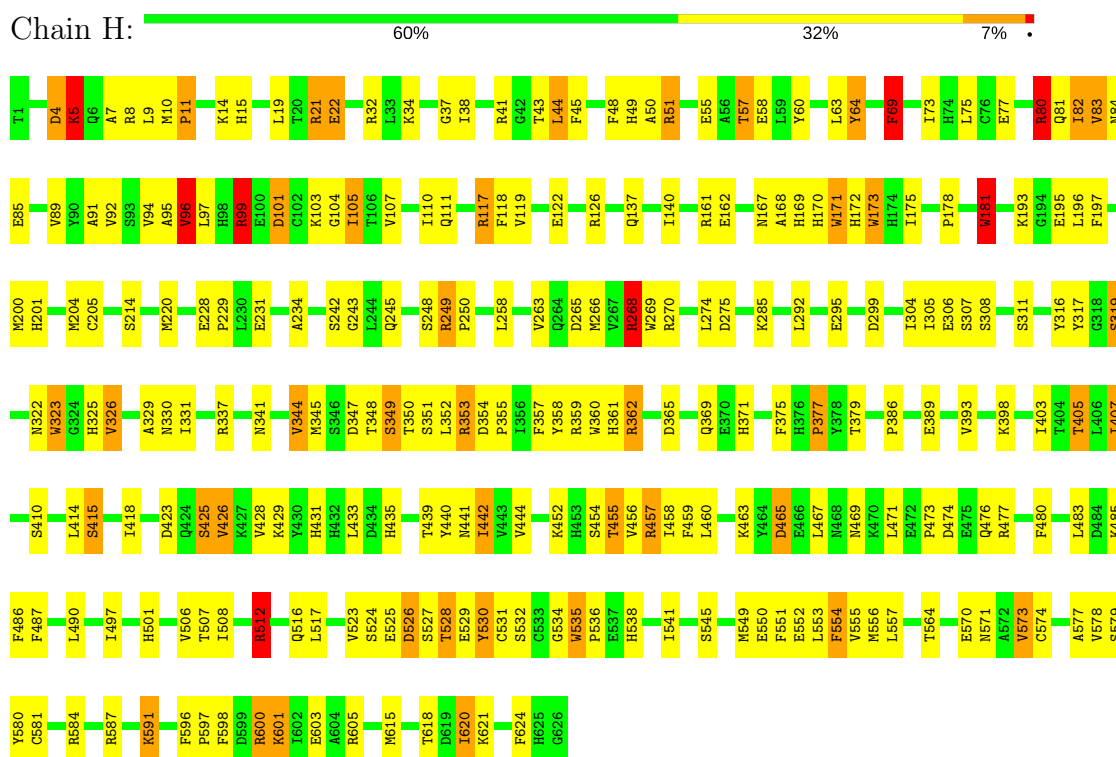
• Molecule 1: Hemocyanin AA6 chain

Chain G: 59% 33% 7% •

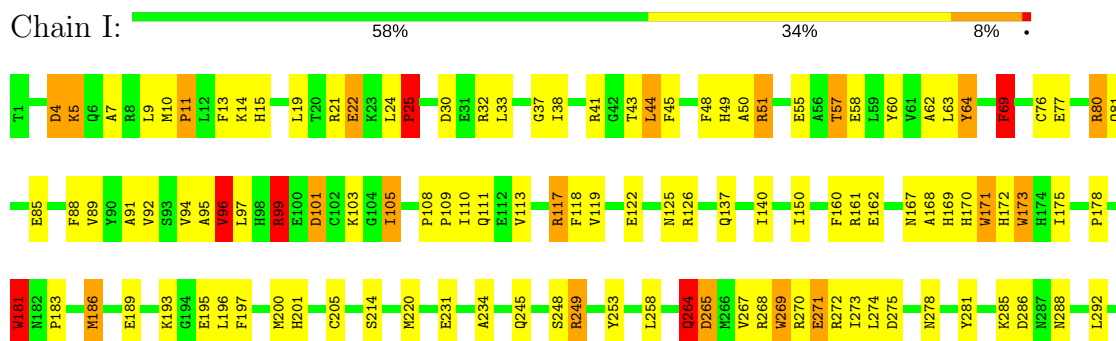




• Molecule 1: Hemocyanin AA6 chain

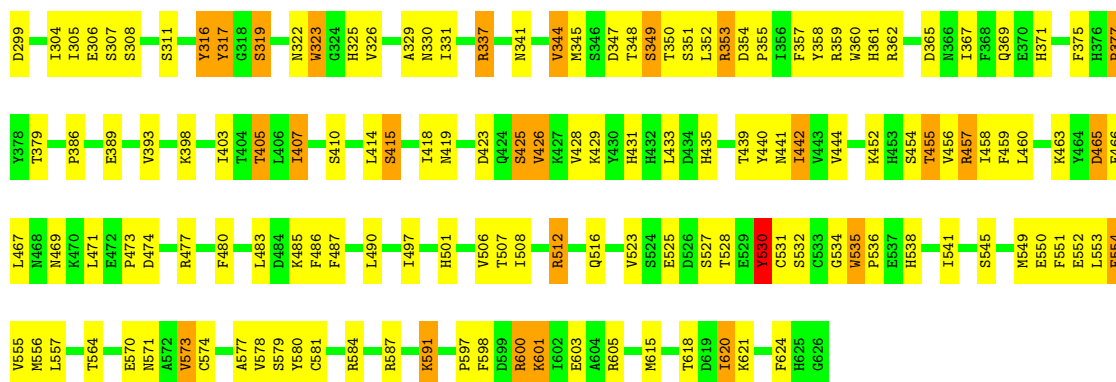


• Molecule 1: Hemocyanin AA6 chain

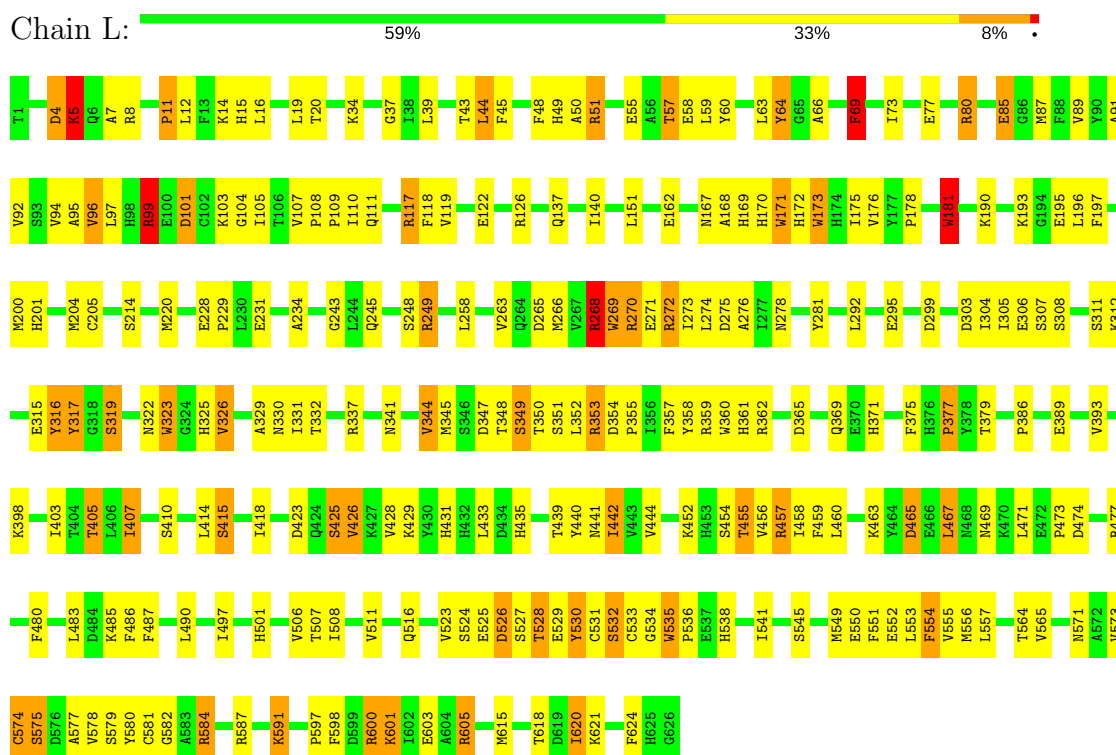




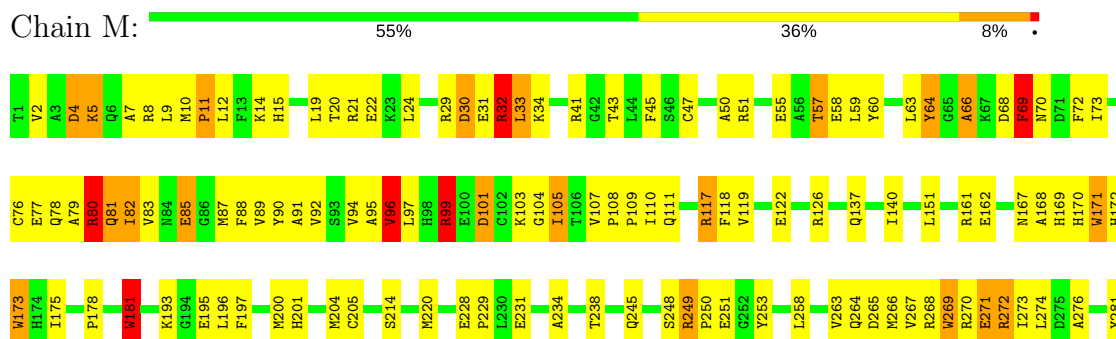


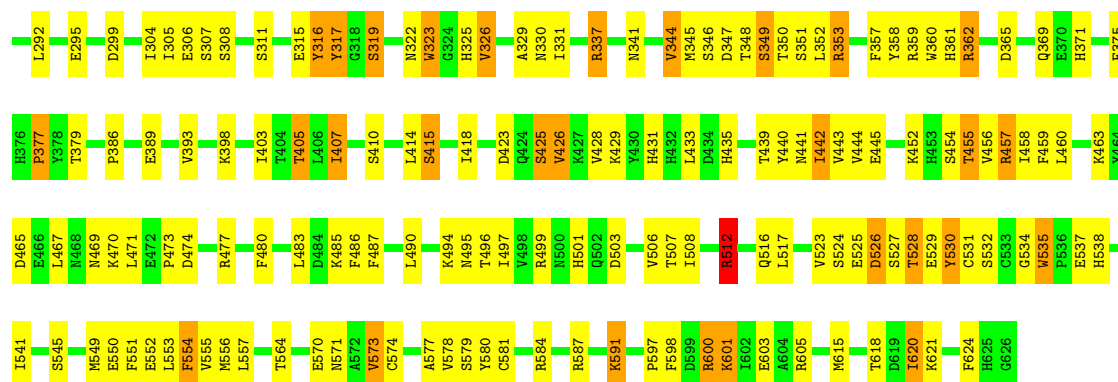


• Molecule 1: Hemocyanin AA6 chain



• Molecule 1: Hemocyanin AA6 chain





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C	Depositor
Number of particles used	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:H:69:PHE:CE1	1:H:69:PHE:CD1	1.96	1.53
1:K:69:PHE:CG	1:K:69:PHE:CD2	1.97	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: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:L:69:PHE:CG	1:L:69:PHE:CD1	1.97	1.52
1:M:69:PHE:CE1	1:M:69:PHE:CD1	1.97	1.51
1:E:69:PHE:CG	1:E:69:PHE:CD1	1.98	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:A:69:PHE:CD2	1:A:69:PHE:CE2	1.98	1.51
1:C:69:PHE:CE1	1:C:69:PHE:CD1	1.99	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:J:69:PHE:CZ	1:J:69:PHE:CE2	1.99	1.51
1:A:69:PHE:CG	1:A:69:PHE:CD1	1.98	1.51
1:J:69:PHE:CE2	1:J:69:PHE:CD2	1.98	1.51
1:A:69:PHE:CZ	1:A:69:PHE:CE2	1.99	1.51
1:K:69:PHE:CD1	1:K:69:PHE:CE1	1.96	1.51
1:C:69:PHE:CZ	1:C:69:PHE:CE2	1.99	1.50
1:E:69:PHE:CE2	1:E:69:PHE:CD2	1.98	1.50
1:I:69:PHE:CD1	1:I:69:PHE:CG	1.96	1.50
1:M:69:PHE:CD2	1:M:69:PHE:CE2	1.96	1.50
1:A:69:PHE:CD1	1:A:69:PHE:CE1	1.99	1.50
1:J:69:PHE:CD1	1:J:69:PHE:CE1	1.99	1.50
1:K:69:PHE:CE2	1:K:69:PHE:CZ	1.96	1.50
1:E:69:PHE:CZ	1:E:69:PHE:CE2	1.99	1.50
1:G:69:PHE:CE1	1:G:69:PHE:CZ	1.96	1.50
1:I:69:PHE:CE1	1:I:69:PHE:CZ	1.96	1.50
1:L:69:PHE:CD2	1:L:69:PHE:CE2	1.96	1.50
1:F:69:PHE:CD2	1:F:69:PHE:CE2	1.98	1.50
1:I:69:PHE:CD1	1:I:69:PHE:CE1	1.96	1.50
1:L:69:PHE:CE1	1:L:69:PHE:CD1	1.96	1.50
1:E:69:PHE:CD1	1:E:69:PHE:CE1	1.99	1.50
1:M:69:PHE:CD2	1:M:69:PHE:CG	1.98	1.50
1:A:79:ALA:HB3	1:A:88:PHE:CE1	1.45	1.49
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:F:69:PHE:CE1	1:F:69:PHE:CD1	1.99	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:L:69:PHE:CG	1:L:69:PHE:CD2	1.97	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: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: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:F:69:PHE:CD2	1:F: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: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:J:69:PHE:CZ	1:J:69:PHE:CE1	1.98	1.48
1:G:69:PHE:CD2	1:G:69:PHE:CG	1.97	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:H:104:GLY:CA	1:H:525:GLU:HB3	1.41	1.46
1:M:69:PHE:CE1	1:M:69:PHE:CZ	2.01	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:F:104:GLY:HA3	1:F:525:GLU:HB3	1.21	1.13
1:J:175:ILE:HG21	1:J:528:THR:HG21	1.24	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:G:204:MET:HG2	1:G:535:TRP:CH2	1.88	1.08
1:L:204:MET:HG2	1:L:535:TRP:CH2	1.89	1.08
1:G:24:LEU:HD13	1:G:81:GLN:NE2	1.68	1.07
1:H:467:LEU:CD1	1:J:151:LEU:CA	2.32	1.07
1:A:24:LEU:CB	1:A:24:LEU:HG	1.84	1.07
1:J:175:ILE:CG2	1:J:528:THR:CG2	2.33	1.07
1:J:5:LYS:NZ	1:J:69:PHE:CZ	2.23	1.07
1:D:204:MET:HG2	1:D:535:TRP:CH2	1.88	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:LYS:NZ	1:E:69:PHE:CZ	2.23	1.07
1:K:175:ILE:CG2	1:K:528:THR:CG2	2.32	1.07
1:K:59:LEU:HD11	1:K:87:MET:HE3	1.08	1.07
1:C:5:LYS:NZ	1:C:69:PHE:CG	2.23	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:A:72:PHE:CE2	1:A:96:VAL:HG23	1.89	1.06
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:F:104:GLY:HA2	1:F:525:GLU:HB3	1.27	1.06
1:F:5:LYS:NZ	1:F:69:PHE:CZ	2.23	1.06
1:H:204:MET:HG2	1:H:535:TRP:CH2	1.89	1.06
1:C:5:LYS:NZ	1:C:69:PHE:CE1	2.23	1.06
1:E:5:LYS:NZ	1:E:69:PHE:CD1	2.24	1.06
1:J:5:LYS:NZ	1:J:69:PHE:CD1	2.24	1.06
1:M:64:TYR:OH	1:M:94:VAL:HG12	1.54	1.06
1:C:5:LYS:NZ	1:C:69:PHE:CD1	2.24	1.06
1:F:5:LYS:NZ	1:F:69:PHE:CD1	2.24	1.06
1:G:5:LYS:NZ	1:G:69:PHE:CZ	2.23	1.06
1:I:5:LYS:NZ	1:I:69:PHE:CZ	2.23	1.06
1:K:5:LYS:NZ	1:K:69:PHE:CG	2.24	1.06
1:A:5:LYS:NZ	1:A:69:PHE:CZ	2.23	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:CE2	2.23	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:A:5:LYS:NZ	1:A:69:PHE:CG	2.23	1.06
1:H:5:LYS:NZ	1:H:69:PHE:CG	2.24	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:CE1	2.24	1.06
1:I:5:LYS:NZ	1:I:69:PHE:CE1	2.24	1.06
1:F:5:LYS:NZ	1:F:69:PHE:CE1	2.23	1.06
1:H:5:LYS:NZ	1:H:69:PHE:CE2	2.24	1.06
1:J:5:LYS:NZ	1:J:69:PHE:CE2	2.23	1.06
1:E:5:LYS:NZ	1:E:69:PHE:CG	2.23	1.06
1:C:5:LYS:NZ	1:C:69:PHE:CD2	2.24	1.05
1:D:104:GLY:HA3	1:D:525:GLU:HB3	1.09	1.05
1:F:5:LYS:NZ	1:F: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:CG	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:CD2	2.24	1.05
1:I:5:LYS:NZ	1:I:69:PHE:CE2	2.24	1.05
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:M:104:GLY:HA3	1:M:525:GLU:HB3	1.10	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:I:5:LYS:NZ	1:I:69:PHE:CD1	2.24	1.05
1:J:5:LYS:NZ	1:J:69:PHE:CD2	2.24	1.05
1:K:5:LYS:NZ	1:K:69:PHE:CZ	2.24	1.05
1:M:5:LYS:NZ	1:M:69:PHE:CZ	2.23	1.05
1:A:5:LYS:NZ	1:A:69:PHE:CE1	2.23	1.05
1:A:76:CYS:HA	1:A:88:PHE:CZ	1.91	1.05
1:E:5:LYS:NZ	1:E: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:A:5:LYS:NZ	1:A:69:PHE:CD1	2.24	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:K:5:LYS:NZ	1:K:69:PHE:CD2	2.25	1.05
1:L:5:LYS:NZ	1:L:69:PHE:CZ	2.24	1.05
1:A:5:LYS:NZ	1:A:69:PHE:CD2	2.24	1.05
1:G:5:LYS:NZ	1:G:69:PHE:CE2	2.24	1.05
1:F:5:LYS:NZ	1:F:69:PHE:CE2	2.23	1.05
1:M:5:LYS:NZ	1:M:69:PHE:CD1	2.25	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:A:79:ALA:CB	1:A:88:PHE:CE1	2.39	1.04
1:G:5:LYS:NZ	1:G:69:PHE:CD2	2.24	1.04
1:L:104:GLY:HA3	1:L:525:GLU:CB	1.83	1.04
1:M:5:LYS:NZ	1:M:69:PHE:CG	2.25	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:G:64:TYR:OH	1:G:94:VAL:HG12	1.57	1.02
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: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:D:9:LEU:CD1	1:D:72:PHE:HE2	1.74	1.00
1:F:104:GLY:CA	1:F:525:GLU:CB	2.37	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:H:467:LEU:HD11	1:J:151:LEU:HA	1.45	0.94
1:J:97:LEU:HD11	1:J:528:THR:CB	1.97	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:H:274:LEU:HB2	1:K:268:ARG:HH12	1.31	0.93
1:M:9:LEU:CD1	1:M:73:ILE:CD1	2.46	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:I:10:MET:SD	1:I:517:LEU:CB	2.59	0.91
1:M:5:LYS:CE	1:M:69:PHE:CE2	2.54	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:H:467:LEU:CG	1:J:151:LEU:HD13	2.01	0.90
1:M:5:LYS:CE	1:M:69:PHE:CD2	2.55	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:50:ALA:HB2	1:K:323:TRP:CH2	2.07	0.89
1:K:107:VAL:HG21	1:K:528:THR:OG1	1.73	0.89
1:D:8:ARG:CZ	1:D:73:ILE:HG21	2.02	0.89
1:M:5:LYS:CE	1:M:69:PHE:CG	2.55	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:F:5:LYS:CE	1:F:69:PHE:CD1	2.57	0.88
1:K:5:LYS:CE	1:K:69:PHE:CD1	2.56	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:24:LEU:HD13	1:G:81:GLN:HE22	1.39	0.88
1:G:5:LYS:CE	1:G:69:PHE:CD1	2.57	0.88
1:G:5:LYS:CE	1:G:69:PHE:CD2	2.57	0.88
1:A:76:CYS:HA	1:A:88:PHE:HZ	1.33	0.88
1:C:5:LYS:CE	1:C:69:PHE:CD2	2.56	0.88
1:E:5:LYS:CE	1:E:69:PHE:CD2	2.57	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:290:ILE:HD12	1:J:300:ILE:CD1	2.03	0.88
1:J:5:LYS:CE	1:J:69:PHE:CD2	2.56	0.88
1:L:5:LYS:CE	1:L:69:PHE:CG	2.57	0.88
1:L:63:LEU:HD22	1:L:91:ALA:HB1	1.52	0.88
1:H:5:LYS:CE	1:H:69:PHE:CG	2.57	0.87
1:I:5:LYS:CE	1:I:69:PHE:CD2	2.56	0.87
1:K:5:LYS:CE	1:K:69:PHE:CG	2.56	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:G:63:LEU:CD2	1:G:91:ALA:CB	2.52	0.87
1:J:5:LYS:CE	1:J:69:PHE:CD1	2.57	0.87
1:L:5:LYS:CE	1:L:69:PHE:CD2	2.57	0.87
1:A:5:LYS:CE	1:A:69:PHE:CG	2.58	0.87
1:C:5:LYS:CE	1:C:69:PHE:CG	2.58	0.87
1:H:5:LYS:CE	1:H:69:PHE:CE2	2.57	0.87
1:E:5:LYS:CE	1:E:69:PHE:CG	2.58	0.87
1:H:5:LYS:CE	1:H:69:PHE:CD1	2.57	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: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:M:5:LYS:HE2	1:M:69:PHE:CD2	2.10	0.87
1:A:5:LYS:CE	1:A:69:PHE:CD1	2.57	0.87
1:A:5:LYS:CE	1:A:69:PHE:CE2	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: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:A:5:LYS:CE	1:A:69:PHE:CD2	2.57	0.87
1:H:467:LEU:HD12	1:J:151:LEU:N	1.90	0.87
1:I:5:LYS:CE	1:I:69:PHE:CE2	2.57	0.87
1:L:5:LYS:CE	1:L:69:PHE:CE2	2.57	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:H:19:LEU:HB3	1:H:80:ARG:HD3	1.56	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:L:5:LYS:CE	1:L:69:PHE:CE1	2.59	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:H:5:LYS:CE	1:H:69:PHE:CE1	2.58	0.86
1:K:5:LYS:CE	1:K:69:PHE:CE2	2.58	0.86
1:L:19:LEU:HB3	1:L:80:ARG:HD2	1.56	0.86
1:I:5:LYS:CE	1:I:69:PHE:CG	2.58	0.86
1:J:5:LYS:CE	1:J:69:PHE:CE1	2.58	0.86
1:K:5:LYS:CE	1:K:69:PHE:CZ	2.59	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:G:32:ARG:HH21	1:G:75:LEU:HD13	1.41	0.86
1:K:5:LYS:CE	1:K:69:PHE:CE1	2.58	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:F:5:LYS:CE	1:F:69:PHE:CZ	2.59	0.85
1:G:5:LYS:CE	1:G: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:C:14:LYS:HE2	1:C:514:PHE:CZ	2.11	0.85
1:F:5:LYS:HE2	1:F:69:PHE:CD2	2.12	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:A:204:MET:HG2	1:A:535:TRP:CZ3	2.12	0.84
1:C:5:LYS:HE2	1:C:69:PHE:CD2	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:A:66:ALA:HB3	1:A:99:ARG:HH21	1.45	0.81
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:E:97:LEU:CD1	1:E:528:THR:CB	2.57	0.81
1:D:9:LEU:CD2	1:D:72:PHE:CZ	2.63	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: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:J:268:ARG:HH22	1:L:274:LEU:HD12	1.46	0.81
1:M:5:LYS:HE3	1:M:69:PHE:CD1	2.14	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:F:529:GLU:HG3	1:F:574:CYS:SG	2.21	0.80
1:M:22:GLU:HB2	1:M:81:GLN:HB3	1.61	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:D:9:LEU:HD21	1:D:72:PHE:CE2	2.17	0.79
1:C:151:LEU:CA	1:G:467:LEU:CD1	2.58	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:H:8:ARG:HH21	1:H:73:ILE:HG13	1.44	0.79
1:I:272:ARG:HH11	1:I:316:TYR:HA	1.47	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:G:63:LEU:HD23	1:G:91:ALA:HB1	1.66	0.78
1:L:5:LYS:HE2	1:L:69:PHE:CE2	2.19	0.78
1:C:5:LYS:HE3	1:C:69:PHE:CD1	2.17	0.78
1:M:8:ARG:NE	1:M:73:ILE:HG21	1.98	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:A:129:LYS:NZ	1:C:243:GLY:HA3	1.99	0.77
1:G:50:ALA:HB2	1:G:323:TRP:HH2	1.49	0.77
1:M:9:LEU:HD12	1:M:73:ILE:CD1	2.14	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:A:268:ARG:HH12	1:G:274:LEU:HB2	1.49	0.77
1:K:274:LEU:HD12	1:M:268:ARG:HH22	1.50	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:D:12:LEU:HD13	1:D:76:CYS:SG	2.25	0.76
1:G:24:LEU:HB2	1:G:81:GLN:NE2	2.00	0.76
1:L:63:LEU:HD21	1:L:91:ALA:HB1	1.65	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:132:SER:HB2	1:K:419:ASN:HD22	1.47	0.76
1:J:290:ILE:HD11	1:J:300:ILE:HD12	1.68	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:E:96:VAL:HG22	1:E:105:ILE:HG21	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:304:ILE:HD11	1:G:312:LYS:HB2	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:A:76:CYS:O	1:A:88:PHE:HE2	1.70	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: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:A:80:ARG:HB2	1:A:88:PHE:CE2	2.23	0.73
1:K:5:LYS:HE3	1:K:69:PHE:CD1	2.22	0.73
1:A:76:CYS:O	1:A:88:PHE:CE2	2.41	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:I:272:ARG:CB	1:I:316:TYR:CZ	2.70	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:J:204:MET:HG2	1:J:535:TRP:HH2	1.50	0.72
1:L:63:LEU:HD21	1:L:91:ALA:CB	2.19	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:F:24:LEU:HD11	1:F:29:ARG:HG3	1.72	0.71
1:H:5:LYS:HE3	1:H:69:PHE:CG	2.24	0.71
1:K:249:ARG:HE	1:K:331:ILE:HG21	1.56	0.71
1:M:204:MET:HG2	1:M:535:TRP:HH2	1.51	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:G:249:ARG:HE	1:G:331:ILE:HG21	1.56	0.70
1:H:204:MET:HG2	1:H:535:TRP:HH2	1.52	0.70
1:A:129:LYS:HZ2	1:C:243:GLY:CA	2.04	0.70
1:C:249:ARG:HE	1:C:331:ILE:HG21	1.55	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: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:E:63:LEU:CD2	1:E:91:ALA:HB1	2.22	0.70
1:F:511:VAL:HA	1:F:531:CYS:HB2	1.72	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: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:J:375:PHE:HB2	1:J:600:ARG:HD3	1.74	0.70
1:M:5:LYS:HE3	1:M:69:PHE:CG	2.27	0.70
1:E:21:ARG:HD3	1:E:41:ARG:CD	2.22	0.70
1:G:307:SER:H	1:G:319:SER:HB3	1.56	0.70
1:I:63:LEU:CD2	1:I:91:ALA:HB1	2.22	0.70
1:L:64:TYR:OH	1:L:94:VAL:CG1	2.40	0.70
1:J:26:LEU:HB3	1:J:28:GLN:HG3	1.74	0.69
1:K:8:ARG:CZ	1:K:73:ILE:CG2	2.69	0.69
1:C:21:ARG:HD3	1:C:41:ARG:CD	2.22	0.69
1:A:274:LEU:HD12	1:E:268:ARG:HH22	1.56	0.69
1:D:19:LEU:HD22	1:D:80:ARG:HD3	1.74	0.69
1:H:21:ARG:HD3	1:H:41:ARG:CD	2.22	0.69
1:J:307:SER:H	1:J:319:SER:HB3	1.56	0.69
1:L:249:ARG:HE	1:L:331:ILE:HG21	1.57	0.69
1:A:24:LEU:HD23	1:A:82:ILE:CG2	2.21	0.69
1:A:24:LEU:CD1	1:A:81:GLN:NE2	2.55	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:A:175:ILE:HG21	1:A:528:THR:HG21	1.75	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:344:VAL:HB	1:A:350:THR:HB	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:169:HIS:HE1	1:I:581:CYS:SG	2.16	0.69
1:G:375:PHE:HB2	1:G:600:ARG:HD3	1.74	0.69
1:I:10:MET:CE	1:I:517:LEU:O	2.39	0.69
1:A:375:PHE:HB2	1:A:600:ARG:HD3	1.74	0.69
1:E:169:HIS:HE1	1:E:581:CYS:SG	2.16	0.69
1:K:375:PHE:HB2	1:K:600:ARG:HD3	1.74	0.69
1:G:32:ARG:NH2	1:G:75:LEU:HD13	2.07	0.69
1:H:344:VAL:HB	1:H:350:THR:HB	1.75	0.69
1:H:96:VAL:HG22	1:H:105:ILE:HG21	1.75	0.69
1:I:21:ARG:HD3	1:I:41:ARG:CD	2.22	0.69
1:K:344:VAL:HB	1:K:350:THR:HB	1.75	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:K:204:MET:HG2	1:K:535:TRP:HH2	1.50	0.69
1:J:122:GLU:HG2	1:K:242:SER:OG	1.92	0.69
1:F:169:HIS:HE1	1:F:581:CYS:SG	2.16	0.68
1:G:344:VAL:HB	1:G:350:THR:HB	1.75	0.68
1:G:169:HIS:HE1	1:G:581:CYS:SG	2.16	0.68
1:I:96:VAL:HG22	1:I:105:ILE:HG21	1.76	0.68
1:I:375:PHE:HB2	1:I:600:ARG:HD3	1.74	0.68
1:M:96:VAL:HG22	1:M:105:ILE:HG21	1.75	0.68
1:A:129:LYS:HZ2	1:C:243:GLY:HA2	1.56	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:D:169:HIS:HE1	1:D:581:CYS:SG	2.16	0.68
1:E:375:PHE:HB2	1:E:600:ARG:HD3	1.74	0.68
1:H:63:LEU:CD2	1:H:91:ALA:HB1	2.22	0.68
1:J:169:HIS:HE1	1:J:581:CYS:SG	2.16	0.68
1:M:375:PHE:HB2	1:M:600:ARG:HD3	1.74	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:E:344:VAL:HB	1:E:350:THR:HB	1.75	0.68
1:H:249:ARG:HE	1:H:331:ILE:HG21	1.57	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:A:59:LEU:HD11	1:A:87:MET:HE3	1.74	0.68
1:D:344:VAL:HB	1:D:350:THR:HB	1.75	0.68
1:F:375:PHE:HB2	1:F:600:ARG:HD3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:512:ARG:HB2	1:J:531:CYS:SG	2.34	0.68
1:L:169:HIS:HE1	1:L:581:CYS:SG	2.16	0.68
1:A:24:LEU:HA	1:A:81:GLN:NE2	2.08	0.68
1:F:344:VAL:HB	1:F:350:THR:HB	1.75	0.68
1:H:467:LEU:HD13	1:J:150:ILE:O	1.94	0.68
1:L:103:LYS:CG	1:L:525:GLU:O	2.42	0.68
1:M:169:HIS:HE1	1:M:581:CYS:SG	2.16	0.68
1:A:169:HIS:HE1	1:A:581:CYS:SG	2.16	0.67
1:C:344:VAL:HB	1:C:350:THR:HB	1.75	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: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: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:K:5:LYS:HA	1:K:69:PHE:CE2	2.29	0.67
1:J:162:GLU:HG2	1:J:353:ARG:HB3	1.76	0.67
1:J:249:ARG:HE	1:J:331:ILE:HG21	1.58	0.67
1:L:162:GLU:HG2	1:L:353:ARG:HB3	1.77	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:F:405:THR:HA	1:F:435:HIS:HA	1.76	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:G:24:LEU:CD1	1:G:81:GLN:HE22	2.07	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:J:5:LYS:HE3	1:J:69:PHE:CG	2.29	0.67
1:M:344:VAL:HB	1:M:350:THR:HB	1.75	0.67
1:C:151:LEU:HD13	1:G:467:LEU:CG	2.23	0.67
1:G:5:LYS:HE3	1:G:69:PHE:CG	2.30	0.67
1:F:96:VAL:HG22	1:F:105:ILE:HG21	1.75	0.67
1:I:264:GLN:HE22	1:J:270:ARG:HH12	1.43	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:M:19:LEU:O	1:M:81:GLN:HA	1.93	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:C:162:GLU:HG2	1:C:353:ARG:HB3	1.77	0.67
1:E:19:LEU:HD13	1:E:80:ARG:HH11	1.60	0.67
1:H:405:THR:HA	1:H:435:HIS:HA	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:A:5:LYS:HE3	1:A:69:PHE:CG	2.29	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:E:5:LYS:HE3	1:E:69:PHE:CG	2.30	0.67
1:L:204:MET:HG2	1:L:535:TRP:HH2	1.52	0.67
1:L:5:LYS:HE2	1:L:69:PHE:CD2	2.30	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: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:H:467:LEU:HD11	1:J:151:LEU:CG	2.22	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:L:405:THR:HA	1:L:435:HIS:HA	1.77	0.66
1:M:162:GLU:HG2	1:M:353:ARG:HB3	1.77	0.66
1:G:64:TYR:HH	1:G:181:TRP:HZ3	1.44	0.66
1:M:69:PHE:O	1:M:72:PHE:HB3	1.94	0.66
1:A:162:GLU:HG2	1:A:353:ARG:HB3	1.77	0.65
1:K:22:GLU:HB2	1:K:81:GLN:HA	1.78	0.65
1:E:405:THR:HA	1:E:435:HIS:HA	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: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:I:405:THR:HG23	1:I:624:PHE:HA	1.78	0.65
1:D:405:THR:HA	1:D:435:HIS:HA	1.77	0.65
1:D:8:ARG:CZ	1:D:73:ILE:HG13	2.26	0.65
1:D:9:LEU:CD2	1:D:72:PHE:CE2	2.80	0.65
1:F:32:ARG:HH21	1:F:75:LEU:HD13	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:405:THR:HG23	1:L:624:PHE:HA	1.78	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:E:19:LEU:HD13	1:E:80:ARG:NH1	2.12	0.65
1:M:30:ASP:HB2	1:M:33:LEU:HB2	1.79	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: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:K:57:THR:HA	1:K:60:TYR:CD2	2.30	0.64
1:A:24:LEU:CG	1:A:81:GLN:HE21	2.10	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:M:405:THR:HG23	1:M: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:405:THR:HG23	1:A:624:PHE:HA	1.78	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:C:150:ILE:C	1:G:467:LEU:HD12	2.18	0.64
1:D:9:LEU:CD2	1:D:72:PHE:HZ	2.09	0.64
1:H:467:LEU:HD21	1:J:151:LEU:CD1	2.28	0.64
1:H:242:SER:C	1:I:125:ASN:ND2	2.52	0.64
1:C:268:ARG:NE	1:C:272:ARG:HH21	1.96	0.64
1:E:405:THR:HG23	1:E:624:PHE:HA	1.79	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:5:LYS:HE2	1:I:69:PHE:CE2	2.33	0.64
1:I:19:LEU:HD13	1:I:80:ARG:NH1	2.12	0.64
1:M:512:ARG:HB2	1:M:531:CYS:SG	2.37	0.64
1:C:19:LEU:HD13	1:C:80:ARG:NH1	2.12	0.63
1:C:416:HIS:CE1	1:C:514:PHE:CB	2.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:THR:HG23	1:C:624:PHE:HA	1.78	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:G:59:LEU:HD11	1:G:87:MET:HE1	1.81	0.63
1:J:175:ILE:HG23	1:J:528:THR:CG2	2.15	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:H:377:PRO:HG3	1:H:601:LYS:HB3	1.81	0.63
1:J:442:ILE:HG23	1:J:497:ILE:HB	1.81	0.63
1:F:97:LEU:HG	1:F:528:THR:OG1	1.99	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:M:63:LEU:CD2	1:M:91:ALA:CB	2.77	0.63
1:C:270:ARG:HH12	1:F:264:GLN:NE2	1.97	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: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:C:377:PRO:HG3	1:C:601:LYS:HB3	1.81	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:A:377:PRO:HG3	1:A:601:LYS:HB3	1.81	0.62
1:K:377:PRO:HG3	1:K:601:LYS:HB3	1.81	0.62
1:M:107:VAL:HG21	1:M:528:THR:OG1	1.98	0.62
1:A:24:LEU:CD2	1:A:81:GLN:HE21	2.12	0.62
1:C:442:ILE:HG23	1:C:497:ILE:HB	1.81	0.62
1:C:525:GLU:HA	1:C:572:ALA:HB1	1.79	0.62
1:H:107:VAL:HG21	1:H:528:THR:OG1	1.99	0.62
1:K:8:ARG:O	1:K:12:LEU:HG	1.99	0.62
1:L:329:ALA:HB2	1:L:345:MET:HB3	1.82	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:I:273:ILE:HA	1:I:317:TYR:HE1	1.62	0.62
1:M:20:THR:HA	1:M:80:ARG:O	1.99	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:D:329:ALA:HB2	1:D:345:MET:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:329:ALA:HB2	1:F:345:MET:HB3	1.81	0.62
1:E:377:PRO:HG3	1:E:601:LYS:HB3	1.81	0.62
1:F:442:ILE:HG23	1:F:497:ILE:HB	1.81	0.62
1:L:377:PRO:HG3	1:L:601:LYS:HB3	1.81	0.62
1:D:4:ASP:HA	1:D:7:ALA:HB3	1.82	0.62
1:H:63:LEU:HD23	1:H:91:ALA:HB1	1.81	0.62
1:I:63:LEU:HD23	1:I:91:ALA:HB1	1.81	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:A:329:ALA:HB2	1:A:345:MET:HB3	1.82	0.61
1:F:110:ILE:HD11	1:F:168:ALA:HA	1.82	0.61
1:G:329:ALA:HB2	1:G:345:MET:HB3	1.81	0.61
1:H:32:ARG:NH2	1:H:75:LEU:HD22	2.15	0.61
1:H:442:ILE:HG23	1:H:497:ILE:HB	1.81	0.61
1:J:329:ALA:HB2	1:J:345:MET:HB3	1.81	0.61
1:M:329:ALA:HB2	1:M:345:MET:HB3	1.82	0.61
1:M:59:LEU:HD11	1:M:87:MET:HE1	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:M:19:LEU:HB2	1:M:80:ARG:HD2	1.81	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:G:107:VAL:HG21	1:G:528:THR:OG1	1.99	0.61
1:J:21:ARG:HD3	1:J:41:ARG:HD2	1.80	0.61
1:A:407:ILE:HD11	1:A:431:HIS:HD2	1.65	0.61
1:E:63:LEU:HD23	1:E:91:ALA:HB1	1.81	0.61
1:F:407:ILE:HD11	1:F:431:HIS:HD2	1.66	0.61
1:K:442:ILE:HG23	1:K:497:ILE:HB	1.81	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:M:5:LYS:HE2	1:M:69:PHE:CE2	2.35	0.61
1:D:23:LYS:O	1:D:81:GLN:HB3	1.99	0.61
1:H:110:ILE:HD11	1:H:168:ALA:HA	1.82	0.61
1:L:442:ILE:HG23	1:L:497:ILE:HB	1.81	0.61
1:D:307:SER:H	1:D:319:SER:HB3	1.64	0.61
1:D:103:LYS:HD2	1:D:526:ASP:OD1	2.01	0.61
1:D:377:PRO:HG3	1:D:601:LYS:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:LEU:HG	1:D:72:PHE:CE2	2.34	0.61
1:E:442:ILE:HG23	1:E:497:ILE:HB	1.81	0.61
1:G:110:ILE:HD11	1:G:168:ALA:HA	1.82	0.61
1:H:103:LYS:HD2	1:H:526:ASP:OD1	2.01	0.61
1:H:80:ARG:HA	1:H:83:VAL:HG22	1.83	0.61
1:C:416:HIS:CE1	1:C:514:PHE:HB2	2.36	0.61
1:D:205:CYS:HG	1:D:358:TYR:HD1	1.49	0.61
1:E:329:ALA:HB2	1:E:345:MET:HB3	1.81	0.61
1:F:63:LEU:HD23	1:F:91:ALA:HB1	1.81	0.61
1:J:377:PRO:HG3	1:J:601:LYS: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:A:64:TYR:OH	1:A:94:VAL:HG12	2.01	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:442:ILE:HG23	1:A:497:ILE:HB	1.81	0.60
1:L:268:ARG:CZ	1:L:272:ARG:HH21	2.15	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:110:ILE:HD11	1:A:168:ALA:HA	1.83	0.60
1:A:24:LEU:HG	1:A:24:LEU:HB3	1.80	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:E:275:ASP:N	1:G:268:ARG:HH12	1.97	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: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: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:K:278:ASN:HB3	1:M:315:GLU:HG3	1.83	0.60
1:C:89:VAL:HA	1:C:92:VAL:HG22	1.84	0.60
1:D:63:LEU:HD23	1:D:91:ALA:HB1	1.81	0.60
1:I:307:SER:H	1:I:319:SER:HB3	1.67	0.60
1:I:4:ASP:HA	1:I:7:ALA:HB3	1.84	0.60
1:K:59:LEU:HD13	1:K:87:MET:SD	2.41	0.60
1:L:272:ARG:HB3	1:L:316:TYR:CE2	2.36	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:E:307:SER:H	1:E:319:SER:HB3	1.67	0.60
1:G:103:LYS:HD2	1:G:526:ASP:OD1	2.02	0.60
1:G:554:PHE:HE1	1:G:615:MET:HB3	1.67	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: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: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: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: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:A:76:CYS:HA	1:A:88:PHE:CE2	2.37	0.59
1:C:76:CYS:HA	1:C:88:PHE:HZ	1.67	0.59
1:H:89:VAL:HA	1:H:92:VAL:HG22	1.84	0.59
1:I:10:MET:CE	1:I:517:LEU:C	2.70	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:HE1	1:I:517:LEU:C	2.21	0.59
1:M:72:PHE:CZ	1:M:96:VAL:CG2	2.85	0.59
1:A:64:TYR:HH	1:A:181:TRP:HZ3	1.49	0.59
1:E:554:PHE:HE1	1:E:615:MET:HB3	1.67	0.59
1:F:89:VAL:HA	1:F:92:VAL:HG22	1.84	0.59
1:I:10:MET:HB3	1:I:514:PHE:CE1	2.37	0.59
1:I:554:PHE:HE1	1:I:615:MET:HB3	1.67	0.59
1:M:554:PHE:HE1	1:M:615:MET:HB3	1.67	0.59
1:G:205:CYS:HG	1:G:358:TYR:HD1	1.50	0.59
1:G:89:VAL:HA	1:G:92:VAL:HG22	1.84	0.59
1:I:205:CYS:HG	1:I:358:TYR:HD1	1.50	0.59
1:K:407:ILE:HD11	1:K:431:HIS:HD2	1.66	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:J:76:CYS:HA	1:J:88:PHE:HZ	1.67	0.59
1:M:307:SER:H	1:M:319:SER:HB3	1.67	0.59
1:F:175:ILE:HG21	1:F:528:THR:HG21	1.85	0.59
1:F:5:LYS:HE2	1:F:69:PHE:CE2	2.38	0.59
1:J:554:PHE:HE1	1:J:615:MET:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:103:LYS:HD2	1:M:526:ASP:OD1	2.03	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:M:64:TYR:HH	1:M:94:VAL:HG12	1.68	0.59
1:A:304:ILE:HA	1:A:311:SER:OG	2.03	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:C:304:ILE:HA	1:C:311:SER:OG	2.03	0.58
1:E:5:LYS:NZ	1:E:5:LYS:CE	2.66	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: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: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:J:529:GLU:HG3	1:J:574:CYS:SG	2.42	0.58
1:M:24:LEU:HD22	1:M:82:ILE:HG21	1.84	0.58
1:M:29:ARG:HG3	1:M:78:GLN:HE22	1.69	0.58
1:A:508:ILE:HD11	1:A:531:CYS:HA	1.84	0.58
1:A:79:ALA:HB3	1:A:88:PHE:HE1	0.89	0.58
1:A:69:PHE:HE1	1:A:96:VAL:CG2	2.16	0.58
1:H:304:ILE:HA	1:H:311:SER:OG	2.03	0.58
1:J:125:ASN:ND2	1:K:242:SER:O	2.37	0.58
1:K:32:ARG:NH2	1:K:75:LEU:HD22	2.18	0.58
1:M:5:LYS:NZ	1:M:5:LYS:CE	2.66	0.58
1:A:554:PHE:HE1	1:A:615:MET:HB3	1.67	0.58
1:I:272:ARG:CD	1:I:316:TYR:CE1	2.84	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:214:SER:HA	1:A:549:MET:SD	2.44	0.58
1:A:5:LYS:CE	1:A:5:LYS:NZ	2.66	0.58
1:C:307:SER:H	1:C:319:SER:HB3	1.67	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:H:512:ARG:HB2	1:H:531:CYS:SG	2.43	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:A:119:VAL:HG11	1:A:428:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:CD1	1:A:87:MET:SD	2.91	0.58
1:E:214:SER:HA	1:E:549:MET:SD	2.44	0.58
1:E:76:CYS:HA	1:E:88:PHE:HZ	1.67	0.58
1:H:467:LEU:HD11	1:J:151:LEU:CB	2.33	0.58
1:I:304:ILE:HA	1:I:311:SER:OG	2.03	0.58
1:K:97:LEU:HG	1:K:528:THR:OG1	2.04	0.58
1:C:214:SER:HA	1:C:549:MET:SD	2.44	0.58
1:C:77:GLU:HA	1:C:80:ARG:NH2	2.19	0.58
1:D:8:ARG:NH1	1:D:73:ILE:HG21	2.18	0.58
1:F:304:ILE:HA	1:F:311:SER:OG	2.03	0.58
1:K:24:LEU:CD1	1:K:81:GLN:NE2	2.58	0.58
1:I:271:GLU:HA	1:L:268:ARG:NH1	2.18	0.58
1:E:304:ILE:HA	1:E:311:SER:OG	2.03	0.58
1:F:5:LYS:CE	1:F:5:LYS:NZ	2.66	0.58
1:F:76:CYS:HA	1:F:88:PHE:HZ	1.67	0.58
1:G:214:SER:HA	1:G:549:MET:SD	2.44	0.58
1:G:77:GLU:HA	1:G:80:ARG:NH2	2.19	0.58
1:H:270:ARG:O	1:H:274:LEU:HG	2.04	0.58
1:I:214:SER:HA	1:I:549:MET:SD	2.44	0.58
1:K:554:PHE:HE1	1:K:615:MET:HB3	1.68	0.58
1:K:77:GLU:HA	1:K:80:ARG:NH2	2.19	0.58
1:A:5:LYS:HE2	1:A:69:PHE:CE2	2.38	0.57
1:J:77:GLU:HA	1:J:80:ARG:NH2	2.19	0.57
1:L:529:GLU:HB2	1:L:574:CYS:HB3	1.85	0.57
1:L:77:GLU:HA	1:L: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: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:M:59:LEU:CD1	1:M:87:MET:CE	2.82	0.57
1:A:128:ASN:OD1	1:A:426:VAL:HB	2.04	0.57
1:K:13:PHE:HD1	1:K:108:PRO:HG2	1.69	0.57
1:L:19:LEU:HD13	1:L:80:ARG:HD3	1.86	0.57
1:L:5:LYS:HE3	1:L:69:PHE:CD1	2.40	0.57
1:F:77:GLU:HA	1:F:80:ARG:NH2	2.19	0.57
1:G:512:ARG:HH22	1:G:523:VAL:HG21	1.70	0.57
1:D:214:SER:HA	1:D:549:MET:SD	2.44	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:H:214:SER:HA	1:H:549:MET:SD	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:214:SER:HA	1:M:549:MET:SD	2.44	0.57
1:E:77:GLU:HA	1:E:80:ARG:NH2	2.19	0.57
1:F:214:SER:HA	1:F:549:MET:SD	2.44	0.57
1:G:270:ARG:O	1:G:274:LEU:HG	2.05	0.57
1:C:296:HIS:HE1	1:I:566:ALA:O	1.87	0.57
1:K:50:ALA:HB2	1:K:323:TRP:HH2	1.66	0.57
1:K:64:TYR:OH	1:K:181:TRP:HZ3	1.88	0.57
1:G:553:LEU:HB2	1:G:620:ILE:HD12	1.87	0.57
1:J:214:SER:HA	1:J:549:MET:SD	2.44	0.57
1:J:5:LYS:HE2	1:J:69:PHE:CE2	2.38	0.57
1:D:77:GLU:HA	1:D:80:ARG:NH2	2.19	0.56
1:M:69:PHE:CE2	1:M:73:ILE:HG12	2.40	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:J:553:LEU:HB2	1:J:620:ILE:HD12	1.87	0.56
1:M:444:VAL:HG11	1:M:490:LEU:HD23	1.87	0.56
1:D:9:LEU:CD1	1:D:72:PHE:CE2	2.61	0.56
1:J:273:ILE:HG12	1:J:317:TYR:HD1	1.71	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:H:4:ASP:HA	1:H:7:ALA:HB3	1.87	0.56
1:I:183:PRO:HB3	1:I:189:GLU:HB3	1.88	0.56
1:I:77:GLU:HA	1:I:80:ARG:NH2	2.19	0.56
1:K:553:LEU:HB2	1:K:620:ILE:HD12	1.87	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:H:389:GLU:O	1:H:444:VAL:HA	2.05	0.56
1:J:306:GLU:N	1:J:307:SER:HA	2.20	0.56
1:K:389:GLU:O	1:K:444:VAL:HA	2.05	0.56
1:C:389:GLU:O	1:C:444:VAL:HA	2.05	0.56
1:C:553:LEU:HB2	1:C:620:ILE:HD12	1.87	0.56
1:K:9:LEU:CD1	1:K:73:ILE:HD11	2.35	0.56
1:L:389:GLU:O	1:L:444:VAL:HA	2.05	0.56
1:M:389:GLU:O	1:M:444:VAL:HA	2.05	0.56
1:M:4:ASP:HA	1:M:7:ALA:HB3	1.87	0.56
1:D:268:ARG:NH1	1:F:271:GLU:HA	2.21	0.56
1:E:553:LEU:HB2	1:E:620:ILE:HD12	1.87	0.56
1:E:4:ASP:HA	1:E:7:ALA:HB3	1.87	0.56
1:F:205:CYS:HG	1:F:358:TYR:HD1	1.51	0.56
1:F:389:GLU:O	1:F:444:VAL:HA	2.05	0.56
1:H:172:HIS:HA	1:H:175:ILE:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:238:THR:CG2	1:K:243:GLY:O	2.46	0.56
1:J:389:GLU:O	1:J:444:VAL:HA	2.05	0.56
1:K:172:HIS:HA	1:K:175:ILE:HG22	1.88	0.56
1:A:172:HIS:HA	1:A:175:ILE:HG22	1.88	0.56
1:F:22:GLU:HB2	1:F:81:GLN:HB3	1.87	0.56
1:C:151:LEU:CA	1:G:467:LEU:HD11	2.31	0.56
1:H:410:SER:O	1:H:429:LYS:HA	2.06	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:C:5:LYS:HE2	1:C:69:PHE:CE2	2.38	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:G:172:HIS:HA	1:G:175:ILE:HG22	1.88	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:G:410:SER:O	1:G:429:LYS:HA	2.06	0.56
1:K:8:ARG:HE	1:K:73:ILE:HG21	1.61	0.56
1:L:553:LEU:HB2	1:L:620:ILE:HD12	1.87	0.56
1:A:118:PHE:HA	1:A:353:ARG:HH12	1.71	0.56
1:H:553:LEU:HB2	1:H:620:ILE:HD12	1.87	0.56
1:K:96:VAL:HG22	1:K:105:ILE:HG21	1.88	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:M:95:ALA:HB1	1:M:99:ARG:HD2	1.88	0.56
1:A:410:SER:O	1:A:429:LYS:HA	2.06	0.55
1:E:172:HIS:HA	1:E:175:ILE:HG22	1.88	0.55
1:E:389:GLU:O	1:E:444:VAL:HA	2.05	0.55
1:E:97:LEU:HG	1:E:528:THR:OG1	2.05	0.55
1:A:4:ASP:HA	1:A:7:ALA:HB3	1.87	0.55
1:J:167:ASN:HB3	1:J:349:SER:O	2.07	0.55
1:K:410:SER:O	1:K:429:LYS:HA	2.06	0.55
1:M:172:HIS:HA	1:M:175:ILE:HG22	1.88	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:C:95:ALA:HB1	1:C:99:ARG:HD2	1.88	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:F:107:VAL:HG21	1:F:528:THR:OG1	2.05	0.55
1:H:167:ASN:HB3	1:H:349:SER:O	2.07	0.55
1:I:389:GLU:O	1:I:444:VAL:HA	2.05	0.55
1:J:97:LEU:HG	1:J:528:THR:OG1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:573:VAL:CG1	1:L:584:ARG:HB2	2.36	0.55
1:A:167:ASN:HB3	1:A:349:SER:O	2.07	0.55
1:A:59:LEU:HD21	1:A:87:MET:HE3	1.88	0.55
1:C:560:HIS:O	1:C:564:THR:HB	2.05	0.55
1:E:263:VAL:O	1:E:266:MET:HB2	2.07	0.55
1:E:226:PHE:CE1	1:E:270:ARG:NH2	2.75	0.55
1:F:167:ASN:HB3	1:F:349:SER:O	2.07	0.55
1:G:24:LEU:CB	1:G:81:GLN:NE2	2.70	0.55
1:G:508:ILE:HD11	1:G:531:CYS:HA	1.88	0.55
1:I:553:LEU:HB2	1:I:620:ILE:HD12	1.87	0.55
1:L:5:LYS:HA	1:L:69:PHE:CE2	2.42	0.55
1:A:127:ALA:HB2	1:A:142:VAL:HG21	1.86	0.55
1:C:167:ASN:HB3	1:C:349:SER:O	2.07	0.55
1:D:172:HIS:HA	1:D:175:ILE:HG22	1.88	0.55
1:F:410:SER:O	1:F:429:LYS:HA	2.06	0.55
1:I:172:HIS:HA	1:I:175:ILE:HG22	1.88	0.55
1:K:2:VAL:HG11	1:K:103:LYS:O	2.07	0.55
1:C:410:SER:O	1:C:429:LYS:HA	2.06	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:I:167:ASN:HB3	1:I:349:SER:O	2.07	0.55
1:J:95:ALA:HB1	1:J:99:ARG:HD2	1.88	0.55
1:M:69:PHE:CZ	1:M:72:PHE:HD2	2.25	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: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: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: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:L:50:ALA:HB2	1:L:323:TRP:HH2	1.72	0.55
1:M:410:SER:O	1:M:429:LYS:HA	2.06	0.55
1:M:553:LEU:HB2	1:M:620:ILE:HD12	1.87	0.55
1:F:172:HIS:HA	1:F:175:ILE:HG22	1.88	0.55
1:I:234:ALA:HA	1:I:248:SER:HB2	1.89	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: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:A:234:ALA:HA	1:A:248:SER:HB2	1.89	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:K:4:ASP:HA	1:K:7:ALA:HB3	1.88	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:F:173:TRP:HZ2	1:F:196:LEU:HG	1.73	0.54
1:I:173:TRP:HZ2	1:I:196:LEU:HG	1.73	0.54
1:J:245:GLN:CG	1:K:245:GLN:HG2	2.36	0.54
1:K:456:VAL:HG22	1:K:557:LEU:HG	1.89	0.54
1:L:167:ASN:HB3	1:L:349:SER:O	2.07	0.54
1:M:167:ASN:HB3	1:M:349:SER:O	2.07	0.54
1:D:234:ALA:HA	1:D:248:SER:HB2	1.89	0.54
1:F:50:ALA:HB2	1:F:323:TRP:HH2	1.73	0.54
1:G:307:SER:N	1:G:319:SER:HB3	2.22	0.54
1:G:167:ASN:HB3	1:G:349:SER:O	2.07	0.54
1:I:456:VAL:HG22	1:I:557:LEU:HG	1.90	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:K:95:ALA:HB1	1:K:99:ARG:HD2	1.89	0.54
1:L:322:ASN:O	1:L:325:HIS:HB2	2.08	0.54
1:A:322:ASN:O	1:A:325:HIS:HB2	2.08	0.54
1:D:167:ASN:HB3	1:D:349:SER:O	2.07	0.54
1:E:456:VAL:HG22	1:E:557:LEU:HG	1.89	0.54
1:E:5:LYS:HE2	1:E:69:PHE:CE2	2.38	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:L:511:VAL:HA	1:L:531:CYS:HB2	1.89	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:E:410:SER:O	1:E:429:LYS:HA	2.06	0.54
1:I:50:ALA:HB2	1:I:323:TRP:HH2	1.72	0.54
1:J:410:SER:O	1:J:429:LYS:HA	2.06	0.54
1:K:175:ILE:HG23	1:K:528:THR:CG2	2.15	0.54
1:H:268:ARG:NH1	1:M:274:LEU:HB2	2.23	0.54
1:M:82:ILE:HG23	1:M:83:VAL:HG13	1.88	0.54
1:M:72:PHE:HZ	1:M:96:VAL:HB	1.72	0.54
1:A:173:TRP:HZ2	1:A:196:LEU:HG	1.73	0.54
1:A:456:VAL:HG22	1:A:557:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ALA:HA	1:C:248:SER:HB2	1.89	0.54
1:G:173:TRP:HZ2	1:G:196:LEU:HG	1.73	0.54
1:J:173:TRP:HZ2	1:J:196:LEU:HG	1.73	0.54
1:L:173:TRP:HZ2	1:L:196:LEU:HG	1.73	0.54
1:L:176:VAL:HG11	1:L:529:GLU:HB3	1.89	0.54
1:M:234:ALA:HA	1:M:248:SER:HB2	1.89	0.54
1:A:50:ALA:HB2	1:A:323:TRP:HH2	1.72	0.54
1:A:107:VAL:HG21	1:A:528:THR:OG1	2.08	0.54
1:D:249:ARG:HG2	1:D:250:PRO:O	2.07	0.54
1:H:77:GLU:HA	1:H:80:ARG:NH2	2.23	0.54
1:J:263:VAL:O	1:J:266:MET:HB2	2.08	0.54
1:A:59:LEU:HD21	1:A:87:MET:HE2	1.90	0.54
1:D:48:PHE:CB	1:D:326:VAL:HG22	2.38	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:E:97:LEU:CD1	1:E:528:THR:OG1	2.56	0.54
1:F:322:ASN:O	1:F:325:HIS:HB2	2.08	0.54
1:I:48:PHE:CB	1:I:326:VAL:HG22	2.38	0.54
1:A:136:ASP:O	1:A:423:ASP:HB3	2.08	0.53
1:C:50:ALA:HB2	1:C:323:TRP:HH2	1.72	0.53
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:I:95:ALA:HB1	1:I:99:ARG:HD2	1.88	0.53
1:L:444:VAL:HG11	1:L:490:LEU:HD23	1.90	0.53
1:C:444:VAL:HG11	1:C:490:LEU:HD23	1.91	0.53
1:C:38:ILE:HD13	1:D:605:ARG:HH12	1.73	0.53
1:E:322:ASN:O	1:E:325:HIS:HB2	2.08	0.53
1:E:529:GLU:HG3	1:E:574:CYS:SG	2.48	0.53
1:C:274:LEU:HB2	1:F:268:ARG:HH22	1.74	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:K:59:LEU:CD1	1:K:87:MET:SD	2.96	0.53
1:M:456:VAL:HG22	1:M:557:LEU:HG	1.90	0.53
1:M:69:PHE:CE2	1:M:73:ILE:CG1	2.90	0.53
1:C:322:ASN:O	1:C:325:HIS:HB2	2.08	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
1:E:118:PHE:HA	1:E:353:ARG:HH12	1.74	0.53
1:I:444:VAL:HG11	1:I:490:LEU:HD23	1.91	0.53
1:J:444:VAL:HG11	1:J:490:LEU:HD23	1.91	0.53
1:J:121:ALA:HB1	1:K:243:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:21:ARG:HD3	1:K:41:ARG:HD2	1.89	0.53
1:A:69:PHE:CE1	1:A:96:VAL:CG2	2.92	0.53
1:F:444:VAL:HG11	1:F:490:LEU:HD23	1.91	0.53
1:K:270:ARG:O	1:K:274:LEU:HG	2.09	0.53
1:A:268:ARG:HD2	1:A:272:ARG:HE	1.73	0.53
1:A:444:VAL:HG11	1:A:490:LEU:HD23	1.91	0.53
1:A:84:ASN:HD22	1:A:84:ASN:N	2.07	0.53
1:A:76:CYS:CA	1:A:88:PHE:CZ	2.79	0.53
1:D:50:ALA:HB2	1:D:323:TRP:HH2	1.72	0.53
1:F:117:ARG:HB2	1:F:350:THR:HG23	1.91	0.53
1:G:322:ASN:O	1:G:325:HIS:HB2	2.08	0.53
1:G:95:ALA:HB1	1:G:99:ARG:HD2	1.88	0.53
1:J:573:VAL:HG22	1:J:574:CYS:H	1.74	0.53
1:L:465:ASP:HB3	1:L:467:LEU:H	1.74	0.53
1:M:269:TRP:O	1:M:273:ILE:HG13	2.08	0.53
1:A:48:PHE:CB	1:A:326:VAL:HG22	2.38	0.53
1:C:270:ARG:O	1:C:274:LEU:HG	2.08	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:H:8:ARG:NH2	1:H:73:ILE:CG1	2.66	0.53
1:K:444:VAL:HG11	1:K:490:LEU:HD23	1.91	0.53
1:K:97:LEU:CD1	1:K:528:THR:OG1	2.56	0.53
1:M:72:PHE:CE2	1:M:96:VAL:CG2	2.91	0.53
1:C:14:LYS:HG3	1:C:514:PHE:CZ	2.44	0.53
1:D:118:PHE:HA	1:D:353:ARG:HH12	1.74	0.53
1:D:444:VAL:HG11	1:D:490:LEU:HD23	1.91	0.53
1:G:118:PHE:HA	1:G:353:ARG:HH12	1.74	0.53
1:I:268:ARG:NH1	1:J:271:GLU:HA	2.24	0.53
1:M:9:LEU:HD12	1:M:73:ILE:HD12	1.89	0.53
1:C:118:PHE:HA	1:C:353:ARG:HH12	1.74	0.53
1:E:173:TRP:HZ2	1:E:196:LEU:HG	1.73	0.53
1:F:573:VAL:HG22	1:F:574:CYS:H	1.74	0.53
1:H:118:PHE:HA	1:H:353:ARG:HH12	1.74	0.53
1:J:30:ASP:O	1:J:33:LEU:N	2.42	0.53
1:K:173:TRP:HZ2	1:K: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:C:456:VAL:HG22	1:C:557:LEU:HG	1.89	0.53
1:E:444:VAL:HG11	1:E:490:LEU:HD23	1.90	0.53
1:F:118:PHE:HA	1:F:353:ARG:HH12	1.74	0.53
1:F:456:VAL:HG22	1:F:557:LEU:HG	1.89	0.53

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:322:ASN:O	1:M:325:HIS:HB2	2.08	0.52
1:A:59:LEU:HD11	1:A:87:MET:CE	2.40	0.52
1:C:64:TYR:OH	1:C:94:VAL:HG12	2.09	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:30:ASP:HB3	1:I:33:LEU:HD13	1.90	0.52
1:I:13:PHE:HB2	1:I:514:PHE:HZ	1.74	0.52
1:C:473:PRO:O	1:C:477:ARG:HG3	2.10	0.52
1:G:460:LEU:HA	1:G:552:GLU:O	2.09	0.52
1:I:64:TYR:OH	1:I:94:VAL:HG12	2.09	0.52
1:J:459:PHE:O	1:J:553:LEU:HA	2.10	0.52
1:I:38:ILE:HD12	1:J:605:ARG:HH22	1.75	0.52
1:K:117:ARG:HB2	1:K:350:THR:HG23	1.91	0.52
1:M:178:PRO:HG2	1:M:181:TRP:HB2	1.92	0.52
1:M:60:TYR:HH	1:M:90:TYR:HD2	1.54	0.52
1:E:178:PRO:HG2	1:E:181:TRP:HB2	1.92	0.52
1:F:433:LEU:O	1:F:538:HIS:HB2	2.10	0.52
1:H:48:PHE:CB	1:H:326:VAL:HG22	2.38	0.52
1:I:178:PRO:HG2	1:I:181:TRP:HB2	1.92	0.52
1:J:460:LEU:HA	1:J:552:GLU:O	2.09	0.52
1:L:433:LEU:O	1:L:538:HIS:HB2	2.09	0.52
1:A:178:PRO:HG2	1:A:181:TRP:HB2	1.91	0.52
1:A:170:HIS:CG	1:A:352:LEU:HD11	2.45	0.52
1:A:473:PRO:O	1:A:477:ARG:HG3	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:F:459:PHE:O	1:F:553:LEU:HA	2.10	0.52
1:G:433:LEU:O	1:G:538:HIS:HB2	2.10	0.52
1:H:170:HIS:CG	1:H:352:LEU:HD11	2.45	0.52
1:I:118:PHE:HA	1:I:353:ARG:HH12	1.74	0.52
1:I:433:LEU:O	1:I:538:HIS:HB2	2.09	0.52
1:J:508:ILE:HD11	1:J:531:CYS:HA	1.91	0.52
1:L:117:ARG:HB2	1:L:350:THR:HG23	1.91	0.52
1:L:456:VAL:O	1:L:485:LYS:HA	2.10	0.52
1:M:253:TYR:HD2	1:M:331:ILE:HG13	1.75	0.52
1:M:118:PHE:HA	1:M:353:ARG:HH12	1.74	0.52
1:M:72:PHE:CZ	1:M:96:VAL:HG23	2.45	0.52
1:C:456:VAL:O	1:C:485:LYS:HA	2.10	0.52
1:E:573:VAL:HG22	1:E:574:CYS:H	1.74	0.52
1:G:64:TYR:OH	1:G:181:TRP:HZ3	1.92	0.52
1:H:573:VAL:HG22	1:H:574:CYS:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:178:PRO:HG2	1:J:181:TRP:HB2	1.92	0.52
1:I:268:ARG:HH11	1:J:271:GLU:HA	1.74	0.52
1:J:473:PRO:O	1:J:477:ARG:HG3	2.10	0.52
1:K:263:VAL:O	1:K:266:MET:HB2	2.09	0.52
1:K:456:VAL:O	1:K:485:LYS:HA	2.10	0.52
1:A:456:VAL:O	1:A:485:LYS:HA	2.10	0.52
1:C:14:LYS:HE2	1:C:514:PHE:CE1	2.44	0.52
1:C:151:LEU:N	1:G:467:LEU:HD12	2.25	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:E:64:TYR:OH	1:E:94:VAL:HG12	2.09	0.52
1:F:170:HIS:CG	1:F:352:LEU:HD11	2.45	0.52
1:G:456:VAL:O	1:G:485:LYS:HA	2.09	0.52
1:G:473:PRO:O	1:G:477:ARG:HG3	2.10	0.52
1:H:433:LEU:O	1:H:538:HIS:HB2	2.10	0.52
1:I:473:PRO:O	1:I:477:ARG:HG3	2.10	0.52
1:J:97:LEU:CG	1:J:528:THR:HB	2.40	0.52
1:K:460:LEU:HA	1:K:552:GLU:O	2.09	0.52
1:M:170:HIS:CG	1:M:352:LEU:HD11	2.45	0.52
1:M:66:ALA:HB3	1:M:99:ARG:HH21	1.74	0.52
1:M:69:PHE:CZ	1:M:72:PHE:CD2	2.98	0.52
1:A:104:GLY:HA2	1:A:525:GLU:HB2	1.85	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:D:473:PRO:O	1:D:477:ARG:HG3	2.10	0.52
1:E:170:HIS:CG	1:E:352:LEU:HD11	2.45	0.52
1:E:97:LEU:CG	1:E:528:THR:HB	2.40	0.52
1:F:263:VAL:O	1:F:266:MET:HB2	2.09	0.52
1:C:278:ASN:O	1:F:315:GLU:OE2	2.28	0.52
1:F:64:TYR:OH	1:F:94:VAL:HG12	2.09	0.52
1:I:456:VAL:O	1:I:485:LYS:HA	2.10	0.52
1:J:107:VAL:HG21	1:J:528:THR:HG1	1.71	0.52
1:J:433:LEU:O	1:J:538:HIS:HB2	2.10	0.52
1:J:419:ASN:HD22	1:K:132:SER:HB2	1.74	0.52
1:L:170:HIS:CG	1:L:352:LEU:HD11	2.45	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:A:130:GLU:HA	1:A:133:ASN:HB2	1.91	0.51
1:A:137:GLN:HA	1:A:423:ASP:HA	1.92	0.51
1:A:573:VAL:HG22	1:A:574:CYS:H	1.74	0.51

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:THR:HA	1:A:486:PHE:O	2.11	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: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:J:132:SER:HB3	1:K:419:ASN:HD22	1.74	0.51
1:K:455:THR:HA	1:K:486:PHE:O	2.11	0.51
1:L:455:THR:HA	1:L:486:PHE:O	2.11	0.51
1:M:55:GLU:O	1:M:58:GLU:HB3	2.11	0.51
1:C:178:PRO:HG2	1:C:181:TRP:HB2	1.92	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:E:55:GLU:O	1:E:58:GLU:HB3	2.11	0.51
1:H:275:ASP:OD1	1:K:316:TYR:CE1	2.52	0.51
1:H:455:THR:HA	1:H:486:PHE:O	2.11	0.51
1:H:55:GLU:O	1:H:58:GLU:HB3	2.11	0.51
1:K:170:HIS:CG	1:K:352:LEU:HD11	2.45	0.51
1:K:9:LEU:HD12	1:K:73:ILE:HD11	1.92	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:M:407:ILE:HD11	1:M:431:HIS:CD2	2.46	0.51
1:C:55:GLU:O	1:C:58:GLU:HB3	2.11	0.51
1:E:117:ARG:HB2	1:E:350:THR:HG23	1.91	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:A:123:THR:HG21	1:A:144:ALA:HA	1.93	0.51
1:E:456:VAL:O	1:E:485:LYS:HA	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:F:477:ARG:HG2	1:F:598:PHE:HB3	1.93	0.50
1:G:455:THR:HA	1:G:486:PHE:O	2.11	0.50
1:C:150:ILE:O	1:G:467:LEU:CD1	2.59	0.50
1:I:467:LEU:HD22	1:I:470:LYS:HE3	1.94	0.50
1:I:5:LYS:CE	1:I:5:LYS:NZ	2.74	0.50
1:J:170:HIS:CG	1:J:352:LEU:HD11	2.45	0.50
1:K:126:ARG:HD3	1:K:142:VAL:HG11	1.93	0.50
1:L:103:LYS:HD2	1:L:526:ASP:OD1	2.11	0.50
1:C:268:ARG:HD2	1:C:272:ARG:HE	1.76	0.50
1:C:477:ARG:HG2	1:C:598:PHE:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:PHE:HB3	1:D:326:VAL:HG22	1.94	0.50
1:F:125:ASN:ND2	1:G:242:SER:C	2.65	0.50
1:G:5:LYS:NZ	1:G:5:LYS:CE	2.75	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:L:5:LYS:CE	1:L:5:LYS:NZ	2.74	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:L:178:PRO:HG2	1:L:181:TRP:HB2	1.92	0.50
1:L:473:PRO:O	1:L:477:ARG:HG3	2.10	0.50
1:M:477:ARG:HG2	1:M:598:PHE:HB3	1.94	0.50
1:C:275:ASP:HB2	1:F:268:ARG:HH11	1.77	0.50
1:C:455:THR:HA	1:C:486:PHE:O	2.11	0.50
1:D:68:ASP:CG	1:D:70:ASN:HB2	2.31	0.50
1:G:55:GLU:O	1:G:58:GLU:HB3	2.11	0.50
1:J:107:VAL:CG2	1:J:528:THR:OG1	2.54	0.50
1:K:477:ARG:HG2	1:K:598:PHE:HB3	1.94	0.50
1:H:268:ARG:HH12	1:M:274:LEU:HB2	1.77	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:D:455:THR:HA	1:D:486:PHE:O	2.11	0.50
1:E:477:ARG:HG2	1:E:598:PHE:HB3	1.94	0.50
1:A:407:ILE:HD11	1:A:431:HIS:CD2	2.46	0.50
1:D:9:LEU:HD21	1:D:72:PHE:HZ	1.59	0.50
1:F:55:GLU:O	1:F:58:GLU:HB3	2.11	0.50
1:H:477:ARG:HA	1:H:480:PHE:HD2	1.77	0.50
1:J:477:ARG:HA	1:J:480:PHE:HD2	1.77	0.50
1:K:55:GLU:O	1:K:58:GLU:HB3	2.11	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:D:477:ARG:HG2	1:D:598:PHE:HB3	1.94	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:I:264:GLN:NE2	1:J:270:ARG:HH12	2.08	0.50
1:M:272:ARG:HH11	1:M:316:TYR:HA	1.76	0.50
1:A:477:ARG:HG2	1:A:598:PHE:HB3	1.94	0.50
1:A:19:LEU:HB3	1:A:80:ARG:HD2	1.93	0.50
1:D:477:ARG:HA	1:D:480:PHE:HD2	1.77	0.50
1:E:407:ILE:HD11	1:E:431:HIS:CD2	2.46	0.50
1:E:477:ARG:HA	1:E:480:PHE:HD2	1.77	0.50
1:F:407:ILE:HD11	1:F:431:HIS:CD2	2.46	0.50

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:79:ALA:HB3	1:M:88:PHE:HE1	1.68	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:G:477:ARG:HG2	1:G:598:PHE:HB3	1.93	0.49
1:H:249:ARG:HG2	1:H:250:PRO:O	2.13	0.49
1:L:414:LEU:HB2	1:L:426:VAL:HG23	1.95	0.49
1:A:477:ARG:HA	1:A:480:PHE:HD2	1.77	0.49
1:A:48:PHE:HB3	1:A:326:VAL:HG22	1.93	0.49
1:C:463:LYS:HD3	1:C:550:GLU:HG2	1.95	0.49
1:C:48:PHE:HB3	1:C:326:VAL:HG22	1.94	0.49
1:D:119:VAL:HG11	1:D:428:VAL:HG11	1.95	0.49
1:D:454:SER:O	1:D: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:M:454:SER:O	1:M:487:PHE:HA	2.13	0.49
1:A:38:ILE:HG12	1:G:605:ARG:HH22	1.78	0.49
1:F:119:VAL:HG11	1:F:428:VAL:HG11	1.95	0.49
1:I:527:SER:HA	1:I:584:ARG:HB3	1.94	0.49
1:K:12:LEU:HD13	1:K:80:ARG:NH2	2.27	0.49
1:K:407:ILE:HD11	1:K:431:HIS:CD2	2.46	0.49
1:K:59:LEU:HD13	1:K:87:MET:CE	2.42	0.49
1:L:573:VAL:HG12	1:L:584:ARG:HB2	1.95	0.49
1:E:151:LEU:HA	1:F:467:LEU:HD22	1.95	0.49
1:A:454:SER:O	1:A:487:PHE:HA	2.13	0.49
1:D:268:ARG:HH11	1:F:271:GLU:HA	1.77	0.49
1:E:454:SER:O	1:E:487:PHE:HA	2.13	0.49
1:E:463:LYS:HD3	1:E:550:GLU:HG2	1.95	0.49
1:E:2:VAL:HA	1:E:5:LYS:HB3	1.95	0.49
1:E:22:GLU:HB2	1:E:81:GLN:HB3	1.95	0.49
1:G:407:ILE:HD11	1:G:431:HIS:CD2	2.46	0.49
1:G:465:ASP:HB3	1:G:467:LEU:H	1.78	0.49
1:J:22:GLU:HB2	1:J:81:GLN:HB3	1.95	0.49
1:J:407:ILE:HD11	1:J:431:HIS:CD2	2.46	0.49
1:L:454:SER:O	1:L:487:PHE:HA	2.13	0.49
1:E:414:LEU:HB2	1:E:426:VAL:HG23	1.95	0.48
1:H:454:SER:O	1:H:487:PHE:HA	2.13	0.48
1:I:38:ILE:HD11	1:I:55:GLU:HG2	1.94	0.48
1:L:48:PHE:HB3	1:L:326:VAL:HG22	1.93	0.48
1:M:119:VAL:HG11	1:M:428:VAL:HG11	1.95	0.48
1:A:59:LEU:HD22	1:A:87:MET:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ILE:HD11	1:C:431:HIS:CD2	2.46	0.48
1:C:414:LEU:HB2	1:C:426:VAL:HG23	1.95	0.48
1:D:232:GLY:HA3	1:E:338:PHE:HZ	1.78	0.48
1:E:19:LEU:HB3	1:E:80:ARG:HD2	1.94	0.48
1:F:36:VAL:HG11	1:F:59:LEU:HD11	1.94	0.48
1:F:477:ARG:HA	1:F:480:PHE:HD2	1.77	0.48
1:G:463:LYS:HD3	1:G:550:GLU:HG2	1.95	0.48
1:H:119:VAL:HG11	1:H:428:VAL:HG11	1.95	0.48
1:H:32:ARG:HH22	1:H:75:LEU:HD22	1.78	0.48
1:J:414:LEU:HB2	1:J:426:VAL:HG23	1.95	0.48
1:M:2:VAL:HA	1:M:5:LYS:HB3	1.95	0.48
1:M:463:LYS:HD3	1:M:550:GLU:HG2	1.95	0.48
1:E:267:VAL:HA	1:E:270:ARG:HH21	1.79	0.48
1:F:414:LEU:HB2	1:F:426:VAL:HG23	1.95	0.48
1:C:151:LEU:HD12	1:G:467:LEU:HD11	1.76	0.48
1:H:48:PHE:HB3	1:H:326:VAL:HG22	1.94	0.48
1:I:275:ASP:HA	1:I:278:ASN:ND2	2.28	0.48
1:I:119:VAL:HG11	1:I:428:VAL:HG11	1.95	0.48
1:I:477:ARG:HG2	1:I:598:PHE:HB3	1.94	0.48
1:K:119:VAL:HG11	1:K:428:VAL:HG11	1.95	0.48
1:M:10:MET:SD	1:M:517:LEU:HB3	2.54	0.48
1:M:249:ARG:HG2	1:M:250:PRO:O	2.13	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:K:271:GLU:HA	1:M:268:ARG:HH11	1.77	0.48
1:K:45:PHE:HE1	1:K:52:HIS:HB3	1.78	0.48
1:M:245:GLN:O	1:M:341:ASN:HB2	2.14	0.48
1:A:24:LEU:CD2	1:A:81:GLN:HB2	2.44	0.48
1:C:169:HIS:CE1	1:C:581:CYS:SG	3.04	0.48
1:C:2:VAL:HA	1:C:5:LYS:HB3	1.94	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:J:2:VAL:HA	1:J:5:LYS:HB3	1.95	0.48
1:K:463:LYS:HD3	1:K:550:GLU:HG2	1.95	0.48
1:A:365:ASP:O	1:A:369:GLN:HG2	2.14	0.48
1:A:66:ALA:HB1	1:A:99:ARG:NH2	2.06	0.48
1:D:365:ASP:O	1:D:369:GLN:HG2	2.14	0.48
1:E:169:HIS:CE1	1:E:581:CYS:SG	3.04	0.48
1:F:2:VAL:HA	1:F:5:LYS:HB3	1.95	0.48
1:G:249:ARG:NE	1:G:331:ILE:HG21	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:GLU:H	1:H:299:ASP:HA	1.79	0.48
1:H:365:ASP:O	1:H:369:GLN:HG2	2.14	0.48
1:H:467:LEU:HD12	1:J:150:ILE:O	2.06	0.48
1:H:477:ARG:HG2	1:H:598:PHE:HB3	1.94	0.48
1:J:477:ARG:HG2	1:J:598:PHE:HB3	1.94	0.48
1:A:249:ARG:NE	1:A:331:ILE:HG21	2.24	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:G:365:ASP:O	1:G:369:GLN:HG2	2.14	0.48
1:H:414:LEU:HB2	1:H:426:VAL:HG23	1.95	0.48
1:I:407:ILE:HD11	1:I:431:HIS:CD2	2.46	0.48
1:I:169:HIS:CE1	1:I:581:CYS:SG	3.04	0.48
1:K:23:LYS:O	1:K:81:GLN:HB3	2.14	0.48
1:L:463:LYS:HD3	1:L:550:GLU:HG2	1.95	0.48
1:A:24:LEU:CB	1:A:81:GLN:NE2	2.76	0.48
1:A:263:VAL:O	1:A:266:MET:HB2	2.14	0.48
1:D:169:HIS:CE1	1:D:581:CYS:SG	3.04	0.48
1:E:119:VAL:HG11	1:E:428:VAL:HG11	1.95	0.48
1:G:195:GLU:HB2	1:G:298:THR:HB	1.94	0.48
1:G:179:ALA:O	1:G:308:SER:HA	2.13	0.48
1:I:22:GLU:HB2	1:I:81:GLN:HB3	1.95	0.48
1:I:463:LYS:HG3	1:I:471:LEU:HD21	1.96	0.48
1:J:549:MET:HB3	1:J:551:PHE:HE1	1.79	0.48
1:K:454:SER:O	1:K:487:PHE:HA	2.13	0.48
1:C:463:LYS:HG3	1:C:471:LEU:HD21	1.96	0.48
1:C:454:SER:O	1:C:487:PHE:HA	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:I:414:LEU:HB2	1:I:426:VAL:HG23	1.95	0.48
1:J:34:LYS:HD2	1:J:35:GLY:N	2.28	0.48
1:J:365:ASP:O	1:J:369:GLN:HG2	2.14	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:L:249:ARG:NE	1:L:331:ILE:HG21	2.26	0.48
1:L:103:LYS:HG3	1:L:525:GLU:O	2.13	0.48
1:M:195:GLU:H	1:M:299:ASP:HA	1.79	0.48
1:M:365:ASP:O	1:M:369:GLN:HG2	2.14	0.48
1:A:274:LEU:CD2	1:A:367:ILE:HG23	2.44	0.48
1:A:76:CYS:SG	1:A:92:VAL:HG21	2.54	0.48
1:C:22:GLU:HB2	1:C:81:GLN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ARG:NE	1:C:331:ILE:HG21	2.26	0.48
1:A:467:LEU:HG	1:D:150:ILE:O	2.14	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:I:365:ASP:O	1:I:369:GLN:HG2	2.14	0.48
1:L:195:GLU:H	1:L:299:ASP:HA	1.79	0.48
1:L:365:ASP:O	1:L:369:GLN:HG2	2.14	0.48
1:L:463:LYS:HG3	1:L:471:LEU:HD21	1.96	0.48
1:M:22:GLU:HB2	1:M:81:GLN:CB	2.41	0.48
1:M:414:LEU:HB2	1:M:426:VAL:HG23	1.95	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: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:M:72:PHE:CZ	1:M:96:VAL:HB	2.49	0.47
1:D:414:LEU:HB2	1:D:426:VAL:HG23	1.95	0.47
1:F:108:PRO:HA	1:F:109:PRO:HD3	1.81	0.47
1:H:463:LYS:HG3	1:H:471:LEU:HD21	1.96	0.47
1:I:549:MET:HB3	1:I:551:PHE:HE1	1.79	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:A:549:MET:HB3	1:A:551:PHE:HE1	1.79	0.47
1:C:365:ASP:O	1:C:369:GLN:HG2	2.14	0.47
1:C:119:VAL:HG11	1:C:428:VAL:HG11	1.95	0.47
1:D:463:LYS:HD3	1:D:550:GLU:HG2	1.95	0.47
1:E:365:ASP:O	1:E:369:GLN:HG2	2.14	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: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:L:119:VAL:HG11	1:L:428:VAL:HG11	1.95	0.47
1:F:549:MET:HB3	1:F:551:PHE:HE1	1.79	0.47
1:G:454:SER:O	1:G:487:PHE:HA	2.13	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:A:512:ARG:HH22	1:A:523:VAL:HG21	1.80	0.47
1:G:304:ILE:HA	1:G:311:SER:OG	2.14	0.47
1:H:467:LEU:HB3	1:J:149:ASN:OD1	2.15	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:C:38:ILE:HD13	1:D:605:ARG:NH1	2.30	0.47
1:G:414:LEU:HB2	1:G:426:VAL:HG23	1.95	0.47
1:G:39:LEU:HD21	1:G:45:PHE:HB2	1.97	0.47
1:H:19:LEU:HD22	1:H:80:ARG:HH11	1.79	0.47
1:K:467:LEU:HD22	1:L:151:LEU:HA	1.97	0.47
1:M:463:LYS:HG3	1:M:471:LEU:HD21	1.96	0.47
1:A:150:ILE:O	1:D:467:LEU:HG	2.15	0.47
1:A:258:LEU:HD22	1:A:330:ASN:HD21	1.80	0.47
1:C:549:MET:HB3	1:C:551:PHE:HE1	1.79	0.47
1:G:119:VAL:HG11	1:G:428:VAL:HG11	1.95	0.47
1:I:57:THR:HA	1:I:60:TYR:CD2	2.50	0.47
1:J:63:LEU:HA	1:J:75:LEU:CD2	2.33	0.47
1:K:365:ASP:O	1:K:369:GLN:HG2	2.14	0.47
1:M:249:ARG:NE	1:M:331:ILE:HG21	2.26	0.47
1:H:38:ILE:HD12	1:M:605:ARG:NH2	2.30	0.47
1:M:64:TYR:OH	1:M:94:VAL:CG1	2.45	0.47
1:G:549:MET:HB3	1:G:551:PHE:HE1	1.79	0.47
1:H:258:LEU:HD22	1:H:330:ASN:HD21	1.80	0.47
1:I:32:ARG:NH2	1:I:62:ALA:HA	2.30	0.47
1:J:267:VAL:O	1:J:271:GLU:HG2	2.15	0.47
1:C:587:ARG:NH2	1:I:568:LEU:HB2	2.30	0.47
1:A:278:ASN:HB3	1:E:315:GLU:HG3	1.96	0.47
1:E:463:LYS:HG3	1:E:471:LEU:HD21	1.96	0.47
1:F:249:ARG:HG2	1:F:250:PRO:O	2.15	0.47
1:F:365:ASP:O	1:F:369:GLN:HG2	2.14	0.47
1:L:107:VAL:HG21	1:L:528:THR:OG1	2.15	0.47
1:M:19:LEU:HD13	1:M:80:ARG:HH11	1.80	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:M:30:ASP:HB3	1:M:32:ARG:HB2	1.95	0.47
1:A:169:HIS:CE1	1:A:581:CYS:SG	3.04	0.47
1:D:403:ILE:HG21	1:D:541:ILE:HG21	1.97	0.47
1:E:200:MET:SD	1:E:580:TYR:HB3	2.55	0.47
1:C:275:ASP:N	1:F:268:ARG:HH12	2.12	0.47
1:I:193:LYS:NZ	1:I:308:SER:OG	2.48	0.47
1:I:200:MET:SD	1:I:580:TYR:HB3	2.55	0.47
1:J:463:LYS:HG3	1:J:471:LEU:HD21	1.96	0.47
1:K:268:ARG:HD2	1:K:272:ARG:HE	1.79	0.47
1:K:273:ILE:HG12	1:K:317:TYR:HD1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:549:MET:HB3	1:M:551:PHE:HE1	1.79	0.47
1:M:20:THR:HG23	1:M:83:VAL:O	2.15	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:D:549:MET:HB3	1:D:551:PHE:HE1	1.79	0.46
1:E:108:PRO:HA	1:E:109:PRO:HD3	1.81	0.46
1:E:549:MET:HB3	1:E:551:PHE:HE1	1.79	0.46
1:I:103:LYS:NZ	1:I:525:GLU:O	2.49	0.46
1:I:528:THR:O	1:I:574:CYS:HB2	2.15	0.46
1:M:258:LEU:HD22	1:M:330:ASN:HD21	1.80	0.46
1:M:24:LEU:HD22	1:M:82:ILE:CG2	2.45	0.46
1:F:195:GLU:H	1:F:299:ASP:HA	1.79	0.46
1:G:23:LYS:O	1:G:81:GLN:NE2	2.48	0.46
1:J:200:MET:SD	1:J:580:TYR:HB3	2.55	0.46
1:L:258:LEU:HD22	1:L:330:ASN:HD21	1.80	0.46
1:L:200:MET:SD	1:L:580:TYR:HB3	2.55	0.46
1:A:195:GLU:H	1:A:299:ASP:HA	1.79	0.46
1:D:200:MET:SD	1:D:580:TYR:HB3	2.55	0.46
1:E:226:PHE:HE1	1:E:270:ARG:NH2	2.12	0.46
1:F:13:PHE:CD2	1:F:16:LEU:HD22	2.51	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: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: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:K:249:ARG:HG2	1:K:250:PRO:O	2.15	0.46
1:K:274:LEU:CD2	1:K:367:ILE:HG23	2.45	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:I:5:LYS:HG3	1:I:69:PHE:CZ	2.49	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:32:ARG:NH2	1:G:75:LEU:CD2	2.68	0.46
1:K:107:VAL:CG2	1:K:528:THR:OG1	2.55	0.46
1:A:386:PRO:O	1:A:452:LYS:NZ	2.49	0.46
1:C:200:MET:SD	1:C:580:TYR:HB3	2.55	0.46
1:G:24:LEU:HD11	1:G:78:GLN:HE21	1.80	0.46

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:9:LEU:HD11	1:H:69:PHE:HZ	1.81	0.45
1:J:556:MET:SD	1:J:597:PRO:HG3	2.56	0.45
1:K:99:ARG:HH12	1:K:101:ASP:CG	2.19	0.45
1:K:200:MET:SD	1:K:580:TYR:HB3	2.56	0.45
1:K:5:LYS:HB2	1:K:5:LYS:HE2	1.36	0.45
1:L:59:LEU:HD11	1:L:87:MET:HE1	1.97	0.45
1:M:5:LYS:NZ	1:M:69:PHE:O	2.50	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:A:556:MET:SD	1:A:597:PRO:HG3	2.57	0.45
1:C:11:PRO:HA	1:C:14:LYS:HE3	1.99	0.45
1:E:556:MET:SD	1:E:597:PRO:HG3	2.56	0.45
1:H:549:MET:O	1:H:621:LYS:HA	2.17	0.45
1:I:258:LEU:HD22	1:I:330:ASN:HD21	1.80	0.45
1:J:55:GLU:O	1:J:58:GLU:HB3	2.16	0.45
1:K:9:LEU:HD11	1:K:73:ILE:HD11	1.99	0.45
1:L:549:MET:O	1:L:621:LYS:HA	2.17	0.45
1:A:128:ASN:HD22	1:A:414:LEU:HD12	1.79	0.45
1:D:171:TRP:HA	1:D:348:THR:HG23	1.99	0.45
1:E:171:TRP:HA	1:E:348:THR:HG23	1.99	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:I:275:ASP:HA	1:I:278:ASN:HD22	1.82	0.45
1:J:249:ARG:HG2	1:J:250:PRO:O	2.17	0.45
1:J:258:LEU:HD22	1:J:330:ASN:HD21	1.80	0.45
1:J:245:GLN:O	1:J:341:ASN:HB2	2.16	0.45
1:K:20:THR:HG23	1:K:83:VAL:O	2.16	0.45
1:K:393:VAL:HB	1:K:618:THR:OG1	2.17	0.45
1:K:556:MET:SD	1:K:597:PRO:HG3	2.57	0.45
1:I:271:GLU:HA	1:L:268:ARG:HH12	1.81	0.45
1:M:169:HIS:CE1	1:M:581:CYS:SG	3.04	0.45
1:A:24:LEU:CD2	1:A:82:ILE:CG2	2.92	0.45
1:D:556:MET:SD	1:D:597:PRO:HG3	2.56	0.45
1:G:245:GLN:O	1:G:341:ASN:HB2	2.16	0.45
1:G:59:LEU:HD11	1:G:87:MET:CE	2.45	0.45
1:H:362:ARG:HA	1:H:362:ARG:HD3	1.84	0.45
1:H:8:ARG:NH1	1:H:73:ILE:HG21	2.30	0.45
1:I:549:MET:O	1:I:621:LYS:HA	2.16	0.45
1:J:290:ILE:HD12	1:J:300:ILE:HD13	1.95	0.45
1:J:171:TRP:HA	1:J:348:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:354:ASP:HA	1:J:355:PRO:HD3	1.85	0.45
1:L:8:ARG:NH2	1:L:73:ILE:CB	2.80	0.45
1:M:549:MET:O	1:M:621:LYS:HA	2.17	0.45
1:C:245:GLN:O	1:C:341:ASN:HB2	2.17	0.45
1:C:354:ASP:HA	1:C:355:PRO:HD3	1.85	0.45
1:D:393:VAL:HB	1:D:618:THR:OG1	2.17	0.45
1:E:393:VAL:HB	1:E:618:THR:OG1	2.17	0.45
1:E:549:MET:O	1:E:621:LYS:HA	2.16	0.45
1:J:393:VAL:HB	1:J:618:THR:OG1	2.17	0.45
1:K:549:MET:O	1:K:621:LYS:HA	2.17	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:M:228:GLU:HA	1:M:229:PRO:HD3	1.88	0.45
1:A:393:VAL:HB	1:A:618:THR:OG1	2.17	0.45
1:C:228:GLU:HA	1:C:229:PRO:HD3	1.88	0.45
1:D:549:MET:O	1:D:621:LYS:HA	2.17	0.45
1:E:245:GLN:O	1:E:341:ASN:HB2	2.16	0.45
1:G:11:PRO:HA	1:G:14:LYS:HE3	1.99	0.45
1:G:549:MET:O	1:G:621:LYS:HA	2.17	0.45
1:H:386:PRO:O	1:H:452:LYS:NZ	2.49	0.45
1:H:243:GLY:N	1:I:125:ASN:HD21	2.00	0.45
1:I:270:ARG:HD3	1:I:320:LEU:HD21	1.98	0.45
1:J:9:LEU:HD22	1:J:105:ILE:HD11	1.99	0.45
1:J:549:MET:O	1:J:621:LYS:HA	2.17	0.45
1:H:270:ARG:NH1	1:K:264:GLN:OE1	2.49	0.45
1:K:193:LYS:NZ	1:K:308:SER:OG	2.48	0.45
1:A:528:THR:O	1:A:532:SER:HB3	2.16	0.45
1:H:10:MET:SD	1:H:517:LEU:HB3	2.57	0.45
1:I:171:TRP:HA	1:I:348:THR:HG23	1.99	0.45
1:J:467:LEU:HD22	1:J:470:LYS:HE3	1.98	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:M:263:VAL:O	1:M:266:MET:HB2	2.17	0.45
1:M:171:TRP:HA	1:M:348:THR:HG23	1.99	0.45
1:E:268:ARG:O	1:E:272:ARG:HG3	2.17	0.45
1:E:273:ILE:HG12	1:E:317:TYR:HD1	1.81	0.45
1:G:304:ILE:HA	1:G:311:SER:CB	2.47	0.45
1:H:393:VAL:HB	1:H:618:THR:OG1	2.17	0.45
1:I:556:MET:SD	1:I:597:PRO:HG3	2.56	0.45
1:K:171:TRP:HA	1:K:348:THR:HG23	1.99	0.45
1:K:403:ILE:HG21	1:K:541:ILE:HG21	1.99	0.45

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:458:ILE:HG23	1:E:555:VAL:HG22	2.00	0.44
1:F:97:LEU:CD2	1:F:528:THR:H	2.30	0.44
1:H:263:VAL:O	1:H:266:MET:HB2	2.17	0.44
1:H:205:CYS:SG	1:H:358:TYR:HD1	2.41	0.44
1:J:386:PRO:O	1:J:452:LYS:NZ	2.49	0.44
1:L:108:PRO:HA	1:L:109:PRO:HD3	1.81	0.44
1:A:11:PRO:HA	1:A:14:LYS:HE3	1.99	0.43
1:A:197:PHE:O	1:A:201:HIS:ND1	2.51	0.43
1:D:310:GLU:O	1:D:312:LYS:NZ	2.51	0.43
1:G:386:PRO:O	1:G:452:LYS:NZ	2.49	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:M:197:PHE:O	1:M:201:HIS:ND1	2.51	0.43
1:D:11:PRO:HA	1:D:14:LYS:HE3	1.99	0.43
1:F:393:VAL:HB	1:F:618:THR:OG1	2.17	0.43
1:H:534:GLY:HA2	1:H:577:ALA:CB	2.48	0.43
1:K:197:PHE:O	1:K:201:HIS:ND1	2.51	0.43
1:A:34:LYS:NZ	1:A:58:GLU:OE1	2.48	0.43
1:C:549:MET:O	1:C:621:LYS:HA	2.17	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: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:M:205:CYS:SG	1:M:358:TYR:HD1	2.40	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:E:386:PRO:O	1:E:452:LYS:NZ	2.49	0.43
1:F:205:CYS:SG	1:F:358:TYR:HD1	2.41	0.43
1:G:197:PHE:O	1:G:201:HIS:ND1	2.51	0.43
1:G:205:CYS:SG	1:G:358:TYR:HD1	2.40	0.43
1:G:458:ILE:HG23	1:G:555:VAL:HG22	2.00	0.43
1:G:63:LEU:HD23	1:G:91:ALA:CB	2.38	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:250:PRO:HG2	1:C:253:TYR:CZ	2.54	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:F:49:HIS:CE1	1:F:51:ARG:HG2	2.54	0.43
1:I:197:PHE:O	1:I:201:HIS:ND1	2.51	0.43
1:J:33:LEU:HD21	1:J:79:ALA:HB1	2.00	0.43
1:M:108:PRO:HA	1:M:109:PRO:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:276:ALA:HB1	1:M:281:TYR:O	2.19	0.43
1:M:72:PHE:CE2	1:M:96:VAL:HG21	2.54	0.43
1:A:25:PRO:C	1:A:26:LEU:HG	2.38	0.43
1:A:266:MET:HB3	1:A:266:MET:HE3	1.86	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:H:193:LYS:NZ	1:H:308:SER:OG	2.48	0.43
1:H:467:LEU:HD21	1:J:151:LEU:HD12	1.99	0.43
1:J:403:ILE:HG21	1:J:541:ILE:HG21	1.99	0.43
1:L:107:VAL:HB	1:L:528:THR:HG23	1.99	0.43
1:M:458:ILE:HG23	1:M:555:VAL:HG22	2.00	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:E:49:HIS:CE1	1:E:51:ARG:HG2	2.54	0.43
1:G:375:PHE:CB	1:G:600:ARG:HD3	2.48	0.43
1:H:49:HIS:CE1	1:H:51:ARG:HG2	2.54	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:K:20:THR:OG1	1:K:85:GLU:HB3	2.18	0.43
1:L:137:GLN:HA	1:L:423:ASP:HA	2.01	0.43
1:A:49:HIS:CE1	1:A:51:ARG:HG2	2.54	0.43
1:C:49:HIS:CE1	1:C:51:ARG:HG2	2.54	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:E:197:PHE:O	1:E:201:HIS:ND1	2.52	0.43
1:E:97:LEU:CG	1:E:528:THR:CB	2.96	0.43
1:F:197:PHE:O	1:F:201:HIS:ND1	2.51	0.43
1:F:169:HIS:CE1	1:F:581:CYS:SG	3.04	0.43
1:G:221:ILE:HA	1:G:222:PRO:HD2	1.92	0.43
1:H:393:VAL:HA	1:H:441:ASN:O	2.19	0.43
1:I:103:LYS:NZ	1:I:524:SER:OG	2.46	0.43
1:K:269:TRP:O	1:K:273:ILE:HG13	2.18	0.43
1:K:97:LEU:HG	1:K:528:THR:CB	2.49	0.43
1:M:12:LEU:HD22	1:M:80:ARG:HH12	1.84	0.43
1:M:267:VAL:HG22	1:M:270:ARG:NH2	2.34	0.43
1:C:263:VAL:O	1:C:266:MET:HB2	2.19	0.43
1:F:393:VAL:HA	1:F:441:ASN:O	2.19	0.43
1:H:197:PHE:O	1:H:201:HIS:ND1	2.51	0.43
1:J:250:PRO:HB2	1:J:253:TYR:CE1	2.54	0.43
1:K:393:VAL:HA	1:K:441:ASN:O	2.19	0.43
1:M:443:VAL:HA	1:M:495:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:50:ALA:HB2	1:M:323:TRP:CH2	2.53	0.43
1:C:386:PRO:O	1:C:452:LYS:NZ	2.49	0.43
1:D:162:GLU:HG2	1:D:353:ARG:CB	2.47	0.43
1:D:193:LYS:NZ	1:D:308:SER:OG	2.47	0.43
1:D:49:HIS:CE1	1:D:51:ARG:HG2	2.54	0.43
1:I:393:VAL:HA	1:I:441:ASN:O	2.19	0.43
1:I:527:SER:HB3	1:I:573:VAL:HG21	2.01	0.43
1:J:76:CYS:HG	1:J:88:PHE:HE2	1.65	0.43
1:L:19:LEU:HD13	1:L:80:ARG:CD	2.49	0.43
1:L:228:GLU:HA	1:L:229:PRO:HD3	1.88	0.43
1:M:79:ALA:CB	1:M:88:PHE:HE1	2.26	0.43
1:A:354:ASP:HA	1:A:355:PRO:HD3	1.85	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: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:K:458:ILE:HG23	1:K:555:VAL:HG22	2.00	0.42
1:I:271:GLU:HB3	1:L:268:ARG:HH11	1.84	0.42
1:M:76:CYS:O	1:M:80:ARG:NH2	2.49	0.42
1:A:276:ALA:HB1	1:A:281:TYR:O	2.19	0.42
1:A:316:TYR:CE1	1:G:275:ASP:OD1	2.72	0.42
1:A:529:GLU:O	1:A:531:CYS:N	2.52	0.42
1:A:591:LYS:HE3	1:A:591:LYS:HA	2.02	0.42
1:C:458:ILE:HG23	1:C:555:VAL:HG22	2.00	0.42
1:C:527:SER:HB3	1:C:573:VAL:HG23	2.00	0.42
1:E:303:ASP:OD2	1:E:312:LYS:NZ	2.52	0.42
1:E:97:LEU:HG	1:E:528:THR:CB	2.49	0.42
1:G:263:VAL:O	1:G:266:MET:HB2	2.19	0.42
1:G:529:GLU:O	1:G:531:CYS:N	2.51	0.42
1:G:5:LYS:HG3	1:G:69:PHE:CZ	2.54	0.42
1:H:228:GLU:HA	1:H:229:PRO:HD3	1.88	0.42
1:J:228:GLU:HA	1:J:229:PRO:HD3	1.88	0.42
1:L:263:VAL:O	1:L:266:MET:HB2	2.19	0.42
1:M:137:GLN:HA	1:M:423:ASP:HA	2.01	0.42
1:C:357:PHE:O	1:C:361:HIS:ND1	2.53	0.42
1:D:137:GLN:HA	1:D:423:ASP:HA	2.01	0.42
1:D:231:GLU:O	1:D:249:ARG:HD2	2.19	0.42
1:D:534:GLY:HA2	1:D:577:ALA:CB	2.49	0.42
1:D:8:ARG:HH21	1:D:73:ILE:HG13	1.83	0.42
1:J:197:PHE:O	1:J:201:HIS:ND1	2.51	0.42
1:J:393:VAL:HA	1:J:441:ASN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TYR:O	1:A:94:VAL:HG23	2.20	0.42
1:E:266:MET:HE3	1:E:266:MET:HB3	1.91	0.42
1:F:506:VAL:HG12	1:F:579:SER:HB2	2.01	0.42
1:H:467:LEU:CB	1:J:149:ASN:OD1	2.66	0.42
1:H:529:GLU:O	1:H:531:CYS:N	2.52	0.42
1:I:137:GLN:HA	1:I:423:ASP:HA	2.01	0.42
1:I:50:ALA:HB2	1:I:323:TRP:CH2	2.53	0.42
1:H:467:LEU:CD2	1:J:151:LEU:CD1	2.97	0.42
1:J:137:GLN:HA	1:J:423:ASP:HA	2.01	0.42
1:J:591:LYS:HE3	1:J:591:LYS:HA	2.02	0.42
1:J:5:LYS:HG2	1:J:105:ILE:HB	2.01	0.42
1:J:96:VAL:HG22	1:J:105:ILE:HG21	2.01	0.42
1:L:393:VAL:HA	1:L:441:ASN:O	2.19	0.42
1:A:108:PRO:HA	1:A:109:PRO:HD3	1.81	0.42
1:A:79:ALA:CB	1:A:88:PHE:CD1	2.97	0.42
1:A:9:LEU:HD22	1:A:105:ILE:HD11	2.02	0.42
1:D:529:GLU:O	1:D:531:CYS:N	2.52	0.42
1:D:591:LYS:HE3	1:D:591:LYS:HA	2.02	0.42
1:C:275:ASP:OD1	1:F:316:TYR:HE1	2.03	0.42
1:F:357:PHE:O	1:F:361:HIS:ND1	2.53	0.42
1:G:303:ASP:HB2	1:G:310:GLU:HB2	2.01	0.42
1:G:34:LYS:HG3	1:G:35:GLY:H	1.85	0.42
1:G:393:VAL:HA	1:G:441:ASN:O	2.19	0.42
1:I:357:PHE:O	1:I:361:HIS:ND1	2.53	0.42
1:J:303:ASP:C	1:J:311:SER:HA	2.39	0.42
1:J:97:LEU:CG	1:J:528:THR:CB	2.97	0.42
1:K:231:GLU:O	1:K:249:ARG:HD2	2.19	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: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:A:303:ASP:OD2	1:A:312:LYS:NZ	2.52	0.42
1:A:467:LEU:HD23	1:D:149:ASN:OD1	2.19	0.42
1:D:357:PHE:O	1:D:361:HIS:ND1	2.53	0.42
1:D:393:VAL:HA	1:D:441:ASN:O	2.19	0.42
1:F:137:GLN:HA	1:F:423:ASP:HA	2.01	0.42
1:H:107:VAL:HG21	1:H:528:THR:HG1	1.85	0.42
1:H:403:ILE:HG21	1:H:541:ILE:HG21	1.99	0.42
1:I:267:VAL:HG13	1:I:270:ARG:NH2	2.34	0.42
1:J:162:GLU:HG2	1:J:353:ARG:CB	2.47	0.42
1:J:282:ILE:HD12	1:J:304:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:357:PHE:O	1:J:361:HIS:ND1	2.53	0.42
1:H:605:ARG:NH1	1:K:38:ILE:HB	2.35	0.42
1:K:465:ASP:HB3	1:K:467:LEU:H	1.84	0.42
1:M:529:GLU:O	1:M:531:CYS:N	2.52	0.42
1:M:591:LYS:HA	1:M:591:LYS:HE3	2.02	0.42
1:M:5:LYS:CD	1:M:69:PHE:CZ	3.02	0.42
1:A:267:VAL:HG13	1:A:270:ARG:NH2	2.34	0.42
1:E:357:PHE:O	1:E:361:HIS:ND1	2.52	0.42
1:E:50:ALA:HB2	1:E:323:TRP:CH2	2.53	0.42
1:F:375:PHE:CB	1:F:600:ARG:HD3	2.47	0.42
1:G:534:GLY:HA2	1:G:577:ALA:CB	2.49	0.42
1:L:357:PHE:O	1:L:361:HIS:ND1	2.52	0.42
1:M:393:VAL:HA	1:M:441:ASN:O	2.19	0.42
1:A:357:PHE:O	1:A:361:HIS:ND1	2.52	0.42
1:C:137:GLN:HA	1:C:423:ASP:HA	2.01	0.42
1:D:232:GLY:HA3	1:E:338:PHE:CZ	2.55	0.42
1:E:76:CYS:HG	1:E:88:PHE:HE2	1.66	0.42
1:F:415:SER:OG	1:F:425:SER:HA	2.20	0.42
1:F:97:LEU:HD11	1:F:528:THR:OG1	2.18	0.42
1:F:588:TYR:HA	1:F:589:PRO:HD3	1.91	0.42
1:G:591:LYS:HA	1:G:591:LYS:HE3	2.01	0.42
1:H:137:GLN:HA	1:H:423:ASP:HA	2.01	0.42
1:H:140:ILE:HB	1:H:426:VAL:HG12	2.02	0.42
1:I:162:GLU:HG2	1:I:353:ARG:CB	2.47	0.42
1:I:48:PHE:HB2	1:I:326:VAL:HG22	2.02	0.42
1:I:508:ILE:HD13	1:I:533:CYS:O	2.20	0.42
1:J:140:ILE:HB	1:J:426:VAL:HG12	2.02	0.42
1:J:534:GLY:HA2	1:J:577:ALA:CB	2.49	0.42
1:K:162:GLU:HG2	1:K:353:ARG:CB	2.47	0.42
1:K:8:ARG:NE	1:K:73:ILE:CG2	2.43	0.42
1:M:362:ARG:HD3	1:M:362:ARG:HA	1.84	0.42
1:M:415:SER:OG	1:M:425:SER:HA	2.20	0.42
1:A:231:GLU:O	1:A:249:ARG:HD2	2.20	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:E:266:MET:SD	1:E:323:TRP:HB3	2.60	0.42
1:E:137:GLN:HA	1:E:423:ASP:HA	2.01	0.42
1:I:99:ARG:HH12	1:I:101:ASP:CG	2.24	0.42
1:J:458:ILE:HG23	1:J:555:VAL:HG22	2.00	0.42
1:K:357:PHE:O	1:K:361:HIS:ND1	2.53	0.42
1:D:304:ILE:HD11	1:D:312:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ALA:HB2	1:D:323:TRP:CH2	2.53	0.42
1:D:605:ARG:HA	1:D:605:ARG:HD3	1.90	0.42
1:E:393:VAL:HA	1:E:441:ASN:O	2.19	0.42
1:F:221:ILE:HA	1:F:222:PRO:HD2	1.92	0.42
1:F:193:LYS:NZ	1:F:308:SER:OG	2.48	0.42
1:F:140:ILE:HB	1:F:426:VAL:HG12	2.02	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:K:292:LEU:HB3	1:K:371:HIS:CE1	2.55	0.42
1:L:269:TRP:O	1:L:273:ILE:HG13	2.19	0.42
1:L:276:ALA:HB1	1:L:281:TYR:O	2.20	0.42
1:M:107:VAL:HB	1:M:528:THR:HG23	2.02	0.42
1:M:69:PHE:CE1	1:M:72:PHE:HD2	2.33	0.42
1:A:84:ASN:ND2	1:A:84:ASN:N	2.68	0.41
1:C:416:HIS:ND1	1:C:514:PHE:HB2	2.35	0.41
1:D:415:SER:OG	1:D:425:SER:HA	2.20	0.41
1:E:354:ASP:HA	1:E:355:PRO:HD3	1.85	0.41
1:E:529:GLU:HB2	1:E:533:CYS:HB2	2.01	0.41
1:E:5:LYS:HG3	1:E:69:PHE:CZ	2.55	0.41
1:F:48:PHE:HB2	1:F:326:VAL:HG22	2.02	0.41
1:H:357:PHE:O	1:H:361:HIS:ND1	2.52	0.41
1:I:140:ILE:HB	1:I:426:VAL:HG12	2.02	0.41
1:J:97:LEU:HG	1:J:528:THR:CB	2.49	0.41
1:J:529:GLU:O	1:J:531:CYS:N	2.53	0.41
1:J:60:TYR:O	1:J:64:TYR:HD2	2.04	0.41
1:K:140:ILE:HB	1:K:426:VAL:HG12	2.02	0.41
1:A:162:GLU:HG2	1:A:353:ARG:CB	2.47	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:C:271:GLU:HB3	1:F:268:ARG:HD3	2.02	0.41
1:F:591:LYS:HE3	1:F:591:LYS:HA	2.01	0.41
1:G:231:GLU:O	1:G:249:ARG:HD2	2.19	0.41
1:G:137:GLN:HA	1:G:423:ASP:HA	2.01	0.41
1:J:362:ARG:HD3	1:J:362:ARG:HA	1.84	0.41
1:L:8:ARG:HH21	1:L:73:ILE:CG1	2.20	0.41
1:M:140:ILE:HB	1:M:426:VAL:HG12	2.02	0.41
1:A:415:SER:OG	1:A:425:SER:HA	2.20	0.41
1:C:292:LEU:HB3	1:C:371:HIS:CE1	2.56	0.41
1:D:474:ASP:HA	1:D:477:ARG:HE	1.86	0.41
1:E:228:GLU:HA	1:E:229:PRO:HD3	1.88	0.41
1:E:97:LEU:HG	1:E:528:THR:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:THR:HA	1:E:60:TYR:CD2	2.56	0.41
1:F:276:ALA:HB1	1:F:281:TYR:O	2.20	0.41
1:F:76:CYS:HG	1:F:88:PHE:HE2	1.65	0.41
1:I:271:GLU:HG3	1:L:268:ARG:HG3	2.02	0.41
1:I:591:LYS:HE3	1:I:591:LYS:HA	2.01	0.41
1:M:99:ARG:HH12	1:M:101:ASP:CG	2.24	0.41
1:A:292:LEU:HB3	1:A:371:HIS:CE1	2.55	0.41
1:A:588:TYR:HA	1:A:589:PRO:HD3	1.92	0.41
1:D:161:ARG:HB3	1:D:353:ARG:HA	2.03	0.41
1:D:270:ARG:HD3	1:D:363:PHE:HZ	1.85	0.41
1:E:231:GLU:O	1:E:249:ARG:HD2	2.19	0.41
1:G:474:ASP:HA	1:G:477:ARG:HE	1.85	0.41
1:I:231:GLU:O	1:I:249:ARG:HD2	2.19	0.41
1:L:140:ILE:HB	1:L:426:VAL:HG12	2.02	0.41
1:L:48:PHE:HB2	1:L:326:VAL:HG22	2.02	0.41
1:M:474:ASP:HA	1:M:477:ARG:HE	1.86	0.41
1:M:59:LEU:CD1	1:M:87:MET:HE3	2.50	0.41
1:A:499:ARG:NH1	1:A:503:ASP:O	2.53	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:D:57:THR:HA	1:D:60:TYR:CD2	2.56	0.41
1:E:161:ARG:HB3	1:E:353:ARG:HA	2.03	0.41
1:E:474:ASP:HA	1:E:477:ARG:HE	1.85	0.41
1:E:375:PHE:CB	1:E:600:ARG:HD3	2.48	0.41
1:H:591:LYS:HA	1:H:591:LYS:HE3	2.02	0.41
1:I:474:ASP:HA	1:I:477:ARG:HE	1.86	0.41
1:I:506:VAL:HG12	1:I:579:SER:HB2	2.02	0.41
1:J:415:SER:OG	1:J:425:SER:HA	2.20	0.41
1:K:24:LEU:CD1	1:K:81:GLN:HE21	2.20	0.41
1:L:272:ARG:NH1	1:L:315:GLU:O	2.53	0.41
1:L:332:THR:OG1	1:M:250:PRO:HG2	2.21	0.41
1:L:12:LEU:HD22	1:L:80:ARG:CZ	2.51	0.41
1:M:442:ILE:O	1:M:496:THR:HA	2.21	0.41
1:M:534:GLY:HA2	1:M:577:ALA:CB	2.51	0.41
1:M:375:PHE:CB	1:M:600:ARG:HD3	2.48	0.41
1:M:59:LEU:HD11	1:M:87:MET:CE	2.44	0.41
1:A:161:ARG:HB3	1:A:353:ARG:HA	2.03	0.41
1:A:24:LEU:CG	1:A:27:ASP:N	2.83	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:F:474:ASP:HA	1:F:477:ARG:HE	1.86	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:G:161:ARG:HB3	1:G:353:ARG:HA	2.03	0.41
1:G:415:SER:OG	1:G:425:SER:HA	2.20	0.41
1:G:99:ARG:HH12	1:G:101:ASP:CG	2.24	0.41
1:I:108:PRO:HA	1:I:109:PRO:HD3	1.81	0.41
1:I:354:ASP:HA	1:I:355:PRO:HD3	1.85	0.41
1:K:80:ARG:HA	1:K:83:VAL:HG22	2.02	0.41
1:D:266:MET:SD	1:D:323:TRP:HB3	2.60	0.41
1:D:9:LEU:HG	1:D:72:PHE:HE2	1.68	0.41
1:E:99:ARG:HH12	1:E:101:ASP:CG	2.24	0.41
1:E:60:TYR:O	1:E:64:TYR:HD2	2.04	0.41
1:H:415:SER:OG	1:H:425:SER:HA	2.20	0.41
1:I:24:LEU:HG	1:I:25:PRO:HD2	2.02	0.41
1:I:292:LEU:HB3	1:I:371:HIS:CE1	2.56	0.41
1:I:415:SER:OG	1:I:425:SER:HA	2.20	0.41
1:J:48:PHE:CB	1:J:326:VAL:HG22	2.50	0.41
1:K:6:GLN:NE2	1:K:105:ILE:HA	2.35	0.41
1:K:22:GLU:O	1:K:81:GLN:O	2.38	0.41
1:K:415:SER:OG	1:K:425:SER:HA	2.20	0.41
1:K:9:LEU:HD11	1:K:69:PHE:CZ	2.56	0.41
1:K:88:PHE:O	1:K:92:VAL:HG22	2.20	0.41
1:L:591:LYS:HA	1:L:591:LYS:HE3	2.02	0.41
1:M:161:ARG:HB3	1:M:353:ARG:HA	2.03	0.41
1:M:499:ARG:NH1	1:M:503:ASP:O	2.53	0.41
1:C:474:ASP:HA	1:C:477:ARG:HE	1.86	0.41
1:D:140:ILE:HB	1:D:426:VAL:HG12	2.02	0.41
1:D:499:ARG:NH1	1:D:503:ASP:O	2.53	0.41
1:D:107:VAL:HB	1:D:528:THR:HG23	2.03	0.41
1:E:140:ILE:HB	1:E:426:VAL:HG12	2.02	0.41
1:E:534:GLY:HA2	1:E:577:ALA:CB	2.50	0.41
1:F:231:GLU:O	1:F:249:ARG:HD2	2.20	0.41
1:C:275:ASP:HB2	1:F:268:ARG:NH1	2.36	0.41
1:F:5:LYS:HG3	1:F:69:PHE:CZ	2.55	0.41
1:G:21:ARG:HD3	1:G:41:ARG:HD3	2.02	0.41
1:H:162:GLU:HG2	1:H:353:ARG:CB	2.47	0.41
1:H:292:LEU:HB3	1:H:371:HIS:CE1	2.56	0.41
1:H:50:ALA:HB2	1:H:323:TRP:CH2	2.53	0.41
1:I:161:ARG:HB3	1:I:353:ARG:HA	2.03	0.41
1:J:99:ARG:HH12	1:J:101:ASP:CG	2.24	0.41
1:J:243:GLY:HA2	1:K:125:ASN:HB2	2.02	0.41
1:J:5:LYS:HG3	1:J:69:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:591:LYS:HA	1:K:591:LYS:HE3	2.02	0.41
1:L:303:ASP:OD2	1:L:312:LYS:NZ	2.52	0.41
1:L:415:SER:OG	1:L:425:SER:HA	2.20	0.41
1:L:506:VAL:HG12	1:L:579:SER:HB2	2.02	0.41
1:L:534:GLY:HA2	1:L:577:ALA:CB	2.51	0.41
1:A:24:LEU:CG	1:A:81:GLN:NE2	2.79	0.41
1:A:596:PHE:HA	1:A:597:PRO:C	2.41	0.41
1:C:5:LYS:HG3	1:C:69:PHE:CZ	2.56	0.41
1:D:48:PHE:HB2	1:D:326:VAL:HG22	2.02	0.41
1:E:596:PHE:HA	1:E:597:PRO:C	2.41	0.41
1:G:107:VAL:HB	1:G:528:THR:HG23	2.03	0.41
1:H:268:ARG:HH11	1:M:271:GLU:HA	1.85	0.41
1:I:272:ARG:HB3	1:I:316:TYR:CE1	2.50	0.41
1:J:499:ARG:NH1	1:J:503:ASP:O	2.53	0.41
1:K:5:LYS:HA	1:K:69:PHE:HE2	1.83	0.41
1:L:575:SER:HA	1:L:582:GLY:O	2.21	0.41
1:A:474:ASP:HA	1:A:477:ARG:HE	1.86	0.41
1:A:512:ARG:CB	1:A:531:CYS:SG	3.08	0.41
1:A:5:LYS:HG3	1:A:69:PHE:CZ	2.55	0.41
1:A:24:LEU:CD2	1:A:82:ILE:HG22	2.40	0.41
1:C:99:ARG:HH12	1:C:101:ASP:CG	2.24	0.41
1:C:473:PRO:HA	1:C:476:GLN:HB2	2.03	0.41
1:C:511:VAL:HG22	1:C:512:ARG:H	1.86	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:E:48:PHE:HB2	1:E:326:VAL:HG22	2.02	0.41
1:F:362:ARG:HD3	1:F:362:ARG:HA	1.84	0.41
1:J:385:PHE:HA	1:J:386:PRO:HD3	1.90	0.41
1:K:534:GLY:HA2	1:K:577:ALA:CB	2.50	0.41
1:L:104:GLY:HA2	1:L:525:GLU:C	2.42	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:C:415:SER:OG	1:C:425:SER:HA	2.20	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:292:LEU:HB3	1:F:371:HIS:CE1	2.55	0.41
1:F:99:ARG:HH12	1:F:101:ASP:CG	2.24	0.41
1:G:272:ARG:HD3	1:G:316:TYR:CE1	2.56	0.41
1:G:555:VAL:O	1:G:615:MET:HA	2.21	0.41
1:G:60:TYR:O	1:G:64:TYR:HD2	2.04	0.41
1:H:474:ASP:HA	1:H:477:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:THR:HA	1:H:60:TYR:CD2	2.56	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
1:I:303:ASP:OD2	1:I:312:LYS:NZ	2.52	0.41
1:J:261:VAL:HG12	1:J:262:ASP:O	2.21	0.41
1:K:474:ASP:HA	1:K:477:ARG:HE	1.86	0.41
1:M:292:LEU:HB3	1:M:371:HIS:CE1	2.55	0.41
1:A:57:THR:HA	1:A:60:TYR:CD2	2.56	0.40
1:C:303:ASP:OD2	1:C:312:LYS:NZ	2.52	0.40
1:C:140:ILE:HB	1:C:426:VAL:HG12	2.02	0.40
1:C:57:THR:HA	1:C:60:TYR:CD2	2.56	0.40
1:D:267:VAL:HG13	1:D:270:ARG:NH2	2.36	0.40
1:E:274:LEU:HB2	1:G:268:ARG:NH1	2.37	0.40
1:E:415:SER:OG	1:E:425:SER:HA	2.20	0.40
1:E:473:PRO:HA	1:E:476:GLN:HB2	2.03	0.40
1:F:161:ARG:HB3	1:F:353:ARG:HA	2.02	0.40
1:F:69:PHE:CD1	1:F:102:CYS:SG	3.14	0.40
1:G:323:TRP:O	1:G:326:VAL:HG23	2.22	0.40
1:G:530:TYR:CD2	1:G:531:CYS:SG	3.12	0.40
1:H:231:GLU:O	1:H:249:ARG:HD2	2.21	0.40
1:H:473:PRO:HA	1:H:476:GLN:HB2	2.03	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:H:99:ARG:HH12	1:H:101:ASP:CG	2.24	0.40
1:I:186:MET:SD	1:I:186:MET:N	2.94	0.40
1:I:555:VAL:O	1:I:615:MET:HA	2.21	0.40
1:J:30:ASP:HB3	1:J:32:ARG:HB2	2.03	0.40
1:J:97:LEU:HG	1:J:528:THR:H	1.86	0.40
1:J:530:TYR:CD2	1:J:531:CYS:SG	3.14	0.40
1:K:2:VAL:C	1:K:5:LYS:HB3	2.41	0.40
1:L:292:LEU:HB3	1:L:371:HIS:CE1	2.55	0.40
1:L:474:ASP:HA	1:L:477:ARG:HE	1.86	0.40
1:M:104:GLY:HA2	1:M:525:GLU:C	2.42	0.40
1:A:140:ILE:HB	1:A:426:VAL:HG12	2.02	0.40
1:A:473:PRO:HA	1:A:476:GLN:HB2	2.03	0.40
1:A:48:PHE:HB2	1:A:326:VAL:HG22	2.02	0.40
1:A:555:VAL:O	1:A:615:MET:HA	2.21	0.40
1:C:517:LEU:HA	1:C:520:GLY:N	2.36	0.40
1:C:24:LEU:HD11	1:C:78:GLN:HE21	1.87	0.40
1:D:172:HIS:CD2	1:D:532:SER:HG	2.39	0.40
1:D:99:ARG:HH12	1:D:101:ASP:CG	2.24	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:G:267:VAL:HG13	1:G:270:ARG:NH2	2.36	0.40
1:G:140:ILE:HB	1:G:426:VAL:HG12	2.02	0.40
1:G:57:THR:HA	1:G:60:TYR:CD2	2.56	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:K:97:LEU:HD11	1:K:528:THR:CG2	2.51	0.40
1:K:150:ILE:O	1:L:467:LEU:HD22	2.21	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:C:362:ARG:HA	1:C:362:ARG:HD3	1.84	0.40
1:D:190:LYS:HD3	1:D:190:LYS:HA	1.88	0.40
1:D:473:PRO:HA	1:D:476:GLN:HB2	2.03	0.40
1:E:16:LEU:HD12	1:E:19:LEU:HD12	2.04	0.40
1:F:60:TYR:O	1:F:64:TYR:HD2	2.03	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:272:ARG:HB3	1:J:316:TYR:CE2	2.57	0.40
1:J:474:ASP:HA	1:J:477:ARG:HE	1.86	0.40
1:J:555:VAL:O	1:J:615:MET:HA	2.21	0.40
1:J:337:ARG:NH2	1:K:251:GLU:OE1	2.55	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:M:323:TRP:O	1:M:326:VAL:HG23	2.22	0.40
1:A:69:PHE:CE1	1:A:96:VAL:HG23	2.57	0.40
1:D:16:LEU:HD12	1:D:19:LEU:HD12	2.04	0.40
1:E:162:GLU:HG2	1:E:353:ARG:CB	2.47	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:E:99:ARG:O	1:E:99:ARG:NH1	2.55	0.40
1:F:107:VAL:HG21	1:F:528:THR:HG1	1.85	0.40
1:F:269:TRP:O	1:F:273:ILE:HG13	2.21	0.40
1:H:161:ARG:HB3	1:H:353:ARG:HA	2.03	0.40
1:H:323:TRP:O	1:H:326:VAL:HG23	2.22	0.40
1:L:323:TRP:O	1:L:326:VAL:HG23	2.22	0.40
1:A:323:TRP:O	1:A:326:VAL:HG23	2.22	0.40
1:C:161:ARG:HB3	1:C:353:ARG:HA	2.03	0.40
1:C:555:VAL:O	1:C:615:MET:HA	2.21	0.40
1:D:323:TRP:O	1:D:326:VAL:HG23	2.22	0.40
1:F:529:GLU:HA	1:F:533:CYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:ARG:O	1:F:99:ARG:NH1	2.55	0.40
1:G:175:ILE:HG21	1:G:528:THR:HG21	2.02	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:H:506:VAL:HG12	1:H:579:SER:HB2	2.03	0.40
1:I:160:PHE:HD1	1:I:539:MET:HE2	1.86	0.40
1:I:362:ARG:HA	1:I:362:ARG:HD3	1.84	0.40
1:I:473:PRO:HA	1:I:476:GLN:HB2	2.03	0.40
1:J:231:GLU:O	1:J:249:ARG:HD2	2.21	0.40
1:J:506:VAL:HG12	1:J:579:SER:HB2	2.04	0.40
1:K:67:LYS:HB3	1:K:71:ASP:HB3	2.03	0.40
1:L:16:LEU:HD12	1:L:19:LEU:HD12	2.04	0.40
1:L:190:LYS:HD3	1:L:190:LYS:HA	1.88	0.40
1:L:531:CYS:SG	1:L:532:SER:N	2.95	0.40
1:L:555:VAL:O	1:L:615:MET:HA	2.21	0.40
1:L:5:LYS:CD	1:L:69:PHE:CE1	3.04	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	36
1	C	622/626 (99%)	526 (85%)	84 (14%)	12 (2%)	9	47
1	D	624/626 (100%)	526 (84%)	82 (13%)	16 (3%)	6	40
1	E	624/626 (100%)	529 (85%)	81 (13%)	14 (2%)	8	44
1	F	624/626 (100%)	529 (85%)	77 (12%)	18 (3%)	5	38
1	G	624/626 (100%)	532 (85%)	76 (12%)	16 (3%)	6	40
1	H	624/626 (100%)	528 (85%)	78 (12%)	18 (3%)	5	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	622/626 (99%)	529 (85%)	79 (13%)	14 (2%)	7	43
1	J	624/626 (100%)	533 (85%)	75 (12%)	16 (3%)	6	40
1	K	624/626 (100%)	532 (85%)	81 (13%)	11 (2%)	10	49
1	L	624/626 (100%)	531 (85%)	81 (13%)	12 (2%)	9	47
1	M	624/626 (100%)	526 (84%)	82 (13%)	16 (3%)	6	40
All	All	7484/7512 (100%)	6348 (85%)	953 (13%)	183 (2%)	11	42

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%)	7	31
1	C	556/556 (100%)	508 (91%)	48 (9%)	12	42
1	D	556/556 (100%)	503 (90%)	53 (10%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	556/556 (100%)	506 (91%)	50 (9%)	11	38
1	F	556/556 (100%)	505 (91%)	51 (9%)	11	37
1	G	556/556 (100%)	508 (91%)	48 (9%)	12	42
1	H	556/556 (100%)	505 (91%)	51 (9%)	11	37
1	I	556/556 (100%)	504 (91%)	52 (9%)	10	36
1	J	556/556 (100%)	503 (90%)	53 (10%)	10	36
1	K	556/556 (100%)	505 (91%)	51 (9%)	11	37
1	L	556/556 (100%)	504 (91%)	52 (9%)	10	36
1	M	556/556 (100%)	504 (91%)	52 (9%)	10	36
All	All	6672/6672 (100%)	6051 (91%)	621 (9%)	15	37

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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.