



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Sep 5, 2017 – 12:26 AM EDT

PDB ID : 5NMS
EMDB ID: : EMD-3459
Title : Hsp21 dodecamer, structural model based on cryo-EM and homology modelling
Authors : Rutsdottir, G.; Harmark, J.; Koeck, P.J.B.; Hebert, H.; Soderberg, C.A.G.; Emanuelsson, C.
Deposited on : unknown
Resolution : 10.00 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

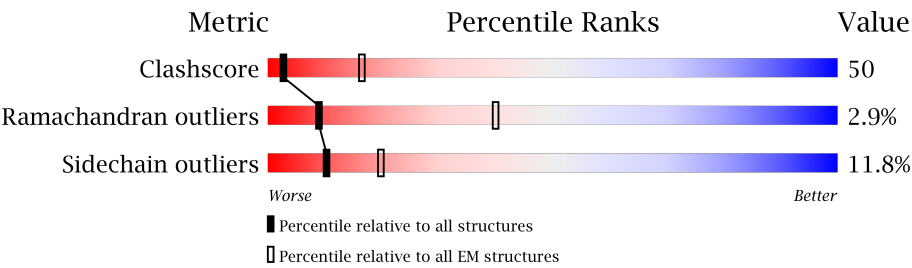
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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 ≥ 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	143	<div><div>44%</div><div>36%</div><div>15%</div><div>5%</div></div>
1	C	143	<div><div>45%</div><div>36%</div><div>15%</div><div>5%</div></div>
1	D	143	<div><div>43%</div><div>36%</div><div>15%</div><div>5%</div></div>
1	G	143	<div><div>43%</div><div>36%</div><div>15%</div><div>5%</div></div>
1	I	143	<div><div>45%</div><div>35%</div><div>15%</div><div>6%</div></div>
1	J	143	<div><div>44%</div><div>36%</div><div>15%</div><div>5%</div></div>
2	B	102	<div><div>48%</div><div>31%</div><div>9%</div><div>12%</div></div>
2	E	102	<div><div>49%</div><div>32%</div><div>8%</div><div>11%</div></div>
2	F	102	<div><div>48%</div><div>31%</div><div>9%</div><div>12%</div></div>

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Mol	Chain	Length	Quality of chain
2	H	102	<div><div></div><div>50%</div><div>30%</div><div>9%</div><div>11%</div></div>
2	K	102	<div><div></div><div>49%</div><div>32%</div><div>9%</div><div>10%</div></div>
2	L	102	<div><div></div><div>48%</div><div>30%</div><div>11%</div><div>11%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23808 atoms, of which 12006 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 25.3 kDa heat shock protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	143	Total	C	H	N	O	S	0	0
			2301	707	1159	200	226	9		
1	C	143	Total	C	H	N	O	S	0	0
			2301	707	1159	200	226	9		
1	D	143	Total	C	H	N	O	S	0	0
			2301	707	1159	200	226	9		
1	G	143	Total	C	H	N	O	S	0	0
			2301	707	1159	200	226	9		
1	I	143	Total	C	H	N	O	S	0	0
			2301	707	1159	200	226	9		
1	J	143	Total	C	H	N	O	S	0	0
			2301	707	1159	200	226	9		

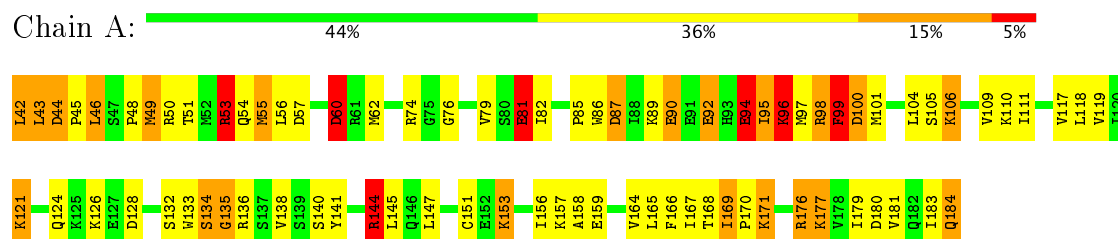
- Molecule 2 is a protein called 25.3 kDa heat shock protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	102	Total	C	H	N	O	S	0	0
			1667	516	842	142	164	3		
2	E	102	Total	C	H	N	O	S	0	0
			1667	516	842	142	164	3		
2	F	102	Total	C	H	N	O	S	0	0
			1667	516	842	142	164	3		
2	H	102	Total	C	H	N	O	S	0	0
			1667	516	842	142	164	3		
2	K	102	Total	C	H	N	O	S	0	0
			1667	516	842	142	164	3		
2	L	102	Total	C	H	N	O	S	0	0
			1667	516	842	142	164	3		

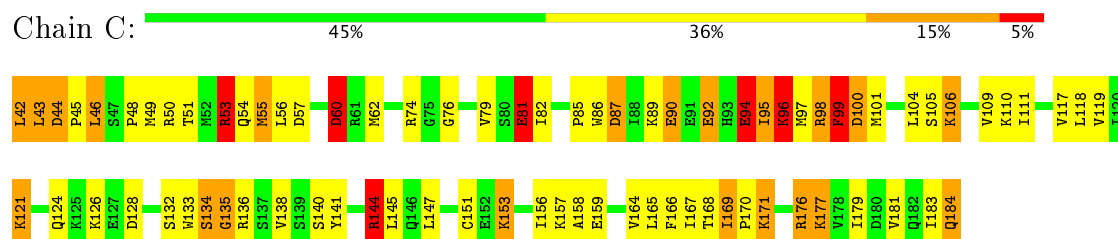
3 Residue-property plots

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.

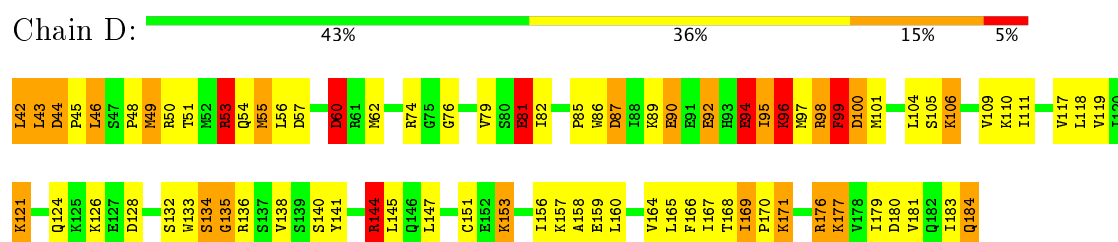
- Molecule 1: 25.3 kDa heat shock protein, chloroplastic



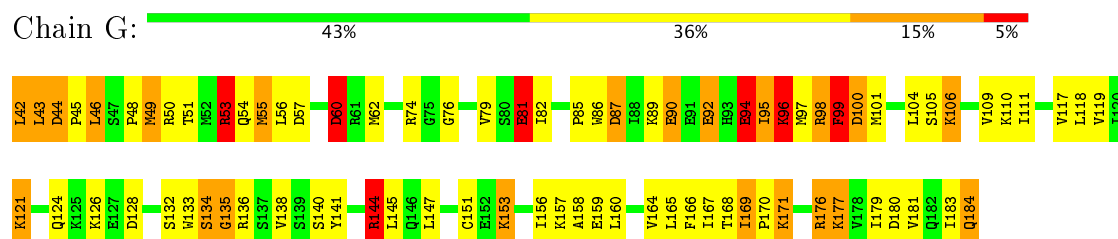
- Molecule 1: 25.3 kDa heat shock protein, chloroplastic



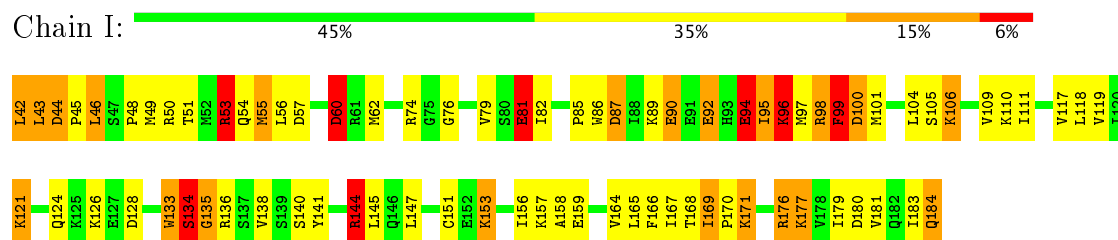
- Molecule 1: 25.3 kDa heat shock protein, chloroplastic



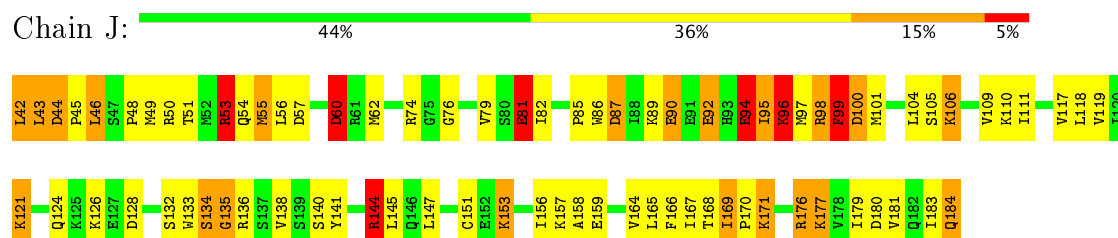
- Molecule 1: 25.3 kDa heat shock protein, chloroplastic



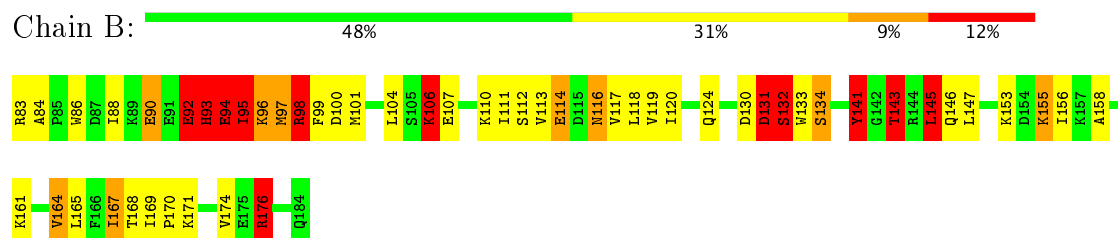
- Molecule 1: 25.3 kDa heat shock protein, chloroplastic



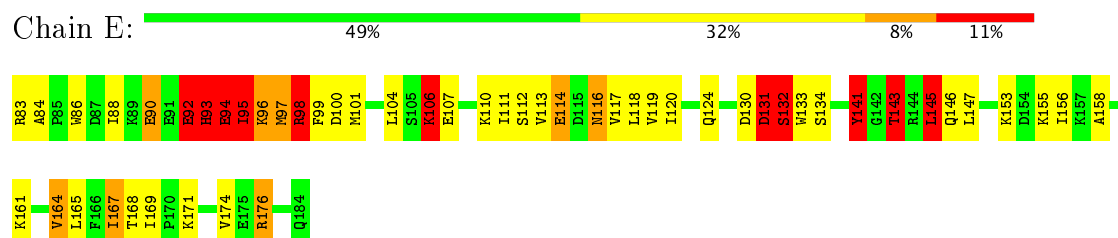
- Molecule 1: 25.3 kDa heat shock protein, chloroplastic



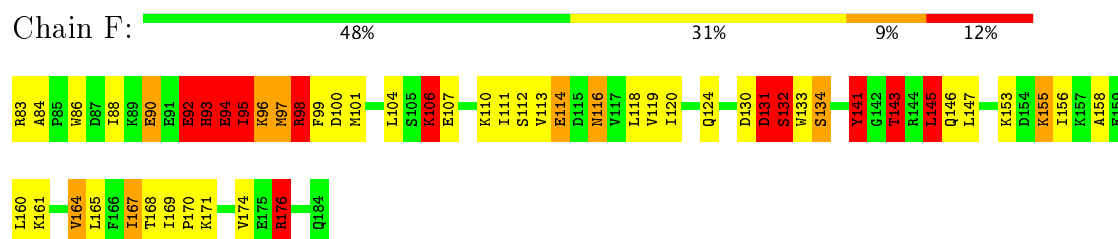
- Molecule 2: 25.3 kDa heat shock protein, chloroplastic



- Molecule 2: 25.3 kDa heat shock protein, chloroplastic

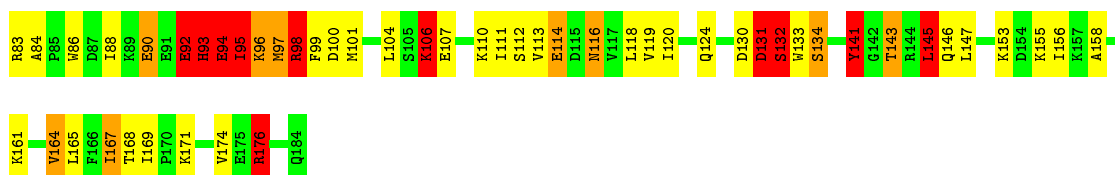


- Molecule 2: 25.3 kDa heat shock protein, chloroplastic



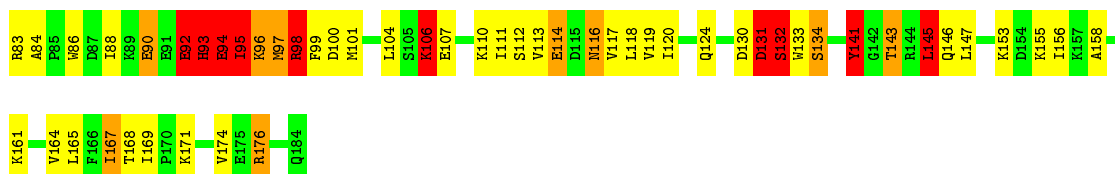
- Molecule 2: 25.3 kDa heat shock protein, chloroplastic





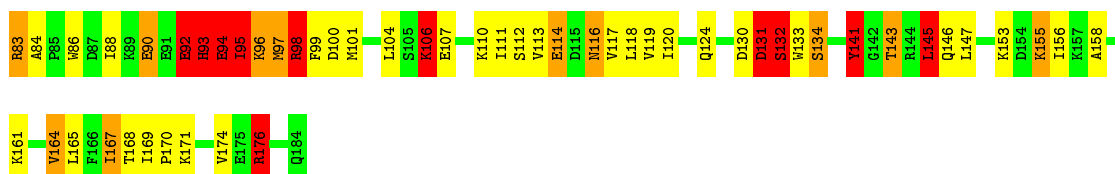
- Molecule 2: 25.3 kDa heat shock protein, chloroplastic

Chain K: 49% 32% 9% 10%



- Molecule 2: 25.3 kDa heat shock protein, chloroplastic

Chain L: 48% 30% 11% 11%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	18407	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL 2100F	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.4	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	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	0.76	0/1157	1.51	22/1549 (1.4%)
1	C	0.76	0/1157	1.51	22/1549 (1.4%)
1	D	0.75	0/1157	1.51	22/1549 (1.4%)
1	G	0.77	0/1157	1.51	22/1549 (1.4%)
1	I	0.77	0/1157	1.52	22/1549 (1.4%)
1	J	0.77	0/1157	1.51	22/1549 (1.4%)
2	B	0.76	0/836	2.00	15/1119 (1.3%)
2	E	0.76	0/836	2.03	15/1119 (1.3%)
2	F	0.75	0/836	2.02	14/1119 (1.3%)
2	H	0.77	0/836	2.07	13/1119 (1.2%)
2	K	0.79	0/836	1.89	15/1119 (1.3%)
2	L	0.78	0/836	1.99	15/1119 (1.3%)
All	All	0.77	0/11958	1.73	219/16008 (1.4%)

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	17
1	C	0	17
1	D	0	17
1	G	0	17
1	I	0	20
1	J	0	17
2	B	0	12
2	E	0	14
2	F	0	12
2	H	0	14
2	K	0	14
2	L	0	13
All	All	0	184

There are no bond length outliers.

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	98	ARG	NE-CZ-NH1	37.70	139.15	120.30
2	F	98	ARG	NE-CZ-NH1	35.83	138.21	120.30
2	E	98	ARG	NE-CZ-NH1	35.53	138.07	120.30
2	B	98	ARG	NE-CZ-NH1	35.22	137.91	120.30
2	L	98	ARG	NE-CZ-NH1	34.52	137.56	120.30
2	K	98	ARG	NE-CZ-NH1	28.21	134.40	120.30
2	H	98	ARG	NH1-CZ-NH2	-20.89	96.42	119.40
2	F	98	ARG	NH1-CZ-NH2	-20.79	96.53	119.40
2	E	98	ARG	NH1-CZ-NH2	-20.26	97.12	119.40
2	B	98	ARG	NH1-CZ-NH2	-19.93	97.48	119.40
2	L	98	ARG	NH1-CZ-NH2	-19.34	98.12	119.40
2	K	132	SER	CA-CB-OG	14.91	151.47	111.20
2	H	132	SER	CA-CB-OG	14.74	150.99	111.20
2	E	132	SER	CA-CB-OG	14.51	150.37	111.20
2	K	98	ARG	NH1-CZ-NH2	-14.35	103.61	119.40
2	F	132	SER	CA-CB-OG	13.63	148.01	111.20
2	B	132	SER	CA-CB-OG	13.60	147.92	111.20
2	L	132	SER	CA-CB-OG	13.58	147.87	111.20
1	C	98	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	I	98	ARG	NE-CZ-NH1	12.26	126.43	120.30
1	G	98	ARG	NE-CZ-NH1	11.97	126.28	120.30
1	A	98	ARG	NE-CZ-NH1	11.97	126.28	120.30
1	J	98	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	D	98	ARG	NE-CZ-NH1	11.92	126.26	120.30
2	L	141	TYR	CB-CG-CD2	-10.36	114.78	121.00
2	K	141	TYR	CB-CG-CD2	-10.32	114.81	121.00
2	F	141	TYR	CB-CG-CD2	-10.30	114.82	121.00
2	H	141	TYR	CB-CG-CD2	-10.29	114.83	121.00
2	H	98	ARG	CD-NE-CZ	10.22	137.91	123.60
2	F	98	ARG	CD-NE-CZ	9.71	137.20	123.60
2	E	98	ARG	CD-NE-CZ	9.63	137.09	123.60
2	F	106	LYS	CA-CB-CG	9.62	134.55	113.40
2	K	106	LYS	CA-CB-CG	9.60	134.51	113.40
2	L	106	LYS	CA-CB-CG	9.59	134.51	113.40
2	E	106	LYS	CA-CB-CG	9.59	134.50	113.40
2	B	106	LYS	CA-CB-CG	9.56	134.44	113.40
2	B	141	TYR	CB-CG-CD2	-9.56	115.26	121.00
2	H	106	LYS	CA-CB-CG	9.55	134.41	113.40
2	B	98	ARG	CD-NE-CZ	9.43	136.80	123.60
2	E	141	TYR	CB-CG-CD2	-9.40	115.36	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	132	SER	N-CA-CB	9.25	124.38	110.50
2	L	98	ARG	CD-NE-CZ	9.18	136.46	123.60
2	K	132	SER	N-CA-CB	9.12	124.17	110.50
2	K	98	ARG	CD-NE-CZ	8.92	136.09	123.60
2	B	95	ILE	CA-CB-CG1	8.71	127.55	111.00
2	K	95	ILE	CA-CB-CG1	8.70	127.54	111.00
2	E	95	ILE	CA-CB-CG1	8.69	127.50	111.00
2	L	95	ILE	CA-CB-CG1	8.67	127.48	111.00
2	H	95	ILE	CA-CB-CG1	8.34	126.85	111.00
2	F	95	ILE	CA-CB-CG1	8.31	126.79	111.00
2	H	145	LEU	CB-CG-CD2	8.24	125.00	111.00
2	F	145	LEU	CB-CG-CD2	8.21	124.95	111.00
1	D	55	MET	CA-CB-CG	8.13	127.12	113.30
1	G	55	MET	CA-CB-CG	8.12	127.10	113.30
2	B	145	LEU	CB-CG-CD2	8.11	124.79	111.00
2	E	145	LEU	CB-CG-CD2	8.10	124.78	111.00
2	K	145	LEU	CB-CG-CD2	8.10	124.76	111.00
2	L	145	LEU	CB-CG-CD2	8.10	124.77	111.00
1	C	55	MET	CA-CB-CG	8.09	127.05	113.30
1	I	55	MET	CA-CB-CG	8.08	127.04	113.30
1	I	100	ASP	CB-CG-OD1	-7.86	111.23	118.30
2	L	106	LYS	CG-CD-CE	7.83	135.38	111.90
2	B	106	LYS	CG-CD-CE	7.83	135.38	111.90
2	F	106	LYS	CG-CD-CE	7.83	135.38	111.90
2	K	106	LYS	CG-CD-CE	7.83	135.38	111.90
2	H	106	LYS	CG-CD-CE	7.82	135.35	111.90
2	E	106	LYS	CG-CD-CE	7.81	135.34	111.90
1	A	55	MET	CA-CB-CG	7.81	126.57	113.30
1	G	100	ASP	CB-CG-OD1	-7.80	111.28	118.30
1	J	55	MET	CA-CB-CG	7.77	126.51	113.30
2	B	131	ASP	CB-CG-OD2	-7.39	111.65	118.30
2	L	131	ASP	CB-CG-OD2	-7.39	111.65	118.30
2	E	131	ASP	CB-CG-OD2	-7.30	111.73	118.30
2	H	131	ASP	CB-CG-OD2	-7.25	111.77	118.30
2	K	131	ASP	CB-CG-OD2	-7.21	111.81	118.30
2	F	131	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	A	60	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	J	100	ASP	CB-CG-OD1	-7.17	111.84	118.30
1	D	60	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	C	60	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	D	176	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	A	100	ASP	CB-CG-OD1	-7.05	111.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	60	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	G	176	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	J	60	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	A	184	GLN	CA-CB-CG	6.95	128.69	113.40
1	J	184	GLN	CA-CB-CG	6.95	128.69	113.40
1	A	176	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	G	184	GLN	CA-CB-CG	6.94	128.67	113.40
1	I	184	GLN	CA-CB-CG	6.94	128.67	113.40
1	D	184	GLN	CA-CB-CG	6.93	128.65	113.40
1	C	184	GLN	CA-CB-CG	6.91	128.60	113.40
1	J	53	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	G	53	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	J	176	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	G	60	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	C	100	ASP	CB-CG-OD1	-6.82	112.17	118.30
1	C	176	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	I	53	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	I	176	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	C	96	LYS	CB-CA-C	6.75	123.89	110.40
1	C	53	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	J	96	LYS	CB-CA-C	6.71	123.81	110.40
1	A	44	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	53	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	96	LYS	CB-CA-C	6.68	123.75	110.40
1	D	44	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	D	96	LYS	CB-CA-C	6.65	123.69	110.40
1	G	96	LYS	CB-CA-C	6.64	123.68	110.40
1	I	96	LYS	CB-CA-C	6.60	123.61	110.40
1	J	184	GLN	CB-CG-CD	6.58	128.71	111.60
1	I	184	GLN	CB-CG-CD	6.56	128.65	111.60
1	G	184	GLN	CB-CG-CD	6.56	128.65	111.60
1	C	44	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	A	184	GLN	CB-CG-CD	6.55	128.63	111.60
1	D	184	GLN	CB-CG-CD	6.55	128.63	111.60
1	C	184	GLN	CB-CG-CD	6.53	128.57	111.60
1	I	44	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	D	53	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	J	44	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	G	44	ASP	CB-CG-OD2	-6.44	112.50	118.30
2	H	131	ASP	CB-CG-OD1	-6.38	112.56	118.30
2	K	131	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	A	95	ILE	N-CA-C	-6.34	93.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	95	ILE	N-CA-C	-6.33	93.90	111.00
1	D	100	ASP	CB-CG-OD1	-6.32	112.62	118.30
2	F	131	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	J	95	ILE	N-CA-C	-6.31	93.97	111.00
1	C	95	ILE	N-CA-C	-6.31	93.97	111.00
1	I	95	ILE	N-CA-C	-6.30	93.98	111.00
2	B	131	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	G	95	ILE	N-CA-C	-6.30	94.00	111.00
2	L	131	ASP	CB-CG-OD1	-6.26	112.66	118.30
2	E	131	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	A	95	ILE	N-CA-CB	6.13	124.91	110.80
1	I	95	ILE	N-CA-CB	6.12	124.86	110.80
1	J	95	ILE	N-CA-CB	6.11	124.86	110.80
1	D	95	ILE	N-CA-CB	6.11	124.85	110.80
1	C	95	ILE	N-CA-CB	6.11	124.85	110.80
1	G	95	ILE	N-CA-CB	6.09	124.81	110.80
2	F	164	VAL	CG1-CB-CG2	5.98	120.47	110.90
2	H	164	VAL	CG1-CB-CG2	5.95	120.41	110.90
2	E	164	VAL	CG1-CB-CG2	5.92	120.37	110.90
1	I	134	SER	CB-CA-C	5.91	121.33	110.10
1	A	184	GLN	OE1-CD-NE2	-5.88	108.37	121.90
1	G	184	GLN	OE1-CD-NE2	-5.87	108.41	121.90
1	J	184	GLN	OE1-CD-NE2	-5.85	108.44	121.90
1	I	184	GLN	OE1-CD-NE2	-5.84	108.47	121.90
1	C	184	GLN	OE1-CD-NE2	-5.82	108.53	121.90
1	D	184	GLN	OE1-CD-NE2	-5.81	108.54	121.90
1	J	166	PHE	CB-CG-CD1	-5.81	116.73	120.80
2	L	164	VAL	CG1-CB-CG2	5.77	120.13	110.90
1	G	166	PHE	CB-CG-CD1	-5.76	116.77	120.80
2	B	164	VAL	CG1-CB-CG2	5.76	120.12	110.90
1	A	166	PHE	CB-CG-CD1	-5.74	116.78	120.80
1	C	98	ARG	NH1-CZ-NH2	-5.73	113.09	119.40
1	C	166	PHE	CB-CG-CD1	-5.72	116.80	120.80
1	I	98	ARG	NH1-CZ-NH2	-5.67	113.16	119.40
1	I	166	PHE	CB-CG-CD1	-5.66	116.84	120.80
1	D	166	PHE	CB-CG-CD1	-5.65	116.84	120.80
2	K	176	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	L	176	ARG	NE-CZ-NH2	-5.57	117.52	120.30
2	H	176	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	D	98	ARG	NH1-CZ-NH2	-5.56	113.29	119.40
1	J	98	ARG	NH1-CZ-NH2	-5.55	113.29	119.40
1	G	98	ARG	NH1-CZ-NH2	-5.55	113.29	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	176	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	G	144	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	E	176	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	55	MET	CB-CA-C	-5.53	99.34	110.40
1	A	98	ARG	NH1-CZ-NH2	-5.52	113.32	119.40
1	J	55	MET	CB-CA-C	-5.50	99.39	110.40
1	I	144	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	43	LEU	CB-CG-CD1	5.43	120.23	111.00
1	C	43	LEU	CB-CG-CD1	5.42	120.21	111.00
1	C	99	PHE	CB-CA-C	5.42	121.23	110.40
1	D	144	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	144	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	J	43	LEU	CB-CG-CD1	5.40	120.18	111.00
1	C	144	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	D	99	PHE	CB-CA-C	5.39	121.18	110.40
1	I	99	PHE	CB-CA-C	5.38	121.17	110.40
1	D	74	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	43	LEU	CB-CG-CD1	5.38	120.14	111.00
1	C	74	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	G	43	LEU	CB-CG-CD1	5.36	120.12	111.00
1	I	43	LEU	CB-CG-CD1	5.36	120.11	111.00
1	J	99	PHE	CB-CA-C	5.34	121.09	110.40
1	J	144	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	99	PHE	CB-CA-C	5.34	121.07	110.40
1	I	74	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	G	99	PHE	CB-CA-C	5.33	121.05	110.40
2	F	176	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	55	MET	CB-CA-C	-5.31	99.77	110.40
1	D	55	MET	CB-CA-C	-5.31	99.78	110.40
1	G	55	MET	CB-CA-C	-5.28	99.83	110.40
1	I	55	MET	CB-CA-C	-5.28	99.83	110.40
1	J	74	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	74	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	J	134	SER	CB-CA-C	5.27	120.11	110.10
1	G	74	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	134	SER	CB-CA-C	5.20	119.97	110.10
1	C	134	SER	CB-CA-C	5.19	119.97	110.10
1	C	96	LYS	N-CA-CB	-5.13	101.37	110.60
1	D	134	SER	CB-CA-C	5.12	119.83	110.10
1	G	134	SER	CB-CA-C	5.12	119.83	110.10
1	I	96	LYS	N-CA-CB	-5.10	101.42	110.60
2	B	98	ARG	NE-CZ-NH2	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	LYS	N-CA-CB	-5.07	101.47	110.60
2	K	98	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	G	96	LYS	N-CA-CB	-5.06	101.49	110.60
1	J	96	LYS	N-CA-CB	-5.05	101.51	110.60
2	L	141	TYR	CB-CG-CD1	5.04	124.02	121.00
2	K	141	TYR	CB-CG-CD1	5.02	124.01	121.00
2	L	83	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	E	143	THR	N-CA-CB	5.02	119.83	110.30
2	F	143	THR	N-CA-CB	5.01	119.82	110.30
1	A	96	LYS	N-CA-CB	-5.00	101.60	110.60
2	B	143	THR	N-CA-CB	5.00	119.80	110.30

There are no chirality outliers.

All (184) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ASP	Sidechain
1	A	128	ASP	Sidechain
1	A	135	GLY	Mainchain
1	A	159	GLU	Sidechain
1	A	169	ILE	Mainchain
1	A	42	LEU	Mainchain
1	A	44	ASP	Sidechain,Mainchain
1	A	49	MET	Mainchain
1	A	51	THR	Peptide
1	A	53	ARG	Sidechain
1	A	60	ASP	Sidechain
1	A	81	GLU	Mainchain
1	A	90	GLU	Sidechain
1	A	92	GLU	Peptide
1	A	94	GLU	Mainchain,Peptide
2	B	100	ASP	Sidechain
2	B	114	GLU	Sidechain
2	B	131	ASP	Sidechain
2	B	90	GLU	Sidechain
2	B	92	GLU	Sidechain
2	B	93	HIS	Sidechain,Peptide
2	B	94	GLU	Mainchain
2	B	96	LYS	Mainchain
2	B	97	MET	Peptide
2	B	98	ARG	Sidechain,Mainchain
1	C	100	ASP	Sidechain

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Mol	Chain	Res	Type	Group
1	C	128	ASP	Sidechain
1	C	135	GLY	Mainchain
1	C	159	GLU	Sidechain
1	C	169	ILE	Mainchain
1	C	42	LEU	Mainchain
1	C	44	ASP	Sidechain,Mainchain
1	C	49	MET	Mainchain
1	C	51	THR	Peptide
1	C	53	ARG	Sidechain
1	C	60	ASP	Sidechain
1	C	81	GLU	Mainchain
1	C	90	GLU	Sidechain
1	C	92	GLU	Peptide
1	C	94	GLU	Mainchain,Peptide
1	D	100	ASP	Sidechain
1	D	128	ASP	Sidechain
1	D	135	GLY	Mainchain
1	D	159	GLU	Sidechain
1	D	169	ILE	Mainchain
1	D	42	LEU	Mainchain
1	D	44	ASP	Sidechain,Mainchain
1	D	49	MET	Mainchain
1	D	51	THR	Peptide
1	D	53	ARG	Sidechain
1	D	60	ASP	Sidechain
1	D	81	GLU	Mainchain
1	D	90	GLU	Sidechain
1	D	92	GLU	Peptide
1	D	94	GLU	Mainchain,Peptide
2	E	100	ASP	Sidechain
2	E	114	GLU	Sidechain
2	E	131	ASP	Sidechain
2	E	132	SER	Mainchain
2	E	90	GLU	Sidechain
2	E	92	GLU	Sidechain
2	E	93	HIS	Sidechain,Mainchain,Peptide
2	E	94	GLU	Mainchain
2	E	96	LYS	Mainchain
2	E	97	MET	Peptide
2	E	98	ARG	Sidechain,Mainchain
2	F	100	ASP	Sidechain
2	F	114	GLU	Sidechain

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Mol	Chain	Res	Type	Group
2	F	131	ASP	Sidechain
2	F	90	GLU	Sidechain
2	F	92	GLU	Sidechain
2	F	93	HIS	Sidechain,Peptide
2	F	94	GLU	Mainchain
2	F	96	LYS	Mainchain
2	F	97	MET	Peptide
2	F	98	ARG	Sidechain,Mainchain
1	G	100	ASP	Sidechain
1	G	128	ASP	Sidechain
1	G	135	GLY	Mainchain
1	G	159	GLU	Sidechain
1	G	169	ILE	Mainchain
1	G	42	LEU	Mainchain
1	G	44	ASP	Sidechain,Mainchain
1	G	49	MET	Mainchain
1	G	51	THR	Peptide
1	G	53	ARG	Sidechain
1	G	60	ASP	Sidechain
1	G	81	GLU	Mainchain
1	G	90	GLU	Sidechain
1	G	92	GLU	Peptide
1	G	94	GLU	Mainchain,Peptide
2	H	100	ASP	Sidechain
2	H	114	GLU	Sidechain
2	H	131	ASP	Sidechain
2	H	132	SER	Mainchain
2	H	90	GLU	Sidechain
2	H	92	GLU	Sidechain
2	H	93	HIS	Sidechain,Peptide
2	H	94	GLU	Mainchain
2	H	96	LYS	Mainchain
2	H	97	MET	Mainchain,Peptide
2	H	98	ARG	Sidechain,Mainchain
1	I	100	ASP	Sidechain
1	I	128	ASP	Sidechain
1	I	133	TRP	Peptide
1	I	134	SER	Peptide
1	I	135	GLY	Mainchain,Peptide
1	I	159	GLU	Sidechain
1	I	169	ILE	Mainchain
1	I	42	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	I	44	ASP	Sidechain,Mainchain
1	I	49	MET	Mainchain
1	I	51	THR	Peptide
1	I	53	ARG	Sidechain
1	I	60	ASP	Sidechain
1	I	81	GLU	Mainchain
1	I	90	GLU	Sidechain
1	I	92	GLU	Peptide
1	I	94	GLU	Mainchain,Peptide
1	J	100	ASP	Sidechain
1	J	128	ASP	Sidechain
1	J	135	GLY	Mainchain
1	J	159	GLU	Sidechain
1	J	169	ILE	Mainchain
1	J	42	LEU	Mainchain
1	J	44	ASP	Sidechain,Mainchain
1	J	49	MET	Mainchain
1	J	51	THR	Peptide
1	J	53	ARG	Sidechain
1	J	60	ASP	Sidechain
1	J	81	GLU	Mainchain
1	J	90	GLU	Sidechain
1	J	92	GLU	Peptide
1	J	94	GLU	Mainchain,Peptide
2	K	100	ASP	Sidechain
2	K	114	GLU	Sidechain
2	K	131	ASP	Sidechain
2	K	132	SER	Mainchain
2	K	90	GLU	Sidechain
2	K	92	GLU	Sidechain
2	K	93	HIS	Sidechain,Mainchain,Peptide
2	K	94	GLU	Mainchain
2	K	96	LYS	Mainchain
2	K	97	MET	Peptide
2	K	98	ARG	Sidechain,Mainchain
2	L	100	ASP	Sidechain
2	L	114	GLU	Sidechain
2	L	131	ASP	Sidechain
2	L	90	GLU	Sidechain
2	L	92	GLU	Sidechain
2	L	93	HIS	Sidechain,Mainchain,Peptide
2	L	94	GLU	Mainchain

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Mol	Chain	Res	Type	Group
2	L	96	LYS	Mainchain
2	L	97	MET	Peptide
2	L	98	ARG	Sidechain,Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1142	1159	1156	145	0
1	C	1142	1159	1156	144	0
1	D	1142	1159	1156	145	0
1	G	1142	1159	1156	150	0
1	I	1142	1159	1156	147	0
1	J	1142	1159	1156	141	0
2	B	825	842	839	120	0
2	E	825	842	839	115	0
2	F	825	842	839	115	0
2	H	825	842	839	119	0
2	K	825	842	839	122	0
2	L	825	842	839	118	0
All	All	11802	12006	11970	1195	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 50.

All (1195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ARG:HH21	2:B:164:VAL:HG21	1.21	1.05
2:H:98:ARG:HH21	2:H:164:VAL:HG21	1.20	1.05
2:F:98:ARG:HH21	2:F:164:VAL:HG21	1.21	1.04
2:E:98:ARG:HH21	2:E:164:VAL:HG21	1.23	1.04
2:L:98:ARG:HH21	2:L:164:VAL:HG21	1.24	1.00
2:K:98:ARG:NH2	2:K:164:VAL:HG21	1.80	0.96
2:H:98:ARG:NH2	2:H:164:VAL:HG21	1.86	0.91
2:F:98:ARG:NH2	2:F:164:VAL:HG21	1.86	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:98:ARG:NH2	2:L:164:VAL:HG21	1.85	0.90
2:E:98:ARG:NH2	2:E:164:VAL:HG21	1.86	0.90
1:I:135:GLY:HA2	2:K:98:ARG:HH11	1.35	0.90
2:B:98:ARG:NH2	2:B:164:VAL:HG21	1.85	0.89
2:H:143:THR:HB	1:J:53:ARG:HG3	1.60	0.82
1:A:53:ARG:HG3	2:F:143:THR:HB	1.61	0.82
2:H:99:PHE:CE1	2:H:143:THR:HG21	2.14	0.82
2:F:99:PHE:CE1	2:F:143:THR:HG21	2.14	0.82
2:B:143:THR:HB	1:C:53:ARG:HG3	1.60	0.81
2:E:143:THR:HB	1:D:53:ARG:HG3	1.61	0.81
1:G:53:ARG:HG3	2:K:143:THR:HB	1.61	0.81
2:B:118:LEU:HB2	2:B:147:LEU:HD21	1.62	0.81
1:I:53:ARG:HG3	2:L:143:THR:HB	1.60	0.81
2:L:118:LEU:HB2	2:L:147:LEU:HD21	1.62	0.81
2:K:99:PHE:CE1	2:K:143:THR:HG21	2.15	0.81
2:E:99:PHE:CE1	2:E:143:THR:HG21	2.15	0.81
2:B:99:PHE:CE1	2:B:143:THR:HG21	2.14	0.81
2:H:118:LEU:HB2	2:H:147:LEU:HD21	1.62	0.81
2:L:99:PHE:CE1	2:L:143:THR:HG21	2.15	0.80
2:F:118:LEU:HB2	2:F:147:LEU:HD21	1.62	0.80
1:I:55:MET:SD	2:L:97:MET:HE3	2.22	0.80
2:K:118:LEU:HB2	2:K:147:LEU:HD21	1.62	0.80
2:E:118:LEU:HB2	2:E:147:LEU:HD21	1.62	0.80
2:E:118:LEU:HD12	2:E:145:LEU:HD23	1.65	0.79
2:B:118:LEU:HD12	2:B:145:LEU:HD23	1.65	0.79
2:K:118:LEU:HD12	2:K:145:LEU:HD23	1.65	0.79
2:L:118:LEU:HD12	2:L:145:LEU:HD23	1.65	0.79
2:H:84:ALA:HB1	2:H:97:MET:SD	2.23	0.79
2:F:84:ALA:HB1	2:F:97:MET:SD	2.23	0.78
2:B:97:MET:HE3	1:C:55:MET:SD	2.24	0.78
1:I:96:LYS:HE2	2:K:132:SER:N	1.97	0.78
2:K:84:ALA:HB1	2:K:97:MET:SD	2.23	0.78
1:C:96:LYS:HE2	2:E:132:SER:N	1.97	0.78
2:E:84:ALA:HB1	2:E:97:MET:SD	2.24	0.78
2:L:84:ALA:HB1	2:L:97:MET:SD	2.23	0.77
2:E:97:MET:HE3	1:D:55:MET:SD	2.25	0.77
2:F:118:LEU:HD12	2:F:145:LEU:HD23	1.65	0.77
1:A:96:LYS:HE2	2:B:132:SER:N	2.00	0.77
2:B:84:ALA:HB1	2:B:97:MET:SD	2.24	0.77
2:H:118:LEU:HD12	2:H:145:LEU:HD23	1.65	0.77
1:G:96:LYS:HE2	2:H:132:SER:N	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:96:LYS:HE2	2:L:132:SER:N	2.01	0.76
2:B:98:ARG:CZ	2:B:164:VAL:HG11	2.15	0.76
1:I:135:GLY:HA2	2:K:98:ARG:NH1	2.01	0.76
2:F:98:ARG:CZ	2:F:164:VAL:HG11	2.16	0.75
2:L:98:ARG:CZ	2:L:164:VAL:HG11	2.17	0.75
1:D:96:LYS:HE2	2:F:132:SER:N	2.00	0.75
1:J:98:ARG:HB2	2:L:132:SER:HB3	1.69	0.75
2:H:98:ARG:CZ	2:H:164:VAL:HG11	2.17	0.74
2:E:98:ARG:CZ	2:E:164:VAL:HG11	2.18	0.74
2:K:98:ARG:CZ	2:K:164:VAL:HG11	2.19	0.73
1:G:55:MET:SD	2:K:97:MET:HE3	2.29	0.73
1:G:98:ARG:HG3	2:H:132:SER:HB2	1.70	0.72
1:C:135:GLY:HA2	2:E:98:ARG:HH11	1.54	0.72
1:I:106:LYS:HD3	1:I:106:LYS:H	1.55	0.72
1:J:135:GLY:HA2	2:L:98:ARG:HH11	1.55	0.72
1:C:106:LYS:H	1:C:106:LYS:HD3	1.55	0.72
1:I:134:SER:HB3	2:K:98:ARG:HH21	1.54	0.72
1:I:184:GLN:HA	2:L:106:LYS:HD2	1.70	0.72
2:H:106:LYS:HD2	1:J:184:GLN:HA	1.70	0.72
1:A:184:GLN:HA	2:F:106:LYS:HD2	1.71	0.71
1:A:179:ILE:HG22	2:F:112:SER:HB2	1.72	0.71
1:G:106:LYS:HD3	1:G:106:LYS:H	1.55	0.71
1:G:53:ARG:HH12	2:K:141:TYR:HB2	1.55	0.71
2:B:106:LYS:HD2	1:C:184:GLN:HA	1.70	0.71
1:D:106:LYS:HD3	1:D:106:LYS:H	1.55	0.71
1:G:184:GLN:HA	2:K:106:LYS:HD2	1.70	0.71
2:H:112:SER:HB2	1:J:179:ILE:HG22	1.72	0.71
2:H:141:TYR:HB2	1:J:53:ARG:HH12	1.54	0.71
2:E:106:LYS:HD2	1:D:184:GLN:HA	1.70	0.71
1:A:53:ARG:HH12	2:F:141:TYR:HB2	1.55	0.71
2:E:141:TYR:HB2	1:D:53:ARG:HH12	1.56	0.70
2:E:112:SER:HB2	1:D:179:ILE:HG22	1.72	0.70
1:I:53:ARG:HH12	2:L:141:TYR:HB2	1.55	0.70
1:I:179:ILE:HG22	2:L:112:SER:HB2	1.72	0.70
2:B:112:SER:HB2	1:C:179:ILE:HG22	1.72	0.70
1:J:106:LYS:HD3	1:J:106:LYS:H	1.55	0.70
1:G:179:ILE:HG22	2:K:112:SER:HB2	1.72	0.70
2:B:145:LEU:HD12	1:C:55:MET:HG2	1.73	0.70
1:D:99:PHE:CZ	1:D:109:VAL:HG21	2.26	0.70
1:G:99:PHE:CZ	1:G:109:VAL:HG21	2.26	0.70
2:H:120:ILE:HB	2:H:143:THR:HG23	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:55:MET:HG2	2:L:145:LEU:HD12	1.73	0.70
1:A:106:LYS:HD3	1:A:106:LYS:H	1.55	0.69
2:B:141:TYR:HB2	1:C:53:ARG:HH12	1.56	0.69
1:C:99:PHE:CZ	1:C:109:VAL:HG21	2.26	0.69
2:B:92:GLU:HG3	2:B:168:THR:CG2	2.22	0.69
2:E:92:GLU:HG3	2:E:168:THR:CG2	2.22	0.69
2:F:120:ILE:HB	2:F:143:THR:HG23	1.73	0.69
2:H:145:LEU:HD12	1:J:55:MET:HG2	1.74	0.69
1:I:99:PHE:CZ	1:I:109:VAL:HG21	2.26	0.69
1:A:99:PHE:CZ	1:A:109:VAL:HG21	2.26	0.69
1:J:99:PHE:CZ	1:J:109:VAL:HG21	2.26	0.69
2:K:92:GLU:HG3	2:K:168:THR:CG2	2.22	0.69
2:L:92:GLU:HG3	2:L:168:THR:CG2	2.22	0.69
1:A:55:MET:HG2	2:F:145:LEU:HD12	1.74	0.69
1:D:135:GLY:HA2	2:F:98:ARG:HH11	1.56	0.69
2:L:120:ILE:HB	2:L:143:THR:HG23	1.73	0.69
2:E:145:LEU:HD12	1:D:55:MET:HG2	1.73	0.69
1:G:55:MET:HG2	2:K:145:LEU:HD12	1.73	0.69
2:B:120:ILE:HB	2:B:143:THR:HG23	1.73	0.69
2:F:92:GLU:HG3	2:F:168:THR:CG2	2.22	0.69
2:E:120:ILE:HB	2:E:143:THR:HG23	1.73	0.69
2:K:120:ILE:HB	2:K:143:THR:HG23	1.73	0.69
2:K:98:ARG:HH21	2:K:164:VAL:HG21	1.55	0.69
2:H:92:GLU:HG3	2:H:168:THR:CG2	2.22	0.68
1:I:151:CYS:SG	1:I:169:ILE:HG23	2.34	0.68
1:C:151:CYS:SG	1:C:169:ILE:HG23	2.34	0.68
1:A:151:CYS:SG	1:A:169:ILE:HG23	2.34	0.68
1:J:151:CYS:SG	1:J:169:ILE:HG23	2.34	0.68
1:D:98:ARG:HB2	2:F:132:SER:HB3	1.76	0.68
1:J:86:TRP:CE3	1:J:145:LEU:HD21	2.29	0.68
1:A:86:TRP:CE3	1:A:145:LEU:HD21	2.29	0.68
1:A:56:LEU:HD11	1:A:62:MET:CE	2.24	0.67
1:G:56:LEU:HD11	1:G:62:MET:CE	2.24	0.67
1:C:86:TRP:CE3	1:C:145:LEU:HD21	2.29	0.67
1:J:56:LEU:HD11	1:J:62:MET:CE	2.24	0.67
1:D:56:LEU:HD11	1:D:62:MET:CE	2.24	0.67
1:I:53:ARG:HG3	2:L:143:THR:CB	2.24	0.67
1:I:86:TRP:CE3	1:I:145:LEU:HD21	2.30	0.67
1:A:111:ILE:HD11	1:A:165:LEU:CD2	2.25	0.67
1:A:98:ARG:HB2	2:B:132:SER:HB3	1.75	0.67
1:D:151:CYS:SG	1:D:169:ILE:HG23	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97:MET:HE3	1:J:55:MET:SD	2.33	0.67
2:E:143:THR:CB	1:D:53:ARG:HG3	2.24	0.67
1:G:53:ARG:HG3	2:K:143:THR:CB	2.24	0.67
2:B:143:THR:CB	1:C:53:ARG:HG3	2.24	0.67
1:C:111:ILE:HD11	1:C:165:LEU:CD2	2.25	0.67
1:I:111:ILE:HD11	1:I:165:LEU:CD2	2.25	0.67
1:J:111:ILE:HD11	1:J:165:LEU:CD2	2.25	0.67
1:D:111:ILE:HD11	1:D:165:LEU:CD2	2.25	0.67
1:G:111:ILE:HD11	1:G:165:LEU:CD2	2.25	0.67
1:D:86:TRP:CE3	1:D:145:LEU:HD21	2.29	0.67
1:A:55:MET:SD	2:F:97:MET:HE3	2.34	0.66
1:G:86:TRP:CE3	1:G:145:LEU:HD21	2.29	0.66
1:C:56:LEU:HD11	1:C:62:MET:CE	2.24	0.66
1:I:56:LEU:HD11	1:I:62:MET:CE	2.24	0.66
1:C:135:GLY:N	2:E:98:ARG:HD2	2.11	0.66
2:E:111:ILE:HD13	2:E:158:ALA:HB2	1.78	0.66
1:A:53:ARG:HG3	2:F:143:THR:CB	2.24	0.66
2:H:143:THR:CB	1:J:53:ARG:HG3	2.24	0.66
1:I:153:LYS:HE2	1:I:156:ILE:CG2	2.26	0.66
2:K:111:ILE:HD13	2:K:158:ALA:HB2	1.78	0.66
1:C:153:LYS:HE2	1:C:156:ILE:CG2	2.26	0.66
1:A:135:GLY:N	2:B:98:ARG:HD2	2.11	0.65
1:A:153:LYS:HE2	1:A:156:ILE:CG2	2.26	0.65
1:I:184:GLN:HA	2:L:106:LYS:CD	2.26	0.65
1:C:82:ILE:HD11	1:C:101:MET:HG3	1.79	0.65
1:D:96:LYS:HE2	2:F:131:ASP:C	2.17	0.65
2:B:106:LYS:CD	1:C:184:GLN:HA	2.26	0.65
1:D:82:ILE:HD11	1:D:101:MET:HG3	1.79	0.65
1:G:96:LYS:HE2	2:H:131:ASP:C	2.17	0.65
1:J:153:LYS:HE2	1:J:156:ILE:CG2	2.27	0.65
1:D:153:LYS:HE2	1:D:156:ILE:CG2	2.26	0.65
1:C:96:LYS:HE2	2:E:132:SER:CA	2.26	0.65
1:D:135:GLY:N	2:F:98:ARG:HD2	2.10	0.65
1:I:82:ILE:HD11	1:I:101:MET:HG3	1.79	0.65
1:I:96:LYS:HE2	2:K:132:SER:CA	2.26	0.65
2:E:106:LYS:CD	1:D:184:GLN:HA	2.27	0.65
1:G:153:LYS:HE2	1:G:156:ILE:CG2	2.26	0.65
1:J:135:GLY:N	2:L:98:ARG:HD2	2.11	0.65
1:G:184:GLN:HA	2:K:106:LYS:CD	2.26	0.65
1:G:82:ILE:HD11	1:G:101:MET:HG3	1.79	0.65
1:J:96:LYS:HE2	2:L:131:ASP:C	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LYS:HE2	2:B:131:ASP:C	2.17	0.65
1:D:98:ARG:HG3	2:F:132:SER:HB2	1.79	0.65
2:H:98:ARG:NH2	2:H:164:VAL:HG11	2.12	0.65
1:I:96:LYS:HE2	2:K:131:ASP:C	2.17	0.65
2:F:98:ARG:NH2	2:F:164:VAL:HG11	2.12	0.64
1:G:96:LYS:HE2	2:H:132:SER:CA	2.26	0.64
2:B:111:ILE:HD13	2:B:158:ALA:HB2	1.78	0.64
1:C:96:LYS:HE2	2:E:131:ASP:C	2.17	0.64
2:L:111:ILE:HD13	2:L:158:ALA:HB2	1.78	0.64
2:F:111:ILE:HD13	2:F:158:ALA:HB2	1.78	0.64
2:H:111:ILE:HD13	2:H:158:ALA:HB2	1.78	0.64
1:G:92:GLU:HB3	1:G:94:GLU:H	1.63	0.64
2:H:106:LYS:CD	1:J:184:GLN:HA	2.27	0.64
1:J:92:GLU:HB3	1:J:94:GLU:H	1.63	0.64
1:A:92:GLU:HB3	1:A:94:GLU:H	1.63	0.64
1:D:92:GLU:HB3	1:D:94:GLU:H	1.63	0.64
2:E:98:ARG:NH2	2:E:164:VAL:HG11	2.12	0.64
1:A:184:GLN:HA	2:F:106:LYS:CD	2.26	0.64
1:D:96:LYS:HE2	2:F:132:SER:CA	2.28	0.64
1:J:104:LEU:HD11	1:J:109:VAL:HB	1.80	0.64
1:J:95:ILE:HD12	1:J:167:ILE:HG23	1.79	0.63
1:A:104:LEU:HD11	1:A:109:VAL:HB	1.80	0.63
1:A:82:ILE:HD11	1:A:101:MET:HG3	1.79	0.63
1:A:95:ILE:HD12	1:A:167:ILE:HG23	1.79	0.63
1:I:92:GLU:CB	1:I:94:GLU:H	2.11	0.63
1:I:92:GLU:HB3	1:I:94:GLU:H	1.63	0.63
1:A:96:LYS:HE2	2:B:132:SER:CA	2.28	0.63
1:A:98:ARG:HG3	2:B:132:SER:HB2	1.80	0.63
1:C:92:GLU:HB3	1:C:94:GLU:H	1.63	0.63
1:G:95:ILE:HD12	1:G:167:ILE:HG23	1.79	0.63
1:J:82:ILE:HD11	1:J:101:MET:HG3	1.79	0.63
1:J:92:GLU:CB	1:J:94:GLU:H	2.12	0.63
1:D:81:GLU:CD	1:D:138:VAL:HG13	2.20	0.63
1:A:92:GLU:CB	1:A:94:GLU:H	2.12	0.62
2:B:97:MET:SD	1:C:55:MET:SD	2.96	0.62
1:C:95:ILE:HD12	1:C:167:ILE:HG23	1.79	0.62
1:D:95:ILE:HD12	1:D:167:ILE:HG23	1.79	0.62
1:D:92:GLU:CB	1:D:94:GLU:H	2.12	0.62
1:G:92:GLU:CB	1:G:94:GLU:H	2.12	0.62
1:A:55:MET:SD	2:F:95:ILE:CG2	2.87	0.62
1:C:92:GLU:CB	1:C:94:GLU:H	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:LEU:HD11	1:D:109:VAL:HB	1.80	0.62
2:E:97:MET:SD	1:D:55:MET:SD	2.97	0.62
1:G:55:MET:SD	2:K:97:MET:SD	2.97	0.62
1:J:96:LYS:HE2	2:L:132:SER:CA	2.28	0.62
2:B:118:LEU:HD13	2:B:119:VAL:N	2.15	0.62
1:G:135:GLY:N	2:H:98:ARG:HD2	2.13	0.62
1:C:104:LEU:HD11	1:C:109:VAL:HB	1.80	0.62
1:D:95:ILE:HD11	1:D:169:ILE:CD1	2.29	0.62
2:L:118:LEU:HD13	2:L:119:VAL:N	2.15	0.62
1:A:95:ILE:HD11	1:A:169:ILE:CD1	2.29	0.62
1:I:95:ILE:HD12	1:I:167:ILE:HG23	1.79	0.62
1:J:95:ILE:HD11	1:J:169:ILE:CD1	2.29	0.62
1:G:95:ILE:HD11	1:G:169:ILE:CD1	2.29	0.62
1:I:104:LEU:HD11	1:I:109:VAL:HB	1.80	0.62
1:I:55:MET:SD	2:L:97:MET:SD	2.97	0.62
2:H:145:LEU:HD12	1:J:55:MET:CG	2.29	0.62
1:A:55:MET:CG	2:F:145:LEU:HD12	2.29	0.62
1:G:104:LEU:HD11	1:G:109:VAL:HB	1.81	0.62
1:G:81:GLU:CD	1:G:138:VAL:HG13	2.20	0.62
1:I:95:ILE:HD11	1:I:169:ILE:CD1	2.30	0.62
2:L:98:ARG:NH2	2:L:164:VAL:HG11	2.14	0.62
1:C:81:GLU:CD	1:C:138:VAL:HG13	2.20	0.62
2:H:95:ILE:CG2	1:J:55:MET:SD	2.88	0.62
1:I:81:GLU:CD	1:I:138:VAL:HG13	2.21	0.61
1:I:85:PRO:HG2	2:K:132:SER:HB3	1.82	0.61
1:I:135:GLY:N	2:K:98:ARG:HD2	2.15	0.61
2:K:118:LEU:HD13	2:K:119:VAL:N	2.15	0.61
1:C:95:ILE:HD11	1:C:169:ILE:CD1	2.30	0.61
2:E:118:LEU:HD13	2:E:119:VAL:N	2.15	0.61
1:G:55:MET:CG	2:K:145:LEU:HD12	2.31	0.61
1:C:135:GLY:HA2	2:E:98:ARG:NH1	2.16	0.61
2:E:145:LEU:HD12	1:D:55:MET:CG	2.31	0.61
2:B:145:LEU:HD12	1:C:55:MET:CG	2.30	0.61
2:E:112:SER:CB	1:D:179:ILE:HG22	2.31	0.61
1:A:95:ILE:H	1:A:168:THR:HA	1.65	0.61
1:G:179:ILE:HG22	2:K:112:SER:CB	2.31	0.61
1:I:55:MET:CG	2:L:145:LEU:HD12	2.31	0.61
1:A:81:GLU:CD	1:A:138:VAL:HG13	2.21	0.61
1:G:95:ILE:H	1:G:168:THR:HA	1.65	0.61
2:H:118:LEU:HD13	2:H:119:VAL:N	2.15	0.61
1:J:95:ILE:H	1:J:168:THR:HA	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ILE:HD13	2:B:168:THR:N	2.16	0.60
2:F:118:LEU:HD13	2:F:119:VAL:N	2.15	0.60
2:L:167:ILE:HD13	2:L:168:THR:N	2.16	0.60
1:D:95:ILE:H	1:D:168:THR:HA	1.65	0.60
1:J:81:GLU:CD	1:J:138:VAL:HG13	2.21	0.60
1:I:95:ILE:H	1:I:168:THR:HA	1.65	0.60
1:J:135:GLY:HA2	2:L:98:ARG:NH1	2.16	0.60
1:C:95:ILE:H	1:C:168:THR:HA	1.65	0.60
1:G:135:GLY:CA	2:H:98:ARG:HH11	2.14	0.60
2:B:94:GLU:HG3	2:B:147:LEU:HD22	1.83	0.60
2:B:92:GLU:HG3	2:B:168:THR:HG23	1.83	0.60
1:G:151:CYS:SG	1:G:169:ILE:HG23	2.42	0.60
2:K:98:ARG:NH1	2:K:164:VAL:HG11	2.17	0.60
2:L:94:GLU:HG3	2:L:147:LEU:HD22	1.83	0.60
1:A:179:ILE:HG22	2:F:112:SER:CB	2.31	0.60
2:B:112:SER:CB	1:C:179:ILE:HG22	2.31	0.60
2:H:112:SER:CB	1:J:179:ILE:HG22	2.31	0.60
2:K:167:ILE:HD13	2:K:168:THR:N	2.17	0.60
1:I:179:ILE:HG22	2:L:112:SER:CB	2.31	0.60
2:L:92:GLU:HG3	2:L:168:THR:HG23	1.84	0.60
2:E:167:ILE:HD13	2:E:168:THR:N	2.17	0.60
2:B:98:ARG:NH2	2:B:164:VAL:HG11	2.16	0.59
1:A:56:LEU:HD11	1:A:62:MET:HE3	1.83	0.59
1:A:99:PHE:HZ	1:A:109:VAL:HG21	1.66	0.59
1:D:135:GLY:CA	2:F:98:ARG:HH11	2.15	0.59
1:I:95:ILE:CD1	1:I:118:LEU:HD22	2.33	0.59
2:L:104:LEU:HD21	2:L:124:GLN:HG2	1.85	0.59
1:A:92:GLU:HA	1:A:171:LYS:HG3	1.84	0.59
1:C:95:ILE:CD1	1:C:118:LEU:HD22	2.33	0.59
1:D:99:PHE:CE2	1:D:165:LEU:HD22	2.38	0.59
1:J:92:GLU:HA	1:J:171:LYS:HG3	1.84	0.59
1:J:99:PHE:HZ	1:J:109:VAL:HG21	1.66	0.59
1:C:99:PHE:HZ	1:C:109:VAL:HG21	1.66	0.59
1:D:92:GLU:HA	1:D:171:LYS:HG3	1.84	0.59
2:F:167:ILE:HD13	2:F:168:THR:N	2.17	0.59
1:G:99:PHE:CE2	1:G:165:LEU:HD22	2.38	0.59
2:B:104:LEU:HD21	2:B:124:GLN:HG2	1.85	0.59
1:C:99:PHE:CE2	1:C:165:LEU:HD22	2.38	0.59
1:C:92:GLU:HA	1:C:171:LYS:HG3	1.84	0.59
1:G:92:GLU:HA	1:G:171:LYS:HG3	1.84	0.59
2:H:167:ILE:HD13	2:H:168:THR:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:99:PHE:CE2	1:I:165:LEU:HD22	2.38	0.59
2:F:94:GLU:HG3	2:F:147:LEU:HD22	1.84	0.59
2:F:92:GLU:HG3	2:F:168:THR:HG23	1.83	0.59
1:I:92:GLU:HA	1:I:171:LYS:HG3	1.84	0.59
2:B:143:THR:HB	1:C:53:ARG:CG	2.32	0.59
2:E:92:GLU:HG3	2:E:168:THR:HG23	1.84	0.59
2:H:92:GLU:HG3	2:H:168:THR:HG23	1.83	0.59
1:I:99:PHE:HZ	1:I:109:VAL:HG21	1.66	0.59
1:A:55:MET:HE1	2:F:97:MET:HB2	1.85	0.59
1:D:95:ILE:CD1	1:D:118:LEU:HD22	2.33	0.59
1:G:124:GLN:HB2	1:G:138:VAL:HG11	1.85	0.59
1:D:86:TRP:CD2	1:D:145:LEU:HD21	2.38	0.58
1:G:86:TRP:CD2	1:G:145:LEU:HD21	2.38	0.58
1:G:95:ILE:CD1	1:G:118:LEU:HD22	2.33	0.58
2:H:94:GLU:HG3	2:H:147:LEU:HD22	1.85	0.58
2:H:97:MET:HB2	1:J:55:MET:HE1	1.85	0.58
1:I:53:ARG:CG	2:L:143:THR:HB	2.32	0.58
1:C:135:GLY:CA	2:E:98:ARG:HH11	2.16	0.58
1:D:135:GLY:HA2	2:F:98:ARG:NH1	2.18	0.58
2:K:94:GLU:HG3	2:K:147:LEU:HD22	1.83	0.58
1:A:156:ILE:HG12	1:A:167:ILE:HD11	1.85	0.58
1:A:95:ILE:CD1	1:A:118:LEU:HD22	2.32	0.58
1:D:124:GLN:HB2	1:D:138:VAL:HG11	1.85	0.58
1:J:156:ILE:HG12	1:J:167:ILE:HD11	1.85	0.58
1:I:86:TRP:CD2	1:I:145:LEU:HD21	2.38	0.58
1:J:99:PHE:CE2	1:J:165:LEU:HD22	2.38	0.58
1:A:99:PHE:CE2	1:A:165:LEU:HD22	2.38	0.58
1:C:86:TRP:CD2	1:C:145:LEU:HD21	2.39	0.58
2:E:94:GLU:HG3	2:E:147:LEU:HD22	1.83	0.58
2:K:92:GLU:HG3	2:K:168:THR:HG23	1.84	0.58
1:J:95:ILE:CD1	1:J:118:LEU:HD22	2.33	0.58
2:H:97:MET:SD	1:J:55:MET:SD	3.01	0.58
1:C:157:LYS:HB2	1:C:168:THR:HG22	1.86	0.58
1:D:81:GLU:OE1	1:D:138:VAL:HG13	2.04	0.58
1:A:55:MET:SD	2:F:95:ILE:HG22	2.44	0.58
1:D:156:ILE:HG12	1:D:167:ILE:HD11	1.85	0.58
2:E:143:THR:HB	1:D:53:ARG:CG	2.32	0.58
2:F:99:PHE:HE1	2:F:143:THR:HG21	1.67	0.58
1:G:156:ILE:HG12	1:G:167:ILE:HD11	1.85	0.58
1:G:53:ARG:CG	2:K:143:THR:HB	2.32	0.58
1:J:86:TRP:CD2	1:J:145:LEU:HD21	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TRP:CD2	1:A:145:LEU:HD21	2.38	0.58
2:B:120:ILE:HD12	2:B:165:LEU:CD2	2.34	0.58
1:C:101:MET:HG2	1:C:104:LEU:HB2	1.85	0.58
1:G:101:MET:HG2	1:G:104:LEU:HB2	1.85	0.58
1:I:101:MET:HG2	1:I:104:LEU:HB2	1.85	0.58
1:I:157:LYS:HB2	1:I:168:THR:HG22	1.86	0.58
2:L:120:ILE:HD12	2:L:165:LEU:CD2	2.34	0.58
1:I:55:MET:SD	2:L:95:ILE:CG2	2.92	0.58
1:D:101:MET:HG2	1:D:104:LEU:HB2	1.85	0.58
1:A:55:MET:SD	2:F:97:MET:SD	3.01	0.58
2:H:143:THR:HB	1:J:53:ARG:CG	2.32	0.58
1:I:98:ARG:HB2	2:K:132:SER:HB2	1.84	0.58
1:J:101:MET:HG2	1:J:104:LEU:HB2	1.86	0.58
1:A:53:ARG:CG	2:F:143:THR:HB	2.32	0.57
2:B:95:ILE:CG2	1:C:55:MET:SD	2.92	0.57
2:H:111:ILE:HD12	2:H:120:ILE:HD11	1.86	0.57
1:I:55:MET:SD	2:L:95:ILE:HG22	2.44	0.57
1:A:101:MET:HG2	1:A:104:LEU:HB2	1.86	0.57
1:G:55:MET:SD	2:K:95:ILE:HG22	2.44	0.57
2:H:104:LEU:HD21	2:H:124:GLN:HG2	1.85	0.57
1:G:55:MET:SD	2:K:95:ILE:CG2	2.92	0.57
2:B:95:ILE:HG22	1:C:55:MET:SD	2.44	0.57
2:E:104:LEU:HD21	2:E:124:GLN:HG2	1.85	0.57
1:G:183:ILE:HG23	2:K:107:GLU:OE2	2.05	0.57
2:B:118:LEU:HD11	2:B:120:ILE:HG12	1.86	0.57
2:E:107:GLU:OE2	1:D:183:ILE:HG23	2.05	0.57
2:E:116:ASN:HB3	1:D:177:LYS:HZ1	1.70	0.57
2:E:120:ILE:HD12	2:E:165:LEU:CD2	2.34	0.57
2:F:111:ILE:HD12	2:F:120:ILE:HD11	1.87	0.57
1:G:177:LYS:HZ1	2:K:116:ASN:HB3	1.70	0.57
1:G:81:GLU:OE1	1:G:138:VAL:HG13	2.05	0.57
2:H:99:PHE:HE1	2:H:143:THR:HG21	1.68	0.57
2:H:120:ILE:HD12	2:H:165:LEU:CD2	2.34	0.57
2:H:95:ILE:HG22	1:J:55:MET:SD	2.44	0.57
2:E:95:ILE:CG2	1:D:55:MET:SD	2.92	0.57
2:H:98:ARG:NH2	2:H:164:VAL:CG2	2.66	0.57
2:K:104:LEU:HD21	2:K:124:GLN:HG2	1.85	0.57
2:K:120:ILE:HD12	2:K:165:LEU:CD2	2.34	0.57
1:A:124:GLN:HB2	1:A:138:VAL:HG11	1.85	0.57
2:F:104:LEU:HD21	2:F:124:GLN:HG2	1.85	0.57
1:I:124:GLN:HB2	1:I:138:VAL:HG11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:124:GLN:HB2	1:J:138:VAL:HG11	1.85	0.57
2:L:118:LEU:HD11	2:L:120:ILE:HG12	1.86	0.57
1:C:124:GLN:HB2	1:C:138:VAL:HG11	1.85	0.57
1:D:157:LYS:HB2	1:D:168:THR:HG22	1.86	0.57
2:E:95:ILE:HG22	1:D:55:MET:SD	2.44	0.57
2:F:120:ILE:HD12	2:F:165:LEU:CD2	2.34	0.57
1:G:55:MET:SD	2:K:97:MET:CE	2.92	0.57
1:A:53:ARG:HH22	2:F:141:TYR:HB2	1.70	0.57
1:G:157:LYS:HB2	1:G:168:THR:HG22	1.86	0.57
2:H:141:TYR:HB2	1:J:53:ARG:HH22	1.70	0.57
1:I:156:ILE:HG12	1:I:167:ILE:HD11	1.86	0.57
1:J:98:ARG:HG3	2:L:132:SER:HB2	1.86	0.57
1:C:156:ILE:HG12	1:C:167:ILE:HD11	1.86	0.57
2:E:141:TYR:HB2	1:D:53:ARG:HH22	1.69	0.56
1:D:99:PHE:HZ	1:D:109:VAL:HG21	1.66	0.56
2:F:98:ARG:NH2	2:F:164:VAL:CG2	2.66	0.56
2:F:118:LEU:HD11	2:F:120:ILE:HG12	1.86	0.56
2:H:118:LEU:HD11	2:H:120:ILE:HG12	1.86	0.56
1:A:81:GLU:OE1	1:A:138:VAL:HG13	2.05	0.56
2:B:107:GLU:OE2	1:C:183:ILE:HG23	2.05	0.56
1:G:99:PHE:HZ	1:G:109:VAL:HG21	1.66	0.56
1:G:98:ARG:NH2	2:H:133:TRP:CZ2	2.73	0.56
1:J:157:LYS:HB2	1:J:168:THR:HG22	1.86	0.56
1:G:53:ARG:HH22	2:K:141:TYR:HB2	1.70	0.56
1:I:183:ILE:HG23	2:L:107:GLU:OE2	2.05	0.56
1:A:135:GLY:CA	2:B:98:ARG:HH11	2.19	0.56
1:A:157:LYS:HB2	1:A:168:THR:HG22	1.86	0.56
1:A:183:ILE:HG23	2:F:107:GLU:OE2	2.05	0.56
1:A:98:ARG:NH2	2:B:133:TRP:CZ2	2.73	0.56
1:D:98:ARG:NH2	2:F:133:TRP:CZ2	2.73	0.56
1:I:53:ARG:HH22	2:L:141:TYR:HB2	1.70	0.56
2:H:107:GLU:OE2	1:J:183:ILE:HG23	2.05	0.56
1:J:98:ARG:NH2	2:L:133:TRP:CZ2	2.73	0.56
2:K:111:ILE:HD12	2:K:120:ILE:HD11	1.87	0.56
2:L:99:PHE:HE1	2:L:143:THR:HG21	1.68	0.56
2:B:116:ASN:HB3	1:C:177:LYS:HZ1	1.70	0.56
2:B:99:PHE:HE1	2:B:143:THR:HG21	1.68	0.56
1:C:81:GLU:OE1	1:C:138:VAL:HG13	2.04	0.56
2:E:111:ILE:HD12	2:E:120:ILE:HD11	1.86	0.56
1:C:98:ARG:NH2	2:E:133:TRP:CZ2	2.74	0.56
1:J:81:GLU:OE1	1:J:138:VAL:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:177:LYS:HZ1	2:L:116:ASN:HB3	1.70	0.56
1:A:95:ILE:HD11	1:A:169:ILE:HD12	1.88	0.56
2:B:141:TYR:HB2	1:C:53:ARG:HH22	1.70	0.56
2:E:156:ILE:HD12	2:E:169:ILE:HD11	1.88	0.56
1:I:81:GLU:OE1	1:I:138:VAL:HG13	2.05	0.56
1:I:98:ARG:NH2	2:K:133:TRP:CZ2	2.74	0.56
2:B:111:ILE:HD12	2:B:120:ILE:HD11	1.87	0.56
1:D:95:ILE:HD11	1:D:169:ILE:HD12	1.88	0.56
1:D:82:ILE:HD11	1:D:101:MET:CG	2.36	0.56
1:J:95:ILE:HD11	1:J:169:ILE:HD12	1.88	0.56
1:I:55:MET:SD	2:L:97:MET:CE	2.93	0.56
1:C:82:ILE:HD11	1:C:101:MET:CG	2.36	0.56
2:H:116:ASN:HB3	1:J:177:LYS:HZ1	1.70	0.56
2:K:156:ILE:HD12	2:K:169:ILE:HD11	1.88	0.56
2:L:111:ILE:HD12	2:L:120:ILE:HD11	1.87	0.56
1:A:177:LYS:HZ1	2:F:116:ASN:HB3	1.70	0.56
2:F:156:ILE:HD12	2:F:169:ILE:HD11	1.88	0.55
2:H:156:ILE:HD12	2:H:169:ILE:HD11	1.88	0.55
2:K:118:LEU:HD11	2:K:120:ILE:HG12	1.86	0.55
1:I:82:ILE:HD11	1:I:101:MET:CG	2.36	0.55
2:E:110:LYS:NZ	1:D:179:ILE:HD12	2.22	0.55
2:E:118:LEU:HD11	2:E:120:ILE:HG12	1.86	0.55
1:G:82:ILE:HD11	1:G:101:MET:CG	2.36	0.55
2:B:104:LEU:HD11	2:B:141:TYR:CE2	2.41	0.55
1:G:95:ILE:HD11	1:G:169:ILE:HD12	1.88	0.55
1:A:82:ILE:HD11	1:A:101:MET:CG	2.36	0.55
2:E:104:LEU:HD11	2:E:141:TYR:CE2	2.41	0.55
1:G:179:ILE:HD12	2:K:110:LYS:NZ	2.22	0.55
1:I:179:ILE:HD12	2:L:110:LYS:NZ	2.22	0.55
1:A:135:GLY:HA2	2:B:98:ARG:HH11	1.71	0.55
2:B:110:LYS:NZ	1:C:179:ILE:HD12	2.22	0.55
1:J:82:ILE:HD11	1:J:101:MET:CG	2.36	0.55
1:A:55:MET:N	2:F:145:LEU:CD1	2.70	0.55
2:H:145:LEU:CD1	1:J:55:MET:N	2.70	0.55
2:E:145:LEU:CD1	1:D:55:MET:N	2.70	0.55
1:G:55:MET:N	2:K:145:LEU:CD1	2.70	0.55
1:I:55:MET:N	2:L:145:LEU:CD1	2.70	0.55
2:L:156:ILE:HD12	2:L:169:ILE:HD11	1.88	0.55
2:B:145:LEU:CD1	1:C:55:MET:N	2.70	0.54
1:G:156:ILE:HD12	1:G:169:ILE:HG12	1.89	0.54
1:A:89:LYS:HD3	1:A:90:GLU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:LYS:HZ1	1:C:179:ILE:HG13	1.71	0.54
2:B:156:ILE:HD12	2:B:169:ILE:HD11	1.88	0.54
2:B:88:ILE:HG23	2:B:93:HIS:NE2	2.23	0.54
1:C:89:LYS:HD3	1:C:90:GLU:H	1.72	0.54
1:G:111:ILE:HD11	1:G:165:LEU:HD22	1.90	0.54
1:I:89:LYS:HD3	1:I:90:GLU:H	1.72	0.54
1:D:111:ILE:HD11	1:D:165:LEU:HD22	1.90	0.54
1:D:89:LYS:HD3	1:D:90:GLU:H	1.72	0.54
2:H:110:LYS:NZ	1:J:179:ILE:HD12	2.22	0.54
1:J:89:LYS:HD3	1:J:90:GLU:H	1.72	0.54
1:A:179:ILE:HD12	2:F:110:LYS:NZ	2.22	0.54
2:E:90:GLU:C	2:E:174:VAL:HG23	2.28	0.54
1:G:89:LYS:HD3	1:G:90:GLU:H	1.72	0.54
2:H:104:LEU:HD11	2:H:141:TYR:CE2	2.42	0.54
2:L:104:LEU:HD11	2:L:141:TYR:CE2	2.42	0.54
2:B:111:ILE:HD11	2:B:167:ILE:CG1	2.38	0.54
2:E:97:MET:CE	1:D:55:MET:SD	2.95	0.54
2:F:90:GLU:C	2:F:174:VAL:HG23	2.28	0.54
2:H:111:ILE:HD11	2:H:167:ILE:CG1	2.38	0.54
2:H:90:GLU:C	2:H:174:VAL:HG23	2.28	0.54
2:K:90:GLU:C	2:K:174:VAL:HG23	2.28	0.54
2:L:88:ILE:HG23	2:L:93:HIS:NE2	2.23	0.54
2:B:90:GLU:C	2:B:174:VAL:HG23	2.28	0.54
2:F:104:LEU:HD11	2:F:141:TYR:CE2	2.42	0.54
2:F:111:ILE:HD11	2:F:167:ILE:CG1	2.38	0.54
1:I:179:ILE:HG13	2:L:110:LYS:HZ1	1.71	0.54
2:H:110:LYS:HZ1	1:J:179:ILE:HG13	1.73	0.54
2:K:104:LEU:HD11	2:K:141:TYR:CE2	2.42	0.54
2:L:90:GLU:C	2:L:174:VAL:HG23	2.28	0.54
2:H:120:ILE:HD12	2:H:165:LEU:HD21	1.90	0.54
1:I:111:ILE:HD11	1:I:165:LEU:HD22	1.90	0.54
2:L:111:ILE:HD11	2:L:167:ILE:CG1	2.38	0.54
1:C:85:PRO:HG2	2:E:132:SER:HB2	1.89	0.54
1:I:95:ILE:HD11	1:I:169:ILE:HD12	1.88	0.54
2:K:99:PHE:HE1	2:K:143:THR:HG21	1.68	0.54
1:C:111:ILE:HD11	1:C:165:LEU:HD22	1.90	0.54
1:D:156:ILE:HD12	1:D:169:ILE:HG12	1.90	0.54
2:B:97:MET:CE	1:C:55:MET:SD	2.95	0.54
2:E:111:ILE:HD11	2:E:167:ILE:CG1	2.38	0.54
1:C:119:VAL:HG22	1:C:144:ARG:CD	2.38	0.53
1:D:56:LEU:HD11	1:D:62:MET:HE3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:ILE:HD12	2:F:165:LEU:HD21	1.90	0.53
1:G:179:ILE:HG13	2:K:110:LYS:HZ1	1.74	0.53
2:K:111:ILE:HD11	2:K:167:ILE:CG1	2.38	0.53
1:A:98:ARG:NH2	2:B:133:TRP:CE2	2.77	0.53
2:E:99:PHE:HE1	2:E:143:THR:HG21	1.68	0.53
1:A:179:ILE:HG13	2:F:110:LYS:HZ1	1.73	0.53
1:G:119:VAL:HG22	1:G:144:ARG:CD	2.38	0.53
1:I:119:VAL:HG22	1:I:144:ARG:CD	2.38	0.53
1:J:98:ARG:NH2	2:L:133:TRP:CE2	2.77	0.53
1:C:43:LEU:HD12	1:C:145:LEU:CD1	2.38	0.53
1:D:119:VAL:HG22	1:D:144:ARG:CD	2.38	0.53
1:D:42:LEU:N	1:D:42:LEU:HD12	2.24	0.53
1:G:42:LEU:HD12	1:G:42:LEU:N	2.24	0.53
1:I:43:LEU:HD12	1:I:145:LEU:CD1	2.38	0.53
1:A:119:VAL:HG22	1:A:144:ARG:CD	2.38	0.53
1:G:98:ARG:NH2	2:H:133:TRP:CE2	2.77	0.53
1:A:43:LEU:HD12	1:A:145:LEU:CD1	2.38	0.53
1:D:98:ARG:NH2	2:F:133:TRP:CE2	2.77	0.53
1:I:42:LEU:HD12	1:I:42:LEU:N	2.24	0.53
2:K:88:ILE:HG23	2:K:93:HIS:NE2	2.23	0.53
2:L:116:ASN:HB2	2:L:153:LYS:HE3	1.91	0.53
2:L:98:ARG:NH2	2:L:164:VAL:CG2	2.66	0.53
2:B:116:ASN:HB2	2:B:153:LYS:HE3	1.91	0.53
1:C:98:ARG:NH2	2:E:133:TRP:CE2	2.77	0.53
1:J:119:VAL:HG22	1:J:144:ARG:CD	2.39	0.53
2:L:120:ILE:HD12	2:L:165:LEU:HD21	1.90	0.53
1:A:111:ILE:HD11	1:A:165:LEU:HD22	1.90	0.53
1:C:42:LEU:HD12	1:C:42:LEU:N	2.24	0.53
2:E:143:THR:CA	1:D:53:ARG:HG3	2.39	0.53
1:J:43:LEU:HD12	1:J:145:LEU:CD1	2.39	0.53
1:I:98:ARG:NH2	2:K:133:TRP:CE2	2.77	0.53
2:E:88:ILE:HG23	2:E:93:HIS:NE2	2.23	0.53
1:G:53:ARG:NH1	2:K:141:TYR:HB2	2.23	0.53
2:H:88:ILE:HG23	2:H:93:HIS:NE2	2.23	0.53
1:G:53:ARG:HG3	2:K:143:THR:CA	2.39	0.53
2:B:120:ILE:HD12	2:B:165:LEU:HD21	1.90	0.53
1:A:53:ARG:HG3	2:F:143:THR:CA	2.39	0.53
2:F:88:ILE:HG23	2:F:93:HIS:NE2	2.23	0.53
1:G:135:GLY:HA2	2:H:98:ARG:HH11	1.74	0.53
1:J:42:LEU:HD12	1:J:42:LEU:N	2.24	0.53
2:H:143:THR:CA	1:J:53:ARG:HG3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:HD12	1:A:169:ILE:HG12	1.90	0.53
1:A:53:ARG:HH12	2:F:141:TYR:CB	2.22	0.53
2:B:98:ARG:NH2	2:B:164:VAL:CG2	2.67	0.53
1:I:53:ARG:HG3	2:L:143:THR:CA	2.39	0.53
1:J:156:ILE:HD12	1:J:169:ILE:HG12	1.90	0.53
1:A:42:LEU:HD12	1:A:42:LEU:N	2.24	0.52
2:B:143:THR:CA	1:C:53:ARG:HG3	2.39	0.52
1:J:111:ILE:HD11	1:J:165:LEU:HD22	1.90	0.52
2:H:141:TYR:CB	1:J:53:ARG:HH12	2.22	0.52
2:E:110:LYS:HZ1	1:D:179:ILE:HG13	1.75	0.52
2:E:95:ILE:HG12	2:E:167:ILE:HD12	1.91	0.52
1:D:43:LEU:HD12	1:D:145:LEU:CD1	2.38	0.52
2:E:120:ILE:HD12	2:E:165:LEU:HD21	1.90	0.52
1:G:43:LEU:HD12	1:G:145:LEU:CD1	2.39	0.52
1:G:53:ARG:HH12	2:K:141:TYR:CB	2.22	0.52
1:G:45:PRO:HG3	1:G:86:TRP:CZ3	2.45	0.52
1:J:76:GLY:HA2	1:J:79:VAL:HG22	1.92	0.52
1:J:136:ARG:HH21	2:L:83:ARG:HD2	1.75	0.52
1:A:136:ARG:HH21	2:B:83:ARG:HD2	1.75	0.52
1:C:95:ILE:HD11	1:C:169:ILE:HD12	1.89	0.52
1:D:45:PRO:HG3	1:D:86:TRP:CZ3	2.45	0.52
1:J:42:LEU:HD23	1:J:117:VAL:HG11	1.92	0.52
1:A:42:LEU:HD23	1:A:117:VAL:HG11	1.92	0.52
2:B:95:ILE:HG12	2:B:167:ILE:HD12	1.92	0.52
2:E:141:TYR:CB	1:D:53:ARG:HH12	2.23	0.52
2:H:116:ASN:HB2	2:H:153:LYS:HE3	1.91	0.52
2:K:98:ARG:NH2	2:K:164:VAL:CG2	2.65	0.52
1:A:76:GLY:HA2	1:A:79:VAL:HG22	1.92	0.52
2:E:141:TYR:HB2	1:D:53:ARG:NH1	2.24	0.52
2:F:116:ASN:HB2	2:F:153:LYS:HE3	1.91	0.52
1:G:56:LEU:HD11	1:G:62:MET:HE3	1.90	0.52
2:H:94:GLU:HB3	2:H:169:ILE:HB	1.90	0.52
1:C:56:LEU:HD11	1:C:62:MET:HE3	1.90	0.52
1:J:135:GLY:CA	2:L:98:ARG:HH11	2.20	0.52
2:K:120:ILE:HD12	2:K:165:LEU:HD21	1.91	0.52
2:K:95:ILE:HG12	2:K:167:ILE:HD12	1.92	0.52
2:L:95:ILE:HG12	2:L:167:ILE:HD12	1.92	0.52
1:C:76:GLY:HA2	1:C:79:VAL:HG22	1.92	0.52
1:C:45:PRO:HG3	1:C:86:TRP:CZ3	2.45	0.52
1:I:156:ILE:HD12	1:I:169:ILE:HG12	1.90	0.52
1:I:56:LEU:HD11	1:I:62:MET:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ILE:HD12	1:C:169:ILE:HG12	1.90	0.52
1:I:45:PRO:HG3	1:I:86:TRP:CZ3	2.45	0.52
2:K:116:ASN:HB2	2:K:153:LYS:HE3	1.91	0.52
1:I:53:ARG:HH12	2:L:141:TYR:CB	2.22	0.51
1:I:76:GLY:HA2	1:I:79:VAL:HG22	1.92	0.51
1:I:53:ARG:NH1	2:L:141:TYR:HB2	2.24	0.51
2:E:116:ASN:HB2	2:E:153:LYS:HE3	1.91	0.51
2:F:94:GLU:HB3	2:F:169:ILE:HB	1.91	0.51
1:A:92:GLU:HB3	1:A:94:GLU:N	2.25	0.51
1:G:42:LEU:HD23	1:G:117:VAL:HG11	1.92	0.51
1:J:92:GLU:HB3	1:J:94:GLU:N	2.25	0.51
1:D:92:GLU:HB3	1:D:94:GLU:N	2.25	0.51
1:G:92:GLU:HB3	1:G:94:GLU:N	2.25	0.51
1:A:45:PRO:HG3	1:A:86:TRP:CZ3	2.45	0.51
1:D:42:LEU:HD23	1:D:117:VAL:HG11	1.92	0.51
1:J:45:PRO:HG3	1:J:86:TRP:CZ3	2.45	0.51
2:K:120:ILE:HB	2:K:143:THR:CG2	2.41	0.51
2:B:141:TYR:CB	1:C:53:ARG:HH12	2.23	0.51
1:C:136:ARG:HH21	2:E:83:ARG:HD2	1.75	0.51
2:E:120:ILE:HB	2:E:143:THR:CG2	2.41	0.51
2:H:95:ILE:HG12	2:H:167:ILE:HD12	1.93	0.51
2:E:98:ARG:NH2	2:E:164:VAL:CG2	2.66	0.51
2:B:110:LYS:HZ1	1:C:179:ILE:CG1	2.24	0.51
2:F:95:ILE:HG12	2:F:167:ILE:HD12	1.93	0.51
1:G:136:ARG:HH21	2:H:83:ARG:HD2	1.74	0.51
1:D:136:ARG:HH21	2:F:83:ARG:HD2	1.75	0.51
1:G:76:GLY:HA2	1:G:79:VAL:HG22	1.92	0.51
1:I:42:LEU:HD23	1:I:117:VAL:HG11	1.92	0.50
1:C:92:GLU:HB3	1:C:94:GLU:N	2.25	0.50
1:I:92:GLU:HB3	1:I:94:GLU:N	2.25	0.50
1:C:42:LEU:HD23	1:C:117:VAL:HG11	1.92	0.50
1:C:92:GLU:CG	1:C:170:PRO:HA	2.42	0.50
2:E:93:HIS:CD2	2:E:171:LYS:HD2	2.47	0.50
2:K:94:GLU:HB3	2:K:169:ILE:HB	1.93	0.50
2:K:93:HIS:CD2	2:K:171:LYS:HD2	2.47	0.50
2:L:94:GLU:HB3	2:L:169:ILE:HB	1.93	0.50
1:D:76:GLY:HA2	1:D:79:VAL:HG22	1.92	0.50
1:G:147:LEU:HD11	1:G:169:ILE:HD13	1.93	0.50
1:I:147:LEU:HD11	1:I:169:ILE:HD13	1.93	0.50
1:I:179:ILE:CG1	2:L:110:LYS:HZ1	2.24	0.50
2:L:93:HIS:CD2	2:L:171:LYS:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:TYR:HB2	1:C:53:ARG:NH1	2.25	0.50
2:B:94:GLU:HB3	2:B:169:ILE:HB	1.93	0.50
2:E:94:GLU:HB3	2:E:169:ILE:HB	1.93	0.50
1:I:92:GLU:CG	1:I:170:PRO:HA	2.42	0.50
1:I:89:LYS:CD	1:I:90:GLU:H	2.25	0.50
1:C:89:LYS:CD	1:C:90:GLU:H	2.25	0.50
1:J:89:LYS:CD	1:J:90:GLU:H	2.25	0.50
1:A:89:LYS:CD	1:A:90:GLU:H	2.25	0.50
2:B:93:HIS:CD2	2:B:171:LYS:HD2	2.47	0.50
1:J:147:LEU:HD11	1:J:169:ILE:HD13	1.93	0.50
1:A:147:LEU:HD11	1:A:169:ILE:HD13	1.93	0.50
1:A:134:SER:C	2:B:98:ARG:CZ	2.80	0.50
1:D:89:LYS:CD	1:D:90:GLU:H	2.24	0.50
1:D:95:ILE:N	1:D:168:THR:HA	2.27	0.50
2:F:97:MET:HB3	2:F:167:ILE:CG2	2.42	0.50
1:G:89:LYS:CD	1:G:90:GLU:H	2.24	0.50
1:D:87:ASP:HB2	1:D:96:LYS:HB3	1.94	0.50
2:E:95:ILE:HD13	2:E:169:ILE:CG1	2.42	0.50
1:G:95:ILE:N	1:G:168:THR:HA	2.27	0.50
2:B:95:ILE:HD13	2:B:169:ILE:CG1	2.42	0.49
1:D:147:LEU:HD11	1:D:169:ILE:HD13	1.93	0.49
2:F:93:HIS:CD2	2:F:171:LYS:HD2	2.47	0.49
2:H:97:MET:HB3	2:H:167:ILE:CG2	2.42	0.49
2:H:93:HIS:CD2	2:H:171:LYS:HD2	2.47	0.49
2:K:95:ILE:HD13	2:K:169:ILE:CG1	2.42	0.49
2:B:88:ILE:HG23	2:B:93:HIS:CD2	2.47	0.49
1:G:135:GLY:CA	2:H:98:ARG:NH1	2.75	0.49
1:J:95:ILE:N	1:J:168:THR:HA	2.27	0.49
1:A:135:GLY:CA	2:B:98:ARG:NH1	2.75	0.49
1:A:95:ILE:N	1:A:168:THR:HA	2.27	0.49
2:F:94:GLU:HG2	2:F:147:LEU:HA	1.94	0.49
1:J:56:LEU:HD11	1:J:62:MET:HE3	1.93	0.49
2:L:120:ILE:HB	2:L:143:THR:CG2	2.41	0.49
2:L:95:ILE:HD13	2:L:169:ILE:CG1	2.42	0.49
2:E:97:MET:HB3	2:E:167:ILE:CG2	2.43	0.49
1:G:87:ASP:HB2	1:G:96:LYS:HB3	1.94	0.49
2:H:141:TYR:HB2	1:J:53:ARG:NH1	2.23	0.49
2:K:97:MET:HB3	2:K:167:ILE:CG2	2.43	0.49
2:L:88:ILE:HG23	2:L:93:HIS:CD2	2.48	0.49
2:E:99:PHE:CE2	2:E:120:ILE:HG13	2.48	0.49
1:A:184:GLN:HB2	2:F:106:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ILE:HB	2:B:143:THR:CG2	2.41	0.49
1:A:92:GLU:CG	1:A:170:PRO:HA	2.41	0.49
2:E:113:VAL:O	1:D:177:LYS:HB2	2.13	0.49
1:A:177:LYS:HB2	2:F:113:VAL:O	2.13	0.49
1:A:53:ARG:NH1	2:F:141:TYR:HB2	2.23	0.49
2:H:113:VAL:O	1:J:177:LYS:HB2	2.13	0.49
2:H:94:GLU:HG2	2:H:147:LEU:HA	1.95	0.49
1:G:134:SER:C	2:H:98:ARG:CZ	2.80	0.49
1:G:135:GLY:HA3	2:H:98:ARG:HH11	1.77	0.49
2:H:106:LYS:N	1:J:184:GLN:HB2	2.27	0.49
1:G:92:GLU:CG	1:G:170:PRO:HA	2.42	0.49
1:I:133:TRP:HB3	1:I:135:GLY:H	1.77	0.49
2:K:99:PHE:CE2	2:K:120:ILE:HG13	2.48	0.49
1:C:96:LYS:CE	2:E:131:ASP:C	2.81	0.49
1:I:95:ILE:N	1:I:168:THR:HA	2.27	0.49
2:E:106:LYS:H	1:D:184:GLN:HB2	1.78	0.48
2:E:106:LYS:N	1:D:184:GLN:HB2	2.27	0.48
2:E:88:ILE:HG23	2:E:93:HIS:CD2	2.47	0.48
1:A:184:GLN:HB2	2:F:106:LYS:H	1.78	0.48
1:J:134:SER:C	2:L:98:ARG:CZ	2.82	0.48
1:G:184:GLN:HB2	2:K:106:LYS:N	2.27	0.48
1:G:177:LYS:HB2	2:K:113:VAL:O	2.13	0.48
2:K:88:ILE:HG23	2:K:93:HIS:CD2	2.47	0.48
1:C:135:GLY:CA	2:E:98:ARG:NH1	2.75	0.48
2:B:106:LYS:H	1:C:184:GLN:HB2	1.78	0.48
1:C:95:ILE:N	1:C:168:THR:HA	2.27	0.48
1:D:92:GLU:CG	1:D:170:PRO:HA	2.42	0.48
1:G:85:PRO:HG2	2:H:132:SER:HB3	1.95	0.48
1:I:96:LYS:CE	2:K:131:ASP:C	2.81	0.48
1:J:92:GLU:CG	1:J:170:PRO:HA	2.42	0.48
2:B:99:PHE:CE2	2:B:120:ILE:HG13	2.48	0.48
2:H:106:LYS:H	1:J:184:GLN:HB2	1.79	0.48
2:L:97:MET:HB3	2:L:167:ILE:CG2	2.43	0.48
2:B:113:VAL:O	1:C:177:LYS:HB2	2.13	0.48
2:B:97:MET:HB3	2:B:167:ILE:CG2	2.43	0.48
2:B:106:LYS:N	1:C:184:GLN:HB2	2.27	0.48
2:H:88:ILE:HG23	2:H:93:HIS:CD2	2.48	0.48
1:I:177:LYS:HB2	2:L:113:VAL:O	2.13	0.48
1:I:184:GLN:HB2	2:L:106:LYS:N	2.27	0.48
1:A:53:ARG:HB3	2:F:143:THR:HA	1.96	0.48
1:A:87:ASP:HB2	1:A:96:LYS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:PHE:CE1	1:C:101:MET:HB2	2.49	0.48
1:G:53:ARG:HB3	2:K:143:THR:HA	1.96	0.48
1:I:99:PHE:CE1	1:I:101:MET:HB2	2.49	0.48
2:H:143:THR:HA	1:J:53:ARG:HB3	1.96	0.48
2:L:99:PHE:CE2	2:L:120:ILE:HG13	2.48	0.48
1:D:96:LYS:CE	2:F:131:ASP:C	2.82	0.48
2:E:143:THR:HA	1:D:53:ARG:HB3	1.96	0.48
2:F:88:ILE:HG23	2:F:93:HIS:CD2	2.48	0.48
2:F:99:PHE:CE2	2:F:120:ILE:HG13	2.47	0.48
1:G:184:GLN:HB2	2:K:106:LYS:H	1.79	0.48
1:G:96:LYS:CE	2:H:131:ASP:C	2.82	0.48
1:J:87:ASP:HB2	1:J:96:LYS:HB3	1.94	0.48
1:I:184:GLN:HB2	2:L:106:LYS:H	1.79	0.48
2:H:99:PHE:CE2	2:H:120:ILE:HG13	2.47	0.48
1:I:87:ASP:HB2	1:I:96:LYS:HB3	1.94	0.48
1:C:87:ASP:HB2	1:C:96:LYS:HB3	1.94	0.48
2:E:94:GLU:HG2	2:E:147:LEU:HA	1.95	0.48
1:G:135:GLY:HA2	2:H:98:ARG:CD	2.44	0.48
1:I:134:SER:HA	2:K:98:ARG:HD2	1.95	0.48
2:K:94:GLU:HG2	2:K:147:LEU:HA	1.95	0.48
2:B:94:GLU:HG2	2:B:147:LEU:HA	1.95	0.47
1:C:147:LEU:HD11	1:C:169:ILE:HD13	1.95	0.47
1:G:99:PHE:CE1	1:G:101:MET:HB2	2.49	0.47
2:H:120:ILE:HB	2:H:143:THR:CG2	2.41	0.47
1:I:136:ARG:HH21	2:K:83:ARG:HD2	1.77	0.47
2:L:94:GLU:HG2	2:L:147:LEU:HA	1.95	0.47
1:A:43:LEU:HD12	1:A:145:LEU:HD11	1.97	0.47
1:A:96:LYS:HE3	2:B:130:ASP:O	2.14	0.47
2:B:143:THR:HA	1:C:53:ARG:HB3	1.96	0.47
1:C:43:LEU:HD12	1:C:145:LEU:HD11	1.97	0.47
1:I:53:ARG:HB3	2:L:143:THR:HA	1.96	0.47
1:J:99:PHE:CE1	1:J:101:MET:HB2	2.49	0.47
1:A:99:PHE:CE1	1:A:101:MET:HB2	2.49	0.47
1:A:99:PHE:CZ	1:A:165:LEU:HB2	2.50	0.47
1:D:134:SER:C	2:F:98:ARG:CZ	2.82	0.47
1:D:99:PHE:CE1	1:D:101:MET:HB2	2.49	0.47
1:I:96:LYS:HE3	2:K:130:ASP:O	2.14	0.47
1:J:135:GLY:CA	2:L:98:ARG:NH1	2.76	0.47
1:J:43:LEU:HD12	1:J:145:LEU:HD11	1.97	0.47
2:K:104:LEU:HD21	2:K:124:GLN:HA	1.97	0.47
1:A:96:LYS:CE	2:B:131:ASP:C	2.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:ILE:HB	2:F:143:THR:CG2	2.41	0.47
2:F:95:ILE:HD13	2:F:169:ILE:CG1	2.44	0.47
1:I:134:SER:HA	2:K:98:ARG:CD	2.44	0.47
1:I:43:LEU:HD12	1:I:145:LEU:HD11	1.97	0.47
1:J:99:PHE:CZ	1:J:165:LEU:HB2	2.50	0.47
1:J:96:LYS:HE3	2:L:130:ASP:O	2.14	0.47
1:C:134:SER:C	2:E:98:ARG:CZ	2.82	0.47
2:H:95:ILE:HD13	2:H:169:ILE:CG1	2.44	0.47
1:I:134:SER:C	2:K:98:ARG:CZ	2.83	0.47
1:G:55:MET:HE3	2:K:86:TRP:HA	1.96	0.47
2:L:111:ILE:HD11	2:L:167:ILE:HG12	1.96	0.47
1:G:55:MET:HA	2:K:97:MET:HE3	1.96	0.47
1:I:99:PHE:CZ	1:I:165:LEU:HB2	2.49	0.47
2:B:111:ILE:HD11	2:B:167:ILE:HG12	1.97	0.47
1:C:96:LYS:HE3	2:E:130:ASP:O	2.15	0.47
1:C:99:PHE:CZ	1:C:165:LEU:HB2	2.49	0.47
2:E:111:ILE:HD11	2:E:167:ILE:HG12	1.97	0.47
1:G:96:LYS:HE3	2:H:130:ASP:O	2.14	0.47
2:K:111:ILE:HD11	2:K:167:ILE:HG12	1.97	0.47
2:L:104:LEU:HD21	2:L:124:GLN:HA	1.97	0.47
1:G:43:LEU:HD12	1:G:145:LEU:HD11	1.97	0.47
1:J:96:LYS:CE	2:L:131:ASP:C	2.82	0.47
1:D:43:LEU:HD12	1:D:145:LEU:HD11	1.97	0.47
1:D:96:LYS:HE3	2:F:130:ASP:O	2.14	0.47
1:D:99:PHE:CZ	1:D:165:LEU:HB2	2.49	0.47
1:G:99:PHE:CZ	1:G:165:LEU:HB2	2.49	0.47
2:H:97:MET:CE	1:J:55:MET:SD	3.02	0.47
1:C:158:ALA:HB2	1:C:167:ILE:CD1	2.46	0.46
2:E:104:LEU:HD21	2:E:124:GLN:HA	1.97	0.46
1:I:158:ALA:HB2	1:I:167:ILE:CD1	2.46	0.46
1:A:86:TRP:CD1	1:A:95:ILE:CG2	2.99	0.46
1:A:135:GLY:HA2	2:B:98:ARG:CD	2.45	0.46
1:C:82:ILE:CG2	1:C:99:PHE:HB2	2.46	0.46
1:J:96:LYS:C	1:J:96:LYS:HD3	2.36	0.46
1:A:96:LYS:C	1:A:96:LYS:HD3	2.36	0.46
1:C:96:LYS:HD3	1:C:96:LYS:C	2.34	0.46
1:J:98:ARG:HD2	1:J:164:VAL:HG11	1.98	0.46
1:J:86:TRP:CD1	1:J:95:ILE:CG2	2.99	0.46
1:I:86:TRP:CD1	1:I:95:ILE:CG2	2.99	0.46
1:D:158:ALA:HB2	1:D:167:ILE:CD1	2.45	0.46
1:D:135:GLY:CA	2:F:98:ARG:NH1	2.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:55:MET:HE3	2:L:86:TRP:HA	1.96	0.46
1:I:82:ILE:CG2	1:I:99:PHE:HB2	2.46	0.46
2:B:104:LEU:HD21	2:B:124:GLN:HA	1.98	0.46
1:C:86:TRP:CD1	1:C:95:ILE:CG2	2.99	0.46
1:G:158:ALA:HB2	1:G:167:ILE:CD1	2.46	0.46
2:H:111:ILE:HD11	2:H:167:ILE:HG12	1.96	0.46
1:A:158:ALA:HB2	1:A:167:ILE:CD1	2.46	0.46
1:A:98:ARG:HD2	1:A:164:VAL:HG11	1.98	0.46
1:A:82:ILE:CG2	1:A:99:PHE:HB2	2.46	0.46
1:C:98:ARG:HG3	2:E:132:SER:H	1.80	0.46
1:J:158:ALA:HB2	1:J:167:ILE:CD1	2.46	0.46
1:J:82:ILE:CG2	1:J:99:PHE:HB2	2.46	0.46
1:A:55:MET:SD	2:F:97:MET:CE	3.03	0.46
2:F:104:LEU:HD21	2:F:124:GLN:HA	1.97	0.46
2:F:111:ILE:HD11	2:F:167:ILE:HG12	1.97	0.46
2:H:110:LYS:HZ1	1:J:179:ILE:CG1	2.28	0.46
1:J:85:PRO:HG3	2:L:133:TRP:C	2.36	0.46
2:H:104:LEU:HD21	2:H:124:GLN:HA	1.97	0.46
1:J:95:ILE:HD12	1:J:167:ILE:CG2	2.46	0.46
1:A:135:GLY:HA2	2:B:98:ARG:NH1	2.31	0.46
1:A:95:ILE:HD12	1:A:167:ILE:CG2	2.46	0.46
1:G:96:LYS:HD3	1:G:96:LYS:C	2.35	0.46
1:D:86:TRP:CD1	1:D:95:ILE:HG23	2.52	0.45
1:I:96:LYS:HD3	1:I:96:LYS:C	2.35	0.45
2:K:161:LYS:O	2:K:164:VAL:HG22	2.15	0.45
1:A:134:SER:C	2:B:98:ARG:HD2	2.36	0.45
1:D:96:LYS:C	1:D:96:LYS:HD3	2.36	0.45
1:D:82:ILE:CG2	1:D:99:PHE:HB2	2.46	0.45
1:G:82:ILE:CG2	1:G:99:PHE:HB2	2.46	0.45
2:K:114:GLU:CD	2:K:119:VAL:HG21	2.37	0.45
1:I:147:LEU:CD1	1:I:169:ILE:HD13	2.47	0.45
1:A:85:PRO:HG3	2:B:133:TRP:C	2.36	0.45
1:C:157:LYS:HB2	1:C:168:THR:CG2	2.46	0.45
1:C:147:LEU:CD1	1:C:169:ILE:HD13	2.47	0.45
1:D:147:LEU:CD1	1:D:169:ILE:HD13	2.47	0.45
1:G:147:LEU:CD1	1:G:169:ILE:HD13	2.46	0.45
1:G:86:TRP:CD1	1:G:95:ILE:HG23	2.52	0.45
1:I:157:LYS:HB2	1:I:168:THR:CG2	2.46	0.45
1:A:134:SER:HA	2:B:98:ARG:HD2	1.98	0.45
2:B:119:VAL:HA	2:B:143:THR:O	2.17	0.45
2:B:110:LYS:HD3	1:C:181:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:PRO:HG3	2:F:133:TRP:C	2.36	0.45
1:D:86:TRP:CD1	1:D:95:ILE:CG2	2.99	0.45
2:E:114:GLU:CD	2:E:119:VAL:HG21	2.37	0.45
1:G:157:LYS:HB2	1:G:168:THR:CG2	2.46	0.45
1:G:86:TRP:CD1	1:G:95:ILE:CG2	2.99	0.45
1:D:119:VAL:HG22	1:D:144:ARG:HD2	1.98	0.45
1:D:134:SER:C	2:F:98:ARG:HD2	2.37	0.45
1:G:119:VAL:HG22	1:G:144:ARG:HD2	1.98	0.45
2:L:161:LYS:O	2:L:164:VAL:HG22	2.16	0.45
1:A:179:ILE:CG1	2:F:110:LYS:HZ1	2.29	0.45
1:I:95:ILE:HD12	1:I:167:ILE:CG2	2.46	0.45
1:I:181:VAL:HG22	2:L:110:LYS:HD3	1.99	0.45
2:L:119:VAL:HA	2:L:143:THR:O	2.17	0.45
2:L:114:GLU:CD	2:L:119:VAL:HG21	2.37	0.45
1:A:147:LEU:CD1	1:A:169:ILE:HD13	2.47	0.45
1:D:98:ARG:HD2	1:D:164:VAL:HG11	1.98	0.45
2:H:119:VAL:HA	2:H:143:THR:O	2.17	0.45
1:G:134:SER:C	2:H:98:ARG:HD2	2.37	0.45
1:J:147:LEU:CD1	1:J:169:ILE:HD13	2.47	0.45
1:J:86:TRP:CD1	1:J:95:ILE:HG23	2.51	0.45
1:C:95:ILE:HD11	1:C:169:ILE:HD11	1.99	0.45
1:D:157:LYS:HB2	1:D:168:THR:CG2	2.46	0.45
1:I:119:VAL:HG22	1:I:144:ARG:HD2	1.98	0.45
2:L:114:GLU:OE1	2:L:119:VAL:HG21	2.17	0.45
2:B:86:TRP:HA	1:C:55:MET:HE3	1.99	0.45
1:C:177:LYS:H	1:C:177:LYS:HD2	1.82	0.45
1:D:177:LYS:HD2	1:D:177:LYS:H	1.82	0.45
2:F:119:VAL:HA	2:F:143:THR:O	2.17	0.45
2:F:114:GLU:OE1	2:F:119:VAL:HG21	2.17	0.45
1:G:98:ARG:HD2	1:G:164:VAL:HG11	1.99	0.45
1:A:157:LYS:HB2	1:A:168:THR:CG2	2.46	0.44
2:B:114:GLU:CD	2:B:119:VAL:HG21	2.37	0.44
1:C:119:VAL:HG22	1:C:144:ARG:HD2	1.98	0.44
2:E:86:TRP:HA	1:D:55:MET:HE3	1.99	0.44
2:H:114:GLU:OE1	2:H:119:VAL:HG21	2.17	0.44
1:I:177:LYS:H	1:I:177:LYS:HD2	1.82	0.44
1:I:85:PRO:HG2	2:K:132:SER:CB	2.47	0.44
1:I:98:ARG:HG3	2:K:132:SER:H	1.82	0.44
1:A:119:VAL:HG22	1:A:144:ARG:HD2	1.98	0.44
1:A:86:TRP:CD1	1:A:95:ILE:HG23	2.52	0.44
2:B:114:GLU:OE1	2:B:119:VAL:HG21	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:110:LYS:HD3	1:D:181:VAL:HG22	1.98	0.44
2:H:114:GLU:CD	2:H:119:VAL:HG21	2.37	0.44
1:J:157:LYS:HB2	1:J:168:THR:CG2	2.46	0.44
1:J:177:LYS:H	1:J:177:LYS:HD2	1.82	0.44
1:C:119:VAL:HG22	1:C:144:ARG:HD3	1.99	0.44
1:G:55:MET:CE	2:K:86:TRP:HA	2.48	0.44
1:I:46:LEU:H	1:I:46:LEU:HD22	1.83	0.44
1:G:181:VAL:HG22	2:K:110:LYS:HD3	1.99	0.44
1:A:177:LYS:HD2	1:A:177:LYS:H	1.82	0.44
2:F:114:GLU:CD	2:F:119:VAL:HG21	2.37	0.44
1:G:177:LYS:HD2	1:G:177:LYS:H	1.82	0.44
1:G:98:ARG:CG	2:H:132:SER:HB2	2.45	0.44
2:H:110:LYS:HD3	1:J:181:VAL:HG22	1.99	0.44
2:K:98:ARG:NH2	2:K:164:VAL:HG11	2.32	0.44
2:L:93:HIS:HA	2:L:96:LYS:HB2	2.00	0.44
1:C:92:GLU:C	1:C:94:GLU:H	2.21	0.44
2:E:114:GLU:OE1	2:E:119:VAL:HG21	2.17	0.44
2:E:161:LYS:O	2:E:164:VAL:HG22	2.17	0.44
1:I:82:ILE:HG13	1:I:141:TYR:CZ	2.53	0.44
2:K:119:VAL:HA	2:K:143:THR:O	2.17	0.44
1:A:43:LEU:CD2	1:A:50:ARG:HE	2.31	0.44
1:C:82:ILE:HG13	1:C:141:TYR:CZ	2.53	0.44
1:C:46:LEU:H	1:C:46:LEU:HD22	1.83	0.44
2:E:119:VAL:HA	2:E:143:THR:O	2.17	0.44
1:A:181:VAL:HG22	2:F:110:LYS:HD3	1.99	0.44
1:G:179:ILE:CG1	2:K:110:LYS:HZ1	2.30	0.44
1:J:119:VAL:HG22	1:J:144:ARG:HD2	1.98	0.44
1:J:56:LEU:HA	1:J:56:LEU:HD22	1.86	0.44
1:I:184:GLN:CA	2:L:106:LYS:HD2	2.46	0.44
2:B:93:HIS:HA	2:B:96:LYS:HB2	2.00	0.44
1:C:43:LEU:CD2	1:C:50:ARG:HE	2.31	0.44
2:E:111:ILE:HD11	2:E:167:ILE:HG13	2.00	0.44
2:H:161:LYS:O	2:H:164:VAL:HG22	2.16	0.44
1:I:92:GLU:C	1:I:94:GLU:H	2.21	0.44
1:J:43:LEU:CD2	1:J:50:ARG:HE	2.31	0.44
2:K:114:GLU:OE1	2:K:119:VAL:HG21	2.17	0.44
1:I:134:SER:HA	2:K:98:ARG:NE	2.33	0.44
1:A:49:MET:HA	1:A:62:MET:HE1	1.99	0.44
1:A:56:LEU:HD22	1:A:56:LEU:HA	1.86	0.44
1:C:86:TRP:CD1	1:C:95:ILE:HG23	2.52	0.44
1:D:46:LEU:H	1:D:46:LEU:HD22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:LEU:CD2	1:G:50:ARG:HE	2.31	0.44
1:I:119:VAL:HG22	1:I:144:ARG:HD3	2.00	0.44
1:I:43:LEU:CD2	1:I:50:ARG:HE	2.31	0.44
1:I:86:TRP:CD1	1:I:95:ILE:HG23	2.52	0.44
1:I:95:ILE:HD11	1:I:169:ILE:HD11	2.00	0.44
2:B:106:LYS:HD2	1:C:184:GLN:CA	2.46	0.44
1:G:46:LEU:H	1:G:46:LEU:HD22	1.83	0.44
2:H:93:HIS:HA	2:H:96:LYS:HB2	2.00	0.44
2:K:111:ILE:HD11	2:K:167:ILE:HG13	2.00	0.44
1:A:82:ILE:HG13	1:A:141:TYR:CZ	2.52	0.43
1:A:133:TRP:HB3	1:A:135:GLY:H	1.83	0.43
1:D:92:GLU:C	1:D:94:GLU:H	2.21	0.43
2:E:95:ILE:HD13	2:E:169:ILE:HG13	2.00	0.43
2:F:93:HIS:HA	2:F:96:LYS:HB2	2.00	0.43
1:J:82:ILE:HG13	1:J:141:TYR:CZ	2.52	0.43
1:J:92:GLU:C	1:J:94:GLU:H	2.21	0.43
2:K:95:ILE:HD13	2:K:169:ILE:HG13	2.00	0.43
2:B:161:LYS:O	2:B:164:VAL:HG22	2.18	0.43
2:B:111:ILE:HD11	2:B:167:ILE:HG13	2.00	0.43
1:D:43:LEU:CD2	1:D:50:ARG:HE	2.31	0.43
2:F:161:LYS:O	2:F:164:VAL:HG22	2.17	0.43
1:G:82:ILE:HG13	1:G:141:TYR:CZ	2.53	0.43
2:L:118:LEU:CD1	2:L:120:ILE:HG12	2.48	0.43
2:B:118:LEU:CD1	2:B:120:ILE:HG12	2.48	0.43
1:A:104:LEU:HD13	1:A:105:SER:O	2.19	0.43
1:A:119:VAL:HG22	1:A:144:ARG:HD3	2.00	0.43
1:A:158:ALA:HB2	1:A:167:ILE:HD13	2.00	0.43
1:A:46:LEU:H	1:A:46:LEU:HD22	1.83	0.43
1:A:82:ILE:HG21	1:A:99:PHE:HB2	2.00	0.43
2:B:97:MET:HB2	1:C:55:MET:HE1	2.00	0.43
1:C:85:PRO:HG2	2:E:132:SER:CB	2.47	0.43
1:D:104:LEU:HD13	1:D:105:SER:O	2.19	0.43
1:D:82:ILE:HG13	1:D:141:TYR:CZ	2.53	0.43
2:E:86:TRP:HA	1:D:55:MET:CE	2.49	0.43
2:E:97:MET:HB2	1:D:55:MET:HE1	2.00	0.43
1:G:92:GLU:C	1:G:94:GLU:H	2.21	0.43
2:H:97:MET:HE3	1:J:55:MET:CE	2.48	0.43
1:J:119:VAL:HG22	1:J:144:ARG:HD3	2.00	0.43
1:A:92:GLU:C	1:A:94:GLU:H	2.21	0.43
1:C:95:ILE:C	1:C:97:MET:H	2.21	0.43
1:D:110:LYS:HB2	1:D:121:LYS:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:LEU:HD13	1:G:105:SER:O	2.19	0.43
1:I:111:ILE:HD11	1:I:165:LEU:HD21	2.01	0.43
1:I:98:ARG:HD2	1:I:164:VAL:HG11	2.00	0.43
1:J:158:ALA:HB2	1:J:167:ILE:HD13	2.00	0.43
1:J:46:LEU:HD22	1:J:46:LEU:H	1.83	0.43
1:C:111:ILE:HD11	1:C:165:LEU:HD21	2.01	0.43
2:B:86:TRP:HA	1:C:55:MET:CE	2.48	0.43
2:E:110:LYS:HZ1	1:D:179:ILE:CG1	2.31	0.43
1:D:85:PRO:HG3	2:F:134:SER:N	2.34	0.43
1:A:55:MET:CB	2:F:145:LEU:HD12	2.49	0.43
1:G:110:LYS:HB2	1:G:121:LYS:HD3	2.01	0.43
1:G:85:PRO:HG3	2:H:133:TRP:C	2.38	0.43
2:H:118:LEU:HD13	2:H:119:VAL:C	2.39	0.43
1:G:135:GLY:HA2	2:H:98:ARG:HD3	2.00	0.43
1:J:104:LEU:HD13	1:J:105:SER:O	2.19	0.43
1:J:82:ILE:HG21	1:J:99:PHE:HB2	2.00	0.43
1:I:55:MET:CE	2:L:86:TRP:HA	2.48	0.43
1:D:153:LYS:HE2	1:D:156:ILE:HG22	2.01	0.43
1:G:153:LYS:HE2	1:G:156:ILE:HG22	2.01	0.43
2:H:145:LEU:HD12	1:J:55:MET:CB	2.49	0.43
2:F:118:LEU:HD13	2:F:119:VAL:C	2.39	0.43
1:G:158:ALA:HB2	1:G:167:ILE:HD13	2.00	0.43
2:H:86:TRP:HA	1:J:55:MET:CE	2.49	0.43
1:J:95:ILE:C	1:J:97:MET:H	2.23	0.43
1:A:95:ILE:C	1:A:97:MET:H	2.23	0.43
1:C:111:ILE:HG21	1:C:167:ILE:HD13	2.01	0.43
1:D:158:ALA:HB2	1:D:167:ILE:HD13	2.00	0.43
1:D:82:ILE:HG21	1:D:99:PHE:HB2	2.00	0.43
1:C:134:SER:C	2:E:98:ARG:HD2	2.39	0.43
2:F:111:ILE:HD11	2:F:167:ILE:HG13	2.00	0.43
1:G:82:ILE:HG21	1:G:99:PHE:HB2	2.00	0.43
1:I:104:LEU:HD13	1:I:105:SER:O	2.19	0.43
1:J:85:PRO:HG3	2:L:134:SER:N	2.34	0.43
1:C:104:LEU:HD13	1:C:105:SER:O	2.19	0.42
1:D:132:SER:O	1:D:133:TRP:C	2.57	0.42
1:D:95:ILE:HD12	1:D:167:ILE:CG2	2.46	0.42
1:G:92:GLU:HG2	1:G:170:PRO:HA	2.01	0.42
1:G:95:ILE:HD12	1:G:167:ILE:CG2	2.46	0.42
2:H:95:ILE:HD13	2:H:169:ILE:HG13	2.01	0.42
1:G:95:ILE:HD11	1:G:169:ILE:HD11	2.00	0.42
2:H:111:ILE:HD11	2:H:167:ILE:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:111:ILE:HG21	1:I:167:ILE:HD13	2.02	0.42
1:I:95:ILE:C	1:I:97:MET:H	2.22	0.42
2:L:111:ILE:HD11	2:L:167:ILE:HG13	2.00	0.42
1:A:92:GLU:HG2	1:A:170:PRO:HA	2.01	0.42
1:A:55:MET:CE	2:F:86:TRP:HA	2.49	0.42
1:A:85:PRO:HG3	2:B:134:SER:N	2.34	0.42
1:C:156:ILE:HD11	1:C:167:ILE:CG1	2.49	0.42
1:D:119:VAL:HG22	1:D:144:ARG:HD3	2.00	0.42
1:D:95:ILE:C	1:D:97:MET:H	2.22	0.42
1:G:156:ILE:HA	1:G:168:THR:O	2.20	0.42
1:J:156:ILE:HD11	1:J:167:ILE:CG1	2.49	0.42
1:I:96:LYS:NZ	2:K:132:SER:HA	2.33	0.42
1:A:156:ILE:HD11	1:A:167:ILE:CG1	2.49	0.42
1:C:82:ILE:HG21	1:C:99:PHE:HB2	2.00	0.42
1:D:156:ILE:HA	1:D:168:THR:O	2.20	0.42
2:E:141:TYR:HB2	1:D:53:ARG:NH2	2.34	0.42
2:E:93:HIS:HA	2:E:96:LYS:HB2	2.00	0.42
2:F:95:ILE:HD13	2:F:169:ILE:HG13	2.01	0.42
1:G:132:SER:O	1:G:133:TRP:C	2.58	0.42
1:G:119:VAL:HG22	1:G:144:ARG:HD3	2.00	0.42
1:G:95:ILE:C	1:G:97:MET:H	2.23	0.42
2:H:118:LEU:CD1	2:H:120:ILE:HG12	2.48	0.42
1:I:156:ILE:HD11	1:I:167:ILE:CG1	2.49	0.42
2:K:93:HIS:HA	2:K:96:LYS:HB2	2.00	0.42
1:C:110:LYS:HB2	1:C:121:LYS:HD3	2.01	0.42
1:D:92:GLU:HG2	1:D:170:PRO:HA	2.02	0.42
1:I:110:LYS:HB2	1:I:121:LYS:HD3	2.01	0.42
2:L:118:LEU:HD13	2:L:119:VAL:C	2.39	0.42
2:B:118:LEU:HD13	2:B:119:VAL:C	2.39	0.42
1:C:98:ARG:HD2	1:C:164:VAL:HG11	2.01	0.42
1:D:156:ILE:HD11	1:D:167:ILE:CG1	2.49	0.42
2:E:145:LEU:HD12	1:D:55:MET:CB	2.50	0.42
1:G:55:MET:HE3	2:K:86:TRP:CA	2.50	0.42
1:G:85:PRO:HG3	2:H:134:SER:N	2.35	0.42
1:J:132:SER:O	1:J:133:TRP:C	2.57	0.42
1:J:134:SER:C	2:L:98:ARG:HD2	2.39	0.42
1:J:92:GLU:HG2	1:J:170:PRO:HA	2.02	0.42
1:G:53:ARG:NH2	2:K:141:TYR:HB2	2.34	0.42
1:C:132:SER:O	1:C:133:TRP:C	2.57	0.42
2:F:118:LEU:CD1	2:F:120:ILE:HG12	2.48	0.42
1:A:55:MET:CE	2:F:97:MET:HE3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:92:GLU:HG2	1:I:170:PRO:HA	2.02	0.42
1:I:82:ILE:HG21	1:I:99:PHE:HB2	2.00	0.42
1:A:156:ILE:HA	1:A:168:THR:O	2.20	0.42
1:C:92:GLU:HG2	1:C:170:PRO:HA	2.02	0.42
2:E:118:LEU:HD13	2:E:119:VAL:C	2.39	0.42
1:I:158:ALA:HB2	1:I:167:ILE:HD13	2.00	0.42
1:G:55:MET:CB	2:K:145:LEU:HD12	2.50	0.42
1:A:48:PRO:HA	1:A:54:GLN:NE2	2.35	0.42
1:C:98:ARG:HA	1:C:165:LEU:O	2.20	0.42
1:D:95:ILE:HD11	1:D:169:ILE:HD11	2.00	0.42
2:E:92:GLU:HG3	2:E:168:THR:HG22	2.00	0.42
1:G:156:ILE:HD11	1:G:167:ILE:CG1	2.50	0.42
1:J:156:ILE:HA	1:J:168:THR:O	2.20	0.42
1:I:55:MET:HE3	2:L:86:TRP:CA	2.50	0.42
1:A:110:LYS:HB2	1:A:121:LYS:HD3	2.01	0.42
1:D:48:PRO:HA	1:D:54:GLN:NE2	2.35	0.42
1:D:95:ILE:C	1:D:97:MET:N	2.73	0.42
1:A:53:ARG:NH2	2:F:141:TYR:HB2	2.34	0.42
2:H:141:TYR:HB2	1:J:53:ARG:NH2	2.34	0.42
1:J:110:LYS:HB2	1:J:121:LYS:HD3	2.01	0.42
1:J:48:PRO:HA	1:J:54:GLN:NE2	2.35	0.42
2:K:118:LEU:HD13	2:K:119:VAL:C	2.39	0.42
1:A:111:ILE:HG21	1:A:167:ILE:HD13	2.02	0.41
2:B:95:ILE:HD13	2:B:169:ILE:HG12	2.02	0.41
1:A:135:GLY:HA2	2:B:98:ARG:HD3	2.02	0.41
1:C:48:PRO:HA	1:C:54:GLN:NE2	2.35	0.41
1:C:95:ILE:HD12	1:C:167:ILE:CG2	2.46	0.41
2:E:117:VAL:HG21	1:D:46:LEU:HD12	2.02	0.41
1:G:48:PRO:HA	1:G:54:GLN:NE2	2.35	0.41
1:I:48:PRO:HA	1:I:54:GLN:NE2	2.35	0.41
1:J:111:ILE:HG21	1:J:167:ILE:HD13	2.02	0.41
1:J:95:ILE:C	1:J:97:MET:N	2.74	0.41
1:G:46:LEU:HD12	2:K:117:VAL:HG21	2.02	0.41
1:G:55:MET:CG	2:K:95:ILE:HG22	2.50	0.41
1:I:55:MET:CG	2:L:95:ILE:HG22	2.50	0.41
1:A:95:ILE:C	1:A:97:MET:N	2.74	0.41
2:B:146:GLN:HE21	1:C:46:LEU:HB3	1.85	0.41
2:B:95:ILE:HD13	2:B:169:ILE:HG13	2.00	0.41
1:C:158:ALA:HB2	1:C:167:ILE:HD13	2.00	0.41
2:E:95:ILE:HG22	1:D:55:MET:CG	2.50	0.41
2:F:92:GLU:HG3	2:F:168:THR:HG22	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:ILE:C	1:G:97:MET:N	2.73	0.41
2:K:84:ALA:C	2:K:97:MET:HE1	2.41	0.41
2:B:86:TRP:CB	1:C:55:MET:HE3	2.50	0.41
2:B:95:ILE:HG22	1:C:55:MET:CG	2.50	0.41
2:E:86:TRP:CA	1:D:55:MET:HE3	2.51	0.41
2:E:95:ILE:HD13	2:E:169:ILE:HG12	2.02	0.41
1:D:98:ARG:NH2	2:F:131:ASP:HB3	2.35	0.41
2:H:143:THR:HA	1:J:53:ARG:O	2.21	0.41
1:I:46:LEU:HB3	2:L:146:GLN:HE21	1.85	0.41
2:L:95:ILE:HD13	2:L:169:ILE:HG12	2.02	0.41
2:L:95:ILE:HD13	2:L:169:ILE:HG13	2.00	0.41
1:A:180:ASP:O	2:F:110:LYS:HE3	2.21	0.41
1:A:53:ARG:O	2:F:143:THR:HA	2.21	0.41
2:B:141:TYR:HB2	1:C:53:ARG:NH2	2.35	0.41
2:B:90:GLU:HB3	2:B:176:ARG:HB2	2.02	0.41
1:G:111:ILE:HG21	1:G:167:ILE:HD13	2.02	0.41
1:G:98:ARG:NH2	2:H:131:ASP:HB3	2.35	0.41
1:I:153:LYS:HE2	1:I:156:ILE:HG22	2.01	0.41
2:H:110:LYS:HE3	1:J:180:ASP:O	2.21	0.41
2:K:95:ILE:HD13	2:K:169:ILE:HG12	2.02	0.41
1:J:98:ARG:NH2	2:L:131:ASP:HB3	2.35	0.41
2:B:145:LEU:HD12	1:C:55:MET:CB	2.50	0.41
1:C:95:ILE:C	1:C:97:MET:N	2.73	0.41
1:D:111:ILE:HG21	1:D:167:ILE:HD13	2.02	0.41
1:D:49:MET:HA	1:D:62:MET:HE1	2.03	0.41
1:A:46:LEU:HB3	2:F:146:GLN:HE21	1.85	0.41
1:G:98:ARG:HB2	2:H:132:SER:CB	2.51	0.41
1:G:184:GLN:CA	2:K:106:LYS:HD2	2.45	0.41
2:K:92:GLU:HG3	2:K:168:THR:HG22	2.00	0.41
1:I:53:ARG:NH2	2:L:141:TYR:HB2	2.34	0.41
2:L:90:GLU:HB3	2:L:176:ARG:HB2	2.02	0.41
1:A:153:LYS:HE2	1:A:156:ILE:HG22	2.01	0.41
2:B:117:VAL:HG21	1:C:46:LEU:HD12	2.02	0.41
1:A:98:ARG:NH2	2:B:131:ASP:HB3	2.35	0.41
1:C:153:LYS:HE2	1:C:156:ILE:HG22	2.01	0.41
2:F:97:MET:SD	2:F:99:PHE:CZ	3.13	0.41
1:G:180:ASP:O	2:K:110:LYS:HE3	2.21	0.41
2:H:106:LYS:HD2	1:J:184:GLN:CA	2.46	0.41
1:I:95:ILE:C	1:I:97:MET:N	2.73	0.41
1:J:153:LYS:HE2	1:J:156:ILE:HG22	2.01	0.41
2:K:118:LEU:CD1	2:K:120:ILE:HG12	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:ARG:O	2:K:143:THR:HA	2.21	0.41
1:I:46:LEU:HD12	2:L:117:VAL:HG21	2.02	0.41
1:J:96:LYS:HE2	2:L:132:SER:CB	2.51	0.41
1:C:156:ILE:HA	1:C:168:THR:O	2.20	0.41
1:I:156:ILE:HA	1:I:168:THR:O	2.19	0.41
1:I:98:ARG:HA	1:I:165:LEU:O	2.21	0.41
1:A:132:SER:O	1:A:133:TRP:C	2.59	0.41
2:E:106:LYS:HD2	1:D:184:GLN:CA	2.46	0.41
2:E:143:THR:HA	1:D:53:ARG:O	2.21	0.41
1:A:184:GLN:CA	2:F:106:LYS:HD2	2.46	0.41
1:G:134:SER:HA	2:H:98:ARG:HD2	2.02	0.41
2:H:146:GLN:HE21	1:J:46:LEU:HB3	1.85	0.41
2:H:92:GLU:HG3	2:H:168:THR:HG22	2.00	0.41
1:I:56:LEU:HD22	1:I:56:LEU:HA	1.87	0.41
1:I:55:MET:CB	2:L:145:LEU:HD12	2.50	0.41
2:B:86:TRP:CA	1:C:55:MET:HE3	2.50	0.41
1:C:56:LEU:HD22	1:C:56:LEU:HA	1.87	0.41
2:E:110:LYS:HE3	1:D:180:ASP:O	2.21	0.41
2:E:146:GLN:HE21	1:D:46:LEU:HB3	1.85	0.41
1:G:46:LEU:HB3	2:K:146:GLN:HE21	1.85	0.41
2:K:98:ARG:CZ	2:K:164:VAL:CG1	2.96	0.41
2:L:155:LYS:HB3	2:L:170:PRO:HG2	2.03	0.41
2:B:155:LYS:HB3	2:B:170:PRO:HG2	2.03	0.41
2:E:104:LEU:HD21	2:E:124:GLN:CG	2.51	0.41
2:H:95:ILE:HG22	1:J:55:MET:CG	2.51	0.41
2:H:97:MET:SD	2:H:99:PHE:CZ	3.14	0.41
1:J:56:LEU:HD13	1:J:56:LEU:C	2.41	0.41
1:I:85:PRO:HG3	2:K:133:TRP:C	2.42	0.41
2:L:104:LEU:CD2	2:L:124:GLN:HA	2.51	0.41
1:A:55:MET:CG	2:F:95:ILE:HG22	2.51	0.41
1:A:56:LEU:C	1:A:56:LEU:HD13	2.42	0.41
2:B:95:ILE:HG21	2:B:145:LEU:CB	2.51	0.41
1:D:111:ILE:HD11	1:D:165:LEU:HD21	2.01	0.41
1:C:98:ARG:NH2	2:E:131:ASP:HB3	2.35	0.41
1:G:98:ARG:HA	1:G:165:LEU:O	2.21	0.41
1:G:55:MET:HE1	2:K:97:MET:HB2	2.02	0.41
2:L:95:ILE:HG21	2:L:145:LEU:CB	2.51	0.41
2:E:86:TRP:CB	1:D:55:MET:HE3	2.50	0.40
2:F:90:GLU:HB3	2:F:176:ARG:HB2	2.02	0.40
2:H:90:GLU:HB3	2:H:176:ARG:HB2	2.02	0.40
2:K:104:LEU:HD21	2:K:124:GLN:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:ARG:NH2	2:K:131:ASP:HB3	2.35	0.40
1:I:85:PRO:HG3	2:K:134:SER:N	2.36	0.40
2:F:104:LEU:CD2	2:F:124:GLN:HA	2.51	0.40
2:H:104:LEU:CD2	2:H:124:GLN:HA	2.51	0.40
1:A:95:ILE:HD11	1:A:169:ILE:HD11	2.00	0.40
2:B:104:LEU:CD2	2:B:124:GLN:HA	2.52	0.40
2:B:143:THR:HA	1:C:53:ARG:O	2.21	0.40
1:C:99:PHE:CE2	1:C:109:VAL:HG21	2.56	0.40
1:C:82:ILE:HG21	1:C:99:PHE:CG	2.56	0.40
2:E:118:LEU:CD1	2:E:120:ILE:HG12	2.48	0.40
2:F:104:LEU:HD21	2:F:124:GLN:CG	2.51	0.40
1:G:49:MET:HA	1:G:62:MET:HE1	2.04	0.40
1:I:180:ASP:O	2:L:110:LYS:HE3	2.21	0.40
1:I:55:MET:N	2:L:145:LEU:HD12	2.37	0.40
1:I:82:ILE:HG21	1:I:99:PHE:CG	2.57	0.40
1:A:82:ILE:HG21	1:A:99:PHE:CG	2.56	0.40
2:B:117:VAL:HG13	2:B:145:LEU:O	2.22	0.40
2:E:106:LYS:HD3	1:D:184:GLN:HA	2.04	0.40
2:E:95:ILE:HG21	2:E:145:LEU:CB	2.51	0.40
2:F:160:LEU:HD23	2:F:160:LEU:C	2.42	0.40
2:F:155:LYS:HB3	2:F:170:PRO:HG2	2.03	0.40
1:G:111:ILE:HD11	1:G:165:LEU:HD21	2.01	0.40
2:H:104:LEU:HD21	2:H:124:GLN:CG	2.51	0.40
1:I:99:PHE:CE2	1:I:109:VAL:HG21	2.56	0.40
1:J:101:MET:SD	1:J:104:LEU:HG	2.62	0.40
1:J:82:ILE:HG21	1:J:99:PHE:CG	2.56	0.40
2:L:117:VAL:HG13	2:L:145:LEU:O	2.22	0.40
1:A:101:MET:SD	1:A:104:LEU:HG	2.62	0.40
1:C:98:ARG:CZ	1:C:164:VAL:HG11	2.51	0.40
2:B:145:LEU:HD12	1:C:55:MET:N	2.37	0.40
1:D:160:LEU:HD12	1:D:164:VAL:C	2.42	0.40
1:D:56:LEU:HD13	1:D:56:LEU:C	2.42	0.40
1:D:98:ARG:HA	1:D:165:LEU:O	2.22	0.40
1:G:135:GLY:HA2	2:H:98:ARG:NH1	2.35	0.40
1:G:133:TRP:HB3	1:G:135:GLY:H	1.86	0.40
1:G:160:LEU:HD12	1:G:164:VAL:C	2.42	0.40
1:J:96:LYS:HE2	2:L:132:SER:HB2	2.02	0.40
2:K:95:ILE:HG21	2:K:145:LEU:CB	2.51	0.40
1:I:53:ARG:O	2:L:143:THR:HA	2.21	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	141/143 (99%)	131 (93%)	5 (4%)	5 (4%)	4	34
1	C	141/143 (99%)	131 (93%)	5 (4%)	5 (4%)	4	34
1	D	141/143 (99%)	131 (93%)	5 (4%)	5 (4%)	4	34
1	G	141/143 (99%)	131 (93%)	5 (4%)	5 (4%)	4	34
1	I	141/143 (99%)	130 (92%)	6 (4%)	5 (4%)	4	34
1	J	141/143 (99%)	131 (93%)	5 (4%)	5 (4%)	4	34
2	B	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	9	46
2	E	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	9	46
2	F	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	9	46
2	H	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	9	46
2	K	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	9	46
2	L	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	9	46
All	All	1446/1470 (98%)	1337 (92%)	67 (5%)	42 (3%)	9	38

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	GLU
1	A	140	SER
2	B	94	GLU
1	C	94	GLU
1	C	140	SER
2	E	94	GLU
1	D	94	GLU
1	D	140	SER
2	F	94	GLU
1	G	94	GLU
1	G	140	SER
2	H	94	GLU

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Mol	Chain	Res	Type
1	I	94	GLU
1	I	140	SER
2	K	94	GLU
1	J	94	GLU
1	J	140	SER
2	L	94	GLU
1	A	57	ASP
1	A	60	ASP
1	C	57	ASP
1	C	60	ASP
1	D	57	ASP
1	D	60	ASP
1	G	57	ASP
1	G	60	ASP
1	I	57	ASP
1	I	60	ASP
1	J	57	ASP
1	J	60	ASP
1	A	176	ARG
1	C	176	ARG
1	D	176	ARG
1	G	176	ARG
1	I	176	ARG
1	J	176	ARG
2	B	101	MET
2	E	101	MET
2	F	101	MET
2	H	101	MET
2	K	101	MET
2	L	101	MET

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	132/132 (100%)	119 (90%)	13 (10%)	9 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	132/132 (100%)	119 (90%)	13 (10%)	9	34
1	D	132/132 (100%)	119 (90%)	13 (10%)	9	34
1	G	132/132 (100%)	119 (90%)	13 (10%)	9	34
1	I	132/132 (100%)	119 (90%)	13 (10%)	9	34
1	J	132/132 (100%)	119 (90%)	13 (10%)	9	34
2	B	95/95 (100%)	81 (85%)	14 (15%)	3	20
2	E	95/95 (100%)	81 (85%)	14 (15%)	3	20
2	F	95/95 (100%)	81 (85%)	14 (15%)	3	20
2	H	95/95 (100%)	81 (85%)	14 (15%)	3	20
2	K	95/95 (100%)	82 (86%)	13 (14%)	4	23
2	L	95/95 (100%)	81 (85%)	14 (15%)	3	20
All	All	1362/1362 (100%)	1201 (88%)	161 (12%)	10	27

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	53	ARG
1	A	81	GLU
1	A	87	ASP
1	A	96	LYS
1	A	99	PHE
1	A	106	LYS
1	A	121	LYS
1	A	126	LYS
1	A	144	ARG
1	A	153	LYS
1	A	171	LYS
1	A	177	LYS
2	B	92	GLU
2	B	93	HIS
2	B	94	GLU
2	B	95	ILE
2	B	106	LYS
2	B	116	ASN
2	B	132	SER
2	B	134	SER
2	B	141	TYR

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Mol	Chain	Res	Type
2	B	143	THR
2	B	145	LEU
2	B	155	LYS
2	B	167	ILE
2	B	176	ARG
1	C	46	LEU
1	C	53	ARG
1	C	81	GLU
1	C	87	ASP
1	C	96	LYS
1	C	99	PHE
1	C	106	LYS
1	C	121	LYS
1	C	126	LYS
1	C	144	ARG
1	C	153	LYS
1	C	171	LYS
1	C	177	LYS
2	E	92	GLU
2	E	93	HIS
2	E	94	GLU
2	E	95	ILE
2	E	106	LYS
2	E	116	ASN
2	E	132	SER
2	E	134	SER
2	E	141	TYR
2	E	143	THR
2	E	145	LEU
2	E	155	LYS
2	E	167	ILE
2	E	176	ARG
1	D	46	LEU
1	D	53	ARG
1	D	81	GLU
1	D	87	ASP
1	D	96	LYS
1	D	99	PHE
1	D	106	LYS
1	D	121	LYS
1	D	126	LYS
1	D	144	ARG

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Mol	Chain	Res	Type
1	D	153	LYS
1	D	171	LYS
1	D	177	LYS
2	F	92	GLU
2	F	93	HIS
2	F	94	GLU
2	F	95	ILE
2	F	106	LYS
2	F	116	ASN
2	F	132	SER
2	F	134	SER
2	F	141	TYR
2	F	143	THR
2	F	145	LEU
2	F	155	LYS
2	F	167	ILE
2	F	176	ARG
1	G	46	LEU
1	G	53	ARG
1	G	81	GLU
1	G	87	ASP
1	G	96	LYS
1	G	99	PHE
1	G	106	LYS
1	G	121	LYS
1	G	126	LYS
1	G	144	ARG
1	G	153	LYS
1	G	171	LYS
1	G	177	LYS
2	H	92	GLU
2	H	93	HIS
2	H	94	GLU
2	H	95	ILE
2	H	106	LYS
2	H	116	ASN
2	H	132	SER
2	H	134	SER
2	H	141	TYR
2	H	143	THR
2	H	145	LEU
2	H	155	LYS

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Mol	Chain	Res	Type
2	H	167	ILE
2	H	176	ARG
1	I	46	LEU
1	I	53	ARG
1	I	81	GLU
1	I	87	ASP
1	I	96	LYS
1	I	99	PHE
1	I	106	LYS
1	I	121	LYS
1	I	126	LYS
1	I	144	ARG
1	I	153	LYS
1	I	171	LYS
1	I	177	LYS
2	K	92	GLU
2	K	93	HIS
2	K	94	GLU
2	K	95	ILE
2	K	106	LYS
2	K	116	ASN
2	K	134	SER
2	K	141	TYR
2	K	143	THR
2	K	145	LEU
2	K	155	LYS
2	K	167	ILE
2	K	176	ARG
1	J	46	LEU
1	J	53	ARG
1	J	81	GLU
1	J	87	ASP
1	J	96	LYS
1	J	99	PHE
1	J	106	LYS
1	J	121	LYS
1	J	126	LYS
1	J	144	ARG
1	J	153	LYS
1	J	171	LYS
1	J	177	LYS
2	L	92	GLU

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Mol	Chain	Res	Type
2	L	93	HIS
2	L	94	GLU
2	L	95	ILE
2	L	106	LYS
2	L	116	ASN
2	L	132	SER
2	L	134	SER
2	L	141	TYR
2	L	143	THR
2	L	145	LEU
2	L	155	LYS
2	L	167	ILE
2	L	176	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
2	B	146	GLN
1	C	54	GLN
2	E	146	GLN
1	D	54	GLN
2	F	146	GLN
1	G	54	GLN
2	H	146	GLN
1	I	54	GLN
2	K	146	GLN
1	J	54	GLN
2	L	146	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.