



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Aug 17, 2017 – 05:05 PM EDT

PDB ID : 2W49
EMDB ID: : EMD-1561
Title : ISOMETRICALLY CONTRACTING INSECT ASYNCHRONOUS FLIGHT
MUSCLE
Authors : Wu, S.; Liu, J.; Reedy, M.C.; Tregear, R.T.; Winkler, H.; Franzini-Armstrong,
C.; Sasaki, H.; Lucaveche, C.; Goldman, Y.E.; Reedy, M.K.; Taylor, K.A.
Deposited on : unknown
Resolution : 35.00 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

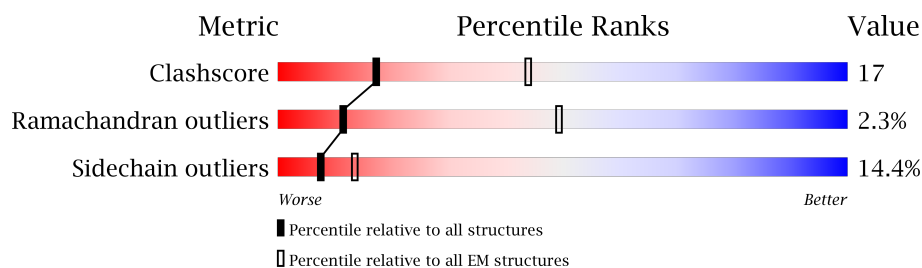
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 35.00 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.




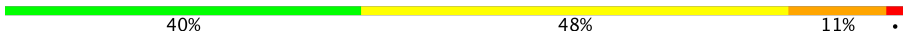
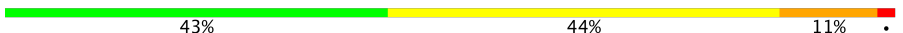






















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	0	159	47% 44% 6% .
1	3	159	46% 45% 6% .
1	6	159	46% 45% 6% .
1	9	159	45% 46% 6% .
2	1	90	51% 37% 12%
2	4	90	51% 38% 11%
2	7	90	52% 39% 9%
2	Y	90	51% 40% 9%
3	2	141	43% 44% 11% .

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Mol	Chain	Length	Quality of chain
3	5	141	 41% 45% 13% .
3	8	141	 40% 48% 11% .
3	Z	141	 43% 44% 11% .
4	A	277	 82% 15% .
4	B	277	 81% 17% .
4	C	277	 11% . . 86%
4	T	277	 9% . . 86%
4	U	277	 81% 17% .
4	V	277	 82% 15% .
4	W	277	 9% . . 86%
4	X	277	 11% . . 86%
5	D	372	 64% 28% 6% .
5	E	372	 64% 28% 7% .
5	F	372	 63% 29% 6% .
5	G	372	 64% 28% 6% .
5	H	372	 64% 28% 7% .
5	I	372	 63% 28% 7% .
5	J	372	 64% 28% 7% .
5	K	372	 63% 29% 7% .
5	L	372	 63% 29% 6% .
5	M	372	 63% 29% 7% .
5	N	372	 63% 28% 7% .
5	O	372	 63% 29% 6% .
5	P	372	 63% 29% 7% .
5	Q	372	 64% 28% 7% .

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Mol	Chain	Length	Quality of chain
5	R	372	<div><div></div><div>64%</div><div>28%</div><div>7%</div><div></div></div>
5	S	372	<div><div></div><div>64%</div><div>28%</div><div>7%</div><div></div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 69376 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TROPONIN C, SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	159	Total	C	N	O	S	0	0
			1252	770	199	272	11		
1	3	159	Total	C	N	O	S	0	0
			1252	770	199	272	11		
1	6	159	Total	C	N	O	S	0	0
			1252	770	199	272	11		
1	9	159	Total	C	N	O	S	0	0
			1252	770	199	272	11		

- Molecule 2 is a protein called TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	90	Total	C	N	O	0	0
			774	486	146	142		
2	4	90	Total	C	N	O	0	0
			774	486	146	142		
2	7	90	Total	C	N	O	0	0
			774	486	146	142		
2	Y	90	Total	C	N	O	0	0
			774	486	146	142		

- Molecule 3 is a protein called TROPONIN I, FAST SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	141	Total	C	N	O	S	0	0
			1140	709	214	212	5		
3	5	141	Total	C	N	O	S	0	0
			1140	709	214	212	5		
3	8	141	Total	C	N	O	S	0	0
			1140	709	214	212	5		
3	Z	141	Total	C	N	O	S	0	0
			1140	709	214	212	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	48	SER	CYS	conflict	UNP P68246
2	64	SER	CYS	conflict	UNP P68246
2	89	ILE	ASN	conflict	UNP P68246
5	48	SER	CYS	conflict	UNP P68246
5	64	SER	CYS	conflict	UNP P68246
5	89	ILE	ASN	conflict	UNP P68246
8	48	SER	CYS	conflict	UNP P68246
8	64	SER	CYS	conflict	UNP P68246
8	89	ILE	ASN	conflict	UNP P68246
Z	48	SER	CYS	conflict	UNP P68246
Z	64	SER	CYS	conflict	UNP P68246
Z	89	ILE	ASN	conflict	UNP P68246

- Molecule 4 is a protein called TROPOMYOSIN ALPHA-1 CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	277	Total	C	N	O	S	0	0
			2230	1362	378	484	6		
4	B	277	Total	C	N	O	S	0	0
			2230	1362	378	484	6		
4	C	39	Total	C	N	O	S	0	0
			316	198	48	69	1		
4	T	39	Total	C	N	O	S	0	0
			316	198	48	69	1		
4	U	277	Total	C	N	O	S	0	0
			2230	1362	378	484	6		
4	V	277	Total	C	N	O	S	0	0
			2230	1362	378	484	6		
4	W	39	Total	C	N	O	S	0	0
			316	198	48	69	1		
4	X	39	Total	C	N	O	S	0	0
			316	198	48	69	1		

- Molecule 5 is a protein called ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	E	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	F	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	G	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	I	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	J	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	K	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	L	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	M	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	N	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	O	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	P	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	Q	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	R	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		
5	S	372	Total	C	N	O	S	0	0
			2907	1836	489	562	20		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	0	4	Total	Ca	0
			4	4	
6	9	4	Total	Ca	0
			4	4	
6	3	4	Total	Ca	0
			4	4	
6	6	4	Total	Ca	0
			4	4	

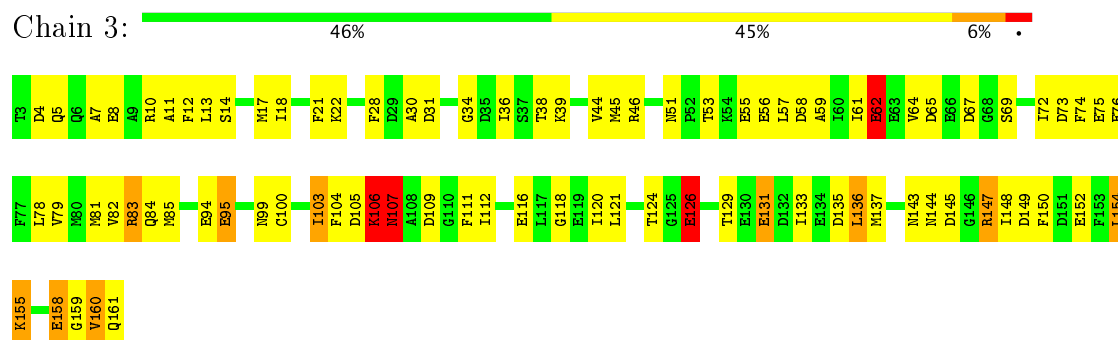
3 Residue-property plots

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.

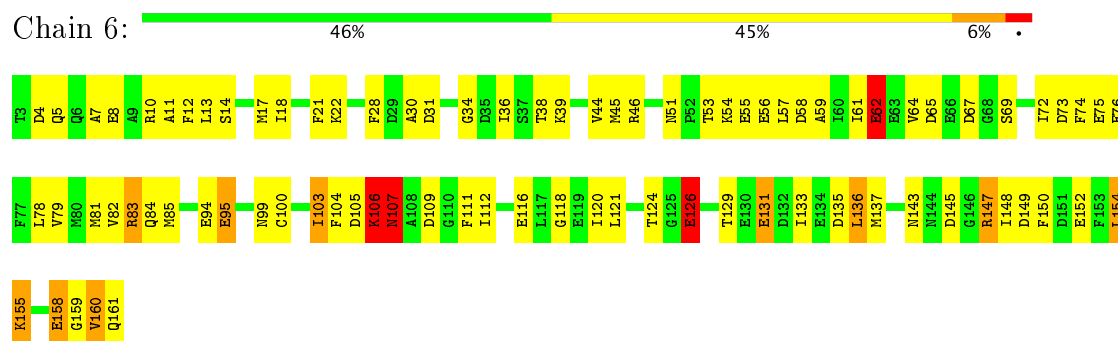
- Molecule 1: TROPONIN C, SKELETAL MUSCLE



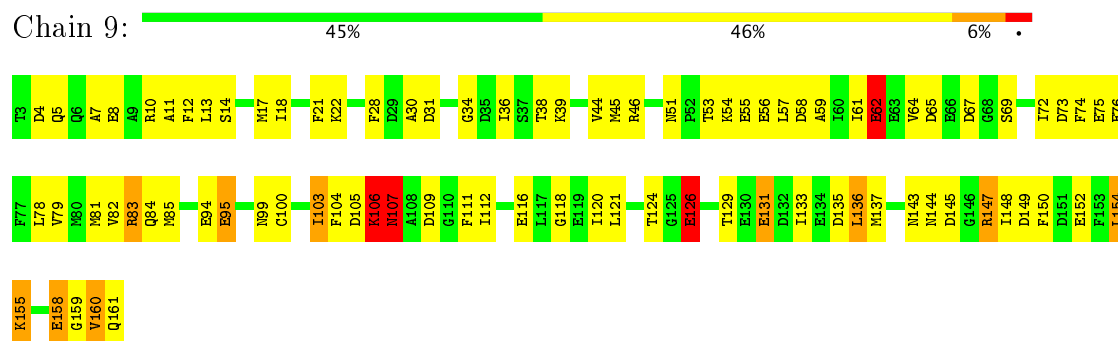
- Molecule 1: TROPONIN C, SKELETAL MUSCLE



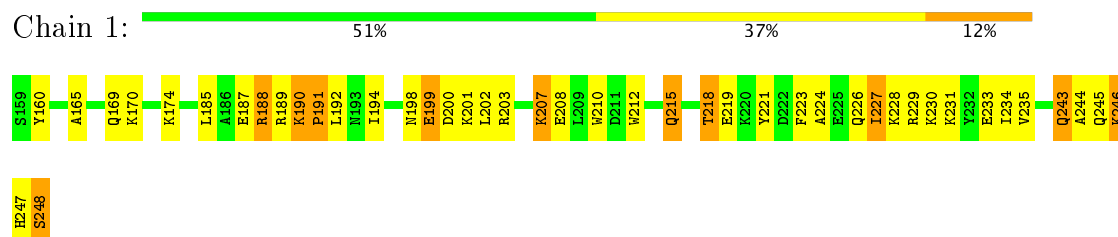
- Molecule 1: TROPONIN C, SKELETAL MUSCLE



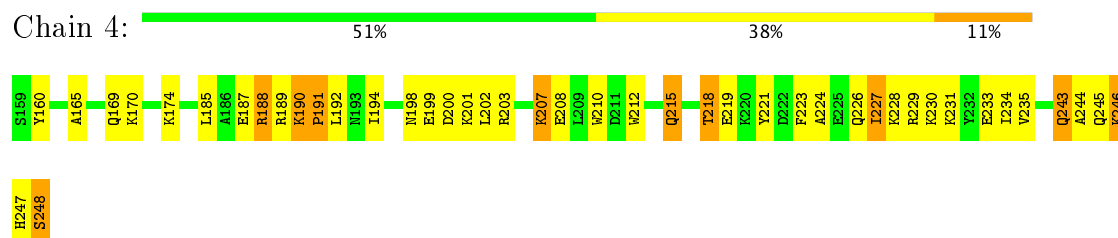
- Molecule 1: TROPONIN C, SKELETAL MUSCLE



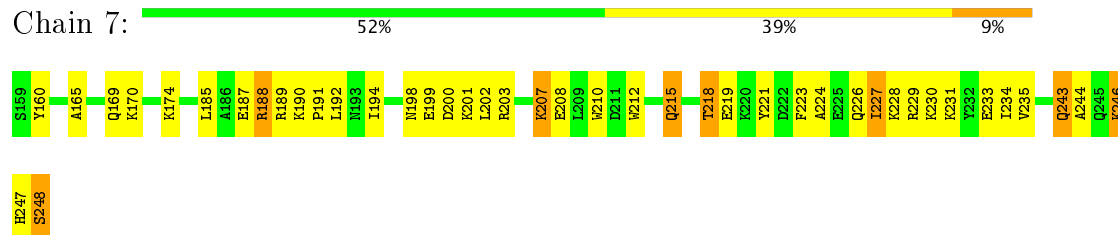
- Molecule 2: TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS



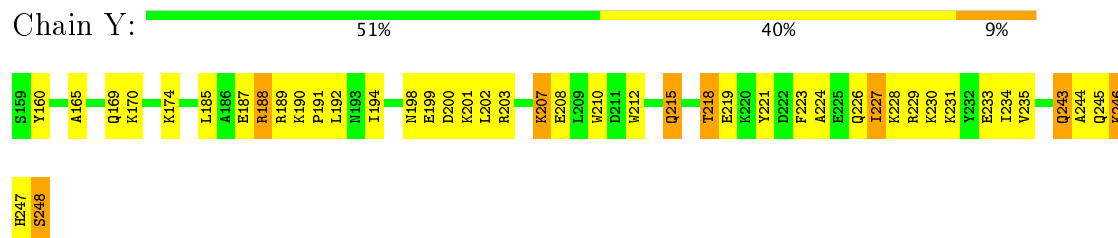
- Molecule 2: TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS



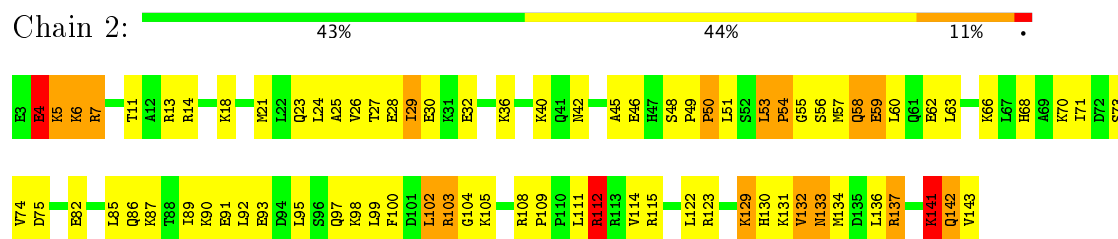
- Molecule 2: TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS



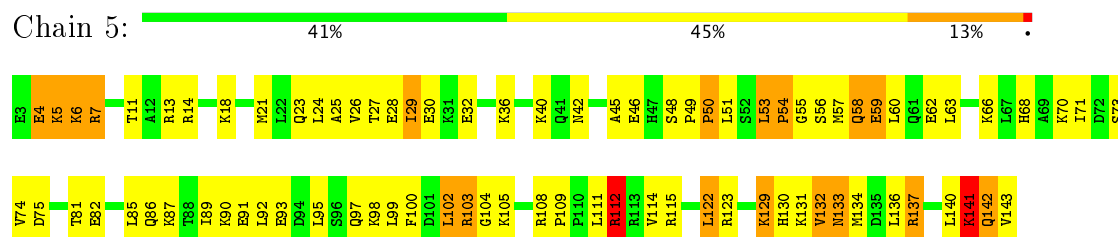
- Molecule 2: TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS



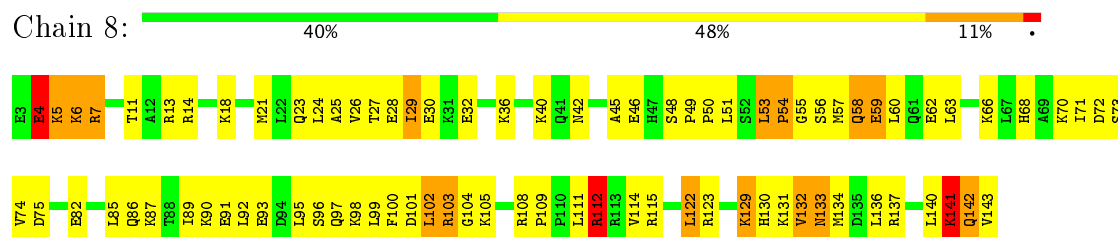
- Molecule 3: TROPONIN I, FAST SKELETAL MUSCLE



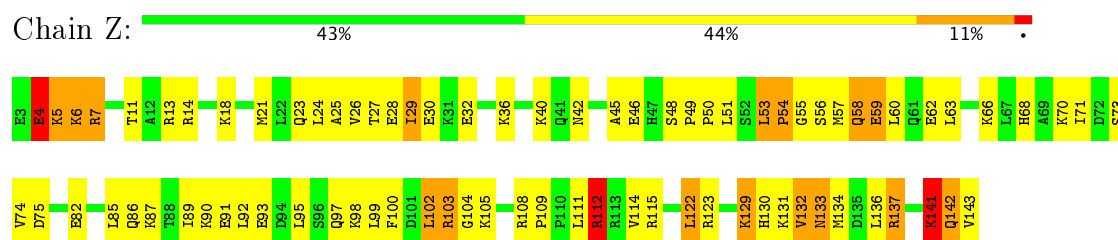
- Molecule 3: TROPONIN I, FAST SKELETAL MUSCLE



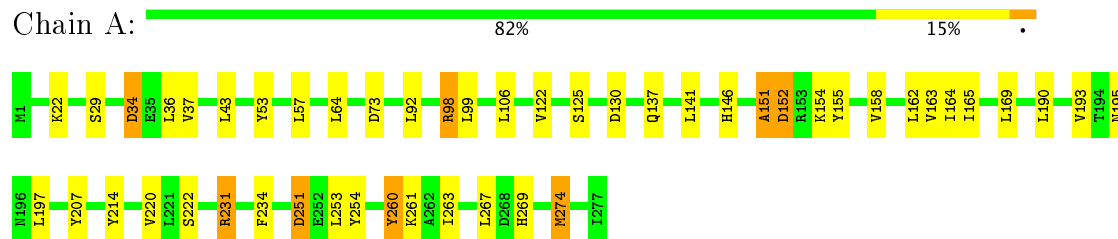
- Molecule 3: TROPONIN I, FAST SKELETAL MUSCLE




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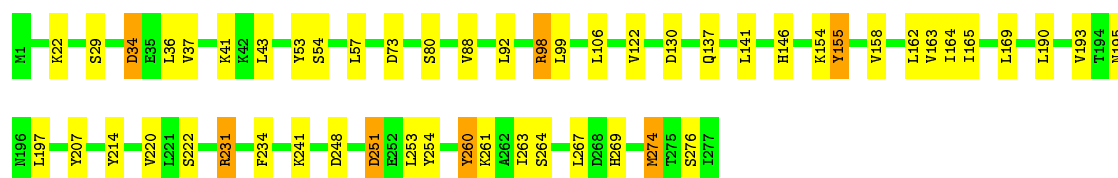


- Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN



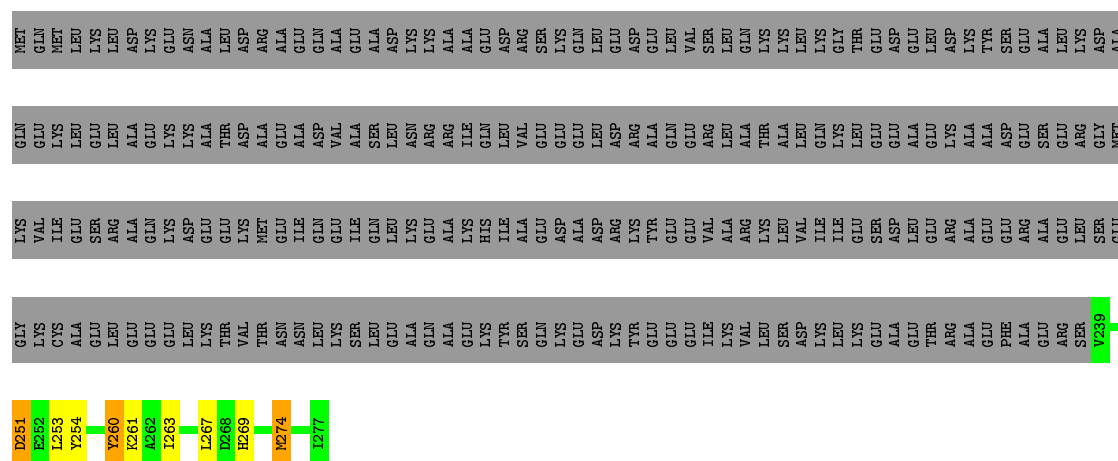
- Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain B:  81% 17% .



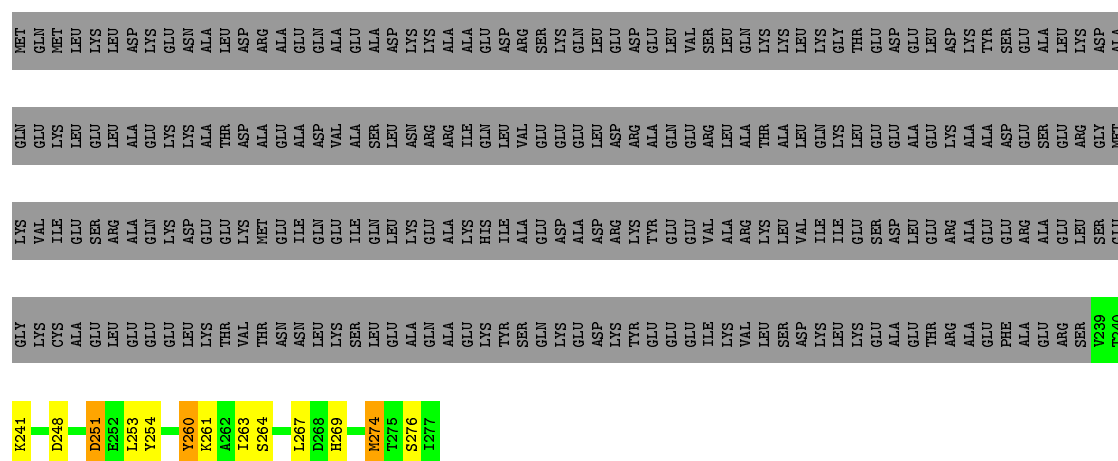
• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain C:  11% .. 86%




• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain T:  9% .. 86%



• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain U:  81% 17% .





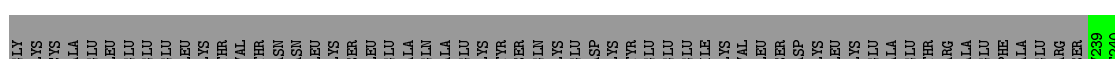
• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain V: 82% 15%



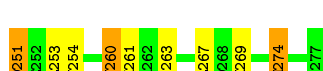
• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain W: 9% 86%

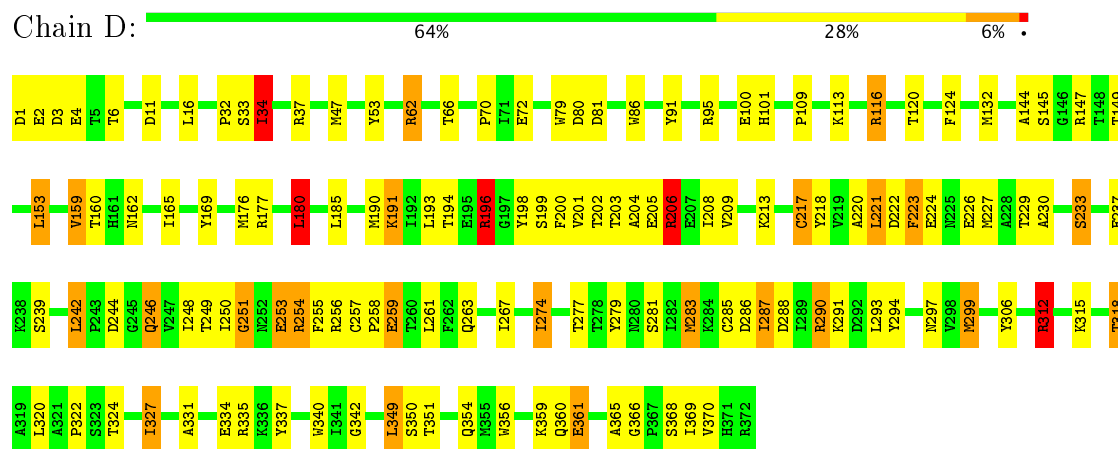


• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

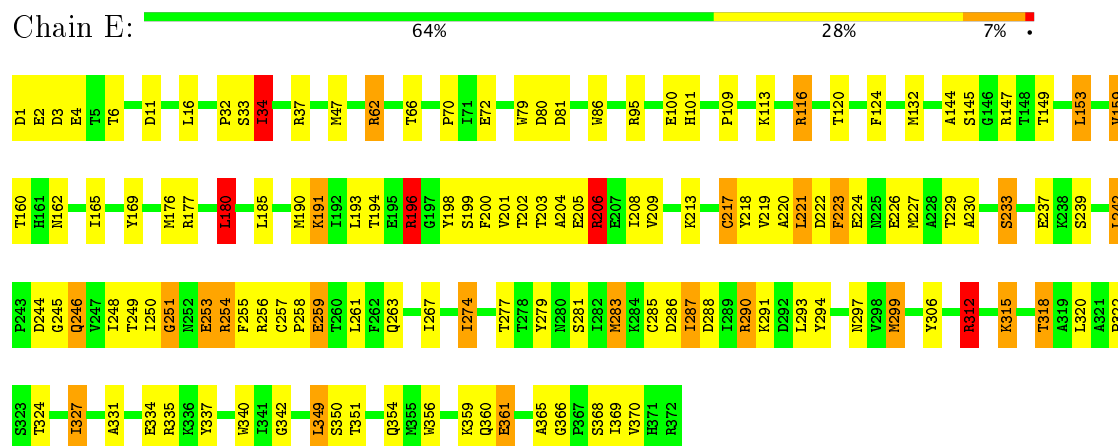
Chain X: 11% 86%



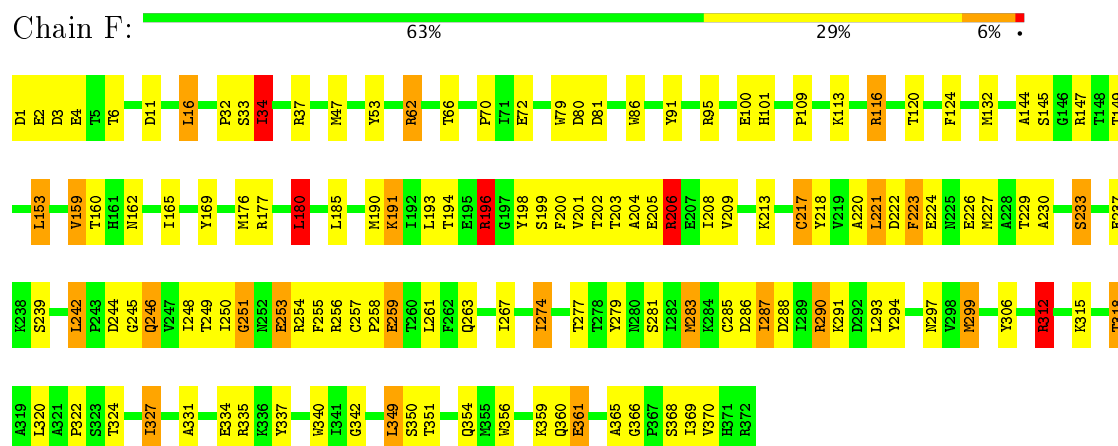
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE



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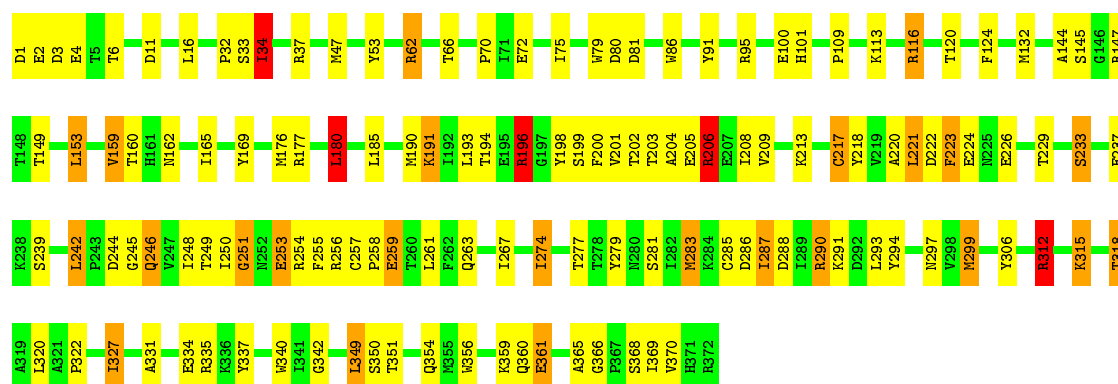


- Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE



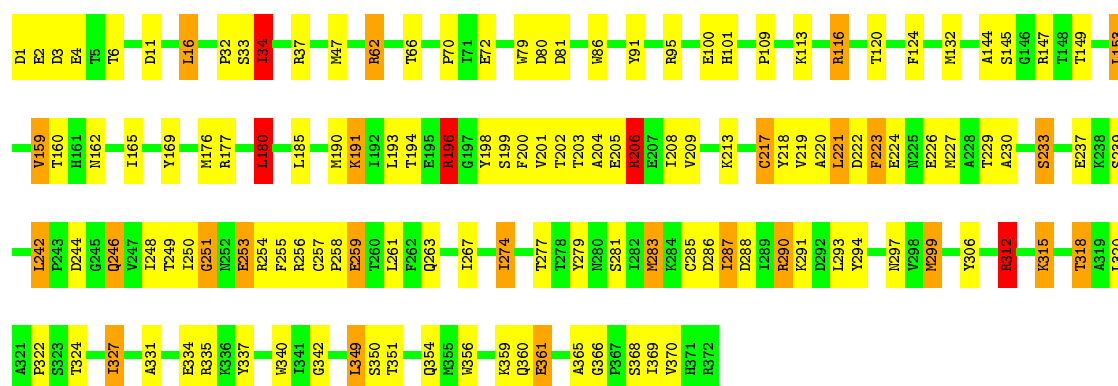
- Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE





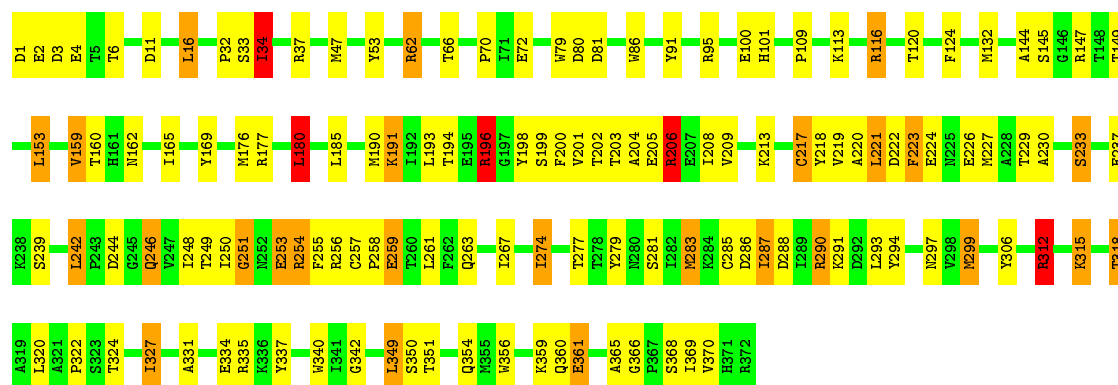
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain H: 64% 28% 7% •



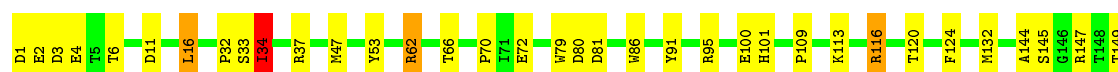
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain I: 63% 28% 7% •



• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

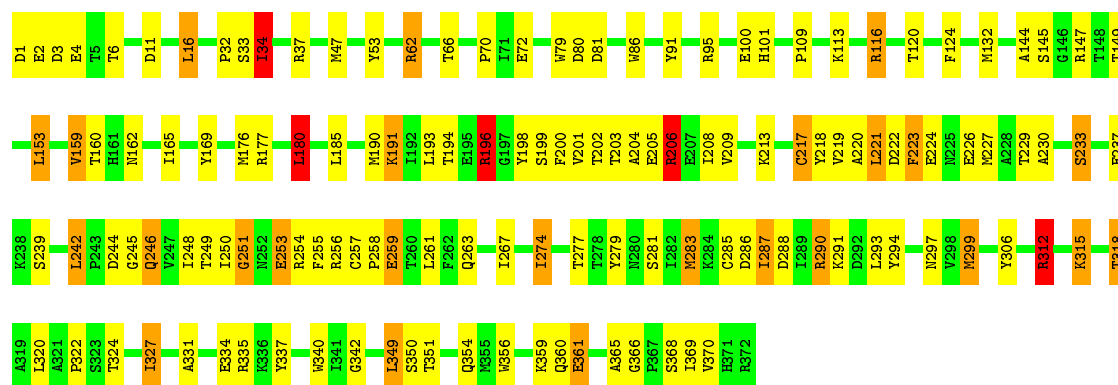
Chain J: 64% 28% 7% •





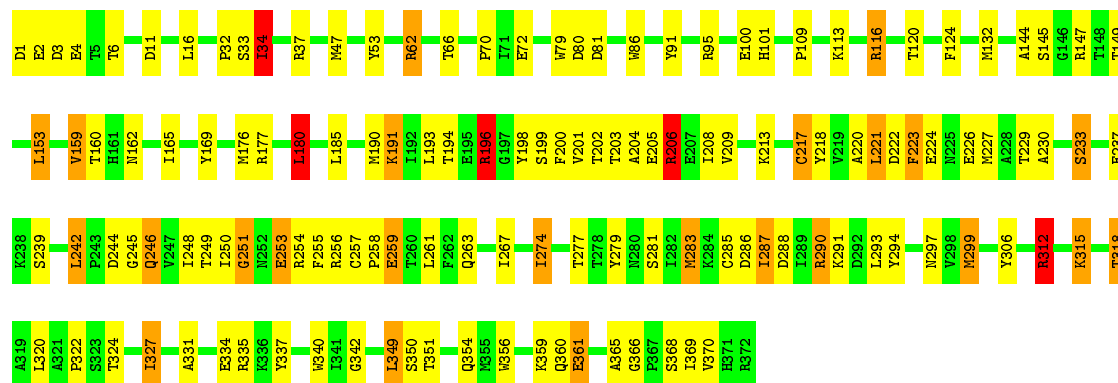
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain K: 63% 29% 7%



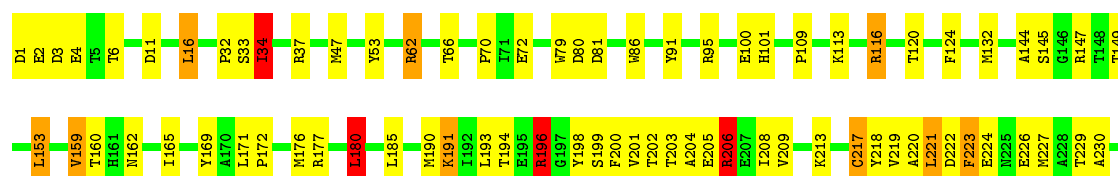
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

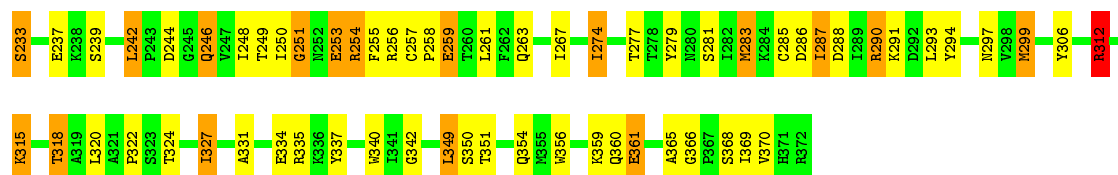
Chain L: 63% 29% 6%



• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

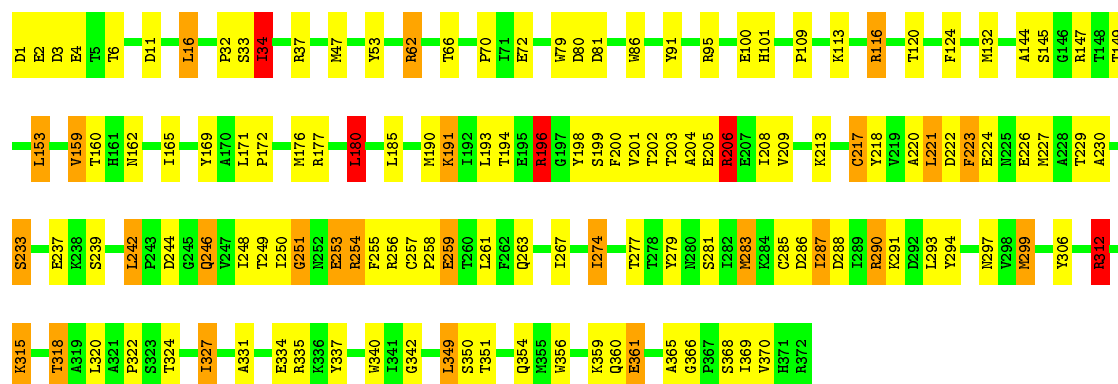
Chain M: 63% 29% 7%





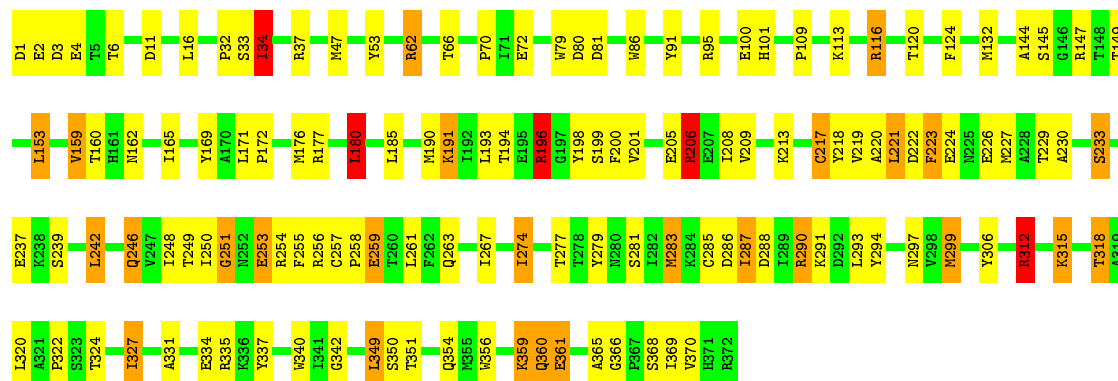
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain N: 63% 28% 7%



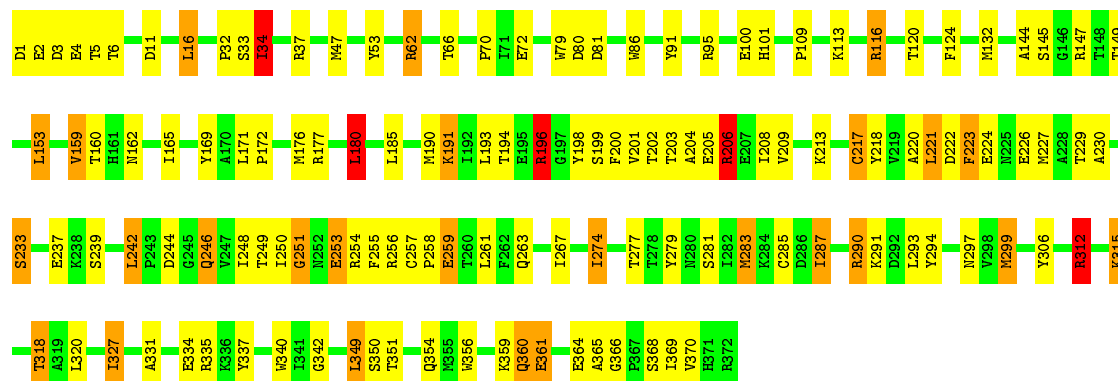
- Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain Q:  64% 28% 7%



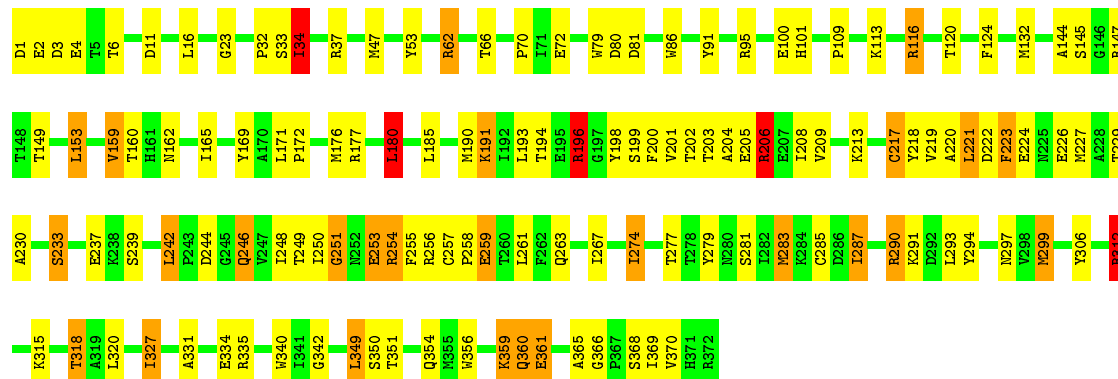
- Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain R: 64% 28% 7%



- Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain S:  64% 28% 7%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	TVIPS TEMCAM-F224 (2k x 2k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	0	0.55	0/1264	0.67	1/1687 (0.1%)
1	3	0.55	0/1264	0.67	1/1687 (0.1%)
1	6	0.55	0/1264	0.67	1/1687 (0.1%)
1	9	0.55	0/1264	0.67	1/1687 (0.1%)
2	1	0.57	0/786	0.59	0/1046
2	4	0.57	0/786	0.59	0/1046
2	7	0.57	0/786	0.59	0/1046
2	Y	0.57	0/786	0.59	0/1046
3	2	0.53	0/1152	0.71	0/1535
3	5	0.53	0/1152	0.70	0/1535
3	8	0.53	0/1152	0.70	0/1535
3	Z	0.53	0/1152	0.70	0/1535
4	A	3.01	15/2238 (0.7%)	1.82	48/2983 (1.6%)
4	B	3.60	9/2238 (0.4%)	1.86	45/2983 (1.5%)
4	C	7.01	7/318 (2.2%)	2.35	13/425 (3.1%)
4	T	7.04	7/318 (2.2%)	2.26	12/425 (2.8%)
4	U	3.60	9/2238 (0.4%)	1.85	46/2983 (1.5%)
4	V	3.01	15/2238 (0.7%)	1.82	48/2983 (1.6%)
4	W	7.04	7/318 (2.2%)	2.26	12/425 (2.8%)
4	X	7.01	7/318 (2.2%)	2.34	13/425 (3.1%)
5	D	0.89	2/2969 (0.1%)	1.64	51/4023 (1.3%)
5	E	0.89	2/2969 (0.1%)	1.64	49/4023 (1.2%)
5	F	0.89	2/2969 (0.1%)	1.64	52/4023 (1.3%)
5	G	0.89	2/2969 (0.1%)	1.64	52/4023 (1.3%)
5	H	0.89	2/2969 (0.1%)	1.64	51/4023 (1.3%)
5	I	0.89	2/2969 (0.1%)	1.64	51/4023 (1.3%)
5	J	0.89	2/2969 (0.1%)	1.64	51/4023 (1.3%)
5	K	0.89	2/2969 (0.1%)	1.64	50/4023 (1.2%)
5	L	0.89	2/2969 (0.1%)	1.64	50/4023 (1.2%)
5	M	0.89	2/2969 (0.1%)	1.64	50/4023 (1.2%)
5	N	0.89	2/2969 (0.1%)	1.64	52/4023 (1.3%)
5	O	0.89	1/2969 (0.0%)	1.64	52/4023 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
5	P	0.89	1/2969 (0.0%)	1.64	51/4023 (1.3%)
5	Q	0.89	2/2969 (0.1%)	1.64	51/4023 (1.3%)
5	R	0.89	2/2969 (0.1%)	1.64	51/4023 (1.3%)
5	S	0.89	2/2969 (0.1%)	1.64	49/4023 (1.2%)
All	All	1.70	106/70536 (0.2%)	1.56	1054/95072 (1.1%)

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
4	A	0	4
4	B	0	5
4	C	0	2
4	T	0	2
4	U	0	5
4	V	0	4
4	W	0	2
4	X	0	2
5	D	0	1
5	E	0	1
5	F	0	1
5	G	0	1
5	H	0	1
5	I	0	1
5	J	0	1
5	K	0	1
5	L	0	1
5	M	0	1
5	N	0	1
5	O	0	1
5	P	0	1
5	Q	0	1
5	R	0	1
5	S	0	1
All	All	0	42

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	260	TYR	CA-CB	110.52	3.97	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	260	TYR	CA-CB	110.51	3.97	1.53
4	B	260	TYR	CA-CB	110.50	3.97	1.53
4	W	260	TYR	CA-CB	110.48	3.97	1.53
4	C	260	TYR	CA-CB	110.21	3.96	1.53
4	V	260	TYR	CA-CB	110.19	3.96	1.53
4	X	260	TYR	CA-CB	110.18	3.96	1.53
4	A	260	TYR	CA-CB	110.16	3.96	1.53
4	U	155	TYR	CA-CB	109.44	3.94	1.53
4	B	155	TYR	CA-CB	109.43	3.94	1.53
4	A	260	TYR	CG-CD1	31.73	1.80	1.39
4	C	260	TYR	CG-CD1	31.71	1.80	1.39
4	X	260	TYR	CG-CD1	31.63	1.80	1.39
4	V	260	TYR	CG-CD1	31.62	1.80	1.39
4	W	260	TYR	CG-CD1	31.59	1.80	1.39
4	B	260	TYR	CG-CD1	31.58	1.80	1.39
4	T	260	TYR	CG-CD1	31.57	1.80	1.39
4	U	260	TYR	CG-CD1	31.55	1.80	1.39
4	A	155	TYR	CG-CD2	26.19	1.73	1.39
4	V	155	TYR	CG-CD2	26.14	1.73	1.39
4	W	260	TYR	CE1-CZ	25.72	1.72	1.38
4	U	260	TYR	CE1-CZ	25.72	1.72	1.38
4	B	260	TYR	CE1-CZ	25.63	1.71	1.38
4	T	260	TYR	CE1-CZ	25.63	1.71	1.38
4	V	155	TYR	CE2-CZ	25.59	1.71	1.38
4	A	155	TYR	CE2-CZ	25.53	1.71	1.38
4	C	260	TYR	CE1-CZ	25.22	1.71	1.38
4	X	260	TYR	CE1-CZ	25.21	1.71	1.38
4	A	260	TYR	CE1-CZ	25.20	1.71	1.38
4	V	260	TYR	CE1-CZ	25.20	1.71	1.38
4	V	155	TYR	CE1-CZ	24.87	1.70	1.38
4	A	155	TYR	CE1-CZ	24.87	1.70	1.38
4	A	155	TYR	CD2-CE2	23.49	1.74	1.39
4	V	155	TYR	CD2-CE2	23.41	1.74	1.39
4	T	260	TYR	CD1-CE1	22.19	1.72	1.39
4	U	260	TYR	CD1-CE1	22.14	1.72	1.39
4	W	260	TYR	CD1-CE1	22.12	1.72	1.39
4	B	260	TYR	CD1-CE1	22.12	1.72	1.39
4	V	260	TYR	CD1-CE1	21.94	1.72	1.39
4	X	260	TYR	CD1-CE1	21.91	1.72	1.39
4	C	260	TYR	CD1-CE1	21.81	1.72	1.39
4	A	260	TYR	CD1-CE1	21.80	1.72	1.39
4	A	155	TYR	CG-CD1	21.64	1.67	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	155	TYR	CG-CD1	21.56	1.67	1.39
4	W	260	TYR	CG-CD2	21.36	1.67	1.39
4	B	260	TYR	CG-CD2	21.35	1.67	1.39
4	T	260	TYR	CG-CD2	21.35	1.67	1.39
4	U	260	TYR	CG-CD2	21.34	1.66	1.39
4	W	260	TYR	CE2-CZ	21.01	1.65	1.38
4	U	260	TYR	CE2-CZ	20.97	1.65	1.38
4	B	260	TYR	CE2-CZ	20.97	1.65	1.38
4	X	260	TYR	CG-CD2	20.97	1.66	1.39
4	T	260	TYR	CE2-CZ	20.94	1.65	1.38
4	V	260	TYR	CG-CD2	20.93	1.66	1.39
4	A	260	TYR	CG-CD2	20.89	1.66	1.39
4	C	260	TYR	CG-CD2	20.89	1.66	1.39
4	A	260	TYR	CE2-CZ	20.43	1.65	1.38
4	C	260	TYR	CE2-CZ	20.43	1.65	1.38
4	V	260	TYR	CE2-CZ	20.43	1.65	1.38
4	X	260	TYR	CE2-CZ	20.41	1.65	1.38
4	A	155	TYR	CD1-CE1	19.48	1.68	1.39
4	V	155	TYR	CD1-CE1	19.43	1.68	1.39
4	B	260	TYR	CD2-CE2	16.93	1.64	1.39
4	T	260	TYR	CD2-CE2	16.92	1.64	1.39
4	U	260	TYR	CD2-CE2	16.86	1.64	1.39
4	W	260	TYR	CD2-CE2	16.81	1.64	1.39
4	V	260	TYR	CD2-CE2	16.57	1.64	1.39
4	X	260	TYR	CD2-CE2	16.56	1.64	1.39
4	A	260	TYR	CD2-CE2	16.52	1.64	1.39
4	C	260	TYR	CD2-CE2	16.50	1.64	1.39
4	V	155	TYR	CA-CB	7.03	1.69	1.53
4	A	155	TYR	CA-CB	7.03	1.69	1.53
5	G	259	GLU	CG-CD	6.27	1.61	1.51
5	M	259	GLU	CG-CD	6.25	1.61	1.51
5	H	259	GLU	CG-CD	6.25	1.61	1.51
5	P	259	GLU	CG-CD	6.24	1.61	1.51
5	J	259	GLU	CG-CD	6.24	1.61	1.51
5	N	259	GLU	CG-CD	6.23	1.61	1.51
5	I	259	GLU	CG-CD	6.23	1.61	1.51
5	E	259	GLU	CG-CD	6.23	1.61	1.51
5	L	259	GLU	CG-CD	6.23	1.61	1.51
5	K	259	GLU	CG-CD	6.21	1.61	1.51
5	O	259	GLU	CG-CD	6.20	1.61	1.51
5	S	259	GLU	CG-CD	6.19	1.61	1.51
5	D	259	GLU	CG-CD	6.18	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	259	GLU	CG-CD	6.17	1.61	1.51
5	R	259	GLU	CG-CD	6.16	1.61	1.51
5	F	259	GLU	CG-CD	6.10	1.61	1.51
4	U	155	TYR	CD1-CE1	-6.00	1.30	1.39
4	B	155	TYR	CD1-CE1	-5.97	1.30	1.39
4	V	155	TYR	CB-CG	5.75	1.60	1.51
4	A	155	TYR	CB-CG	5.73	1.60	1.51
5	D	259	GLU	CB-CG	5.12	1.61	1.52
5	F	259	GLU	CB-CG	5.08	1.61	1.52
5	G	259	GLU	CB-CG	5.08	1.61	1.52
5	S	259	GLU	CB-CG	5.07	1.61	1.52
5	Q	259	GLU	CB-CG	5.06	1.61	1.52
5	E	259	GLU	CB-CG	5.05	1.61	1.52
5	K	259	GLU	CB-CG	5.04	1.61	1.52
5	N	259	GLU	CB-CG	5.04	1.61	1.52
5	M	259	GLU	CB-CG	5.04	1.61	1.52
5	H	259	GLU	CB-CG	5.03	1.61	1.52
5	L	259	GLU	CB-CG	5.03	1.61	1.52
5	R	259	GLU	CB-CG	5.03	1.61	1.52
5	I	259	GLU	CB-CG	5.03	1.61	1.52
5	J	259	GLU	CB-CG	5.02	1.61	1.52

All (1054) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	155	TYR	CB-CG-CD1	-26.75	104.95	121.00
4	U	155	TYR	CB-CG-CD1	-26.69	104.99	121.00
4	V	260	TYR	CB-CG-CD2	-21.14	108.31	121.00
4	X	260	TYR	CB-CG-CD2	-21.11	108.33	121.00
4	C	260	TYR	CB-CG-CD2	-21.07	108.36	121.00
4	A	260	TYR	CB-CG-CD2	-21.02	108.39	121.00
4	U	260	TYR	CB-CG-CD2	-20.34	108.80	121.00
4	W	260	TYR	CB-CG-CD2	-20.30	108.82	121.00
4	T	260	TYR	CB-CG-CD2	-20.27	108.84	121.00
4	B	260	TYR	CB-CG-CD2	-20.26	108.84	121.00
4	B	231	ARG	NE-CZ-NH2	-17.07	111.76	120.30
4	U	231	ARG	NE-CZ-NH2	-16.97	111.81	120.30
4	C	274	MET	CA-CB-CG	16.40	141.18	113.30
4	A	274	MET	CA-CB-CG	16.39	141.17	113.30
4	X	274	MET	CA-CB-CG	16.38	141.15	113.30
4	V	274	MET	CA-CB-CG	16.38	141.14	113.30
4	V	231	ARG	NE-CZ-NH1	15.89	128.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	231	ARG	NE-CZ-NH1	15.88	128.24	120.30
4	T	274	MET	CA-CB-CG	15.38	139.45	113.30
4	B	274	MET	CA-CB-CG	15.37	139.43	113.30
4	W	274	MET	CA-CB-CG	15.35	139.40	113.30
4	U	274	MET	CA-CB-CG	15.35	139.39	113.30
4	B	231	ARG	NE-CZ-NH1	14.06	127.33	120.30
4	U	231	ARG	NE-CZ-NH1	14.05	127.32	120.30
4	U	98	ARG	NE-CZ-NH2	-13.65	113.47	120.30
4	B	98	ARG	NE-CZ-NH2	-13.65	113.47	120.30
4	A	98	ARG	NE-CZ-NH2	-13.50	113.55	120.30
4	V	98	ARG	NE-CZ-NH2	-13.42	113.59	120.30
4	V	231	ARG	CD-NE-CZ	-11.56	107.42	123.60
4	A	231	ARG	CD-NE-CZ	-11.55	107.43	123.60
4	V	231	ARG	NE-CZ-NH2	-11.32	114.64	120.30
4	A	231	ARG	NE-CZ-NH2	-11.30	114.65	120.30
4	T	253	LEU	N-CA-C	10.19	138.51	111.00
4	B	253	LEU	N-CA-C	10.18	138.47	111.00
4	U	155	TYR	CG-CD1-CE1	-10.18	113.16	121.30
4	W	253	LEU	N-CA-C	10.18	138.48	111.00
4	U	253	LEU	N-CA-C	10.17	138.45	111.00
4	B	155	TYR	CG-CD1-CE1	-10.14	113.19	121.30
4	V	155	TYR	CA-CB-CG	10.09	132.57	113.40
4	A	155	TYR	CA-CB-CG	10.08	132.56	113.40
4	V	253	LEU	N-CA-C	9.81	137.49	111.00
4	C	253	LEU	N-CA-C	9.81	137.48	111.00
4	A	253	LEU	N-CA-C	9.80	137.47	111.00
4	X	253	LEU	N-CA-C	9.79	137.44	111.00
5	N	356	TRP	CD1-CG-CD2	9.26	113.71	106.30
5	G	356	TRP	CD1-CG-CD2	9.21	113.67	106.30
5	R	356	TRP	CD1-CG-CD2	9.19	113.65	106.30
5	M	356	TRP	CD1-CG-CD2	9.18	113.64	106.30
5	K	356	TRP	CD1-CG-CD2	9.15	113.62	106.30
5	F	356	TRP	CD1-CG-CD2	9.14	113.61	106.30
5	O	356	TRP	CD1-CG-CD2	9.11	113.59	106.30
5	D	356	TRP	CD1-CG-CD2	9.09	113.58	106.30
5	L	356	TRP	CD1-CG-CD2	9.09	113.57	106.30
5	J	356	TRP	CD1-CG-CD2	9.08	113.56	106.30
5	S	356	TRP	CD1-CG-CD2	9.07	113.56	106.30
4	U	92	LEU	N-CA-C	9.05	135.44	111.00
4	B	92	LEU	N-CA-C	9.05	135.43	111.00
5	E	356	TRP	CD1-CG-CD2	9.05	113.54	106.30
5	P	356	TRP	CD1-CG-CD2	9.04	113.54	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	356	TRP	CD1-CG-CD2	9.03	113.52	106.30
5	I	356	TRP	CD1-CG-CD2	9.02	113.52	106.30
5	H	356	TRP	CD1-CG-CD2	9.02	113.51	106.30
5	I	177	ARG	NE-CZ-NH2	-8.85	115.87	120.30
5	M	177	ARG	NE-CZ-NH2	-8.83	115.88	120.30
4	A	92	LEU	N-CA-C	8.82	134.82	111.00
4	V	92	LEU	N-CA-C	8.81	134.78	111.00
4	V	253	LEU	CB-CG-CD1	-8.77	96.10	111.00
4	X	253	LEU	CB-CG-CD1	-8.76	96.11	111.00
4	A	253	LEU	CB-CG-CD1	-8.75	96.12	111.00
4	C	253	LEU	CB-CG-CD1	-8.75	96.12	111.00
5	O	177	ARG	NE-CZ-NH2	-8.73	115.94	120.30
5	P	177	ARG	NE-CZ-NH2	-8.72	115.94	120.30
5	J	177	ARG	NE-CZ-NH2	-8.71	115.94	120.30
5	Q	177	ARG	NE-CZ-NH2	-8.68	115.96	120.30
5	G	177	ARG	NE-CZ-NH2	-8.67	115.97	120.30
5	H	177	ARG	NE-CZ-NH2	-8.66	115.97	120.30
4	V	260	TYR	CB-CG-CD1	8.66	126.20	121.00
4	C	260	TYR	CB-CG-CD1	8.66	126.19	121.00
4	X	260	TYR	CB-CG-CD1	8.66	126.19	121.00
5	F	177	ARG	NE-CZ-NH2	-8.64	115.98	120.30
4	A	260	TYR	CB-CG-CD1	8.63	126.18	121.00
5	J	86	TRP	CD1-CG-CD2	8.61	113.19	106.30
5	K	177	ARG	NE-CZ-NH2	-8.60	116.00	120.30
5	P	86	TRP	CD1-CG-CD2	8.59	113.17	106.30
5	D	177	ARG	NE-CZ-NH2	-8.57	116.01	120.30
5	L	86	TRP	CD1-CG-CD2	8.56	113.15	106.30
5	E	177	ARG	NE-CZ-NH2	-8.55	116.02	120.30
5	Q	86	TRP	CD1-CG-CD2	8.55	113.14	106.30
5	L	177	ARG	NE-CZ-NH2	-8.55	116.03	120.30
5	H	86	TRP	CD1-CG-CD2	8.53	113.12	106.30
5	O	86	TRP	CD1-CG-CD2	8.52	113.11	106.30
5	E	86	TRP	CD1-CG-CD2	8.50	113.10	106.30
5	D	86	TRP	CD1-CG-CD2	8.49	113.09	106.30
5	S	177	ARG	NE-CZ-NH2	-8.49	116.05	120.30
5	M	86	TRP	CD1-CG-CD2	8.49	113.09	106.30
5	F	86	TRP	CD1-CG-CD2	8.47	113.07	106.30
5	N	86	TRP	CD1-CG-CD2	8.47	113.08	106.30
5	R	86	TRP	CD1-CG-CD2	8.46	113.07	106.30
5	S	86	TRP	CD1-CG-CD2	8.46	113.07	106.30
5	I	86	TRP	CD1-CG-CD2	8.46	113.06	106.30
5	R	177	ARG	NE-CZ-NH2	-8.44	116.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	86	TRP	CD1-CG-CD2	8.44	113.05	106.30
5	G	86	TRP	CD1-CG-CD2	8.43	113.04	106.30
4	V	197	LEU	CB-CG-CD1	-8.39	96.73	111.00
4	U	92	LEU	CB-CG-CD1	-8.34	96.82	111.00
4	A	197	LEU	CB-CG-CD1	-8.34	96.82	111.00
4	B	92	LEU	CB-CG-CD1	-8.34	96.82	111.00
4	A	36	LEU	CD1-CG-CD2	8.25	135.24	110.50
4	A	197	LEU	CD1-CG-CD2	8.24	135.22	110.50
4	V	36	LEU	CD1-CG-CD2	8.23	135.20	110.50
4	V	197	LEU	CD1-CG-CD2	8.23	135.19	110.50
5	N	177	ARG	NE-CZ-NH2	-8.22	116.19	120.30
5	N	356	TRP	CE2-CD2-CG	-8.14	100.78	107.30
5	M	356	TRP	CE2-CD2-CG	-8.08	100.83	107.30
5	G	356	TRP	CE2-CD2-CG	-8.06	100.86	107.30
4	V	155	TYR	N-CA-CB	8.04	125.06	110.60
5	D	356	TRP	CE2-CD2-CG	-8.03	100.88	107.30
4	A	155	TYR	N-CA-CB	8.01	125.02	110.60
5	F	356	TRP	CE2-CD2-CG	-8.01	100.89	107.30
5	L	356	TRP	CE2-CD2-CG	-7.98	100.91	107.30
5	J	356	TRP	CE2-CD2-CG	-7.98	100.91	107.30
4	B	169	LEU	CB-CG-CD1	-7.98	97.44	111.00
5	S	356	TRP	CE2-CD2-CG	-7.97	100.92	107.30
5	R	356	TRP	CE2-CD2-CG	-7.97	100.92	107.30
5	P	356	TRP	CE2-CD2-CG	-7.96	100.94	107.30
5	K	356	TRP	CE2-CD2-CG	-7.95	100.94	107.30
5	Q	356	TRP	CE2-CD2-CG	-7.95	100.94	107.30
4	U	169	LEU	CB-CG-CD1	-7.95	97.48	111.00
5	O	356	TRP	CE2-CD2-CG	-7.95	100.94	107.30
5	E	356	TRP	CE2-CD2-CG	-7.91	100.98	107.30
5	I	356	TRP	CE2-CD2-CG	-7.88	100.99	107.30
4	A	169	LEU	CB-CG-CD1	-7.87	97.63	111.00
4	V	169	LEU	CB-CG-CD1	-7.86	97.64	111.00
4	B	36	LEU	CD1-CG-CD2	7.86	134.07	110.50
4	U	36	LEU	CD1-CG-CD2	7.85	134.06	110.50
5	H	356	TRP	CE2-CD2-CG	-7.85	101.02	107.30
4	V	92	LEU	CB-CG-CD1	-7.84	97.67	111.00
4	U	169	LEU	CD1-CG-CD2	7.83	133.98	110.50
5	J	312	ARG	NE-CZ-NH2	7.82	124.21	120.30
4	B	169	LEU	CD1-CG-CD2	7.82	133.95	110.50
4	A	92	LEU	CB-CG-CD1	-7.81	97.72	111.00
4	A	190	LEU	CD1-CG-CD2	7.77	133.81	110.50
5	S	312	ARG	NE-CZ-NH2	7.77	124.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	312	ARG	NE-CZ-NH2	7.76	124.18	120.30
4	V	190	LEU	CD1-CG-CD2	7.76	133.78	110.50
4	B	92	LEU	CD1-CG-CD2	7.74	133.73	110.50
4	U	92	LEU	CD1-CG-CD2	7.73	133.70	110.50
5	M	312	ARG	NE-CZ-NH2	7.72	124.16	120.30
5	I	312	ARG	NE-CZ-NH2	7.69	124.14	120.30
5	K	312	ARG	NE-CZ-NH2	7.69	124.15	120.30
5	L	312	ARG	NE-CZ-NH2	7.69	124.14	120.30
5	O	312	ARG	NE-CZ-NH2	7.69	124.14	120.30
5	Q	312	ARG	NE-CZ-NH2	7.69	124.14	120.30
5	M	86	TRP	CE2-CD2-CG	-7.66	101.17	107.30
5	E	312	ARG	NE-CZ-NH2	7.66	124.13	120.30
4	V	169	LEU	CD1-CG-CD2	7.66	133.47	110.50
5	L	86	TRP	CE2-CD2-CG	-7.65	101.18	107.30
5	D	312	ARG	NE-CZ-NH2	7.65	124.12	120.30
5	J	86	TRP	CE2-CD2-CG	-7.65	101.18	107.30
5	N	312	ARG	NE-CZ-NH2	7.64	124.12	120.30
5	P	312	ARG	NE-CZ-NH2	7.64	124.12	120.30
5	H	312	ARG	NE-CZ-NH2	7.63	124.11	120.30
5	R	312	ARG	NE-CZ-NH2	7.63	124.11	120.30
4	A	169	LEU	CD1-CG-CD2	7.63	133.38	110.50
5	S	86	TRP	CE2-CD2-CG	-7.62	101.20	107.30
5	P	86	TRP	CE2-CD2-CG	-7.61	101.21	107.30
5	H	86	TRP	CE2-CD2-CG	-7.60	101.22	107.30
5	O	86	TRP	CE2-CD2-CG	-7.56	101.25	107.30
5	D	86	TRP	CE2-CD2-CG	-7.56	101.25	107.30
4	T	260	TYR	CB-CG-CD1	7.56	125.53	121.00
4	B	260	TYR	CB-CG-CD1	7.54	125.52	121.00
5	E	86	TRP	CE2-CD2-CG	-7.54	101.27	107.30
5	G	312	ARG	NE-CZ-NH2	7.54	124.07	120.30
5	R	86	TRP	CE2-CD2-CG	-7.53	101.27	107.30
5	N	86	TRP	CE2-CD2-CG	-7.52	101.28	107.30
5	I	86	TRP	CE2-CD2-CG	-7.51	101.29	107.30
5	K	86	TRP	CE2-CD2-CG	-7.51	101.30	107.30
4	U	260	TYR	CB-CG-CD1	7.51	125.50	121.00
5	Q	86	TRP	CE2-CD2-CG	-7.50	101.30	107.30
5	F	86	TRP	CE2-CD2-CG	-7.49	101.31	107.30
4	W	260	TYR	CB-CG-CD1	7.46	125.47	121.00
4	A	92	LEU	CD1-CG-CD2	7.45	132.86	110.50
5	G	86	TRP	CE2-CD2-CG	-7.45	101.34	107.30
5	S	254	ARG	NE-CZ-NH2	-7.45	116.57	120.30
4	V	92	LEU	CD1-CG-CD2	7.43	132.80	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	233	SER	CA-C-N	-7.41	100.91	117.20
5	D	180	LEU	CA-CB-CG	7.40	132.32	115.30
4	U	197	LEU	CD1-CG-CD2	7.40	132.69	110.50
5	E	254	ARG	NE-CZ-NH2	-7.39	116.60	120.30
5	O	233	SER	CA-C-N	-7.38	100.96	117.20
5	O	254	ARG	NE-CZ-NH2	-7.38	116.61	120.30
5	F	233	SER	CA-C-N	-7.38	100.97	117.20
4	B	197	LEU	CD1-CG-CD2	7.38	132.62	110.50
5	G	180	LEU	CA-CB-CG	7.38	132.26	115.30
5	M	233	SER	CA-C-N	-7.37	100.98	117.20
5	P	233	SER	CA-C-N	-7.37	100.98	117.20
5	S	233	SER	CA-C-N	-7.37	100.99	117.20
5	G	233	SER	CA-C-N	-7.37	100.99	117.20
5	R	180	LEU	CA-CB-CG	7.37	132.25	115.30
5	L	233	SER	CA-C-N	-7.37	101.00	117.20
5	S	180	LEU	CA-CB-CG	7.36	132.24	115.30
5	J	180	LEU	CA-CB-CG	7.36	132.23	115.30
5	I	233	SER	CA-C-N	-7.36	101.01	117.20
5	J	233	SER	CA-C-N	-7.36	101.02	117.20
5	D	233	SER	CA-C-N	-7.36	101.02	117.20
5	E	233	SER	CA-C-N	-7.35	101.02	117.20
5	H	180	LEU	CA-CB-CG	7.35	132.21	115.30
5	Q	233	SER	CA-C-N	-7.35	101.03	117.20
5	F	180	LEU	CA-CB-CG	7.35	132.20	115.30
5	H	254	ARG	NE-CZ-NH2	-7.35	116.63	120.30
5	K	233	SER	CA-C-N	-7.34	101.04	117.20
5	P	180	LEU	CA-CB-CG	7.34	132.19	115.30
5	R	233	SER	CA-C-N	-7.34	101.04	117.20
5	J	254	ARG	NE-CZ-NH2	-7.34	116.63	120.30
5	K	180	LEU	CA-CB-CG	7.34	132.19	115.30
5	O	180	LEU	CA-CB-CG	7.34	132.18	115.30
5	L	180	LEU	CA-CB-CG	7.34	132.18	115.30
5	M	180	LEU	CA-CB-CG	7.33	132.16	115.30
5	G	79	TRP	CD1-CG-CD2	7.33	112.16	106.30
5	N	180	LEU	CA-CB-CG	7.33	132.15	115.30
5	E	180	LEU	CA-CB-CG	7.32	132.14	115.30
5	H	233	SER	CA-C-N	-7.32	101.10	117.20
5	R	79	TRP	CD1-CG-CD2	7.30	112.14	106.30
5	Q	180	LEU	CA-CB-CG	7.30	132.08	115.30
5	L	254	ARG	NE-CZ-NH2	-7.28	116.66	120.30
5	I	180	LEU	CA-CB-CG	7.28	132.05	115.30
5	Q	79	TRP	CD1-CG-CD2	7.28	112.12	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	79	TRP	CD1-CG-CD2	7.27	112.12	106.30
5	J	79	TRP	CD1-CG-CD2	7.27	112.12	106.30
5	K	79	TRP	CD1-CG-CD2	7.27	112.11	106.30
4	B	141	LEU	CD1-CG-CD2	7.27	132.30	110.50
5	Q	254	ARG	NE-CZ-NH2	-7.26	116.67	120.30
4	U	141	LEU	CD1-CG-CD2	7.26	132.28	110.50
5	M	79	TRP	CD1-CG-CD2	7.25	112.10	106.30
5	I	254	ARG	NE-CZ-NH2	-7.25	116.67	120.30
5	N	79	TRP	CD1-CG-CD2	7.24	112.09	106.30
5	F	254	ARG	NE-CZ-NH2	-7.23	116.69	120.30
5	I	79	TRP	CD1-CG-CD2	7.23	112.08	106.30
5	N	254	ARG	NE-CZ-NH2	-7.22	116.69	120.30
5	H	79	TRP	CD1-CG-CD2	7.21	112.07	106.30
5	D	79	TRP	CD1-CG-CD2	7.21	112.07	106.30
4	A	197	LEU	N-CA-C	7.21	130.46	111.00
5	L	79	TRP	CD1-CG-CD2	7.21	112.06	106.30
5	M	254	ARG	NE-CZ-NH2	-7.21	116.70	120.30
5	P	254	ARG	NE-CZ-NH2	-7.20	116.70	120.30
5	Q	340	TRP	CE2-CD2-CG	-7.20	101.54	107.30
5	L	340	TRP	CE2-CD2-CG	-7.19	101.54	107.30
4	V	43	LEU	CD1-CG-CD2	7.19	132.07	110.50
4	A	43	LEU	CD1-CG-CD2	7.19	132.07	110.50
4	V	197	LEU	N-CA-C	7.19	130.41	111.00
5	O	79	TRP	CD1-CG-CD2	7.19	112.05	106.30
5	H	340	TRP	CE2-CD2-CG	-7.18	101.56	107.30
5	S	79	TRP	CD1-CG-CD2	7.17	112.04	106.30
5	F	79	TRP	CD1-CG-CD2	7.17	112.03	106.30
5	G	79	TRP	CE2-CD2-CG	-7.16	101.58	107.30
5	S	340	TRP	CE2-CD2-CG	-7.15	101.58	107.30
5	E	79	TRP	CD1-CG-CD2	7.14	112.02	106.30
5	G	254	ARG	NE-CZ-NH2	-7.14	116.73	120.30
5	L	79	TRP	CE2-CD2-CG	-7.14	101.59	107.30
5	N	340	TRP	CE2-CD2-CG	-7.14	101.59	107.30
5	L	206	ARG	NE-CZ-NH1	7.14	123.87	120.30
5	K	254	ARG	NE-CZ-NH2	-7.13	116.73	120.30
5	J	79	TRP	CE2-CD2-CG	-7.13	101.59	107.30
5	G	340	TRP	CE2-CD2-CG	-7.13	101.60	107.30
5	D	254	ARG	NE-CZ-NH2	-7.12	116.74	120.30
5	K	79	TRP	CE2-CD2-CG	-7.11	101.61	107.30
5	M	340	TRP	CE2-CD2-CG	-7.11	101.61	107.30
4	U	155	TYR	CB-CG-CD2	7.11	125.27	121.00
5	H	206	ARG	NE-CZ-NH1	7.11	123.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	253	LEU	CB-CG-CD1	-7.10	98.92	111.00
5	O	340	TRP	CE2-CD2-CG	-7.10	101.62	107.30
4	W	253	LEU	CB-CG-CD1	-7.10	98.93	111.00
4	U	253	LEU	CB-CG-CD1	-7.10	98.94	111.00
5	E	340	TRP	CE2-CD2-CG	-7.09	101.62	107.30
5	R	79	TRP	CE2-CD2-CG	-7.09	101.63	107.30
5	H	340	TRP	CD1-CG-CD2	7.09	111.97	106.30
4	B	43	LEU	CD1-CG-CD2	7.09	131.76	110.50
5	Q	79	TRP	CE2-CD2-CG	-7.09	101.63	107.30
5	N	79	TRP	CE2-CD2-CG	-7.08	101.63	107.30
5	Q	340	TRP	CD1-CG-CD2	7.08	111.97	106.30
4	B	253	LEU	CB-CG-CD1	-7.08	98.96	111.00
5	S	206	ARG	NE-CZ-NH1	7.08	123.84	120.30
4	A	141	LEU	CD1-CG-CD2	7.07	131.72	110.50
4	V	141	LEU	CD1-CG-CD2	7.07	131.72	110.50
5	F	340	TRP	CE2-CD2-CG	-7.07	101.64	107.30
5	M	206	ARG	NE-CZ-NH1	7.07	123.84	120.30
5	J	47	MET	CA-CB-CG	-7.07	101.28	113.30
5	O	206	ARG	NE-CZ-NH1	7.07	123.83	120.30
4	U	43	LEU	CD1-CG-CD2	7.07	131.71	110.50
4	U	169	LEU	N-CA-C	7.07	130.08	111.00
5	R	340	TRP	CE2-CD2-CG	-7.07	101.65	107.30
5	O	79	TRP	CE2-CD2-CG	-7.06	101.65	107.30
5	P	340	TRP	CE2-CD2-CG	-7.06	101.65	107.30
5	E	47	MET	CA-CB-CG	-7.06	101.30	113.30
5	P	206	ARG	NE-CZ-NH1	7.06	123.83	120.30
5	I	340	TRP	CE2-CD2-CG	-7.06	101.66	107.30
5	P	79	TRP	CE2-CD2-CG	-7.05	101.66	107.30
5	K	340	TRP	CE2-CD2-CG	-7.05	101.66	107.30
5	M	79	TRP	CE2-CD2-CG	-7.05	101.66	107.30
5	S	47	MET	CA-CB-CG	-7.04	101.32	113.30
5	D	340	TRP	CE2-CD2-CG	-7.04	101.67	107.30
4	T	251	ASP	CB-CG-OD1	7.04	124.64	118.30
5	D	47	MET	CA-CB-CG	-7.04	101.33	113.30
5	L	47	MET	CA-CB-CG	-7.04	101.33	113.30
5	P	47	MET	CA-CB-CG	-7.04	101.33	113.30
5	D	79	TRP	CE2-CD2-CG	-7.03	101.67	107.30
5	F	79	TRP	CE2-CD2-CG	-7.03	101.67	107.30
5	O	47	MET	CA-CB-CG	-7.03	101.34	113.30
5	F	206	ARG	NE-CZ-NH1	7.03	123.81	120.30
4	B	169	LEU	N-CA-C	7.02	129.97	111.00
5	I	47	MET	CA-CB-CG	-7.02	101.37	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	190	LEU	CD1-CG-CD2	7.02	131.55	110.50
5	E	79	TRP	CE2-CD2-CG	-7.02	101.69	107.30
4	B	197	LEU	CB-CG-CD1	-7.01	99.08	111.00
5	M	47	MET	CA-CB-CG	-7.01	101.38	113.30
5	K	47	MET	CA-CB-CG	-7.01	101.38	113.30
5	S	79	TRP	CE2-CD2-CG	-7.00	101.70	107.30
4	C	251	ASP	CB-CG-OD1	7.00	124.60	118.30
5	F	340	TRP	CD1-CG-CD2	7.00	111.90	106.30
4	U	190	LEU	CD1-CG-CD2	7.00	131.51	110.50
4	B	251	ASP	CB-CG-OD1	7.00	124.60	118.30
4	U	197	LEU	CB-CG-CD1	-7.00	99.10	111.00
4	U	251	ASP	CB-CG-OD1	7.00	124.60	118.30
4	W	251	ASP	CB-CG-OD1	7.00	124.60	118.30
4	V	251	ASP	CB-CG-OD1	7.00	124.60	118.30
5	G	47	MET	CA-CB-CG	-7.00	101.40	113.30
5	N	47	MET	CA-CB-CG	-7.00	101.40	113.30
5	R	254	ARG	NE-CZ-NH2	-7.00	116.80	120.30
5	H	79	TRP	CE2-CD2-CG	-7.00	101.70	107.30
5	J	206	ARG	NE-CZ-NH1	7.00	123.80	120.30
4	A	251	ASP	CB-CG-OD1	6.99	124.59	118.30
4	X	251	ASP	CB-CG-OD1	6.99	124.59	118.30
5	G	206	ARG	NE-CZ-NH1	6.99	123.80	120.30
5	Q	47	MET	CA-CB-CG	-6.99	101.42	113.30
5	H	47	MET	CA-CB-CG	-6.99	101.42	113.30
5	I	79	TRP	CE2-CD2-CG	-6.98	101.72	107.30
5	R	206	ARG	NE-CZ-NH1	6.98	123.79	120.30
5	I	206	ARG	NE-CZ-NH1	6.98	123.79	120.30
5	N	206	ARG	NE-CZ-NH1	6.98	123.79	120.30
5	E	206	ARG	NE-CZ-NH1	6.98	123.79	120.30
5	R	47	MET	CA-CB-CG	-6.97	101.44	113.30
5	J	340	TRP	CE2-CD2-CG	-6.97	101.72	107.30
5	Q	206	ARG	NE-CZ-NH1	6.97	123.79	120.30
4	B	155	TYR	CB-CG-CD2	6.97	125.18	121.00
5	F	47	MET	CA-CB-CG	-6.96	101.46	113.30
5	R	340	TRP	CD1-CG-CD2	6.96	111.87	106.30
5	K	206	ARG	NE-CZ-NH1	6.96	123.78	120.30
5	G	340	TRP	CD1-CG-CD2	6.94	111.85	106.30
5	M	340	TRP	CD1-CG-CD2	6.94	111.85	106.30
5	O	340	TRP	CD1-CG-CD2	6.94	111.85	106.30
4	V	169	LEU	N-CA-C	6.92	129.70	111.00
5	L	340	TRP	CD1-CG-CD2	6.92	111.84	106.30
5	D	340	TRP	CD1-CG-CD2	6.91	111.83	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	340	TRP	CD1-CG-CD2	6.91	111.83	106.30
5	P	340	TRP	CD1-CG-CD2	6.91	111.83	106.30
5	J	340	TRP	CD1-CG-CD2	6.90	111.82	106.30
5	S	340	TRP	CD1-CG-CD2	6.89	111.81	106.30
4	A	169	LEU	N-CA-C	6.89	129.61	111.00
5	I	340	TRP	CD1-CG-CD2	6.89	111.81	106.30
5	K	340	TRP	CD1-CG-CD2	6.87	111.79	106.30
5	D	206	ARG	NE-CZ-NH1	6.86	123.73	120.30
5	N	340	TRP	CD1-CG-CD2	6.86	111.78	106.30
5	Q	169	TYR	CB-CG-CD2	-6.76	116.94	121.00
5	D	169	TYR	CB-CG-CD2	-6.76	116.94	121.00
5	J	169	TYR	CB-CG-CD2	-6.73	116.96	121.00
5	S	169	TYR	CB-CG-CD2	-6.71	116.97	121.00
4	U	34	ASP	CB-CG-OD1	6.70	124.33	118.30
4	B	34	ASP	CB-CG-OD1	6.68	124.31	118.30
5	O	169	TYR	CB-CG-CD2	-6.67	117.00	121.00
5	H	169	TYR	CB-CG-CD2	-6.64	117.01	121.00
5	F	169	TYR	CB-CG-CD2	-6.61	117.03	121.00
5	L	169	TYR	CB-CG-CD2	-6.60	117.04	121.00
5	E	169	TYR	CB-CG-CD2	-6.58	117.05	121.00
5	N	169	TYR	CB-CG-CD2	-6.57	117.06	121.00
5	E	283	MET	CG-SD-CE	6.56	110.70	100.20
5	M	283	MET	CG-SD-CE	6.55	110.68	100.20
5	D	283	MET	CG-SD-CE	6.54	110.67	100.20
5	L	283	MET	CG-SD-CE	6.54	110.67	100.20
5	S	283	MET	CG-SD-CE	6.54	110.67	100.20
5	F	283	MET	CG-SD-CE	6.54	110.66	100.20
5	N	283	MET	CG-SD-CE	6.54	110.66	100.20
5	K	283	MET	CG-SD-CE	6.53	110.65	100.20
5	R	283	MET	CG-SD-CE	6.53	110.65	100.20
5	H	283	MET	CG-SD-CE	6.53	110.65	100.20
5	P	283	MET	CG-SD-CE	6.53	110.65	100.20
5	R	169	TYR	CB-CG-CD2	-6.53	117.08	121.00
5	D	196	ARG	NE-CZ-NH1	6.52	123.56	120.30
5	I	283	MET	CG-SD-CE	6.52	110.63	100.20
5	Q	283	MET	CG-SD-CE	6.52	110.63	100.20
5	P	169	TYR	CB-CG-CD2	-6.52	117.09	121.00
5	J	283	MET	CG-SD-CE	6.51	110.62	100.20
5	G	283	MET	CG-SD-CE	6.51	110.62	100.20
5	R	196	ARG	NE-CZ-NH1	6.51	123.56	120.30
5	O	283	MET	CG-SD-CE	6.50	110.59	100.20
5	P	159	VAL	CB-CA-C	-6.49	99.08	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	159	VAL	CB-CA-C	-6.48	99.08	111.40
5	K	196	ARG	NE-CZ-NH1	6.48	123.54	120.30
5	O	196	ARG	NE-CZ-NH1	6.48	123.54	120.30
5	R	159	VAL	CB-CA-C	-6.48	99.08	111.40
4	V	34	ASP	CB-CG-OD1	6.48	124.13	118.30
4	A	130	ASP	CA-C-N	6.48	131.45	117.20
5	L	196	ARG	NE-CZ-NH1	6.48	123.54	120.30
5	F	159	VAL	CB-CA-C	-6.47	99.10	111.40
5	D	159	VAL	CB-CA-C	-6.47	99.10	111.40
5	J	159	VAL	CB-CA-C	-6.47	99.11	111.40
5	Q	159	VAL	CB-CA-C	-6.47	99.11	111.40
5	K	169	TYR	CB-CG-CD2	-6.47	117.12	121.00
4	V	130	ASP	CA-C-N	6.46	131.42	117.20
5	H	159	VAL	CB-CA-C	-6.46	99.12	111.40
5	S	196	ARG	NE-CZ-NH1	6.46	123.53	120.30
5	H	34	ILE	CA-CB-CG2	-6.46	97.99	110.90
5	K	159	VAL	CB-CA-C	-6.46	99.13	111.40
5	N	159	VAL	CB-CA-C	-6.46	99.13	111.40
5	M	159	VAL	CB-CA-C	-6.45	99.14	111.40
5	S	159	VAL	CB-CA-C	-6.45	99.14	111.40
5	P	196	ARG	NE-CZ-NH1	6.45	123.53	120.30
5	I	159	VAL	CB-CA-C	-6.44	99.16	111.40
5	G	169	TYR	CB-CG-CD2	-6.44	117.14	121.00
5	L	159	VAL	CB-CA-C	-6.44	99.17	111.40
5	O	159	VAL	CB-CA-C	-6.43	99.17	111.40
5	J	196	ARG	NE-CZ-NH1	6.43	123.52	120.30
5	P	34	ILE	CA-CB-CG2	-6.43	98.05	110.90
5	N	34	ILE	CA-CB-CG2	-6.42	98.05	110.90
5	I	34	ILE	CA-CB-CG2	-6.42	98.05	110.90
5	J	34	ILE	CA-CB-CG2	-6.42	98.06	110.90
4	A	154	LYS	CA-CB-CG	6.41	127.51	113.40
5	S	34	ILE	CA-CB-CG2	-6.41	98.07	110.90
5	E	159	VAL	CB-CA-C	-6.41	99.22	111.40
5	F	34	ILE	CA-CB-CG2	-6.41	98.08	110.90
5	L	34	ILE	CA-CB-CG2	-6.41	98.08	110.90
5	R	34	ILE	CA-CB-CG2	-6.40	98.09	110.90
4	A	34	ASP	CB-CG-OD1	6.40	124.06	118.30
4	V	154	LYS	CA-CB-CG	6.40	127.48	113.40
5	F	196	ARG	NE-CZ-NH1	6.39	123.50	120.30
5	M	34	ILE	CA-CB-CG2	-6.39	98.11	110.90
5	E	34	ILE	CA-CB-CG2	-6.39	98.11	110.90
5	Q	34	ILE	CA-CB-CG2	-6.39	98.12	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	34	ILE	CA-CB-CG2	-6.39	98.12	110.90
5	D	34	ILE	CA-CB-CG2	-6.39	98.13	110.90
5	G	34	ILE	CA-CB-CG2	-6.38	98.14	110.90
5	I	196	ARG	NE-CZ-NH1	6.38	123.49	120.30
5	M	169	TYR	CB-CG-CD2	-6.36	117.18	121.00
4	B	197	LEU	N-CA-C	6.36	128.17	111.00
5	N	196	ARG	NE-CZ-NH1	6.35	123.47	120.30
5	O	34	ILE	CA-CB-CG2	-6.35	98.21	110.90
4	B	155	TYR	CD1-CG-CD2	6.34	124.88	117.90
5	D	217	CYS	CA-CB-SG	-6.34	102.59	114.00
5	E	217	CYS	CA-CB-SG	-6.34	102.59	114.00
5	M	196	ARG	NE-CZ-NH1	6.32	123.46	120.30
4	U	197	LEU	N-CA-C	6.32	128.08	111.00
4	A	154	LYS	N-CA-CB	-6.32	99.23	110.60
5	P	217	CYS	CA-CB-SG	-6.32	102.63	114.00
4	V	154	LYS	N-CA-CB	-6.30	99.25	110.60
5	J	217	CYS	CA-CB-SG	-6.30	102.66	114.00
5	M	217	CYS	CA-CB-SG	-6.30	102.66	114.00
5	E	196	ARG	NE-CZ-NH1	6.30	123.45	120.30
5	Q	217	CYS	CA-CB-SG	-6.29	102.67	114.00
5	I	217	CYS	CA-CB-SG	-6.29	102.67	114.00
5	N	217	CYS	CA-CB-SG	-6.29	102.68	114.00
5	K	217	CYS	CA-CB-SG	-6.28	102.69	114.00
5	R	217	CYS	CA-CB-SG	-6.28	102.70	114.00
4	U	154	LYS	C-N-CA	6.28	137.40	121.70
5	G	217	CYS	CA-CB-SG	-6.28	102.70	114.00
5	H	217	CYS	CA-CB-SG	-6.28	102.70	114.00
5	O	217	CYS	CA-CB-SG	-6.27	102.71	114.00
5	F	217	CYS	CA-CB-SG	-6.26	102.72	114.00
4	B	154	LYS	C-N-CA	6.26	137.35	121.70
4	U	130	ASP	CA-C-N	6.25	130.94	117.20
5	H	196	ARG	NE-CZ-NH1	6.24	123.42	120.30
5	L	217	CYS	CA-CB-SG	-6.24	102.77	114.00
5	S	217	CYS	CA-CB-SG	-6.24	102.77	114.00
4	U	155	TYR	CD1-CG-CD2	6.24	124.76	117.90
5	G	196	ARG	NE-CZ-NH1	6.23	123.41	120.30
4	B	130	ASP	CA-C-N	6.23	130.90	117.20
4	B	155	TYR	CZ-CE2-CD2	-6.18	114.24	119.80
5	Q	196	ARG	NE-CZ-NH1	6.18	123.39	120.30
5	I	169	TYR	CB-CG-CD2	-6.18	117.29	121.00
4	U	155	TYR	CZ-CE2-CD2	-6.16	114.26	119.80
5	F	259	GLU	CA-CB-CG	6.15	126.93	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	259	GLU	CA-CB-CG	6.15	126.92	113.40
5	L	259	GLU	CA-CB-CG	6.13	126.89	113.40
5	K	259	GLU	CA-CB-CG	6.13	126.89	113.40
5	M	259	GLU	CA-CB-CG	6.13	126.89	113.40
5	D	259	GLU	CA-CB-CG	6.13	126.88	113.40
5	G	259	GLU	CA-CB-CG	6.13	126.88	113.40
5	P	259	GLU	CA-CB-CG	6.13	126.88	113.40
5	Q	259	GLU	CA-CB-CG	6.13	126.88	113.40
5	N	259	GLU	CA-CB-CG	6.12	126.87	113.40
5	J	259	GLU	CA-CB-CG	6.12	126.87	113.40
5	O	259	GLU	CA-CB-CG	6.12	126.87	113.40
5	D	335	ARG	NE-CZ-NH2	-6.12	117.24	120.30
5	H	259	GLU	CA-CB-CG	6.12	126.86	113.40
5	R	259	GLU	CA-CB-CG	6.12	126.86	113.40
4	U	155	TYR	CA-CB-CG	6.11	125.01	113.40
5	I	259	GLU	CA-CB-CG	6.11	126.83	113.40
5	E	259	GLU	CA-CB-CG	6.11	126.83	113.40
4	B	155	TYR	CA-CB-CG	6.10	125.00	113.40
5	F	16	LEU	CA-CB-CG	6.08	129.28	115.30
5	M	16	LEU	CA-CB-CG	6.07	129.25	115.30
5	H	335	ARG	NE-CZ-NH2	-6.06	117.27	120.30
5	F	116	ARG	NE-CZ-NH1	6.06	123.33	120.30
5	P	16	LEU	CA-CB-CG	6.06	129.24	115.30
5	D	349	LEU	CA-C-N	-6.06	103.87	117.20
4	V	154	LYS	C-N-CA	6.06	136.84	121.70
4	A	154	LYS	C-N-CA	6.05	136.84	121.70
5	K	349	LEU	CA-C-N	-6.05	103.88	117.20
5	O	16	LEU	CA-CB-CG	6.05	129.22	115.30
5	I	16	LEU	CA-CB-CG	6.05	129.22	115.30
5	D	16	LEU	CA-CB-CG	6.05	129.21	115.30
5	H	349	LEU	CA-C-N	-6.05	103.89	117.20
5	N	16	LEU	CA-CB-CG	6.04	129.20	115.30
5	P	79	TRP	CG-CD2-CE3	6.04	139.34	133.90
5	F	335	ARG	NE-CZ-NH2	-6.04	117.28	120.30
5	N	79	TRP	CG-CD2-CE3	6.04	139.34	133.90
5	H	16	LEU	CA-CB-CG	6.04	129.18	115.30
5	K	16	LEU	CA-CB-CG	6.04	129.18	115.30
5	S	349	LEU	CA-C-N	-6.04	103.92	117.20
5	L	16	LEU	CA-CB-CG	6.03	129.18	115.30
5	R	349	LEU	CA-C-N	-6.03	103.92	117.20
5	J	16	LEU	CA-CB-CG	6.03	129.17	115.30
5	Q	16	LEU	CA-CB-CG	6.03	129.17	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	335	ARG	NE-CZ-NH2	-6.03	117.28	120.30
5	S	16	LEU	CA-CB-CG	6.03	129.16	115.30
5	E	16	LEU	CA-CB-CG	6.02	129.16	115.30
5	I	349	LEU	CA-C-N	-6.02	103.95	117.20
5	R	16	LEU	CA-CB-CG	6.02	129.15	115.30
5	L	349	LEU	CA-C-N	-6.02	103.96	117.20
5	P	349	LEU	CA-C-N	-6.02	103.96	117.20
5	G	16	LEU	CA-CB-CG	6.01	129.13	115.30
5	G	349	LEU	CA-C-N	-6.01	103.98	117.20
5	N	349	LEU	CA-C-N	-6.01	103.98	117.20
5	Q	79	TRP	CG-CD2-CE3	6.01	139.31	133.90
5	J	349	LEU	CA-C-N	-6.01	103.99	117.20
5	O	349	LEU	CA-C-N	-6.01	103.99	117.20
5	K	79	TRP	CG-CD2-CE3	6.00	139.30	133.90
5	K	254	ARG	NE-CZ-NH1	6.00	123.30	120.30
5	E	349	LEU	CA-C-N	-5.99	104.02	117.20
5	O	79	TRP	CG-CD2-CE3	5.99	139.29	133.90
5	F	349	LEU	CA-C-N	-5.99	104.03	117.20
5	E	79	TRP	CG-CD2-CE3	5.98	139.28	133.90
5	G	79	TRP	CG-CD2-CE3	5.98	139.28	133.90
5	K	335	ARG	NE-CZ-NH2	-5.98	117.31	120.30
5	R	335	ARG	NE-CZ-NH2	-5.98	117.31	120.30
5	Q	349	LEU	CA-C-N	-5.97	104.06	117.20
5	R	79	TRP	CG-CD2-CE3	5.97	139.27	133.90
5	M	79	TRP	CG-CD2-CE3	5.96	139.27	133.90
5	Q	335	ARG	NE-CZ-NH2	-5.96	117.32	120.30
5	M	349	LEU	CA-C-N	-5.94	104.12	117.20
5	M	335	ARG	NE-CZ-NH2	-5.94	117.33	120.30
5	J	79	TRP	CG-CD2-CE3	5.93	139.23	133.90
5	K	116	ARG	NE-CZ-NH1	5.92	123.26	120.30
5	F	79	TRP	CG-CD2-CE3	5.92	139.23	133.90
5	H	79	TRP	CG-CD2-CE3	5.91	139.22	133.90
5	I	79	TRP	CG-CD2-CE3	5.91	139.22	133.90
5	S	79	TRP	CG-CD2-CE3	5.91	139.22	133.90
5	E	335	ARG	NE-CZ-NH2	-5.90	117.35	120.30
5	L	79	TRP	CG-CD2-CE3	5.90	139.21	133.90
4	C	274	MET	N-CA-CB	5.90	121.22	110.60
4	A	274	MET	N-CA-CB	5.89	121.20	110.60
5	J	335	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	3	107	ASN	N-CA-C	-5.88	95.12	111.00
5	R	200	PHE	CA-C-N	-5.88	104.26	117.20
5	H	254	ARG	NE-CZ-NH1	5.88	123.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	200	PHE	CA-C-N	-5.88	104.27	117.20
4	V	274	MET	N-CA-CB	5.88	121.18	110.60
5	N	200	PHE	CA-C-N	-5.87	104.28	117.20
4	X	274	MET	N-CA-CB	5.87	121.17	110.60
5	M	200	PHE	CA-C-N	-5.87	104.29	117.20
5	R	116	ARG	NE-CZ-NH1	5.87	123.23	120.30
4	U	22	LYS	CB-CG-CD	-5.87	96.35	111.60
4	B	22	LYS	CB-CG-CD	-5.86	96.36	111.60
5	M	116	ARG	NE-CZ-NH1	5.86	123.23	120.30
5	R	254	ARG	NE-CZ-NH1	5.86	123.23	120.30
5	H	200	PHE	CA-C-N	-5.86	104.31	117.20
5	Q	200	PHE	CA-C-N	-5.86	104.31	117.20
1	0	107	ASN	N-CA-C	-5.85	95.20	111.00
5	F	200	PHE	CA-C-N	-5.85	104.33	117.20
5	G	200	PHE	CA-C-N	-5.85	104.33	117.20
5	E	200	PHE	CA-C-N	-5.84	104.35	117.20
1	6	107	ASN	N-CA-C	-5.84	95.24	111.00
5	J	200	PHE	CA-C-N	-5.84	104.36	117.20
5	O	200	PHE	CA-C-N	-5.84	104.36	117.20
4	V	36	LEU	CB-CG-CD1	-5.84	101.08	111.00
5	D	79	TRP	CG-CD2-CE3	5.83	139.15	133.90
4	A	36	LEU	CB-CG-CD1	-5.83	101.09	111.00
5	D	116	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	9	107	ASN	N-CA-C	-5.83	95.27	111.00
5	L	200	PHE	CA-C-N	-5.83	104.38	117.20
5	E	95	ARG	CA-CB-CG	5.82	126.21	113.40
4	A	151	ALA	CA-C-N	5.82	130.01	117.20
5	O	254	ARG	NE-CZ-NH1	5.82	123.21	120.30
5	D	200	PHE	CA-C-N	-5.82	104.40	117.20
5	P	200	PHE	CA-C-N	-5.82	104.40	117.20
5	I	200	PHE	CA-C-N	-5.82	104.41	117.20
5	O	335	ARG	NE-CZ-NH2	-5.82	117.39	120.30
4	V	151	ALA	CA-C-N	5.82	129.99	117.20
5	L	95	ARG	CA-CB-CG	5.81	126.19	113.40
5	S	95	ARG	CA-CB-CG	5.81	126.19	113.40
5	S	200	PHE	CA-C-N	-5.81	104.41	117.20
5	G	254	ARG	NE-CZ-NH1	5.80	123.20	120.30
5	I	95	ARG	CA-CB-CG	5.80	126.17	113.40
5	E	254	ARG	NE-CZ-NH1	5.80	123.20	120.30
5	M	95	ARG	CA-CB-CG	5.79	126.15	113.40
5	I	335	ARG	NE-CZ-NH2	-5.79	117.40	120.30
5	J	95	ARG	CA-CB-CG	5.79	126.14	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	95	ARG	CA-CB-CG	5.79	126.15	113.40
5	D	95	ARG	CA-CB-CG	5.79	126.13	113.40
4	A	274	MET	CB-CA-C	-5.79	98.83	110.40
4	C	274	MET	CB-CA-C	-5.78	98.83	110.40
5	G	335	ARG	NE-CZ-NH2	-5.78	117.41	120.30
5	Q	95	ARG	CA-CB-CG	5.78	126.12	113.40
5	J	254	ARG	NE-CZ-NH1	5.78	123.19	120.30
5	K	95	ARG	CA-CB-CG	5.77	126.10	113.40
5	F	95	ARG	CA-CB-CG	5.77	126.10	113.40
4	V	274	MET	CB-CA-C	-5.77	98.86	110.40
5	J	116	ARG	NE-CZ-NH1	5.77	123.18	120.30
5	P	95	ARG	CA-CB-CG	5.77	126.09	113.40
5	G	95	ARG	CA-CB-CG	5.76	126.08	113.40
5	O	95	ARG	CA-CB-CG	5.76	126.07	113.40
5	M	254	ARG	NE-CZ-NH1	5.75	123.18	120.30
5	P	335	ARG	NE-CZ-NH2	-5.75	117.43	120.30
4	W	253	LEU	CD1-CG-CD2	5.75	127.74	110.50
4	X	274	MET	CB-CA-C	-5.75	98.90	110.40
4	U	253	LEU	CD1-CG-CD2	5.75	127.73	110.50
5	Q	116	ARG	NE-CZ-NH1	5.74	123.17	120.30
5	N	116	ARG	NE-CZ-NH1	5.74	123.17	120.30
4	T	253	LEU	CD1-CG-CD2	5.74	127.72	110.50
5	H	95	ARG	CA-CB-CG	5.74	126.02	113.40
4	B	253	LEU	CD1-CG-CD2	5.73	127.70	110.50
5	G	116	ARG	NE-CZ-NH1	5.73	123.17	120.30
5	R	95	ARG	CA-CB-CG	5.73	126.01	113.40
5	Q	254	ARG	NE-CZ-NH1	5.73	123.16	120.30
5	P	335	ARG	CA-CB-CG	5.72	125.99	113.40
5	I	335	ARG	CA-CB-CG	5.72	125.98	113.40
5	K	335	ARG	CA-CB-CG	5.72	125.98	113.40
5	P	116	ARG	NE-CZ-NH1	5.72	123.16	120.30
5	Q	335	ARG	CA-CB-CG	5.72	125.98	113.40
5	D	335	ARG	CA-CB-CG	5.71	125.96	113.40
5	R	335	ARG	CA-CB-CG	5.71	125.96	113.40
5	F	254	ARG	NE-CZ-NH1	5.71	123.15	120.30
5	N	335	ARG	CA-CB-CG	5.71	125.95	113.40
5	J	335	ARG	CA-CB-CG	5.71	125.95	113.40
5	N	254	ARG	NE-CZ-NH1	5.70	123.15	120.30
5	O	335	ARG	CA-CB-CG	5.70	125.94	113.40
5	M	335	ARG	CA-CB-CG	5.70	125.93	113.40
5	F	335	ARG	CA-CB-CG	5.69	125.93	113.40
5	S	335	ARG	NE-CZ-NH2	-5.69	117.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	279	TYR	CB-CG-CD2	-5.69	117.58	121.00
5	G	335	ARG	CA-CB-CG	5.69	125.91	113.40
5	S	254	ARG	NE-CZ-NH1	5.68	123.14	120.30
5	E	335	ARG	CA-CB-CG	5.68	125.89	113.40
5	H	335	ARG	CA-CB-CG	5.68	125.89	113.40
5	N	356	TRP	CG-CD2-CE3	5.68	139.01	133.90
5	L	335	ARG	CA-CB-CG	5.67	125.88	113.40
5	D	254	ARG	NE-CZ-NH1	5.67	123.13	120.30
5	S	335	ARG	CA-CB-CG	5.67	125.86	113.40
5	E	294	TYR	CB-CG-CD2	-5.66	117.60	121.00
4	U	155	TYR	CD1-CE1-CZ	5.65	124.89	119.80
5	L	279	TYR	CB-CG-CD2	-5.65	117.61	121.00
5	N	279	TYR	CB-CG-CD2	-5.65	117.61	121.00
5	P	294	TYR	CB-CG-CD2	-5.65	117.61	121.00
5	H	116	ARG	NE-CZ-NH1	5.63	123.12	120.30
5	G	294	TYR	CB-CG-CD2	-5.63	117.62	121.00
5	S	116	ARG	NE-CZ-NH1	5.63	123.11	120.30
5	L	254	ARG	NE-CZ-NH1	5.62	123.11	120.30
5	F	294	TYR	CB-CG-CD2	-5.62	117.63	121.00
5	E	356	TRP	CG-CD2-CE3	5.62	138.96	133.90
5	R	356	TRP	CG-CD2-CE3	5.62	138.96	133.90
5	M	356	TRP	CG-CD2-CE3	5.61	138.95	133.90
5	I	254	ARG	NE-CZ-NH1	5.61	123.11	120.30
5	S	279	TYR	CB-CG-CD2	-5.61	117.63	121.00
5	K	356	TRP	CG-CD2-CE3	5.61	138.95	133.90
5	G	356	TRP	CG-CD2-CE3	5.61	138.95	133.90
5	L	113	LYS	CA-CB-CG	5.61	125.73	113.40
5	S	113	LYS	CA-CB-CG	5.61	125.73	113.40
5	F	356	TRP	CG-CD2-CE3	5.60	138.94	133.90
5	L	116	ARG	NE-CZ-NH1	5.60	123.10	120.30
5	Q	113	LYS	CA-CB-CG	5.60	125.72	113.40
5	F	113	LYS	CA-CB-CG	5.60	125.71	113.40
5	G	113	LYS	CA-CB-CG	5.60	125.71	113.40
5	M	113	LYS	CA-CB-CG	5.59	125.71	113.40
5	H	113	LYS	CA-CB-CG	5.59	125.70	113.40
5	P	254	ARG	NE-CZ-NH1	5.59	123.09	120.30
5	J	113	LYS	CA-CB-CG	5.59	125.69	113.40
5	P	113	LYS	CA-CB-CG	5.59	125.69	113.40
5	D	294	TYR	CB-CG-CD2	-5.58	117.65	121.00
5	L	356	TRP	CG-CD2-CE3	5.58	138.92	133.90
5	D	254	ARG	N-CA-CB	-5.58	100.56	110.60
5	N	113	LYS	CA-CB-CG	5.58	125.67	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	113	LYS	CA-CB-CG	5.58	125.67	113.40
5	O	116	ARG	NE-CZ-NH1	5.57	123.09	120.30
5	I	113	LYS	CA-CB-CG	5.56	125.64	113.40
5	R	254	ARG	N-CA-CB	-5.56	100.59	110.60
5	K	113	LYS	CA-CB-CG	5.56	125.63	113.40
5	O	113	LYS	CA-CB-CG	5.56	125.63	113.40
5	E	116	ARG	NE-CZ-NH1	5.56	123.08	120.30
5	N	294	TYR	CB-CG-CD2	-5.56	117.67	121.00
5	E	113	LYS	CA-CB-CG	5.56	125.63	113.40
5	J	11	ASP	CB-CG-OD1	5.56	123.30	118.30
4	T	267	LEU	N-CA-C	5.56	126.00	111.00
5	L	335	ARG	NE-CZ-NH2	-5.55	117.52	120.30
5	D	356	TRP	CG-CD2-CE3	5.55	138.90	133.90
4	B	267	LEU	N-CA-C	5.55	125.98	111.00
5	J	254	ARG	N-CA-CB	-5.55	100.61	110.60
5	S	356	TRP	CG-CD2-CE3	5.55	138.89	133.90
4	V	197	LEU	CA-CB-CG	-5.55	102.53	115.30
5	K	11	ASP	CB-CG-OD1	5.55	123.29	118.30
5	L	294	TYR	CB-CG-CD2	-5.54	117.67	121.00
5	M	11	ASP	CB-CG-OD1	5.54	123.29	118.30
5	N	254	ARG	N-CA-CB	-5.54	100.62	110.60
5	P	279	TYR	CB-CG-CD2	-5.54	117.67	121.00
5	Q	279	TYR	CB-CG-CD2	-5.54	117.67	121.00
5	M	254	ARG	N-CA-CB	-5.54	100.63	110.60
5	F	254	ARG	N-CA-CB	-5.54	100.63	110.60
5	K	254	ARG	N-CA-CB	-5.54	100.63	110.60
4	A	197	LEU	CA-CB-CG	-5.54	102.57	115.30
5	O	254	ARG	N-CA-CB	-5.54	100.64	110.60
5	H	147	ARG	NE-CZ-NH2	-5.53	117.53	120.30
5	I	279	TYR	CB-CG-CD2	-5.53	117.68	121.00
5	K	279	TYR	CB-CG-CD2	-5.53	117.68	121.00
5	P	254	ARG	N-CA-CB	-5.53	100.64	110.60
5	G	254	ARG	N-CA-CB	-5.53	100.65	110.60
5	S	254	ARG	N-CA-CB	-5.53	100.64	110.60
4	V	253	LEU	CA-CB-CG	-5.53	102.58	115.30
4	X	253	LEU	CA-CB-CG	-5.53	102.58	115.30
4	B	36	LEU	CB-CG-CD1	-5.53	101.60	111.00
5	R	294	TYR	CB-CG-CD2	-5.53	117.68	121.00
5	D	113	LYS	CA-CB-CG	5.53	125.56	113.40
5	J	356	TRP	CG-CD2-CE3	5.53	138.87	133.90
5	Q	254	ARG	N-CA-CB	-5.53	100.66	110.60
5	S	294	TYR	CB-CG-CD2	-5.53	117.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	11	ASP	CB-CG-OD1	5.52	123.27	118.30
4	A	154	LYS	N-CA-C	5.52	125.91	111.00
5	L	254	ARG	N-CA-CB	-5.52	100.66	110.60
5	Q	147	ARG	NE-CZ-NH2	-5.52	117.54	120.30
5	I	116	ARG	NE-CZ-NH1	5.52	123.06	120.30
4	U	267	LEU	N-CA-C	5.52	125.90	111.00
5	F	11	ASP	CB-CG-OD1	5.52	123.27	118.30
5	H	294	TYR	CB-CG-CD2	-5.52	117.69	121.00
5	I	254	ARG	N-CA-CB	-5.52	100.67	110.60
4	U	36	LEU	CB-CG-CD1	-5.52	101.62	111.00
4	C	253	LEU	CA-CB-CG	-5.51	102.62	115.30
5	E	254	ARG	N-CA-CB	-5.51	100.67	110.60
5	O	356	TRP	CG-CD2-CE3	5.51	138.86	133.90
4	B	155	TYR	CD1-CE1-CZ	5.51	124.76	119.80
5	H	11	ASP	CB-CG-OD1	5.51	123.26	118.30
4	W	267	LEU	N-CA-C	5.51	125.88	111.00
4	A	253	LEU	CA-CB-CG	-5.51	102.63	115.30
5	G	279	TYR	CB-CG-CD2	-5.51	117.69	121.00
5	I	294	TYR	CB-CG-CD2	-5.51	117.69	121.00
5	H	254	ARG	N-CA-CB	-5.51	100.69	110.60
5	O	279	TYR	CB-CG-CD2	-5.50	117.70	121.00
4	V	154	LYS	N-CA-C	5.50	125.86	111.00
4	W	274	MET	N-CA-CB	5.49	120.49	110.60
4	U	274	MET	N-CA-CB	5.49	120.49	110.60
5	H	279	TYR	CB-CG-CD2	-5.49	117.70	121.00
5	R	279	TYR	CB-CG-CD2	-5.49	117.71	121.00
5	E	11	ASP	CB-CG-OD1	5.49	123.24	118.30
5	J	279	TYR	CB-CG-CD2	-5.49	117.71	121.00
5	H	356	TRP	CG-CD2-CE3	5.49	138.84	133.90
5	P	11	ASP	CB-CG-OD1	5.48	123.23	118.30
5	M	294	TYR	CB-CG-CD2	-5.48	117.71	121.00
5	K	294	TYR	CB-CG-CD2	-5.48	117.71	121.00
5	S	11	ASP	CB-CG-OD1	5.48	123.23	118.30
5	M	279	TYR	CB-CG-CD2	-5.47	117.72	121.00
4	V	22	LYS	CB-CG-CD	-5.47	97.38	111.60
4	V	73	ASP	CA-CB-CG	5.46	125.42	113.40
5	D	11	ASP	CB-CG-OD1	5.46	123.22	118.30
5	I	356	TRP	CG-CD2-CE3	5.46	138.81	133.90
5	O	335	ARG	NE-CZ-NH1	5.46	123.03	120.30
4	A	22	LYS	CB-CG-CD	-5.46	97.41	111.60
5	D	279	TYR	CB-CG-CD2	-5.46	117.72	121.00
4	B	274	MET	N-CA-CB	5.46	120.42	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	335	ARG	NE-CZ-NH1	5.46	123.03	120.30
4	T	274	MET	N-CA-CB	5.45	120.42	110.60
4	A	73	ASP	CA-CB-CG	5.45	125.39	113.40
5	I	11	ASP	CB-CG-OD1	5.45	123.20	118.30
4	T	274	MET	CB-CA-C	-5.44	99.51	110.40
5	G	356	TRP	CB-CG-CD1	-5.44	119.93	127.00
4	B	274	MET	CB-CA-C	-5.44	99.52	110.40
5	R	356	TRP	CB-CG-CD1	-5.44	119.93	127.00
5	D	147	ARG	NE-CZ-NH2	-5.43	117.58	120.30
5	G	11	ASP	CB-CG-OD1	5.43	123.19	118.30
4	U	274	MET	CB-CA-C	-5.43	99.54	110.40
5	S	356	TRP	CB-CG-CD1	-5.43	119.94	127.00
5	J	294	TYR	CB-CG-CD2	-5.43	117.74	121.00
5	R	79	TRP	CB-CG-CD1	-5.42	119.95	127.00
5	O	294	TYR	CB-CG-CD2	-5.42	117.75	121.00
5	P	356	TRP	CG-CD2-CE3	5.42	138.78	133.90
5	S	147	ARG	NE-CZ-NH2	-5.42	117.59	120.30
5	L	356	TRP	CB-CG-CD1	-5.42	119.95	127.00
5	D	79	TRP	CB-CG-CD1	-5.42	119.95	127.00
5	Q	356	TRP	CG-CD2-CE3	5.42	138.78	133.90
5	S	79	TRP	CB-CG-CD1	-5.42	119.95	127.00
5	K	356	TRP	CB-CG-CD1	-5.42	119.95	127.00
5	R	11	ASP	CB-CG-OD1	5.42	123.18	118.30
4	W	274	MET	CB-CA-C	-5.42	99.56	110.40
5	M	356	TRP	CB-CG-CD1	-5.42	119.96	127.00
4	U	73	ASP	CA-CB-CG	5.42	125.31	113.40
4	B	73	ASP	CA-CB-CG	5.41	125.31	113.40
5	J	356	TRP	CB-CG-CD1	-5.41	119.97	127.00
4	U	169	LEU	CB-CA-C	-5.41	99.92	110.20
5	O	356	TRP	CB-CG-CD1	-5.41	119.97	127.00
5	N	356	TRP	CG-CD1-NE1	-5.41	104.69	110.10
5	G	356	TRP	CG-CD1-NE1	-5.40	104.70	110.10
5	O	11	ASP	CB-CG-OD1	5.40	123.16	118.30
5	Q	294	TYR	CB-CG-CD2	-5.40	117.76	121.00
5	H	79	TRP	CB-CG-CD1	-5.40	119.98	127.00
5	G	79	TRP	CB-CG-CD1	-5.40	119.98	127.00
5	N	356	TRP	CB-CG-CD1	-5.40	119.98	127.00
5	P	356	TRP	CG-CD1-NE1	-5.40	104.70	110.10
5	H	356	TRP	CB-CG-CD1	-5.40	119.99	127.00
5	M	79	TRP	CB-CG-CD1	-5.39	119.99	127.00
4	B	260	TYR	CA-C-O	-5.39	108.78	120.10
5	J	356	TRP	CG-CD1-NE1	-5.39	104.71	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	356	TRP	CG-CD1-NE1	-5.39	104.71	110.10
4	B	169	LEU	CB-CA-C	-5.39	99.96	110.20
5	L	79	TRP	CB-CG-CD1	-5.39	119.99	127.00
5	P	356	TRP	CB-CG-CD1	-5.39	120.00	127.00
5	N	11	ASP	CB-CG-OD1	5.38	123.14	118.30
5	J	251	GLY	CA-C-N	-5.38	105.36	117.20
5	Q	11	ASP	CB-CG-OD1	5.38	123.14	118.30
5	I	79	TRP	CB-CG-CD1	-5.38	120.01	127.00
5	L	356	TRP	CG-CD1-NE1	-5.38	104.72	110.10
5	Q	356	TRP	CB-CG-CD1	-5.38	120.01	127.00
5	Q	356	TRP	CG-CD1-NE1	-5.38	104.72	110.10
5	F	335	ARG	NE-CZ-NH1	5.38	122.99	120.30
5	J	79	TRP	CB-CG-CD1	-5.38	120.01	127.00
5	L	251	GLY	CA-C-N	-5.38	105.37	117.20
5	Q	251	GLY	CA-C-N	-5.37	105.38	117.20
5	S	251	GLY	CA-C-N	-5.37	105.38	117.20
5	O	79	TRP	CB-CG-CD1	-5.37	120.02	127.00
4	X	253	LEU	CD1-CG-CD2	5.37	126.62	110.50
5	E	356	TRP	CB-CG-CD1	-5.37	120.02	127.00
4	T	260	TYR	CA-C-O	-5.37	108.82	120.10
5	G	251	GLY	CA-C-N	-5.37	105.39	117.20
5	P	79	TRP	CB-CG-CD1	-5.37	120.02	127.00
5	P	251	GLY	CA-C-N	-5.37	105.39	117.20
5	K	79	TRP	CB-CG-CD1	-5.37	120.03	127.00
5	M	251	GLY	CA-C-N	-5.37	105.39	117.20
5	R	356	TRP	CG-CD1-NE1	-5.37	104.73	110.10
5	F	356	TRP	CB-CG-CD1	-5.36	120.03	127.00
5	H	356	TRP	CG-CD1-NE1	-5.36	104.74	110.10
5	F	79	TRP	CB-CG-CD1	-5.36	120.03	127.00
4	A	137	GLN	CA-CB-CG	-5.36	101.61	113.40
5	N	335	ARG	NE-CZ-NH1	5.36	122.98	120.30
5	O	251	GLY	CA-C-N	-5.36	105.41	117.20
5	Q	79	TRP	CB-CG-CD1	-5.36	120.03	127.00
5	F	251	GLY	CA-C-N	-5.36	105.41	117.20
4	U	260	TYR	CA-C-O	-5.36	108.86	120.10
4	V	137	GLN	CA-CB-CG	-5.36	101.62	113.40
4	V	253	LEU	CD1-CG-CD2	5.36	126.57	110.50
4	C	253	LEU	CD1-CG-CD2	5.35	126.56	110.50
5	I	356	TRP	CB-CG-CD1	-5.35	120.04	127.00
5	M	356	TRP	CG-CD1-NE1	-5.35	104.75	110.10
5	S	356	TRP	CG-CD1-NE1	-5.35	104.75	110.10
5	G	176	MET	CG-SD-CE	5.35	108.76	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	169	LEU	CB-CA-C	-5.35	100.03	110.20
5	D	251	GLY	CA-C-N	-5.35	105.43	117.20
5	E	251	GLY	CA-C-N	-5.35	105.43	117.20
4	W	260	TYR	CA-C-O	-5.35	108.87	120.10
5	F	279	TYR	CB-CG-CD2	-5.35	117.79	121.00
4	A	253	LEU	CD1-CG-CD2	5.34	126.53	110.50
5	E	356	TRP	CG-CD1-NE1	-5.34	104.76	110.10
5	N	251	GLY	CA-C-N	-5.34	105.45	117.20
5	D	356	TRP	CG-CD1-NE1	-5.34	104.76	110.10
5	F	356	TRP	CG-CD1-NE1	-5.34	104.76	110.10
5	I	251	GLY	CA-C-N	-5.33	105.46	117.20
5	E	147	ARG	NE-CZ-NH2	-5.33	117.63	120.30
5	K	251	GLY	CA-C-N	-5.33	105.47	117.20
5	Q	176	MET	CG-SD-CE	5.33	108.73	100.20
5	R	176	MET	CG-SD-CE	5.33	108.73	100.20
5	O	356	TRP	CG-CD1-NE1	-5.33	104.77	110.10
5	Q	335	ARG	NE-CZ-NH1	5.33	122.97	120.30
5	I	356	TRP	CG-CD1-NE1	-5.33	104.77	110.10
5	J	176	MET	CG-SD-CE	5.33	108.72	100.20
5	H	251	GLY	CA-C-N	-5.32	105.49	117.20
5	K	176	MET	CG-SD-CE	5.32	108.72	100.20
5	R	251	GLY	CA-C-N	-5.32	105.49	117.20
5	O	147	ARG	NE-CZ-NH2	-5.32	117.64	120.30
5	F	176	MET	CG-SD-CE	5.32	108.71	100.20
5	R	147	ARG	NE-CZ-NH2	-5.32	117.64	120.30
5	E	79	TRP	CB-CG-CD1	-5.31	120.10	127.00
5	N	176	MET	CG-SD-CE	5.31	108.70	100.20
5	O	176	MET	CG-SD-CE	5.31	108.70	100.20
4	A	169	LEU	CB-CA-C	-5.31	100.11	110.20
5	D	356	TRP	CB-CG-CD1	-5.31	120.10	127.00
5	N	79	TRP	CB-CG-CD1	-5.31	120.10	127.00
4	C	260	TYR	CA-C-O	-5.31	108.95	120.10
5	M	176	MET	CG-SD-CE	5.31	108.69	100.20
5	D	176	MET	CG-SD-CE	5.30	108.69	100.20
4	X	260	TYR	CA-C-O	-5.30	108.97	120.10
5	Q	337	TYR	CB-CG-CD1	-5.30	117.82	121.00
5	S	176	MET	CG-SD-CE	5.30	108.68	100.20
4	V	260	TYR	CA-C-O	-5.29	108.98	120.10
5	J	91	TYR	CB-CG-CD2	-5.29	117.83	121.00
5	L	176	MET	CG-SD-CE	5.29	108.67	100.20
4	U	155	TYR	CB-CA-C	5.29	120.98	110.40
4	B	155	TYR	CB-CA-C	5.29	120.97	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	335	ARG	NE-CZ-NH1	5.29	122.94	120.30
5	I	176	MET	CG-SD-CE	5.28	108.66	100.20
4	A	260	TYR	CA-C-O	-5.28	109.01	120.10
5	J	147	ARG	NE-CZ-NH2	-5.27	117.66	120.30
5	P	147	ARG	NE-CZ-NH2	-5.27	117.66	120.30
5	M	147	ARG	NE-CZ-NH2	-5.27	117.66	120.30
5	F	91	TYR	CB-CG-CD2	-5.27	117.84	121.00
5	H	176	MET	CG-SD-CE	5.27	108.62	100.20
4	A	152	ASP	N-CA-C	5.26	125.21	111.00
5	Q	91	TYR	CB-CG-CD2	-5.26	117.84	121.00
5	P	176	MET	CG-SD-CE	5.26	108.62	100.20
4	U	137	GLN	CA-CB-CG	-5.26	101.82	113.40
5	G	335	ARG	NE-CZ-NH1	5.26	122.93	120.30
5	I	147	ARG	NE-CZ-NH2	-5.26	117.67	120.30
5	L	147	ARG	NE-CZ-NH2	-5.26	117.67	120.30
4	B	137	GLN	CA-CB-CG	-5.25	101.84	113.40
5	D	53	TYR	CB-CG-CD1	-5.25	117.85	121.00
5	E	176	MET	CG-SD-CE	5.25	108.60	100.20
5	F	53	TYR	CB-CG-CD1	-5.25	117.85	121.00
5	P	335	ARG	NE-CZ-NH1	5.24	122.92	120.30
4	V	152	ASP	N-CA-C	5.23	125.13	111.00
5	G	147	ARG	NE-CZ-NH2	-5.23	117.69	120.30
5	H	335	ARG	NE-CZ-NH1	5.23	122.92	120.30
5	K	147	ARG	NE-CZ-NH2	-5.23	117.69	120.30
4	W	248	ASP	CA-CB-CG	5.22	124.89	113.40
5	D	335	ARG	NE-CZ-NH1	5.22	122.91	120.30
5	D	91	TYR	CB-CG-CD2	-5.22	117.87	121.00
5	I	337	TYR	CB-CG-CD1	-5.21	117.87	121.00
5	L	290	ARG	CA-C-N	5.21	128.66	117.20
5	G	62	ARG	NE-CZ-NH1	5.20	122.90	120.30
5	M	335	ARG	NE-CZ-NH1	5.20	122.90	120.30
5	Q	86	TRP	CG-CD1-NE1	-5.20	104.90	110.10
4	U	248	ASP	CA-CB-CG	5.20	124.84	113.40
5	S	290	ARG	CA-C-N	5.20	128.63	117.20
4	B	248	ASP	CA-CB-CG	5.19	124.82	113.40
5	O	290	ARG	CA-C-N	5.19	128.61	117.20
5	P	290	ARG	CA-C-N	5.18	128.61	117.20
5	R	290	ARG	CA-C-N	5.18	128.60	117.20
5	I	290	ARG	CA-C-N	5.18	128.59	117.20
5	E	290	ARG	CA-C-N	5.18	128.59	117.20
5	G	337	TYR	CB-CG-CD1	-5.18	117.89	121.00
5	N	337	TYR	CB-CG-CD1	-5.18	117.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	248	ASP	CA-CB-CG	5.18	124.79	113.40
5	F	147	ARG	NE-CZ-NH2	-5.17	117.71	120.30
5	F	337	TYR	CB-CG-CD1	-5.17	117.90	121.00
5	Q	290	ARG	CA-C-N	5.17	128.58	117.20
5	H	337	TYR	CB-CG-CD1	-5.17	117.90	121.00
5	K	290	ARG	CA-C-N	5.17	128.56	117.20
4	X	267	LEU	N-CA-C	5.16	124.94	111.00
5	F	290	ARG	CA-C-N	5.16	128.56	117.20
5	J	290	ARG	CA-C-N	5.16	128.55	117.20
5	N	290	ARG	CA-C-N	5.16	128.56	117.20
5	I	335	ARG	NE-CZ-NH1	5.16	122.88	120.30
5	G	290	ARG	CA-C-N	5.16	128.55	117.20
5	Q	53	TYR	CB-CG-CD1	-5.16	117.91	121.00
4	V	267	LEU	N-CA-C	5.16	124.92	111.00
5	F	62	ARG	NE-CZ-NH1	5.15	122.88	120.30
5	O	337	TYR	CB-CG-CD1	-5.15	117.91	121.00
5	I	91	TYR	CB-CG-CD2	-5.15	117.91	121.00
5	M	290	ARG	CA-C-N	5.15	128.52	117.20
5	P	91	TYR	CB-CG-CD2	-5.15	117.91	121.00
5	H	290	ARG	CA-C-N	5.14	128.52	117.20
4	A	267	LEU	N-CA-C	5.14	124.88	111.00
5	J	337	TYR	CB-CG-CD1	-5.14	117.92	121.00
5	O	53	TYR	CB-CG-CD1	-5.14	117.92	121.00
5	R	53	TYR	CB-CG-CD1	-5.14	117.92	121.00
5	D	290	ARG	CA-C-N	5.14	128.50	117.20
5	S	91	TYR	CB-CG-CD2	-5.14	117.92	121.00
5	I	62	ARG	NE-CZ-NH1	5.14	122.87	120.30
4	C	267	LEU	N-CA-C	5.13	124.86	111.00
5	N	147	ARG	NE-CZ-NH2	-5.13	117.73	120.30
4	X	274	MET	CG-SD-CE	5.13	108.41	100.20
4	V	274	MET	CG-SD-CE	5.13	108.41	100.20
5	M	337	TYR	CB-CG-CD1	-5.13	117.92	121.00
5	O	91	TYR	CB-CG-CD2	-5.12	117.93	121.00
5	N	53	TYR	CB-CG-CD1	-5.12	117.93	121.00
4	A	274	MET	CG-SD-CE	5.12	108.39	100.20
4	C	274	MET	CG-SD-CE	5.12	108.39	100.20
5	K	53	TYR	CB-CG-CD1	-5.12	117.93	121.00
5	L	335	ARG	NE-CZ-NH1	5.12	122.86	120.30
5	S	62	ARG	CA-CB-CG	5.11	124.65	113.40
5	E	337	TYR	CB-CG-CD1	-5.11	117.93	121.00
5	N	62	ARG	CA-CB-CG	5.11	124.64	113.40
5	G	53	TYR	CB-CG-CD1	-5.11	117.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	335	ARG	NE-CZ-NH1	5.10	122.85	120.30
4	B	92	LEU	CB-CA-C	-5.10	100.51	110.20
5	P	53	TYR	CB-CG-CD1	-5.10	117.94	121.00
5	S	53	TYR	CB-CG-CD1	-5.10	117.94	121.00
5	R	337	TYR	CB-CG-CD1	-5.10	117.94	121.00
5	J	86	TRP	CG-CD1-NE1	-5.10	105.00	110.10
5	G	86	TRP	CG-CD1-NE1	-5.09	105.00	110.10
5	M	53	TYR	CB-CG-CD1	-5.09	117.94	121.00
5	N	86	TRP	CG-CD1-NE1	-5.09	105.00	110.10
5	N	191	LYS	CA-C-N	5.09	128.41	117.20
5	F	62	ARG	CA-CB-CG	5.09	124.61	113.40
5	L	62	ARG	CA-CB-CG	5.09	124.60	113.40
5	E	62	ARG	CA-CB-CG	5.09	124.60	113.40
5	D	62	ARG	CA-CB-CG	5.09	124.59	113.40
5	F	191	LYS	CA-C-N	5.09	128.39	117.20
5	G	91	TYR	CB-CG-CD2	-5.09	117.95	121.00
5	N	91	TYR	CB-CG-CD2	-5.09	117.95	121.00
5	O	62	ARG	CA-CB-CG	5.09	124.59	113.40
5	J	62	ARG	CA-CB-CG	5.08	124.59	113.40
5	P	86	TRP	CG-CD1-NE1	-5.08	105.02	110.10
5	H	91	TYR	CB-CG-CD2	-5.08	117.95	121.00
5	M	91	TYR	CB-CG-CD2	-5.08	117.95	121.00
5	L	53	TYR	CB-CG-CD1	-5.08	117.95	121.00
5	Q	62	ARG	CA-CB-CG	5.08	124.58	113.40
5	R	62	ARG	CA-CB-CG	5.08	124.58	113.40
5	I	62	ARG	CA-CB-CG	5.08	124.58	113.40
5	D	337	TYR	CB-CG-CD1	-5.08	117.95	121.00
5	K	62	ARG	CA-CB-CG	5.08	124.57	113.40
5	K	335	ARG	NE-CZ-NH1	5.08	122.84	120.30
5	K	337	TYR	CB-CG-CD1	-5.08	117.95	121.00
5	P	62	ARG	CA-CB-CG	5.08	124.57	113.40
5	I	191	LYS	CA-C-N	5.08	128.37	117.20
5	M	62	ARG	CA-CB-CG	5.08	124.57	113.40
5	O	86	TRP	CG-CD1-NE1	-5.08	105.03	110.10
5	H	191	LYS	CA-C-N	5.07	128.36	117.20
5	J	191	LYS	CA-C-N	5.07	128.36	117.20
5	D	86	TRP	CG-CD1-NE1	-5.07	105.03	110.10
5	J	53	TYR	CB-CG-CD1	-5.07	117.96	121.00
5	O	191	LYS	CA-C-N	5.07	128.35	117.20
5	G	62	ARG	CA-CB-CG	5.07	124.54	113.40
5	G	191	LYS	CA-C-N	5.07	128.34	117.20
4	U	92	LEU	CB-CA-C	-5.06	100.58	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	53	TYR	CB-CG-CD1	-5.06	117.96	121.00
5	M	191	LYS	CA-C-N	5.06	128.33	117.20
5	P	337	TYR	CB-CG-CD1	-5.06	117.96	121.00
5	R	86	TRP	CG-CD1-NE1	-5.06	105.04	110.10
4	V	64	LEU	N-CA-C	5.06	124.66	111.00
5	D	191	LYS	CA-C-N	5.06	128.32	117.20
5	H	62	ARG	CA-CB-CG	5.05	124.52	113.40
5	L	191	LYS	CA-C-N	5.05	128.31	117.20
5	R	335	ARG	NE-CZ-NH1	5.05	122.83	120.30
4	A	64	LEU	N-CA-C	5.05	124.63	111.00
5	L	337	TYR	CB-CG-CD1	-5.05	117.97	121.00
5	E	191	LYS	CA-C-N	5.04	128.30	117.20
5	R	191	LYS	CA-C-N	5.04	128.30	117.20
5	K	191	LYS	CA-C-N	5.04	128.30	117.20
5	O	62	ARG	NE-CZ-NH1	5.04	122.82	120.30
5	N	62	ARG	NE-CZ-NH1	5.04	122.82	120.30
5	S	191	LYS	CA-C-N	5.03	128.27	117.20
5	L	91	TYR	CB-CG-CD2	-5.03	117.98	121.00
4	V	155	TYR	N-CA-C	-5.03	97.41	111.00
5	R	91	TYR	CB-CG-CD2	-5.03	117.98	121.00
5	F	86	TRP	CG-CD1-NE1	-5.03	105.07	110.10
4	U	50	LEU	N-CA-C	5.03	124.58	111.00
4	A	155	TYR	N-CA-C	-5.02	97.44	111.00
5	K	91	TYR	CB-CG-CD2	-5.02	117.99	121.00
5	P	191	LYS	CA-C-N	5.02	128.25	117.20
5	Q	191	LYS	CA-C-N	5.02	128.25	117.20
5	H	86	TRP	CG-CD1-NE1	-5.02	105.08	110.10
5	E	86	TRP	CG-CD1-NE1	-5.02	105.08	110.10
5	H	62	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	231	ARG	Sidechain
4	A	260	TYR	Sidechain
4	A	261	LYS	Mainchain
4	A	98	ARG	Sidechain
4	B	155	TYR	Sidechain
4	B	231	ARG	Sidechain
4	B	260	TYR	Sidechain
4	B	261	LYS	Mainchain

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Mol	Chain	Res	Type	Group
4	B	98	ARG	Sidechain
4	C	260	TYR	Sidechain
4	C	261	LYS	Mainchain
5	D	62	ARG	Sidechain
5	E	62	ARG	Sidechain
5	F	62	ARG	Sidechain
5	G	62	ARG	Sidechain
5	H	62	ARG	Sidechain
5	I	62	ARG	Sidechain
5	J	62	ARG	Sidechain
5	K	62	ARG	Sidechain
5	L	62	ARG	Sidechain
5	M	62	ARG	Sidechain
5	N	62	ARG	Sidechain
5	O	62	ARG	Sidechain
5	P	62	ARG	Sidechain
5	Q	62	ARG	Sidechain
5	R	62	ARG	Sidechain
5	S	62	ARG	Sidechain
4	T	260	TYR	Sidechain
4	T	261	LYS	Mainchain
4	U	155	TYR	Sidechain
4	U	231	ARG	Sidechain
4	U	260	TYR	Sidechain
4	U	261	LYS	Mainchain
4	U	98	ARG	Sidechain
4	V	231	ARG	Sidechain
4	V	260	TYR	Sidechain
4	V	261	LYS	Mainchain
4	V	98	ARG	Sidechain
4	W	260	TYR	Sidechain
4	W	261	LYS	Mainchain
4	X	260	TYR	Sidechain
4	X	261	LYS	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	0	1252	0	1172	102	0
1	3	1252	0	1172	80	0
1	6	1252	0	1172	95	0
1	9	1252	0	1172	76	0
2	1	774	0	797	48	0
2	4	774	0	796	51	0
2	7	774	0	797	48	0
2	Y	774	0	791	49	0
3	2	1140	0	1201	104	0
3	5	1140	0	1201	93	0
3	8	1140	0	1199	88	0
3	Z	1140	0	1201	86	0
4	A	2230	0	2227	0	0
4	B	2230	0	2227	0	0
4	C	316	0	314	0	0
4	T	316	0	312	0	0
4	U	2230	0	2227	0	0
4	V	2230	0	2227	0	0
4	W	316	0	307	0	0
4	X	316	0	314	0	0
5	D	2907	0	2862	101	0
5	E	2907	0	2862	101	0
5	F	2907	0	2864	101	0
5	G	2907	0	2864	98	0
5	H	2907	0	2864	103	0
5	I	2907	0	2864	102	0
5	J	2907	0	2864	103	0
5	K	2907	0	2864	103	0
5	L	2907	0	2864	97	0
5	M	2907	0	2864	104	0
5	N	2907	0	2864	105	0
5	O	2907	0	2864	104	0
5	P	2907	0	2860	120	0
5	Q	2907	0	2863	116	0
5	R	2907	0	2863	115	0
5	S	2907	0	2862	94	0
6	0	4	0	0	0	0
6	3	4	0	0	0	0
6	6	4	0	0	0	0
6	9	4	0	0	0	0
All	All	69376	0	68638	2028	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 17.

All (2028) 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)
3:2:100:PHE:CG	5:R:5:THR:HG22	1.40	1.54
3:5:97:GLN:HE22	5:Q:4:GLU:CG	1.19	1.49
1:0:62:GLU:CG	5:P:360:GLN:HB2	1.52	1.40
1:0:62:GLU:CG	5:P:359:LYS:HD2	1.52	1.38
3:5:97:GLN:NE2	5:Q:4:GLU:CG	1.85	1.37
1:9:62:GLU:OE2	5:S:359:LYS:HD3	1.22	1.33
1:0:62:GLU:CB	5:P:359:LYS:CD	1.76	1.32
1:0:62:GLU:HB2	5:P:359:LYS:CD	0.92	1.32
1:0:62:GLU:OE2	5:P:358:THR:HB	1.21	1.31
3:5:97:GLN:NE2	5:Q:4:GLU:HG3	1.45	1.28
1:0:62:GLU:OE1	5:P:359:LYS:CE	1.82	1.26
3:8:97:GLN:HA	5:S:4:GLU:OE2	1.36	1.25
3:2:100:PHE:CG	5:R:5:THR:CG2	2.06	1.24
1:3:59:ALA:N	5:R:360:GLN:HG3	1.50	1.23
1:0:62:GLU:OE1	5:P:359:LYS:HE3	1.36	1.23
5:L:322:PRO:CB	5:N:244:ASP:OD2	1.88	1.22
5:N:322:PRO:CB	5:R:244:ASP:OD2	1.88	1.22
5:E:244:ASP:OD2	5:Q:322:PRO:CB	1.88	1.22
5:O:322:PRO:CB	5:S:244:ASP:OD2	1.88	1.22
5:I:322:PRO:CB	5:K:244:ASP:OD2	1.88	1.21
5:D:322:PRO:CB	5:F:244:ASP:OD2	1.88	1.21
5:F:322:PRO:CB	5:H:244:ASP:OD2	1.88	1.21
5:J:322:PRO:CB	5:L:244:ASP:OD2	1.88	1.21
5:E:322:PRO:CB	5:G:244:ASP:OD2	1.88	1.21
5:K:322:PRO:CB	5:M:244:ASP:OD2	1.88	1.21
5:H:322:PRO:CB	5:J:244:ASP:OD2	1.88	1.20
5:D:322:PRO:HB2	5:F:244:ASP:OD2	1.41	1.20
5:D:244:ASP:OD2	5:P:322:PRO:CB	1.88	1.20
5:M:322:PRO:CB	5:O:244:ASP:OD2	1.88	1.20
5:F:322:PRO:HB2	5:H:244:ASP:OD2	1.41	1.20
5:G:322:PRO:CB	5:I:244:ASP:OD2	1.88	1.19
5:H:322:PRO:HB2	5:J:244:ASP:OD2	1.41	1.19
5:L:322:PRO:HB2	5:N:244:ASP:OD2	1.41	1.19
5:I:322:PRO:HB2	5:K:244:ASP:OD2	1.41	1.19
5:K:322:PRO:HB2	5:M:244:ASP:OD2	1.41	1.18
5:G:322:PRO:HB2	5:I:244:ASP:OD2	1.41	1.18
5:D:244:ASP:OD2	5:P:322:PRO:HB2	1.41	1.18
5:N:322:PRO:HB2	5:R:244:ASP:OD2	1.41	1.17
5:O:322:PRO:HB2	5:S:244:ASP:OD2	1.41	1.17
5:J:322:PRO:HB2	5:L:244:ASP:OD2	1.41	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:322:PRO:HB2	5:O:244:ASP:OD2	1.41	1.17
3:5:97:GLN:NE2	5:Q:4:GLU:CD	1.95	1.17
5:E:322:PRO:HB2	5:G:244:ASP:OD2	1.41	1.17
1:0:62:GLU:HG2	5:P:360:GLN:CB	1.73	1.16
5:F:290:ARG:NH2	5:H:202:THR:HG23	1.61	1.16
5:L:290:ARG:NH2	5:N:202:THR:HG23	1.61	1.16
5:D:290:ARG:NH2	5:F:202:THR:HG23	1.61	1.16
5:H:290:ARG:NH2	5:J:202:THR:HG23	1.61	1.15
5:D:202:THR:HG23	5:P:290:ARG:NH2	1.61	1.15
5:E:244:ASP:OD2	5:Q:322:PRO:HB2	1.41	1.15
1:0:62:GLU:CB	5:P:359:LYS:HD3	1.47	1.15
5:K:290:ARG:NH2	5:M:202:THR:HG23	1.61	1.15
5:M:290:ARG:NH2	5:O:202:THR:HG23	1.61	1.15
5:J:290:ARG:NH2	5:L:202:THR:HG23	1.61	1.15
5:O:290:ARG:NH2	5:S:202:THR:HG23	1.61	1.15
5:E:202:THR:HG23	5:Q:290:ARG:NH2	1.61	1.15
1:6:55:GLU:O	5:Q:360:GLN:NE2	1.78	1.14
5:I:290:ARG:NH2	5:K:202:THR:HG23	1.61	1.14
1:0:62:GLU:CD	5:P:359:LYS:HD2	1.65	1.14
5:N:290:ARG:NH2	5:R:202:THR:HG23	1.61	1.13
5:G:290:ARG:NH2	5:I:202:THR:HG23	1.61	1.13
5:E:290:ARG:NH2	5:G:202:THR:HG23	1.61	1.13
5:E:287:ILE:HG21	5:G:205:GLU:HG2	1.18	1.11
5:F:287:ILE:HG21	5:H:205:GLU:HG2	1.18	1.10
5:H:287:ILE:HG21	5:J:205:GLU:HG2	1.18	1.10
5:N:287:ILE:HG21	5:R:205:GLU:HG2	1.18	1.10
5:D:287:ILE:HG21	5:F:205:GLU:HG2	1.18	1.09
5:G:287:ILE:HG21	5:I:205:GLU:HG2	1.18	1.09
1:0:62:GLU:CB	5:P:359:LYS:HD2	1.53	1.09
5:E:205:GLU:HG2	5:Q:287:ILE:HG21	1.18	1.09
5:N:290:ARG:CZ	5:R:202:THR:HG21	1.83	1.09
5:E:290:ARG:CZ	5:G:202:THR:HG21	1.83	1.09
5:G:290:ARG:CZ	5:I:202:THR:HG21	1.83	1.09
1:0:62:GLU:HG2	5:P:360:GLN:HB2	1.12	1.09
5:L:290:ARG:CZ	5:N:202:THR:HG21	1.83	1.09
5:D:205:GLU:HG2	5:P:287:ILE:HG21	1.18	1.09
5:I:290:ARG:CZ	5:K:202:THR:HG21	1.83	1.09
5:J:287:ILE:HG21	5:L:205:GLU:HG2	1.18	1.09
5:K:290:ARG:CZ	5:M:202:THR:HG21	1.83	1.09
5:E:202:THR:HG21	5:Q:290:ARG:CZ	1.83	1.09
5:P:5:THR:CG2	3:Z:105:LYS:HB2	1.81	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:287:ILE:HG21	5:S:205:GLU:HG2	1.18	1.08
5:O:290:ARG:CZ	5:S:202:THR:HG21	1.83	1.08
5:F:290:ARG:CZ	5:H:202:THR:HG21	1.83	1.08
5:J:290:ARG:CZ	5:L:202:THR:HG21	1.83	1.08
5:D:290:ARG:CZ	5:F:202:THR:HG21	1.83	1.08
5:M:290:ARG:CZ	5:O:202:THR:HG21	1.83	1.08
3:2:105:LYS:HG3	5:R:1:ASP:OD1	1.50	1.08
1:0:58:ASP:O	5:P:360:GLN:HG3	1.54	1.08
5:O:3:ASP:HA	5:O:6:THR:HB	1.36	1.07
5:H:290:ARG:CZ	5:J:202:THR:HG21	1.83	1.07
5:M:3:ASP:HA	5:M:6:THR:HB	1.36	1.07
5:M:287:ILE:HG21	5:O:205:GLU:HG2	1.18	1.07
5:S:3:ASP:HA	5:S:6:THR:HB	1.36	1.07
5:I:287:ILE:HG21	5:K:205:GLU:HG2	1.18	1.07
5:L:287:ILE:HG21	5:N:205:GLU:HG2	1.18	1.07
5:D:202:THR:HG21	5:P:290:ARG:CZ	1.83	1.07
5:K:287:ILE:HG21	5:M:205:GLU:HG2	1.18	1.07
5:K:3:ASP:HA	5:K:6:THR:HB	1.36	1.07
1:0:62:GLU:HG3	5:P:360:GLN:HB2	1.35	1.06
5:H:3:ASP:HA	5:H:6:THR:HB	1.36	1.05
5:F:3:ASP:HA	5:F:6:THR:HB	1.36	1.05
5:I:3:ASP:HA	5:I:6:THR:HB	1.36	1.05
5:D:3:ASP:HA	5:D:6:THR:HB	1.36	1.05
3:8:141:LYS:H	3:8:141:LYS:HD2	1.20	1.04
5:J:3:ASP:HA	5:J:6:THR:HB	1.36	1.04
1:0:62:GLU:HG2	5:P:360:GLN:N	1.72	1.04
5:P:3:ASP:HA	5:P:6:THR:HB	1.36	1.03
3:Z:141:LYS:HD2	3:Z:141:LYS:H	1.20	1.03
3:5:141:LYS:H	3:5:141:LYS:HD2	1.20	1.03
5:N:3:ASP:HA	5:N:6:THR:HB	1.36	1.02
3:2:141:LYS:HD2	3:2:141:LYS:H	1.20	1.02
5:L:3:ASP:HA	5:L:6:THR:HB	1.36	1.02
5:G:290:ARG:CZ	5:I:202:THR:CG2	2.38	1.02
5:Q:3:ASP:HA	5:Q:6:THR:HB	1.36	1.02
5:R:3:ASP:HA	5:R:6:THR:HB	1.36	1.02
5:E:290:ARG:CZ	5:G:202:THR:CG2	2.38	1.02
5:E:3:ASP:HA	5:E:6:THR:HB	1.36	1.02
5:I:290:ARG:CZ	5:K:202:THR:CG2	2.38	1.02
5:P:5:THR:HG22	3:Z:100:PHE:HE1	1.25	1.02
5:G:3:ASP:HA	5:G:6:THR:HB	1.36	1.01
5:N:290:ARG:CZ	5:R:202:THR:CG2	2.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:5:THR:HG21	3:Z:105:LYS:HB2	1.01	1.01
5:E:202:THR:CG2	5:Q:290:ARG:CZ	2.38	1.01
5:F:290:ARG:CZ	5:H:202:THR:CG2	2.38	1.01
1:O:62:GLU:CD	5:P:359:LYS:CD	2.28	1.01
5:K:290:ARG:CZ	5:M:202:THR:CG2	2.38	1.01
5:D:290:ARG:CZ	5:F:202:THR:CG2	2.38	1.01
5:H:290:ARG:CZ	5:J:202:THR:CG2	2.38	1.01
5:O:290:ARG:CZ	5:S:202:THR:CG2	2.38	1.01
5:M:290:ARG:CZ	5:O:202:THR:CG2	2.38	1.00
5:G:287:ILE:HB	5:I:204:ALA:H	1.27	1.00
5:K:287:ILE:HB	5:M:204:ALA:H	1.27	1.00
5:D:202:THR:CG2	5:P:290:ARG:CZ	2.38	1.00
5:F:290:ARG:NH2	5:H:202:THR:CG2	2.25	1.00
5:H:290:ARG:NH2	5:J:202:THR:CG2	2.25	1.00
5:M:290:ARG:NH2	5:O:202:THR:CG2	2.25	1.00
5:D:290:ARG:NH2	5:F:202:THR:CG2	2.25	1.00
5:J:290:ARG:CZ	5:L:202:THR:CG2	2.38	1.00
5:D:204:ALA:H	5:P:287:ILE:HB	1.27	1.00
5:D:202:THR:CG2	5:P:290:ARG:NH2	2.25	1.00
1:O:62:GLU:OE1	5:P:359:LYS:NZ	1.92	1.00
5:O:290:ARG:NH2	5:S:202:THR:CG2	2.25	1.00
5:O:287:ILE:HB	5:S:204:ALA:H	1.27	1.00
3:2:97:GLN:HE22	5:R:4:GLU:HG3	1.26	1.00
5:F:287:ILE:HB	5:H:204:ALA:H	1.27	1.00
5:J:290:ARG:NH2	5:L:202:THR:CG2	2.25	1.00
5:K:290:ARG:NH2	5:M:202:THR:CG2	2.25	1.00
5:L:290:ARG:CZ	5:N:202:THR:CG2	2.38	1.00
5:E:204:ALA:H	5:Q:287:ILE:HB	1.27	1.00
5:L:290:ARG:NH2	5:N:202:THR:CG2	2.25	0.99
5:I:290:ARG:NH2	5:K:202:THR:CG2	2.25	0.99
5:J:287:ILE:HB	5:L:204:ALA:H	1.27	0.99
5:G:290:ARG:NH2	5:I:202:THR:CG2	2.25	0.99
5:N:290:ARG:NH2	5:R:202:THR:CG2	2.25	0.99
5:D:287:ILE:HB	5:F:204:ALA:H	1.26	0.98
5:O:286:ASP:OD1	5:S:203:THR:HG22	1.64	0.98
5:E:286:ASP:OD1	5:G:203:THR:HG22	1.64	0.98
5:N:286:ASP:OD1	5:R:203:THR:HG22	1.64	0.98
5:G:322:PRO:HB3	5:I:244:ASP:OD2	1.64	0.98
5:K:286:ASP:OD1	5:M:203:THR:HG22	1.64	0.98
5:D:322:PRO:HB3	5:F:244:ASP:OD2	1.64	0.98
5:E:322:PRO:HB3	5:G:244:ASP:OD2	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:322:PRO:HB3	5:K:244:ASP:OD2	1.64	0.98
5:D:203:THR:HG22	5:P:286:ASP:OD1	1.64	0.98
1:0:62:GLU:HG2	5:P:360:GLN:CA	1.93	0.98
5:L:287:ILE:HB	5:N:204:ALA:H	1.27	0.98
5:F:286:ASP:OD1	5:H:203:THR:HG22	1.64	0.98
5:H:287:ILE:HB	5:J:204:ALA:H	1.26	0.98
5:I:286:ASP:OD1	5:K:203:THR:HG22	1.64	0.98
5:K:322:PRO:HB3	5:M:244:ASP:OD2	1.64	0.98
5:N:287:ILE:HB	5:R:204:ALA:H	1.27	0.98
5:O:322:PRO:HB3	5:S:244:ASP:OD2	1.64	0.98
5:F:322:PRO:HB3	5:H:244:ASP:OD2	1.64	0.98
5:M:322:PRO:HB3	5:O:244:ASP:OD2	1.64	0.97
5:D:244:ASP:OD2	5:P:322:PRO:HB3	1.64	0.97
5:E:290:ARG:NH2	5:G:202:THR:CG2	2.25	0.97
5:J:286:ASP:OD1	5:L:203:THR:HG22	1.64	0.97
5:I:287:ILE:HB	5:K:204:ALA:H	1.27	0.97
5:H:322:PRO:HB3	5:J:244:ASP:OD2	1.64	0.97
5:E:202:THR:CG2	5:Q:290:ARG:NH2	2.25	0.97
5:L:286:ASP:OD1	5:N:203:THR:HG22	1.64	0.97
5:E:287:ILE:HB	5:G:204:ALA:H	1.27	0.97
1:9:55:GLU:HA	5:S:360:GLN:CD	1.71	0.97
5:E:203:THR:HG22	5:Q:286:ASP:OD1	1.64	0.97
1:9:55:GLU:HA	5:S:360:GLN:OE1	1.64	0.97
5:E:244:ASP:OD2	5:Q:322:PRO:HB3	1.64	0.97
5:M:287:ILE:HB	5:O:204:ALA:H	1.27	0.96
5:G:286:ASP:OD1	5:I:203:THR:HG22	1.64	0.96
5:D:286:ASP:OD1	5:F:203:THR:HG22	1.64	0.96
5:M:286:ASP:OD1	5:O:203:THR:HG22	1.64	0.96
5:J:322:PRO:HB3	5:L:244:ASP:OD2	1.64	0.96
1:6:58:ASP:HB2	5:Q:360:GLN:NE2	1.80	0.96
3:Z:53:LEU:HD13	3:Z:53:LEU:H	1.31	0.95
1:0:62:GLU:CG	5:P:360:GLN:CB	2.38	0.95
1:0:58:ASP:C	5:P:360:GLN:HG3	1.80	0.95
1:0:62:GLU:OE2	5:P:358:THR:CB	2.15	0.95
1:9:62:GLU:OE2	5:S:359:LYS:CD	2.14	0.95
5:J:288:ASP:HA	5:L:204:ALA:HB2	1.49	0.95
1:0:62:GLU:CD	5:P:359:LYS:CE	2.33	0.95
5:H:288:ASP:HA	5:J:204:ALA:HB2	1.49	0.95
5:H:286:ASP:OD1	5:J:203:THR:HG22	1.64	0.95
1:0:62:GLU:HB2	5:P:359:LYS:HD2	1.16	0.95
3:8:53:LEU:H	3:8:53:LEU:HD13	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:288:ASP:HA	5:N:204:ALA:HB2	1.49	0.95
3:5:53:LEU:H	3:5:53:LEU:HD13	1.31	0.95
5:F:288:ASP:HA	5:H:204:ALA:HB2	1.49	0.95
5:L:322:PRO:HB3	5:N:244:ASP:OD2	1.64	0.95
5:M:288:ASP:HA	5:O:204:ALA:HB2	1.49	0.95
5:N:288:ASP:HA	5:R:204:ALA:HB2	1.49	0.95
5:O:288:ASP:HA	5:S:204:ALA:HB2	1.49	0.95
5:D:204:ALA:HB2	5:P:288:ASP:HA	1.49	0.94
5:K:288:ASP:HA	5:M:204:ALA:HB2	1.49	0.94
3:2:53:LEU:HD13	3:2:53:LEU:H	1.31	0.94
5:D:288:ASP:HA	5:F:204:ALA:HB2	1.49	0.94
5:G:288:ASP:HA	5:I:204:ALA:HB2	1.48	0.94
5:I:288:ASP:HA	5:K:204:ALA:HB2	1.49	0.94
5:E:204:ALA:HB2	5:Q:288:ASP:HA	1.49	0.94
5:E:288:ASP:HA	5:G:204:ALA:HB2	1.49	0.94
5:N:322:PRO:HB3	5:R:244:ASP:OD2	1.64	0.94
5:P:5:THR:HG21	3:Z:105:LYS:CB	1.97	0.93
2:Y:198:ASN:HB3	2:Y:201:LYS:HB2	1.54	0.90
2:4:198:ASN:HB3	2:4:201:LYS:HB2	1.53	0.89
1:0:61:ILE:HD12	5:P:360:GLN:HE21	1.35	0.89
1:6:55:GLU:HA	5:Q:360:GLN:NE2	1.88	0.88
2:7:198:ASN:HB3	2:7:201:LYS:HB2	1.54	0.87
1:0:62:GLU:HG2	5:P:360:GLN:H	1.35	0.87
3:2:105:LYS:CG	5:R:1:ASP:OD1	2.21	0.87
2:1:198:ASN:HB3	2:1:201:LYS:HB2	1.54	0.86
3:8:97:GLN:HA	5:S:4:GLU:CD	1.95	0.86
5:L:322:PRO:HB2	5:N:244:ASP:CG	1.96	0.86
5:E:244:ASP:CG	5:Q:322:PRO:HB2	1.96	0.86
3:2:105:LYS:HG3	5:R:1:ASP:CG	1.96	0.85
5:M:322:PRO:HB2	5:O:244:ASP:CG	1.96	0.85
5:N:322:PRO:HB2	5:R:244:ASP:CG	1.96	0.85
5:J:322:PRO:HB2	5:L:244:ASP:CG	1.96	0.85
5:D:244:ASP:CG	5:P:322:PRO:HB2	1.96	0.85
1:6:55:GLU:HA	5:Q:360:GLN:CD	1.97	0.85
3:2:100:PHE:CD1	5:R:5:THR:CG2	0.80	0.85
1:6:55:GLU:CA	5:Q:360:GLN:NE2	2.40	0.85
5:E:322:PRO:HB2	5:G:244:ASP:CG	1.96	0.85
5:I:287:ILE:CG2	5:K:205:GLU:HG2	2.07	0.85
5:N:287:ILE:CG2	5:R:205:GLU:HG2	2.07	0.85
1:6:55:GLU:C	5:Q:360:GLN:NE2	2.30	0.84
5:L:287:ILE:CG2	5:N:205:GLU:HG2	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:322:PRO:HB2	5:H:244:ASP:CG	1.96	0.84
5:H:322:PRO:HB2	5:J:244:ASP:CG	1.96	0.84
5:I:322:PRO:HB2	5:K:244:ASP:CG	1.96	0.84
5:D:322:PRO:HB2	5:F:244:ASP:CG	1.96	0.84
5:O:322:PRO:HB2	5:S:244:ASP:CG	1.96	0.84
5:G:322:PRO:HB2	5:I:244:ASP:CG	1.96	0.84
5:K:322:PRO:HB2	5:M:244:ASP:CG	1.96	0.84
5:N:237:GLU:HA	5:N:251:GLY:HA2	1.60	0.84
1:9:121:LEU:O	1:9:124:THR:HG22	1.78	0.84
5:H:287:ILE:CG2	5:J:205:GLU:HG2	2.07	0.84
5:L:237:GLU:HA	5:L:251:GLY:HA2	1.60	0.84
5:F:237:GLU:HA	5:F:251:GLY:HA2	1.60	0.83
5:M:287:ILE:CG2	5:O:205:GLU:HG2	2.07	0.83
1:0:121:LEU:O	1:0:124:THR:HG22	1.78	0.83
5:H:237:GLU:HA	5:H:251:GLY:HA2	1.60	0.83
5:J:287:ILE:CG2	5:L:205:GLU:HG2	2.07	0.83
5:Q:237:GLU:HA	5:Q:251:GLY:HA2	1.60	0.83
5:R:237:GLU:HA	5:R:251:GLY:HA2	1.60	0.83
1:3:121:LEU:O	1:3:124:THR:HG22	1.78	0.83
5:J:237:GLU:HA	5:J:251:GLY:HA2	1.60	0.83
5:D:237:GLU:HA	5:D:251:GLY:HA2	1.60	0.83
5:G:287:ILE:CG2	5:I:205:GLU:HG2	2.07	0.83
5:K:287:ILE:CG2	5:M:205:GLU:HG2	2.07	0.83
3:2:100:PHE:CD1	5:R:5:THR:HG21	1.41	0.83
5:D:287:ILE:CG2	5:F:205:GLU:HG2	2.07	0.83
5:S:237:GLU:HA	5:S:251:GLY:HA2	1.60	0.83
5:O:287:ILE:CG2	5:S:205:GLU:HG2	2.07	0.83
3:2:100:PHE:CB	5:R:4:GLU:OE2	2.27	0.82
5:E:237:GLU:HA	5:E:251:GLY:HA2	1.60	0.82
5:P:237:GLU:HA	5:P:251:GLY:HA2	1.60	0.82
1:6:121:LEU:O	1:6:124:THR:HG22	1.78	0.82
5:O:237:GLU:HA	5:O:251:GLY:HA2	1.60	0.82
5:F:287:ILE:CG2	5:H:205:GLU:HG2	2.07	0.82
5:H:286:ASP:OD1	5:J:203:THR:CG2	2.28	0.82
5:J:286:ASP:OD1	5:L:203:THR:CG2	2.28	0.81
5:D:205:GLU:HG2	5:P:287:ILE:CG2	2.07	0.81
5:G:237:GLU:HA	5:G:251:GLY:HA2	1.60	0.81
5:M:237:GLU:HA	5:M:251:GLY:HA2	1.60	0.81
5:D:203:THR:CG2	5:P:286:ASP:OD1	2.28	0.81
5:E:205:GLU:HG2	5:Q:287:ILE:CG2	2.07	0.81
5:F:286:ASP:OD1	5:H:203:THR:CG2	2.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:286:ASP:OD1	5:I:203:THR:CG2	2.28	0.81
5:L:286:ASP:OD1	5:N:203:THR:CG2	2.28	0.81
5:I:237:GLU:HA	5:I:251:GLY:HA2	1.60	0.81
5:K:237:GLU:HA	5:K:251:GLY:HA2	1.60	0.81
5:M:286:ASP:OD1	5:O:203:THR:CG2	2.28	0.81
5:D:223:PHE:HE1	5:D:255:PHE:HB2	1.46	0.81
5:E:203:THR:CG2	5:Q:286:ASP:OD1	2.28	0.81
5:F:223:PHE:HE1	5:F:255:PHE:HB2	1.46	0.81
5:E:286:ASP:OD1	5:G:203:THR:CG2	2.28	0.81
5:Q:223:PHE:HE1	5:Q:255:PHE:HB2	1.46	0.81
5:D:286:ASP:OD1	5:F:203:THR:CG2	2.28	0.80
5:K:286:ASP:OD1	5:M:203:THR:CG2	2.28	0.80
5:M:223:PHE:HE1	5:M:255:PHE:HB2	1.46	0.80
3:8:141:LYS:H	3:8:141:LYS:CD	1.94	0.80
1:6:55:GLU:HA	5:Q:360:GLN:OE1	1.82	0.80
3:2:100:PHE:HB2	5:R:4:GLU:OE2	1.81	0.80
5:P:5:THR:HG22	3:Z:100:PHE:CE1	2.13	0.80
5:I:286:ASP:OD1	5:K:203:THR:CG2	2.28	0.80
5:J:290:ARG:NH1	5:L:202:THR:HG21	1.97	0.80
5:N:286:ASP:OD1	5:R:203:THR:CG2	2.28	0.80
5:P:223:PHE:HE1	5:P:255:PHE:HB2	1.46	0.80
5:E:223:PHE:HE1	5:E:255:PHE:HB2	1.46	0.80
5:K:223:PHE:HE1	5:K:255:PHE:HB2	1.46	0.80
5:E:202:THR:HG21	5:Q:290:ARG:NH1	1.97	0.80
5:L:290:ARG:NH1	5:N:202:THR:HG21	1.97	0.80
5:H:290:ARG:NH1	5:J:202:THR:HG21	1.96	0.80
5:O:223:PHE:HE1	5:O:255:PHE:HB2	1.46	0.80
5:O:286:ASP:OD1	5:S:203:THR:CG2	2.28	0.80
5:D:202:THR:HG21	5:P:290:ARG:NH1	1.97	0.80
5:H:223:PHE:HE1	5:H:255:PHE:HB2	1.46	0.80
5:E:290:ARG:NH1	5:G:202:THR:HG21	1.97	0.80
5:O:290:ARG:NH1	5:S:202:THR:HG21	1.97	0.79
5:R:223:PHE:HE1	5:R:255:PHE:HB2	1.46	0.79
5:D:290:ARG:NH1	5:F:202:THR:HG21	1.97	0.79
5:G:290:ARG:NH1	5:I:202:THR:HG21	1.97	0.79
5:N:290:ARG:NH1	5:R:202:THR:HG21	1.97	0.79
3:2:141:LYS:CD	3:2:141:LYS:H	1.94	0.79
5:J:223:PHE:HE1	5:J:255:PHE:HB2	1.46	0.79
5:I:223:PHE:HE1	5:I:255:PHE:HB2	1.46	0.79
5:G:223:PHE:HE1	5:G:255:PHE:HB2	1.46	0.79
5:I:290:ARG:NH1	5:K:202:THR:HG21	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:290:ARG:NH1	5:O:202:THR:HG21	1.97	0.79
5:F:290:ARG:NH1	5:H:202:THR:HG21	1.97	0.79
5:N:223:PHE:HE1	5:N:255:PHE:HB2	1.46	0.79
5:S:223:PHE:HE1	5:S:255:PHE:HB2	1.46	0.79
3:2:97:GLN:HE22	5:R:4:GLU:CG	1.96	0.79
5:K:290:ARG:NH1	5:M:202:THR:HG21	1.97	0.78
5:L:223:PHE:HE1	5:L:255:PHE:HB2	1.46	0.78
3:5:97:GLN:CD	5:Q:4:GLU:CG	2.50	0.78
3:5:142:GLN:HG2	3:5:143:VAL:HG23	1.65	0.78
3:5:141:LYS:H	3:5:141:LYS:CD	1.94	0.78
3:8:142:GLN:HG2	3:8:143:VAL:HG23	1.65	0.78
1:6:58:ASP:HB2	5:Q:360:GLN:CG	2.13	0.78
3:2:142:GLN:HG2	3:2:143:VAL:HG23	1.65	0.78
3:2:141:LYS:HD2	3:2:141:LYS:N	1.99	0.78
3:2:100:PHE:CD1	5:R:5:THR:HG23	0.91	0.78
3:5:141:LYS:HD2	3:5:141:LYS:N	1.99	0.78
5:K:287:ILE:HB	5:M:204:ALA:N	1.99	0.78
5:D:204:ALA:N	5:P:287:ILE:HB	1.99	0.78
5:M:287:ILE:HB	5:O:204:ALA:N	1.99	0.77
5:E:223:PHE:HD2	5:E:312:ARG:HH21	1.32	0.77
3:Z:142:GLN:HG2	3:Z:143:VAL:HG23	1.65	0.77
1:0:61:ILE:HD12	5:P:360:GLN:NE2	1.98	0.77
3:5:97:GLN:HE22	5:Q:4:GLU:HG3	0.61	0.77
5:Q:223:PHE:HD2	5:Q:312:ARG:HH21	1.33	0.77
5:R:223:PHE:HD2	5:R:312:ARG:HH21	1.33	0.77
5:N:223:PHE:HD2	5:N:312:ARG:HH21	1.33	0.77
5:G:223:PHE:HD2	5:G:312:ARG:HH21	1.33	0.77
5:I:223:PHE:HD2	5:I:312:ARG:HH21	1.33	0.77
5:J:223:PHE:HD2	5:J:312:ARG:HH21	1.33	0.77
5:I:287:ILE:HB	5:K:204:ALA:N	1.99	0.77
5:E:287:ILE:HB	5:G:204:ALA:N	1.99	0.77
5:L:223:PHE:HD2	5:L:312:ARG:HH21	1.33	0.77
5:S:223:PHE:HD2	5:S:312:ARG:HH21	1.32	0.77
3:Z:141:LYS:CD	3:Z:141:LYS:H	1.94	0.77
5:E:204:ALA:N	5:Q:287:ILE:HB	1.99	0.76
5:H:223:PHE:HD2	5:H:312:ARG:HH21	1.33	0.76
5:D:287:ILE:HB	5:F:204:ALA:N	1.99	0.76
5:E:287:ILE:CG2	5:G:205:GLU:HG2	2.07	0.76
5:K:223:PHE:HD2	5:K:312:ARG:HH21	1.33	0.76
5:F:223:PHE:HD2	5:F:312:ARG:HH21	1.33	0.76
5:O:223:PHE:HD2	5:O:312:ARG:HH21	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:287:ILE:HB	5:I:204:ALA:N	1.99	0.76
5:M:223:PHE:HD2	5:M:312:ARG:HH21	1.33	0.76
5:H:287:ILE:HB	5:J:204:ALA:N	1.99	0.76
5:J:287:ILE:HB	5:L:204:ALA:N	1.99	0.76
5:O:287:ILE:HB	5:S:204:ALA:N	1.99	0.76
5:L:287:ILE:HB	5:N:204:ALA:N	1.99	0.76
5:P:223:PHE:HD2	5:P:312:ARG:HH21	1.33	0.76
5:D:223:PHE:HD2	5:D:312:ARG:HH21	1.33	0.75
5:N:287:ILE:HB	5:R:204:ALA:N	1.99	0.75
5:P:5:THR:CG2	3:Z:100:PHE:HE1	1.98	0.75
5:F:287:ILE:HB	5:H:204:ALA:N	1.99	0.75
1:6:65:ASP:HA	1:6:76:GLU:OE2	1.86	0.75
1:0:58:ASP:C	5:P:360:GLN:CG	2.53	0.75
5:H:253:GLU:HA	5:H:256:ARG:HG3	1.69	0.75
3:5:97:GLN:OE1	5:Q:4:GLU:HG2	1.87	0.75
5:M:290:ARG:HH22	5:O:202:THR:HG23	1.52	0.74
5:P:253:GLU:HA	5:P:256:ARG:HG3	1.69	0.74
3:Z:141:LYS:N	3:Z:141:LYS:HD2	1.99	0.74
5:S:253:GLU:HA	5:S:256:ARG:HG3	1.70	0.74
1:3:65:ASP:HA	1:3:76:GLU:OE2	1.86	0.74
5:F:253:GLU:HA	5:F:256:ARG:HG3	1.69	0.74
5:J:253:GLU:HA	5:J:256:ARG:HG3	1.69	0.74
5:O:253:GLU:HA	5:O:256:ARG:HG3	1.70	0.74
3:8:141:LYS:N	3:8:141:LYS:HD2	1.99	0.74
5:D:290:ARG:HH22	5:F:202:THR:HG23	1.52	0.74
5:D:202:THR:HG23	5:P:290:ARG:HH22	1.52	0.74
5:D:253:GLU:HA	5:D:256:ARG:HG3	1.70	0.74
1:6:58:ASP:HB2	5:Q:360:GLN:CD	2.08	0.74
5:K:253:GLU:HA	5:K:256:ARG:HG3	1.69	0.74
5:M:253:GLU:HA	5:M:256:ARG:HG3	1.69	0.74
1:0:65:ASP:HA	1:0:76:GLU:OE2	1.86	0.74
1:6:53:THR:OG1	1:6:56:GLU:HG3	1.88	0.74
5:K:290:ARG:NH1	5:M:202:THR:CG2	2.51	0.74
5:N:253:GLU:HA	5:N:256:ARG:HG3	1.69	0.74
1:9:65:ASP:HA	1:9:76:GLU:OE2	1.86	0.74
5:N:290:ARG:NH1	5:R:202:THR:CG2	2.51	0.74
5:D:202:THR:CG2	5:P:290:ARG:NH1	2.51	0.74
5:E:288:ASP:H	5:G:203:THR:HG22	1.53	0.73
5:L:253:GLU:HA	5:L:256:ARG:HG3	1.70	0.73
2:4:207:LYS:HZ2	2:4:208:GLU:HA	1.54	0.73
5:G:290:ARG:NH1	5:I:202:THR:CG2	2.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:290:ARG:NH1	5:J:202:THR:CG2	2.51	0.73
3:2:105:LYS:HA	5:R:1:ASP:OD2	1.88	0.73
1:3:155:LYS:HE3	1:3:155:LYS:HA	1.69	0.73
1:9:155:LYS:HA	1:9:155:LYS:HE3	1.69	0.73
5:E:202:THR:CG2	5:Q:290:ARG:NH1	2.51	0.73
1:6:54:LYS:O	5:Q:360:GLN:NE2	2.21	0.73
5:I:288:ASP:H	5:K:203:THR:HG22	1.54	0.73
5:I:253:GLU:HA	5:I:256:ARG:HG3	1.69	0.73
5:M:288:ASP:H	5:O:203:THR:HG22	1.54	0.73
5:Q:253:GLU:HA	5:Q:256:ARG:HG3	1.69	0.73
3:2:105:LYS:CB	5:R:1:ASP:OD1	2.37	0.73
5:G:253:GLU:HA	5:G:256:ARG:HG3	1.69	0.73
5:J:290:ARG:NH1	5:L:202:THR:CG2	2.51	0.73
5:J:288:ASP:H	5:L:203:THR:HG22	1.54	0.73
5:D:288:ASP:H	5:F:203:THR:HG22	1.53	0.73
5:R:253:GLU:HA	5:R:256:ARG:HG3	1.69	0.73
1:9:53:THR:OG1	1:9:56:GLU:HG3	1.88	0.73
5:K:290:ARG:HH22	5:M:202:THR:HG23	1.52	0.73
2:7:207:LYS:HZ2	2:7:208:GLU:HA	1.53	0.73
5:D:290:ARG:NH1	5:F:202:THR:CG2	2.51	0.73
5:E:253:GLU:HA	5:E:256:ARG:HG3	1.69	0.73
5:M:290:ARG:NH1	5:O:202:THR:CG2	2.51	0.73
5:L:288:ASP:H	5:N:203:THR:HG22	1.54	0.72
5:N:288:ASP:H	5:R:203:THR:HG22	1.54	0.72
5:E:290:ARG:NH1	5:G:202:THR:CG2	2.51	0.72
5:D:203:THR:HG22	5:P:288:ASP:H	1.53	0.72
1:3:59:ALA:H	5:R:360:GLN:HG3	1.53	0.72
5:O:288:ASP:H	5:S:203:THR:HG22	1.53	0.72
1:0:53:THR:OG1	1:0:56:GLU:HG3	1.88	0.72
1:3:59:ALA:N	5:R:360:GLN:CG	2.43	0.72
1:3:53:THR:OG1	1:3:56:GLU:HG3	1.88	0.72
5:R:3:ASP:HA	5:R:6:THR:CB	2.18	0.72
1:6:155:LYS:HA	1:6:155:LYS:HE3	1.69	0.72
5:H:288:ASP:H	5:J:203:THR:HG22	1.53	0.72
5:I:290:ARG:NH1	5:K:202:THR:CG2	2.51	0.72
5:O:3:ASP:HA	5:O:6:THR:CB	2.18	0.72
5:P:3:ASP:HA	5:P:6:THR:CB	2.18	0.72
1:6:58:ASP:HB2	5:Q:360:GLN:HE21	1.54	0.72
2:1:207:LYS:HZ2	2:1:208:GLU:HA	1.55	0.72
5:F:288:ASP:H	5:H:203:THR:HG22	1.53	0.72
5:S:3:ASP:HA	5:S:6:THR:CB	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:155:LYS:HA	1:0:155:LYS:HE3	1.69	0.72
1:6:62:GLU:OE1	5:Q:359:LYS:NZ	2.21	0.72
5:D:3:ASP:HA	5:D:6:THR:CB	2.17	0.72
5:K:288:ASP:H	5:M:203:THR:HG22	1.53	0.72
5:M:3:ASP:HA	5:M:6:THR:CB	2.18	0.72
5:N:290:ARG:HH22	5:R:202:THR:HG23	1.52	0.72
5:G:288:ASP:H	5:I:203:THR:HG22	1.53	0.71
5:E:202:THR:HG23	5:Q:290:ARG:HH22	1.52	0.71
3:2:100:PHE:CG	5:R:5:THR:HG23	2.01	0.71
5:J:290:ARG:HH22	5:L:202:THR:HG23	1.52	0.71
3:2:100:PHE:CD1	5:R:5:THR:HG22	0.81	0.71
5:E:203:THR:HG22	5:Q:288:ASP:H	1.53	0.71
5:K:3:ASP:HA	5:K:6:THR:CB	2.18	0.71
1:3:116:GLU:O	1:3:120:ILE:HG22	1.91	0.71
5:F:3:ASP:HA	5:F:6:THR:CB	2.18	0.71
5:L:290:ARG:NH1	5:N:202:THR:CG2	2.51	0.71
5:Q:3:ASP:HA	5:Q:6:THR:CB	2.17	0.71
2:Y:215:GLN:O	2:Y:218:THR:HG22	1.91	0.71
5:N:3:ASP:HA	5:N:6:THR:CB	2.18	0.71
2:1:215:GLN:O	2:1:218:THR:HG22	1.91	0.71
1:6:116:GLU:O	1:6:120:ILE:HG22	1.91	0.71
1:9:116:GLU:O	1:9:120:ILE:HG22	1.91	0.71
5:F:290:ARG:NH1	5:H:202:THR:CG2	2.51	0.70
2:4:215:GLN:O	2:4:218:THR:HG22	1.91	0.70
5:H:3:ASP:HA	5:H:6:THR:CB	2.18	0.70
5:I:3:ASP:HA	5:I:6:THR:CB	2.17	0.70
5:M:1:ASP:HA	5:M:4:GLU:HB3	1.74	0.70
5:O:1:ASP:HA	5:O:4:GLU:HB3	1.74	0.70
1:0:62:GLU:CG	5:P:359:LYS:CD	2.33	0.70
2:7:215:GLN:O	2:7:218:THR:HG22	1.91	0.70
1:0:39:LYS:H	1:0:39:LYS:HD2	1.57	0.70
1:9:39:LYS:HD2	1:9:39:LYS:H	1.57	0.70
1:3:137:MET:HE1	1:3:148:ILE:HG13	1.72	0.70
5:D:1:ASP:HA	5:D:4:GLU:HB3	1.74	0.70
5:H:1:ASP:HA	5:H:4:GLU:HB3	1.74	0.70
5:P:1:ASP:HA	5:P:4:GLU:HB3	1.74	0.70
5:S:1:ASP:HA	5:S:4:GLU:HB3	1.74	0.70
3:8:70:LYS:O	3:8:74:VAL:HG23	1.92	0.70
5:F:1:ASP:HA	5:F:4:GLU:HB3	1.74	0.70
1:3:58:ASP:C	5:R:360:GLN:HG3	2.11	0.70
5:K:1:ASP:HA	5:K:4:GLU:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:290:ARG:HH22	5:N:202:THR:HG23	1.52	0.70
1:0:116:GLU:O	1:0:120:ILE:HG22	1.91	0.70
3:5:70:LYS:O	3:5:74:VAL:HG23	1.92	0.70
5:H:290:ARG:HH22	5:J:202:THR:HG23	1.52	0.70
5:L:3:ASP:HA	5:L:6:THR:CB	2.18	0.70
5:I:1:ASP:HA	5:I:4:GLU:HB3	1.74	0.70
5:J:1:ASP:HA	5:J:4:GLU:HB3	1.74	0.70
5:G:3:ASP:HA	5:G:6:THR:CB	2.18	0.69
5:G:1:ASP:HA	5:G:4:GLU:HB3	1.74	0.69
5:J:3:ASP:HA	5:J:6:THR:CB	2.18	0.69
5:L:1:ASP:HA	5:L:4:GLU:HB3	1.74	0.69
5:O:290:ARG:NH1	5:S:202:THR:CG2	2.51	0.69
3:2:100:PHE:HD1	5:R:5:THR:CG2	1.35	0.69
1:9:137:MET:HE1	1:9:148:ILE:HG13	1.72	0.69
5:I:290:ARG:HH22	5:K:202:THR:HG23	1.52	0.69
5:N:1:ASP:HA	5:N:4:GLU:HB3	1.74	0.69
1:6:55:GLU:CA	5:Q:360:GLN:HE22	2.05	0.69
5:E:290:ARG:HH22	5:G:202:THR:HG23	1.52	0.69
5:R:1:ASP:HA	5:R:4:GLU:HB3	1.74	0.69
3:2:70:LYS:O	3:2:74:VAL:HG23	1.92	0.69
5:E:3:ASP:HA	5:E:6:THR:CB	2.17	0.69
5:Q:1:ASP:HA	5:Q:4:GLU:HB3	1.74	0.69
3:Z:70:LYS:O	3:Z:74:VAL:HG23	1.92	0.69
5:D:160:THR:HG21	5:D:274:ILE:HD11	1.75	0.69
5:E:1:ASP:HA	5:E:4:GLU:HB3	1.74	0.69
5:H:160:THR:HG21	5:H:274:ILE:HD11	1.75	0.69
5:F:160:THR:HG21	5:F:274:ILE:HD11	1.76	0.68
5:J:160:THR:HG21	5:J:274:ILE:HD11	1.76	0.68
5:P:160:THR:HG21	5:P:274:ILE:HD11	1.76	0.68
5:S:160:THR:HG21	5:S:274:ILE:HD11	1.75	0.68
1:6:39:LYS:HD2	1:6:39:LYS:H	1.57	0.68
5:F:290:ARG:HH22	5:H:202:THR:HG23	1.52	0.68
5:L:160:THR:HG21	5:L:274:ILE:HD11	1.76	0.68
5:O:160:THR:HG21	5:O:274:ILE:HD11	1.76	0.68
1:0:137:MET:HE1	1:0:148:ILE:HG13	1.74	0.68
1:6:137:MET:CE	1:6:148:ILE:HG13	2.24	0.68
5:M:160:THR:HG21	5:M:274:ILE:HD11	1.76	0.68
1:3:59:ALA:CA	5:R:360:GLN:HG3	2.24	0.68
5:G:290:ARG:HH22	5:I:202:THR:HG23	1.52	0.68
5:N:160:THR:HG21	5:N:274:ILE:HD11	1.75	0.68
5:Q:153:LEU:HD11	5:Q:274:ILE:HG13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:137:MET:CE	1:3:148:ILE:HG13	2.24	0.68
3:5:29:ILE:HD11	1:6:99:ASN:HB3	1.76	0.68
1:3:39:LYS:HD2	1:3:39:LYS:H	1.57	0.68
2:4:244:ALA:HB1	3:5:103:ARG:HD2	1.76	0.68
5:G:153:LEU:HD11	5:G:274:ILE:HG13	1.76	0.68
5:K:160:THR:HG21	5:K:274:ILE:HD11	1.75	0.68
5:N:153:LEU:HD11	5:N:274:ILE:HG13	1.76	0.68
1:0:99:ASN:HB3	3:Z:29:ILE:HD11	1.76	0.68
2:1:244:ALA:HB1	3:2:103:ARG:HD2	1.76	0.68
5:E:153:LEU:HD11	5:E:274:ILE:HG13	1.76	0.68
3:2:29:ILE:HD11	1:3:99:ASN:HB3	1.76	0.67
1:6:58:ASP:HB2	5:Q:360:GLN:HG2	1.77	0.67
5:R:160:THR:HG21	5:R:274:ILE:HD11	1.75	0.67
2:Y:244:ALA:HB1	3:Z:103:ARG:HD2	1.76	0.67
1:0:137:MET:CE	1:0:148:ILE:HG13	2.24	0.67
3:5:108:ARG:HG2	1:6:94:GLU:HB3	1.76	0.67
5:I:160:THR:HG21	5:I:274:ILE:HD11	1.75	0.67
1:0:94:GLU:HB3	3:Z:108:ARG:HG2	1.76	0.67
2:7:244:ALA:HB1	3:8:103:ARG:HD2	1.76	0.67
3:8:29:ILE:HD11	1:9:99:ASN:HB3	1.76	0.67
5:R:153:LEU:HD11	5:R:274:ILE:HG13	1.76	0.67
5:I:153:LEU:HD11	5:I:274:ILE:HG13	1.76	0.67
5:L:153:LEU:HD11	5:L:274:ILE:HG13	1.76	0.67
5:Q:160:THR:HG21	5:Q:274:ILE:HD11	1.76	0.67
5:E:160:THR:HG21	5:E:274:ILE:HD11	1.76	0.67
5:J:153:LEU:HD11	5:J:274:ILE:HG13	1.76	0.67
3:8:108:ARG:HG2	1:9:94:GLU:HB3	1.76	0.67
1:9:137:MET:CE	1:9:148:ILE:HG13	2.24	0.67
5:G:160:THR:HG21	5:G:274:ILE:HD11	1.76	0.67
5:K:153:LEU:HD11	5:K:274:ILE:HG13	1.76	0.67
1:6:62:GLU:CD	5:Q:359:LYS:NZ	2.48	0.66
5:D:153:LEU:HD11	5:D:274:ILE:HG13	1.76	0.66
5:O:290:ARG:HH22	5:S:202:THR:HG23	1.52	0.66
1:6:137:MET:HE1	1:6:148:ILE:HG13	1.75	0.66
2:Y:207:LYS:HZ2	2:Y:208:GLU:HG2	1.60	0.66
3:2:108:ARG:HG2	1:3:94:GLU:HB3	1.76	0.66
5:H:153:LEU:HD11	5:H:274:ILE:HG13	1.76	0.66
5:M:153:LEU:HD11	5:M:274:ILE:HG13	1.76	0.66
5:O:153:LEU:HD11	5:O:274:ILE:HG13	1.76	0.66
5:F:153:LEU:HD11	5:F:274:ILE:HG13	1.76	0.66
5:S:153:LEU:HD11	5:S:274:ILE:HG13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:203:ARG:HH21	3:5:53:LEU:HG	1.61	0.66
3:5:97:GLN:CD	5:Q:4:GLU:HG2	2.16	0.65
2:1:203:ARG:HH21	3:2:53:LEU:HG	1.61	0.65
5:P:153:LEU:HD11	5:P:274:ILE:HG13	1.76	0.65
1:3:46:ARG:HH11	1:3:51:ASN:ND2	1.95	0.65
2:7:231:LYS:O	2:7:235:VAL:HG23	1.97	0.65
1:6:46:ARG:HH11	1:6:51:ASN:ND2	1.95	0.65
3:5:5:LYS:HE2	3:5:5:LYS:N	2.12	0.65
2:Y:231:LYS:O	2:Y:235:VAL:HG23	1.97	0.65
1:9:46:ARG:HH11	1:9:51:ASN:ND2	1.95	0.65
3:Z:54:PRO:HB2	3:Z:59:GLU:HB2	1.79	0.65
1:9:55:GLU:CA	5:S:360:GLN:CD	2.41	0.64
3:2:5:LYS:N	3:2:5:LYS:HE2	2.12	0.64
3:5:42:ASN:O	3:5:45:ALA:HB3	1.98	0.64
2:1:231:LYS:O	2:1:235:VAL:HG23	1.97	0.64
2:7:203:ARG:HH21	3:8:53:LEU:HG	1.62	0.64
3:8:54:PRO:HB2	3:8:59:GLU:HB2	1.79	0.64
1:0:46:ARG:HH11	1:0:51:ASN:ND2	1.95	0.64
5:N:190:MET:SD	5:N:209:VAL:HG11	2.38	0.64
1:6:21:PHE:CD1	1:6:81:MET:HG3	2.33	0.64
1:9:21:PHE:CD1	1:9:81:MET:HG3	2.33	0.64
5:R:190:MET:SD	5:R:209:VAL:HG11	2.38	0.64
1:0:21:PHE:CD1	1:0:81:MET:HG3	2.33	0.64
3:2:42:ASN:O	3:2:45:ALA:HB3	1.98	0.64
5:G:190:MET:SD	5:G:209:VAL:HG11	2.38	0.64
2:4:231:LYS:O	2:4:235:VAL:HG23	1.97	0.64
5:H:190:MET:SD	5:H:209:VAL:HG11	2.38	0.64
3:8:70:LYS:O	3:8:73:SER:HB3	1.99	0.63
2:Y:203:ARG:HH21	3:Z:53:LEU:HG	1.61	0.63
3:8:5:LYS:N	3:8:5:LYS:HE2	2.12	0.63
5:L:190:MET:SD	5:L:209:VAL:HG11	2.38	0.63
5:Q:190:MET:SD	5:Q:209:VAL:HG11	2.38	0.63
3:2:97:GLN:NE2	5:R:4:GLU:CG	2.61	0.63
3:Z:70:LYS:O	3:Z:73:SER:HB3	1.99	0.63
3:8:24:LEU:O	3:8:27:THR:HG22	1.99	0.63
5:L:257:CYS:HB3	5:L:258:PRO:HD3	1.81	0.63
5:R:257:CYS:HB3	5:R:258:PRO:HD3	1.81	0.63
3:2:70:LYS:O	3:2:73:SER:HB3	1.98	0.63
5:E:190:MET:SD	5:E:209:VAL:HG11	2.38	0.63
2:Y:207:LYS:HZ2	2:Y:208:GLU:HA	1.61	0.63
3:5:24:LEU:O	3:5:27:THR:HG22	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:24:LEU:O	3:Z:27:THR:HG22	1.99	0.63
3:Z:5:LYS:N	3:Z:5:LYS:HE2	2.13	0.63
1:3:21:PHE:CD1	1:3:81:MET:HG3	2.33	0.63
5:I:190:MET:SD	5:I:209:VAL:HG11	2.38	0.63
5:J:257:CYS:HB3	5:J:258:PRO:HD3	1.81	0.63
5:K:190:MET:SD	5:K:209:VAL:HG11	2.38	0.63
5:Q:257:CYS:HB3	5:Q:258:PRO:HD3	1.81	0.63
3:2:24:LEU:O	3:2:27:THR:HG22	1.99	0.63
3:2:54:PRO:HB2	3:2:59:GLU:HB2	1.79	0.63
5:E:257:CYS:HB3	5:E:258:PRO:HD3	1.81	0.63
5:F:257:CYS:HB3	5:F:258:PRO:HD3	1.81	0.63
5:N:257:CYS:HB3	5:N:258:PRO:HD3	1.81	0.63
1:3:4:ASP:O	1:3:7:ALA:HB3	1.99	0.63
3:5:70:LYS:O	3:5:73:SER:HB3	1.99	0.63
5:J:190:MET:SD	5:J:209:VAL:HG11	2.38	0.63
1:3:55:GLU:O	5:R:360:GLN:NE2	2.31	0.63
3:5:45:ALA:O	3:5:49:PRO:HG3	1.99	0.63
1:6:4:ASP:O	1:6:7:ALA:HB3	1.99	0.63
5:G:257:CYS:HB3	5:G:258:PRO:HD3	1.81	0.63
3:5:54:PRO:HB2	3:5:59:GLU:HB2	1.79	0.62
5:F:190:MET:SD	5:F:209:VAL:HG11	2.38	0.62
5:O:190:MET:SD	5:O:209:VAL:HG11	2.38	0.62
3:Z:42:ASN:O	3:Z:45:ALA:HB3	1.98	0.62
1:9:4:ASP:O	1:9:7:ALA:HB3	1.99	0.62
3:Z:45:ALA:O	3:Z:49:PRO:HG3	1.99	0.62
3:8:45:ALA:O	3:8:49:PRO:HG3	1.99	0.62
5:H:257:CYS:HB3	5:H:258:PRO:HD3	1.81	0.62
1:0:57:LEU:O	1:0:61:ILE:HG13	1.99	0.62
1:6:155:LYS:HE3	1:6:155:LYS:CA	2.30	0.62
5:D:257:CYS:HB3	5:D:258:PRO:HD3	1.81	0.62
5:M:190:MET:SD	5:M:209:VAL:HG11	2.38	0.62
1:6:121:LEU:HD23	1:6:133:ILE:HG12	1.81	0.62
3:5:108:ARG:NH1	1:6:95:GLU:OE1	2.33	0.62
3:8:42:ASN:O	3:8:45:ALA:HB3	1.98	0.62
1:9:57:LEU:O	1:9:61:ILE:HG13	1.99	0.62
5:D:190:MET:SD	5:D:209:VAL:HG11	2.38	0.62
5:E:361:GLU:HB3	5:E:369:ILE:HG12	1.82	0.62
5:I:361:GLU:HB3	5:I:369:ILE:HG12	1.82	0.62
5:J:361:GLU:HB3	5:J:369:ILE:HG12	1.82	0.62
5:K:361:GLU:HB3	5:K:369:ILE:HG12	1.82	0.62
5:L:361:GLU:HB3	5:L:369:ILE:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:361:GLU:HB3	5:R:369:ILE:HG12	1.82	0.62
5:H:361:GLU:HB3	5:H:369:ILE:HG12	1.82	0.62
5:I:257:CYS:HB3	5:I:258:PRO:HD3	1.81	0.62
5:P:190:MET:SD	5:P:209:VAL:HG11	2.38	0.62
5:P:257:CYS:HB3	5:P:258:PRO:HD3	1.81	0.62
1:0:95:GLU:OE1	3:Z:108:ARG:NH1	2.33	0.62
3:2:108:ARG:NH1	1:3:95:GLU:OE1	2.33	0.62
1:9:58:ASP:O	1:9:62:GLU:HG3	2.00	0.62
5:G:361:GLU:HB3	5:G:369:ILE:HG12	1.82	0.62
5:M:361:GLU:HB3	5:M:369:ILE:HG12	1.82	0.62
5:N:361:GLU:HB3	5:N:369:ILE:HG12	1.82	0.62
5:P:361:GLU:HB3	5:P:369:ILE:HG12	1.82	0.62
5:Q:361:GLU:HB3	5:Q:369:ILE:HG12	1.82	0.62
5:S:190:MET:SD	5:S:209:VAL:HG11	2.38	0.62
5:S:257:CYS:HB3	5:S:258:PRO:HD3	1.81	0.62
1:0:155:LYS:CA	1:0:155:LYS:HE3	2.30	0.62
3:8:123:ARG:HG3	3:8:123:ARG:HH11	1.65	0.62
1:9:14:SER:H	1:9:17:MET:HG3	1.65	0.62
5:S:361:GLU:HB3	5:S:369:ILE:HG12	1.82	0.62
1:3:58:ASP:O	1:3:62:GLU:HG3	2.00	0.62
1:6:58:ASP:O	1:6:62:GLU:HG3	1.99	0.62
5:D:361:GLU:HB3	5:D:369:ILE:HG12	1.82	0.62
5:F:361:GLU:HB3	5:F:369:ILE:HG12	1.82	0.62
5:K:257:CYS:HB3	5:K:258:PRO:HD3	1.81	0.62
5:M:257:CYS:HB3	5:M:258:PRO:HD3	1.81	0.62
5:O:257:CYS:HB3	5:O:258:PRO:HD3	1.81	0.62
3:2:123:ARG:HG3	3:2:123:ARG:HH11	1.65	0.62
5:O:361:GLU:HB3	5:O:369:ILE:HG12	1.82	0.62
1:3:57:LEU:O	1:3:61:ILE:HG13	1.99	0.61
1:0:4:ASP:O	1:0:7:ALA:HB3	1.99	0.61
1:0:58:ASP:O	1:0:62:GLU:HG3	2.00	0.61
1:3:121:LEU:HD23	1:3:133:ILE:HG12	1.81	0.61
3:Z:123:ARG:HH11	3:Z:123:ARG:HG3	1.65	0.61
3:2:45:ALA:O	3:2:49:PRO:HG3	1.99	0.61
1:6:57:LEU:O	1:6:61:ILE:HG13	1.99	0.61
1:9:121:LEU:HD23	1:9:133:ILE:HG12	1.81	0.61
1:3:155:LYS:HE3	1:3:155:LYS:CA	2.30	0.61
1:9:155:LYS:HE3	1:9:155:LYS:CA	2.30	0.61
5:P:4:GLU:OE2	3:Z:100:PHE:CD1	2.53	0.61
1:3:14:SER:H	1:3:17:MET:HG3	1.65	0.61
3:5:14:ARG:O	3:5:18:LYS:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:121:LEU:HD23	1:0:133:ILE:HG12	1.81	0.61
2:4:198:ASN:HD21	2:4:200:ASP:CG	2.04	0.61
1:6:14:SER:H	1:6:17:MET:HG3	1.65	0.61
1:0:14:SER:H	1:0:17:MET:HG3	1.65	0.61
3:2:130:HIS:HE1	3:2:134:MET:HE3	1.66	0.61
3:5:123:ARG:HG3	3:5:123:ARG:HH11	1.65	0.61
3:8:48:SER:N	3:8:49:PRO:HD3	2.15	0.61
3:8:108:ARG:NH1	1:9:95:GLU:OE1	2.33	0.61
3:5:97:GLN:HA	5:Q:4:GLU:OE2	2.00	0.61
2:1:198:ASN:HD21	2:1:200:ASP:CG	2.04	0.61
3:2:14:ARG:O	3:2:18:LYS:HG3	2.01	0.61
3:Z:14:ARG:O	3:Z:18:LYS:HG3	2.01	0.61
3:2:48:SER:N	3:2:49:PRO:HD3	2.16	0.61
1:6:62:GLU:CD	5:Q:359:LYS:HZ3	2.02	0.61
3:5:48:SER:N	3:5:49:PRO:HD3	2.16	0.60
5:L:223:PHE:HD2	5:L:312:ARG:NH2	1.99	0.60
5:Q:223:PHE:HD2	5:Q:312:ARG:NH2	1.99	0.60
3:8:14:ARG:O	3:8:18:LYS:HG3	2.01	0.60
5:F:223:PHE:HD2	5:F:312:ARG:NH2	1.99	0.60
1:0:62:GLU:CD	5:P:359:LYS:HE3	2.07	0.60
5:K:223:PHE:HD2	5:K:312:ARG:NH2	1.99	0.60
5:D:223:PHE:HD2	5:D:312:ARG:NH2	2.00	0.60
5:P:5:THR:HA	3:Z:100:PHE:HZ	1.67	0.60
3:2:5:LYS:HE2	3:2:6:LYS:H	1.67	0.60
3:8:132:VAL:HB	3:8:134:MET:HE2	1.83	0.60
5:I:223:PHE:HD2	5:I:312:ARG:NH2	1.99	0.60
5:M:223:PHE:HD2	5:M:312:ARG:NH2	2.00	0.60
3:8:5:LYS:HE2	3:8:6:LYS:H	1.67	0.60
5:D:287:ILE:HD12	5:D:287:ILE:H	1.67	0.60
5:P:287:ILE:HD12	5:P:287:ILE:H	1.67	0.60
5:P:223:PHE:HD2	5:P:312:ARG:NH2	2.00	0.60
5:J:223:PHE:HD2	5:J:312:ARG:NH2	1.99	0.60
2:Y:202:LEU:HB3	3:Z:60:LEU:HB3	1.83	0.60
5:P:5:THR:HA	3:Z:100:PHE:CZ	2.35	0.60
3:Z:132:VAL:HB	3:Z:134:MET:HE2	1.84	0.60
2:1:202:LEU:HB3	3:2:60:LEU:HB3	1.83	0.60
5:F:287:ILE:HD12	5:F:287:ILE:H	1.67	0.60
5:O:223:PHE:HD2	5:O:312:ARG:NH2	1.99	0.60
3:2:97:GLN:NE2	5:R:4:GLU:HG3	2.07	0.60
2:Y:198:ASN:HD21	2:Y:200:ASP:CG	2.04	0.60
3:Z:48:SER:N	3:Z:49:PRO:HD3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:287:ILE:H	5:Q:287:ILE:HD12	1.67	0.60
3:2:132:VAL:HB	3:2:134:MET:HE2	1.83	0.60
2:7:202:LEU:HB3	3:8:60:LEU:HB3	1.83	0.60
5:K:287:ILE:H	5:K:287:ILE:HD12	1.67	0.60
5:M:287:ILE:HD12	5:M:287:ILE:H	1.67	0.60
3:8:130:HIS:HE1	3:8:134:MET:HE3	1.67	0.59
5:H:287:ILE:H	5:H:287:ILE:HD12	1.67	0.59
2:4:202:LEU:HB3	3:5:60:LEU:HB3	1.83	0.59
3:5:132:VAL:HB	3:5:134:MET:HE2	1.84	0.59
5:G:223:PHE:HD2	5:G:312:ARG:NH2	2.00	0.59
2:7:198:ASN:HD21	2:7:200:ASP:CG	2.04	0.59
5:J:287:ILE:H	5:J:287:ILE:HD12	1.67	0.59
5:S:223:PHE:HD2	5:S:312:ARG:NH2	1.99	0.59
2:1:207:LYS:HZ2	2:1:208:GLU:HG2	1.67	0.59
5:E:287:ILE:HD12	5:E:287:ILE:H	1.67	0.59
5:O:287:ILE:H	5:O:287:ILE:HD12	1.67	0.59
1:3:58:ASP:OD2	5:R:364:GLU:OE1	2.20	0.59
1:6:59:ALA:HA	5:Q:359:LYS:HZ2	1.67	0.59
1:0:67:ASP:OD2	1:0:69:SER:HB3	2.03	0.59
5:L:287:ILE:HD12	5:L:287:ILE:H	1.67	0.59
5:R:223:PHE:HD2	5:R:312:ARG:NH2	1.99	0.59
2:Y:170:LYS:O	2:Y:174:LYS:HG2	2.03	0.59
5:I:287:ILE:H	5:I:287:ILE:HD12	1.67	0.59
5:R:287:ILE:H	5:R:287:ILE:HD12	1.67	0.59
1:6:67:ASP:OD2	1:6:69:SER:HB3	2.03	0.59
2:7:170:LYS:O	2:7:174:LYS:HG2	2.03	0.58
5:H:223:PHE:HD2	5:H:312:ARG:NH2	1.99	0.58
2:4:207:LYS:HZ2	2:4:208:GLU:HG2	1.68	0.58
3:5:5:LYS:HE2	3:5:6:LYS:H	1.67	0.58
5:N:287:ILE:H	5:N:287:ILE:HD12	1.67	0.58
5:S:287:ILE:H	5:S:287:ILE:HD12	1.67	0.58
3:Z:5:LYS:HE2	3:Z:6:LYS:H	1.67	0.58
1:3:67:ASP:OD2	1:3:69:SER:HB3	2.03	0.58
1:6:58:ASP:CB	5:Q:360:GLN:NE2	2.62	0.58
1:0:150:PHE:CE2	1:0:154:LEU:HD21	2.39	0.58
5:E:223:PHE:HD2	5:E:312:ARG:NH2	1.99	0.58
2:4:194:ILE:HG21	2:4:201:LYS:HE2	1.86	0.58
3:5:54:PRO:CB	3:5:59:GLU:HB2	2.34	0.58
1:9:150:PHE:CE2	1:9:154:LEU:HD21	2.39	0.58
5:G:287:ILE:H	5:G:287:ILE:HD12	1.67	0.58
2:1:170:LYS:O	2:1:174:LYS:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:194:ILE:HG21	2:1:201:LYS:HE2	1.86	0.58
1:3:150:PHE:CE2	1:3:154:LEU:HD21	2.39	0.58
2:4:210:TRP:CE2	3:5:51:LEU:HB2	2.39	0.58
1:6:150:PHE:CE2	1:6:154:LEU:HD21	2.39	0.58
1:6:55:GLU:HA	5:Q:360:GLN:HE22	1.61	0.58
3:5:133:ASN:N	3:5:133:ASN:HD22	2.02	0.57
1:0:62:GLU:CG	5:P:360:GLN:H	2.13	0.57
1:9:55:GLU:CA	5:S:360:GLN:OE1	2.47	0.57
1:0:62:GLU:HB2	5:P:359:LYS:HD3	0.57	0.57
1:9:67:ASP:OD2	1:9:69:SER:HB3	2.03	0.57
3:2:54:PRO:CB	3:2:59:GLU:HB2	2.34	0.57
2:4:170:LYS:O	2:4:174:LYS:HG2	2.03	0.57
2:7:194:ILE:HG21	2:7:201:LYS:HE2	1.86	0.57
2:7:210:TRP:CE2	3:8:51:LEU:HB2	2.39	0.57
2:Y:194:ILE:HG21	2:Y:201:LYS:HE2	1.86	0.57
2:Y:210:TRP:CE2	3:Z:51:LEU:HB2	2.39	0.57
3:Z:54:PRO:CB	3:Z:59:GLU:HB2	2.34	0.57
3:8:54:PRO:CB	3:8:59:GLU:HB2	2.34	0.57
1:0:28:PHE:HA	1:0:44:VAL:HG21	1.87	0.57
1:9:28:PHE:HA	1:9:44:VAL:HG21	1.87	0.57
5:N:223:PHE:HD2	5:N:312:ARG:NH2	1.99	0.57
3:Z:133:ASN:HD22	3:Z:133:ASN:N	2.02	0.56
1:0:39:LYS:N	1:0:39:LYS:HD2	2.21	0.56
1:3:28:PHE:HA	1:3:44:VAL:HG21	1.87	0.56
1:0:143:ASN:ND2	1:0:145:ASP:CG	2.59	0.56
2:1:210:TRP:CE2	3:2:51:LEU:HB2	2.39	0.56
1:6:143:ASN:ND2	1:6:145:ASP:CG	2.59	0.56
5:H:365:ALA:HB3	5:H:369:ILE:HB	1.88	0.56
1:6:28:PHE:HA	1:6:44:VAL:HG21	1.87	0.56
1:9:39:LYS:HD2	1:9:39:LYS:N	2.21	0.56
5:F:365:ALA:HB3	5:F:369:ILE:HB	1.88	0.56
5:L:365:ALA:HB3	5:L:369:ILE:HB	1.88	0.56
1:3:58:ASP:C	5:R:360:GLN:CG	2.73	0.56
1:9:143:ASN:ND2	1:9:145:ASP:CG	2.59	0.56
5:J:365:ALA:HB3	5:J:369:ILE:HB	1.88	0.56
3:2:133:ASN:N	3:2:133:ASN:HD22	2.02	0.56
5:D:365:ALA:HB3	5:D:369:ILE:HB	1.88	0.56
5:S:365:ALA:HB3	5:S:369:ILE:HB	1.88	0.56
1:6:143:ASN:ND2	1:6:145:ASP:OD1	2.39	0.56
5:O:365:ALA:HB3	5:O:369:ILE:HB	1.88	0.56
5:N:365:ALA:HB3	5:N:369:ILE:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:143:ASN:ND2	1:3:145:ASP:OD1	2.39	0.56
2:7:207:LYS:HZ2	2:7:208:GLU:HG2	1.69	0.56
1:9:143:ASN:ND2	1:9:145:ASP:OD1	2.39	0.56
5:M:365:ALA:HB3	5:M:369:ILE:HB	1.88	0.56
1:0:159:GLY:O	1:0:160:VAL:C	2.44	0.56
5:P:365:ALA:HB3	5:P:369:ILE:HB	1.88	0.56
3:8:97:GLN:C	3:8:99:LEU:H	2.10	0.55
5:R:365:ALA:HB3	5:R:369:ILE:HB	1.88	0.55
2:7:227:ILE:C	2:7:227:ILE:HD12	2.27	0.55
1:9:159:GLY:O	1:9:160:VAL:C	2.44	0.55
5:H:288:ASP:CA	5:J:204:ALA:HB2	2.32	0.55
5:Q:365:ALA:HB3	5:Q:369:ILE:HB	1.88	0.55
1:0:143:ASN:ND2	1:0:145:ASP:OD1	2.39	0.55
2:1:227:ILE:HD12	2:1:227:ILE:C	2.27	0.55
1:3:143:ASN:ND2	1:3:145:ASP:CG	2.59	0.55
5:K:365:ALA:HB3	5:K:369:ILE:HB	1.88	0.55
1:3:105:ASP:O	1:3:106:LYS:C	2.45	0.55
5:E:365:ALA:HB3	5:E:369:ILE:HB	1.88	0.55
5:G:365:ALA:HB3	5:G:369:ILE:HB	1.88	0.55
5:F:288:ASP:CA	5:H:204:ALA:HB2	2.32	0.55
3:8:133:ASN:N	3:8:133:ASN:HD22	2.02	0.55
5:I:365:ALA:HB3	5:I:369:ILE:HB	1.88	0.55
2:Y:227:ILE:HD12	2:Y:227:ILE:C	2.27	0.55
3:5:130:HIS:HE1	3:5:134:MET:HE3	1.70	0.55
1:6:39:LYS:N	1:6:39:LYS:HD2	2.21	0.55
2:1:243:GLN:HE21	1:3:149:ASP:HB3	1.72	0.55
2:7:207:LYS:O	2:7:210:TRP:HB3	2.07	0.55
1:0:46:ARG:NH1	1:0:51:ASN:HD21	2.05	0.55
1:9:105:ASP:O	1:9:106:LYS:C	2.45	0.55
5:D:288:ASP:CA	5:F:204:ALA:HB2	2.32	0.55
2:Y:207:LYS:O	2:Y:210:TRP:HB3	2.07	0.55
2:1:202:LEU:H	2:1:202:LEU:HD22	1.73	0.54
3:2:97:GLN:C	3:2:99:LEU:H	2.10	0.54
1:3:39:LYS:HD2	1:3:39:LYS:N	2.21	0.54
5:E:288:ASP:CA	5:G:204:ALA:HB2	2.32	0.54
3:Z:130:HIS:HE1	3:Z:134:MET:HE3	1.71	0.54
3:2:105:LYS:HB2	5:R:1:ASP:OD1	2.07	0.54
1:3:159:GLY:O	1:3:160:VAL:C	2.44	0.54
3:8:91:GLU:O	3:8:95:LEU:HG	2.08	0.54
1:9:46:ARG:NH1	1:9:51:ASN:HD21	2.06	0.54
5:D:204:ALA:HB2	5:P:288:ASP:CA	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:91:GLU:O	3:2:95:LEU:HG	2.08	0.54
1:6:159:GLY:O	1:6:160:VAL:C	2.44	0.54
2:7:243:GLN:HE21	1:9:149:ASP:HB3	1.72	0.54
5:O:288:ASP:CA	5:S:204:ALA:HB2	2.32	0.54
2:4:202:LEU:H	2:4:202:LEU:HD22	1.73	0.54
3:5:97:GLN:C	3:5:99:LEU:H	2.10	0.54
3:Z:97:GLN:C	3:Z:99:LEU:H	2.09	0.54
5:M:288:ASP:CA	5:O:204:ALA:HB2	2.32	0.54
1:0:149:ASP:HB3	2:Y:243:GLN:HE21	1.72	0.54
1:0:105:ASP:O	1:0:106:LYS:C	2.45	0.54
2:4:207:LYS:O	2:4:210:TRP:HB3	2.07	0.54
5:K:288:ASP:CA	5:M:204:ALA:HB2	2.32	0.54
2:1:207:LYS:O	2:1:210:TRP:HB3	2.07	0.54
1:6:105:ASP:O	1:6:106:LYS:C	2.45	0.54
5:I:288:ASP:CA	5:K:204:ALA:HB2	2.32	0.54
5:P:23:GLY:HA3	3:Z:100:PHE:HE2	1.73	0.54
1:6:46:ARG:NH1	1:6:51:ASN:HD21	2.05	0.54
3:8:100:PHE:HB3	5:S:4:GLU:OE2	2.08	0.54
3:5:103:ARG:HE	3:5:103:ARG:HA	1.73	0.54
1:3:46:ARG:NH1	1:3:51:ASN:HD21	2.05	0.53
2:4:243:GLN:HE21	1:6:149:ASP:HB3	1.72	0.53
5:L:185:LEU:HD23	5:L:306:TYR:OH	2.08	0.53
3:2:103:ARG:HA	3:2:103:ARG:HE	1.74	0.53
3:5:91:GLU:O	3:5:95:LEU:HG	2.08	0.53
2:4:227:ILE:C	2:4:227:ILE:HD12	2.27	0.53
5:N:185:LEU:HD23	5:N:306:TYR:OH	2.09	0.53
1:6:55:GLU:O	5:Q:360:GLN:CD	2.45	0.53
5:G:185:LEU:HD23	5:G:306:TYR:OH	2.09	0.53
2:Y:202:LEU:H	2:Y:202:LEU:HD22	1.73	0.53
3:Z:91:GLU:O	3:Z:95:LEU:HG	2.08	0.53
5:E:185:LEU:HD23	5:E:306:TYR:OH	2.09	0.53
5:R:185:LEU:HD23	5:R:306:TYR:OH	2.08	0.53
2:7:202:LEU:H	2:7:202:LEU:HD22	1.72	0.53
5:P:185:LEU:HD23	5:P:306:TYR:OH	2.08	0.53
2:Y:207:LYS:HZ2	2:Y:208:GLU:CG	2.21	0.53
3:8:103:ARG:HA	3:8:103:ARG:HE	1.73	0.53
1:0:62:GLU:HG3	5:P:360:GLN:CB	2.22	0.53
5:K:185:LEU:HD23	5:K:306:TYR:OH	2.09	0.53
5:O:185:LEU:HD23	5:O:306:TYR:OH	2.09	0.53
5:Q:185:LEU:HD23	5:Q:306:TYR:OH	2.09	0.53
5:S:185:LEU:HD23	5:S:306:TYR:OH	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:84:GLN:O	1:3:85:MET:C	2.47	0.53
5:F:185:LEU:HD23	5:F:306:TYR:OH	2.09	0.53
5:M:185:LEU:HD23	5:M:306:TYR:OH	2.09	0.53
1:6:58:ASP:CB	5:Q:360:GLN:HG2	2.38	0.53
5:F:180:LEU:HD22	5:F:267:ILE:HD11	1.91	0.53
5:J:185:LEU:HD23	5:J:306:TYR:OH	2.09	0.53
5:D:185:LEU:HD23	5:D:306:TYR:OH	2.09	0.52
5:I:180:LEU:HD22	5:I:267:ILE:HD11	1.92	0.52
1:0:84:GLN:O	1:0:85:MET:C	2.47	0.52
5:M:285:CYS:O	5:M:290:ARG:NH1	2.43	0.52
5:D:285:CYS:O	5:D:290:ARG:NH1	2.43	0.52
5:E:180:LEU:HD22	5:E:267:ILE:HD11	1.92	0.52
5:H:180:LEU:HD22	5:H:267:ILE:HD11	1.92	0.52
5:I:185:LEU:HD23	5:I:306:TYR:OH	2.09	0.52
5:J:180:LEU:HD22	5:J:267:ILE:HD11	1.91	0.52
5:N:285:CYS:O	5:N:290:ARG:NH1	2.43	0.52
5:R:285:CYS:O	5:R:290:ARG:NH1	2.42	0.52
3:Z:103:ARG:HA	3:Z:103:ARG:HE	1.74	0.52
3:8:23:GLN:O	3:8:26:VAL:HG12	2.10	0.52
5:M:180:LEU:HD22	5:M:267:ILE:HD11	1.92	0.52
5:O:285:CYS:O	5:O:290:ARG:NH1	2.43	0.52
5:P:180:LEU:HD22	5:P:267:ILE:HD11	1.92	0.52
5:Q:180:LEU:HD22	5:Q:267:ILE:HD11	1.92	0.52
5:D:180:LEU:HD22	5:D:267:ILE:HD11	1.92	0.52
5:H:285:CYS:O	5:H:290:ARG:NH1	2.43	0.52
3:5:100:PHE:CB	5:Q:4:GLU:OE2	2.58	0.52
3:2:23:GLN:O	3:2:26:VAL:HG12	2.10	0.52
3:2:97:GLN:O	3:2:99:LEU:N	2.43	0.52
1:9:84:GLN:O	1:9:85:MET:C	2.47	0.52
5:H:185:LEU:HD23	5:H:306:TYR:OH	2.09	0.52
5:K:180:LEU:HD22	5:K:267:ILE:HD11	1.92	0.52
5:O:180:LEU:HD22	5:O:267:ILE:HD11	1.92	0.52
5:S:180:LEU:HD22	5:S:267:ILE:HD11	1.92	0.52
3:Z:97:GLN:O	3:Z:99:LEU:N	2.43	0.52
5:E:285:CYS:O	5:E:290:ARG:NH1	2.43	0.52
5:G:180:LEU:HD22	5:G:267:ILE:HD11	1.92	0.52
5:I:285:CYS:O	5:I:290:ARG:NH1	2.43	0.52
5:J:285:CYS:O	5:J:290:ARG:NH1	2.43	0.52
5:L:180:LEU:HD22	5:L:267:ILE:HD11	1.92	0.52
3:Z:23:GLN:O	3:Z:26:VAL:HG12	2.10	0.52
1:0:143:ASN:HD21	1:0:145:ASP:CG	2.14	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:93:GLU:HG2	3:2:111:LEU:HD21	1.92	0.52
3:5:23:GLN:O	3:5:26:VAL:HG12	2.10	0.52
5:L:285:CYS:O	5:L:290:ARG:NH1	2.43	0.52
5:N:180:LEU:HD22	5:N:267:ILE:HD11	1.92	0.52
5:S:285:CYS:O	5:S:290:ARG:NH1	2.43	0.52
2:Y:207:LYS:NZ	2:Y:208:GLU:HA	2.25	0.52
1:9:106:LYS:O	1:9:107:ASN:HB3	2.09	0.52
5:K:285:CYS:O	5:K:290:ARG:NH1	2.43	0.52
5:Q:285:CYS:O	5:Q:290:ARG:NH1	2.43	0.52
5:R:180:LEU:HD22	5:R:267:ILE:HD11	1.92	0.52
1:0:106:LYS:O	1:0:107:ASN:HB3	2.09	0.52
3:2:25:ALA:HB1	1:3:100:CYS:SG	2.50	0.52
3:5:25:ALA:HB1	1:6:100:CYS:SG	2.50	0.52
1:3:103:ILE:HG22	1:3:104:PHE:CD1	2.46	0.51
1:9:143:ASN:HD21	1:9:145:ASP:CG	2.14	0.51
2:1:207:LYS:NZ	2:1:208:GLU:HA	2.25	0.51
3:5:93:GLU:HG2	3:5:111:LEU:HD21	1.92	0.51
1:6:143:ASN:HD21	1:6:145:ASP:CG	2.14	0.51
1:6:103:ILE:HG22	1:6:104:PHE:CD1	2.46	0.51
5:G:285:CYS:O	5:G:290:ARG:NH1	2.43	0.51
1:3:106:LYS:O	1:3:107:ASN:HB3	2.09	0.51
5:F:285:CYS:O	5:F:290:ARG:NH1	2.43	0.51
5:G:288:ASP:CA	5:I:204:ALA:HB2	2.32	0.51
5:N:287:ILE:HG22	5:R:204:ALA:HB3	1.92	0.51
1:6:106:LYS:O	1:6:107:ASN:HB3	2.09	0.51
2:7:243:GLN:NE2	1:9:149:ASP:HB3	2.26	0.51
3:8:93:GLU:HG2	3:8:111:LEU:HD21	1.92	0.51
3:8:25:ALA:HB1	1:9:100:CYS:SG	2.50	0.51
5:M:287:ILE:HG22	5:O:204:ALA:HB3	1.92	0.51
5:P:285:CYS:O	5:P:290:ARG:NH1	2.43	0.51
5:E:204:ALA:HB3	5:Q:287:ILE:HG22	1.92	0.51
1:3:143:ASN:HD21	1:3:145:ASP:CG	2.14	0.51
3:5:97:GLN:O	3:5:99:LEU:N	2.43	0.51
5:L:287:ILE:HG22	5:N:204:ALA:HB3	1.92	0.51
1:0:62:GLU:CG	5:P:360:GLN:N	2.59	0.51
3:8:97:GLN:O	3:8:99:LEU:N	2.43	0.51
1:0:149:ASP:HB3	2:Y:243:GLN:NE2	2.26	0.51
3:Z:93:GLU:HG2	3:Z:111:LEU:HD21	1.92	0.51
1:6:84:GLN:O	1:6:85:MET:C	2.47	0.51
5:D:204:ALA:HB3	5:P:287:ILE:HG22	1.92	0.51
3:8:109:PRO:O	3:8:112:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:287:ILE:HG22	5:G:204:ALA:HB3	1.92	0.51
5:K:287:ILE:HG22	5:M:204:ALA:HB3	1.92	0.51
5:O:287:ILE:HG22	5:S:204:ALA:HB3	1.92	0.51
3:Z:109:PRO:O	3:Z:112:ARG:HG2	2.11	0.51
1:O:100:CYS:SG	3:Z:25:ALA:HB1	2.50	0.51
3:8:101:ASP:OD1	5:S:23:GLY:HA3	2.11	0.51
5:D:287:ILE:HG22	5:F:204:ALA:HB3	1.92	0.50
5:I:287:ILE:HG22	5:K:204:ALA:HB3	1.92	0.50
5:J:287:ILE:HG22	5:L:204:ALA:HB3	1.92	0.50
1:O:103:ILE:HG22	1:O:104:PHE:CD1	2.45	0.50
5:G:287:ILE:HG22	5:I:204:ALA:HB3	1.92	0.50
1:9:103:ILE:HG22	1:9:104:PHE:CD1	2.46	0.50
2:4:243:GLN:NE2	1:6:149:ASP:HB3	2.26	0.50
3:5:56:SER:N	3:5:59:GLU:OE1	2.39	0.50
5:L:288:ASP:CA	5:N:204:ALA:HB2	2.32	0.50
2:4:188:ARG:NH1	3:5:75:ASP:OD2	2.45	0.50
5:H:287:ILE:HG22	5:J:204:ALA:HB3	1.92	0.50
5:I:70:PRO:HG3	5:I:81:ASP:HB3	1.93	0.50
3:5:109:PRO:O	3:5:112:ARG:HG2	2.11	0.50
3:Z:97:GLN:C	3:Z:99:LEU:N	2.65	0.50
3:2:109:PRO:O	3:2:112:ARG:HG2	2.11	0.50
5:F:287:ILE:HG22	5:H:204:ALA:HB3	1.92	0.50
5:H:318:THR:HA	5:H:327:ILE:HG12	1.94	0.50
1:6:22:LYS:HA	1:6:74:PHE:CE1	2.47	0.50
1:9:54:LYS:O	5:S:360:GLN:NE2	2.45	0.50
2:1:187:GLU:C	2:1:189:ARG:H	2.16	0.49
1:6:36:ILE:HD12	1:6:72:ILE:HB	1.94	0.49
3:8:97:GLN:C	3:8:99:LEU:N	2.65	0.49
5:E:70:PRO:HG3	5:E:81:ASP:HB3	1.94	0.49
5:K:318:THR:HA	5:K:327:ILE:HG12	1.94	0.49
2:Y:188:ARG:NH1	3:Z:75:ASP:OD2	2.45	0.49
1:9:46:ARG:NH1	1:9:51:ASN:ND2	2.59	0.49
5:E:318:THR:HA	5:E:327:ILE:HG12	1.94	0.49
5:F:318:THR:HA	5:F:327:ILE:HG12	1.94	0.49
5:O:318:THR:HA	5:O:327:ILE:HG12	1.94	0.49
5:S:318:THR:HA	5:S:327:ILE:HG12	1.94	0.49
1:9:22:LYS:HA	1:9:74:PHE:CE1	2.47	0.49
5:G:70:PRO:HG3	5:G:81:ASP:HB3	1.94	0.49
5:I:318:THR:HA	5:I:327:ILE:HG12	1.95	0.49
5:P:318:THR:HA	5:P:327:ILE:HG12	1.94	0.49
5:Q:70:PRO:HG3	5:Q:81:ASP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:318:THR:HA	5:R:327:ILE:HG12	1.94	0.49
2:Y:207:LYS:NZ	2:Y:208:GLU:HG2	2.27	0.49
2:1:188:ARG:NH1	3:2:75:ASP:OD2	2.45	0.49
3:5:26:VAL:HG13	3:5:27:THR:N	2.28	0.49
1:6:149:ASP:OD2	1:6:152:GLU:HG3	2.13	0.49
3:8:56:SER:N	3:8:59:GLU:OE1	2.39	0.49
5:M:318:THR:HA	5:M:327:ILE:HG12	1.94	0.49
5:Q:318:THR:HA	5:Q:327:ILE:HG12	1.94	0.49
1:3:149:ASP:OD2	1:3:152:GLU:HG3	2.13	0.49
5:D:318:THR:HA	5:D:327:ILE:HG12	1.95	0.49
5:I:124:PHE:CZ	5:I:132:MET:HG3	2.48	0.49
5:J:253:GLU:HA	5:J:256:ARG:CG	2.42	0.49
5:K:70:PRO:HG3	5:K:81:ASP:HB3	1.94	0.49
5:N:318:THR:HA	5:N:327:ILE:HG12	1.94	0.49
3:Z:26:VAL:HG13	3:Z:27:THR:N	2.28	0.49
1:0:22:LYS:HA	1:0:74:PHE:CE1	2.47	0.49
2:1:243:GLN:NE2	1:3:149:ASP:HB3	2.26	0.49
2:7:188:ARG:NH1	3:8:75:ASP:OD2	2.45	0.49
3:8:111:LEU:HD22	3:8:111:LEU:N	2.28	0.49
3:8:26:VAL:HG13	3:8:27:THR:N	2.28	0.49
5:G:124:PHE:CZ	5:G:132:MET:HG3	2.48	0.49
5:G:253:GLU:HA	5:G:256:ARG:CG	2.42	0.49
5:J:318:THR:HA	5:J:327:ILE:HG12	1.95	0.49
5:K:124:PHE:CZ	5:K:132:MET:HG3	2.48	0.49
5:L:318:THR:HA	5:L:327:ILE:HG12	1.95	0.49
1:0:103:ILE:HG22	1:0:104:PHE:HD1	1.78	0.49
1:0:46:ARG:NH1	1:0:51:ASN:ND2	2.59	0.49
2:1:207:LYS:HZ2	2:1:208:GLU:CG	2.26	0.49
1:3:118:GLY:HA2	1:3:133:ILE:HD13	1.95	0.49
1:3:22:LYS:HA	1:3:74:PHE:CE1	2.47	0.49
2:4:165:ALA:O	2:4:169:GLN:HG2	2.13	0.49
2:4:207:LYS:NZ	2:4:208:GLU:HG2	2.27	0.49
5:G:318:THR:HA	5:G:327:ILE:HG12	1.95	0.49
5:M:124:PHE:CZ	5:M:132:MET:HG3	2.48	0.49
5:P:124:PHE:CZ	5:P:132:MET:HG3	2.48	0.49
3:Z:56:SER:N	3:Z:59:GLU:OE1	2.39	0.49
3:2:26:VAL:HG13	3:2:27:THR:N	2.28	0.49
1:3:36:ILE:HD12	1:3:72:ILE:HB	1.95	0.49
2:4:187:GLU:C	2:4:189:ARG:H	2.16	0.49
1:9:103:ILE:HG22	1:9:104:PHE:HD1	1.78	0.49
5:D:198:TYR:CZ	5:D:248:ILE:HG13	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:70:PRO:HG3	5:N:81:ASP:HB3	1.94	0.49
5:P:198:TYR:CZ	5:P:248:ILE:HG13	2.48	0.49
5:R:70:PRO:HG3	5:R:81:ASP:HB3	1.94	0.49
5:S:70:PRO:HG3	5:S:81:ASP:HB3	1.94	0.49
3:Z:133:ASN:ND2	3:Z:133:ASN:N	2.61	0.49
2:1:207:LYS:NZ	2:1:208:GLU:HG2	2.27	0.49
1:6:118:GLY:HA2	1:6:133:ILE:HD13	1.95	0.49
2:7:187:GLU:C	2:7:189:ARG:H	2.16	0.49
5:F:70:PRO:HG3	5:F:81:ASP:HB3	1.94	0.49
5:K:198:TYR:CZ	5:K:248:ILE:HG13	2.48	0.49
5:M:198:TYR:CZ	5:M:248:ILE:HG13	2.48	0.49
5:Q:124:PHE:CZ	5:Q:132:MET:HG3	2.48	0.49
5:R:124:PHE:CZ	5:R:132:MET:HG3	2.48	0.49
2:4:194:ILE:HG21	2:4:201:LYS:CE	2.43	0.49
2:7:207:LYS:NZ	2:7:208:GLU:HG2	2.27	0.49
5:D:124:PHE:CZ	5:D:132:MET:HG3	2.48	0.49
5:E:124:PHE:CZ	5:E:132:MET:HG3	2.48	0.49
5:F:213:LYS:O	5:F:217:CYS:HB2	2.13	0.49
5:F:120:THR:HG21	5:F:370:VAL:HG11	1.95	0.49
5:I:198:TYR:CZ	5:I:248:ILE:HG13	2.48	0.49
5:I:287:ILE:HA	5:K:202:THR:HG21	1.58	0.49
5:P:70:PRO:HG3	5:P:81:ASP:HB3	1.94	0.49
3:Z:111:LEU:HD22	3:Z:111:LEU:N	2.28	0.49
3:5:111:LEU:HD22	3:5:111:LEU:N	2.28	0.48
1:6:111:PHE:HB3	1:6:147:ARG:HB3	1.95	0.48
2:7:227:ILE:CD1	2:7:231:LYS:HD3	2.43	0.48
3:8:96:SER:O	5:S:4:GLU:OE1	2.31	0.48
5:F:124:PHE:CZ	5:F:132:MET:HG3	2.48	0.48
5:F:198:TYR:CZ	5:F:248:ILE:HG13	2.48	0.48
5:G:198:TYR:CZ	5:G:248:ILE:HG13	2.48	0.48
5:M:213:LYS:O	5:M:217:CYS:HB2	2.13	0.48
5:Q:213:LYS:O	5:Q:217:CYS:HB2	2.13	0.48
3:2:97:GLN:C	3:2:99:LEU:N	2.65	0.48
5:D:120:THR:HG21	5:D:370:VAL:HG11	1.95	0.48
5:D:70:PRO:HG3	5:D:81:ASP:HB3	1.94	0.48
5:H:120:THR:HG21	5:H:370:VAL:HG11	1.95	0.48
5:H:198:TYR:CZ	5:H:248:ILE:HG13	2.48	0.48
5:K:287:ILE:HA	5:M:202:THR:HG21	1.58	0.48
5:M:287:ILE:HA	5:O:202:THR:HG21	1.58	0.48
5:N:124:PHE:CZ	5:N:132:MET:HG3	2.48	0.48
5:O:124:PHE:CZ	5:O:132:MET:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:198:TYR:CZ	5:O:248:ILE:HG13	2.48	0.48
2:Y:227:ILE:CD1	2:Y:231:LYS:HD3	2.43	0.48
3:2:133:ASN:ND2	3:2:133:ASN:N	2.61	0.48
1:6:38:THR:HA	1:6:61:ILE:HD11	1.95	0.48
1:6:59:ALA:N	5:Q:360:GLN:HG3	2.27	0.48
5:D:213:LYS:O	5:D:217:CYS:HB2	2.13	0.48
5:E:198:TYR:CZ	5:E:248:ILE:HG13	2.48	0.48
5:G:120:THR:HG21	5:G:370:VAL:HG11	1.95	0.48
5:H:124:PHE:CZ	5:H:132:MET:HG3	2.48	0.48
5:H:70:PRO:HG3	5:H:81:ASP:HB3	1.94	0.48
5:J:120:THR:HG21	5:J:370:VAL:HG11	1.95	0.48
5:M:70:PRO:HG3	5:M:81:ASP:HB3	1.94	0.48
5:O:70:PRO:HG3	5:O:81:ASP:HB3	1.94	0.48
5:R:213:LYS:O	5:R:217:CYS:HB2	2.13	0.48
2:1:194:ILE:HG21	2:1:201:LYS:CE	2.43	0.48
1:3:111:PHE:HB3	1:3:147:ARG:HB3	1.96	0.48
1:3:46:ARG:NH1	1:3:51:ASN:ND2	2.59	0.48
2:7:165:ALA:O	2:7:169:GLN:HG2	2.13	0.48
1:9:38:THR:HA	1:9:61:ILE:HD11	1.95	0.48
5:R:198:TYR:CZ	5:R:248:ILE:HG13	2.48	0.48
5:S:120:THR:HG21	5:S:370:VAL:HG11	1.95	0.48
2:1:165:ALA:O	2:1:169:GLN:HG2	2.13	0.48
3:5:123:ARG:HG3	3:5:123:ARG:NH1	2.29	0.48
1:6:103:ILE:HG22	1:6:104:PHE:HD1	1.78	0.48
2:7:207:LYS:NZ	2:7:208:GLU:HA	2.25	0.48
1:9:118:GLY:HA2	1:9:133:ILE:HD13	1.95	0.48
5:E:213:LYS:O	5:E:217:CYS:HB2	2.13	0.48
5:G:213:LYS:O	5:G:217:CYS:HB2	2.13	0.48
5:H:213:LYS:O	5:H:217:CYS:HB2	2.13	0.48
5:J:198:TYR:CZ	5:J:248:ILE:HG13	2.48	0.48
5:Q:198:TYR:CZ	5:Q:248:ILE:HG13	2.48	0.48
5:S:198:TYR:CZ	5:S:248:ILE:HG13	2.48	0.48
2:Y:165:ALA:O	2:Y:169:GLN:HG2	2.13	0.48
2:Y:187:GLU:C	2:Y:189:ARG:H	2.16	0.48
1:0:149:ASP:OD2	1:0:152:GLU:HG3	2.13	0.48
1:0:38:THR:HA	1:0:61:ILE:HD11	1.95	0.48
1:3:103:ILE:HG22	1:3:104:PHE:HD1	1.78	0.48
3:5:97:GLN:C	3:5:99:LEU:N	2.65	0.48
1:6:17:MET:HE2	1:6:17:MET:HA	1.95	0.48
1:9:36:ILE:HD12	1:9:72:ILE:HB	1.95	0.48
5:E:250:ILE:HG23	5:E:253:GLU:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:250:ILE:HG23	5:H:253:GLU:HG2	1.96	0.48
5:J:124:PHE:CZ	5:J:132:MET:HG3	2.48	0.48
5:J:250:ILE:HG23	5:J:253:GLU:HG2	1.96	0.48
5:J:70:PRO:HG3	5:J:81:ASP:HB3	1.94	0.48
5:L:70:PRO:HG3	5:L:81:ASP:HB3	1.94	0.48
5:N:213:LYS:O	5:N:217:CYS:HB2	2.13	0.48
5:P:120:THR:HG21	5:P:370:VAL:HG11	1.95	0.48
3:2:123:ARG:HG3	3:2:123:ARG:NH1	2.28	0.48
3:2:56:SER:N	3:2:59:GLU:OE1	2.39	0.48
2:4:227:ILE:CD1	2:4:231:LYS:HD3	2.43	0.48
3:5:29:ILE:HA	1:6:103:ILE:HD11	1.95	0.48
3:8:102:LEU:O	3:8:102:LEU:HD23	2.14	0.48
1:9:111:PHE:HB3	1:9:147:ARG:HB3	1.95	0.48
5:F:250:ILE:HG23	5:F:253:GLU:HG2	1.96	0.48
5:G:250:ILE:HG23	5:G:253:GLU:HG2	1.96	0.48
5:I:213:LYS:O	5:I:217:CYS:HB2	2.13	0.48
5:I:120:THR:HG21	5:I:370:VAL:HG11	1.95	0.48
5:J:213:LYS:O	5:J:217:CYS:HB2	2.13	0.48
5:K:213:LYS:O	5:K:217:CYS:HB2	2.13	0.48
5:L:124:PHE:CZ	5:L:132:MET:HG3	2.48	0.48
5:L:213:LYS:O	5:L:217:CYS:HB2	2.13	0.48
5:P:253:GLU:HA	5:P:256:ARG:CG	2.42	0.48
5:R:253:GLU:HA	5:R:256:ARG:CG	2.42	0.48
5:S:124:PHE:CZ	5:S:132:MET:HG3	2.48	0.48
5:D:250:ILE:HG23	5:D:253:GLU:HG2	1.96	0.48
5:I:250:ILE:HG23	5:I:253:GLU:HG2	1.96	0.48
5:N:198:TYR:CZ	5:N:248:ILE:HG13	2.48	0.48
5:N:250:ILE:HG23	5:N:253:GLU:HG2	1.96	0.48
5:O:213:LYS:O	5:O:217:CYS:HB2	2.13	0.48
5:O:120:THR:HG21	5:O:370:VAL:HG11	1.95	0.48
3:Z:29:ILE:CG2	3:Z:30:GLU:N	2.77	0.48
1:0:111:PHE:HB3	1:0:147:ARG:HB3	1.95	0.48
1:0:36:ILE:HD12	1:0:72:ILE:HB	1.95	0.48
3:8:133:ASN:N	3:8:133:ASN:ND2	2.61	0.48
3:8:29:ILE:CG2	3:8:30:GLU:N	2.77	0.48
1:9:149:ASP:OD2	1:9:152:GLU:HG3	2.13	0.48
5:E:120:THR:HG21	5:E:370:VAL:HG11	1.95	0.48
5:H:253:GLU:HA	5:H:256:ARG:CG	2.42	0.48
5:L:198:TYR:CZ	5:L:248:ILE:HG13	2.48	0.48
5:Q:250:ILE:HG23	5:Q:253:GLU:HG2	1.96	0.48
5:S:253:GLU:HA	5:S:256:ARG:CG	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:118:GLY:HA2	1:0:133:ILE:HD13	1.95	0.48
3:2:111:LEU:N	3:2:111:LEU:HD22	2.28	0.48
3:2:29:ILE:HG22	3:2:30:GLU:N	2.28	0.48
5:L:120:THR:HG21	5:L:370:VAL:HG11	1.95	0.48
5:Q:120:THR:HG21	5:Q:370:VAL:HG11	1.95	0.48
2:7:194:ILE:HG21	2:7:201:LYS:CE	2.43	0.47
5:K:120:THR:HG21	5:K:370:VAL:HG11	1.95	0.47
5:L:250:ILE:HG23	5:L:253:GLU:HG2	1.96	0.47
1:6:54:LYS:C	5:Q:360:GLN:HE22	2.17	0.47
5:R:250:ILE:HG23	5:R:253:GLU:HG2	1.96	0.47
2:Y:194:ILE:HG21	2:Y:201:LYS:CE	2.43	0.47
2:1:227:ILE:CD1	2:1:231:LYS:HD3	2.43	0.47
2:4:207:LYS:HZ2	2:4:208:GLU:CA	2.25	0.47
2:4:207:LYS:NZ	2:4:208:GLU:HA	2.25	0.47
3:5:102:LEU:O	3:5:102:LEU:HD23	2.14	0.47
3:8:29:ILE:HG22	3:8:30:GLU:N	2.28	0.47
5:E:253:GLU:HA	5:E:256:ARG:CG	2.42	0.47
5:K:250:ILE:HG23	5:K:253:GLU:HG2	1.96	0.47
5:N:120:THR:HG21	5:N:370:VAL:HG11	1.95	0.47
5:S:213:LYS:O	5:S:217:CYS:HB2	2.13	0.47
2:4:223:PHE:O	2:4:227:ILE:HG23	2.15	0.47
2:7:223:PHE:O	2:7:227:ILE:HG23	2.15	0.47
5:M:250:ILE:HG23	5:M:253:GLU:HG2	1.96	0.47
5:M:253:GLU:HA	5:M:256:ARG:CG	2.42	0.47
5:M:120:THR:HG21	5:M:370:VAL:HG11	1.95	0.47
5:P:250:ILE:HG23	5:P:253:GLU:HG2	1.96	0.47
5:R:120:THR:HG21	5:R:370:VAL:HG11	1.95	0.47
3:Z:102:LEU:O	3:Z:102:LEU:HD23	2.14	0.47
2:4:207:LYS:HZ2	2:4:208:GLU:CG	2.27	0.47
3:5:29:ILE:HG22	3:5:30:GLU:N	2.28	0.47
1:6:160:VAL:O	1:6:161:GLN:OXT	2.33	0.47
5:J:162:ASN:OD1	5:J:277:THR:HG22	2.15	0.47
5:L:162:ASN:OD1	5:L:277:THR:HG22	2.15	0.47
5:P:213:LYS:O	5:P:217:CYS:HB2	2.13	0.47
5:S:250:ILE:HG23	5:S:253:GLU:HG2	1.96	0.47
2:Y:223:PHE:O	2:Y:227:ILE:HG23	2.15	0.47
3:Z:100:PHE:O	3:Z:104:GLY:N	2.48	0.47
1:0:17:MET:HE2	1:0:17:MET:HA	1.96	0.47
3:2:102:LEU:O	3:2:102:LEU:HD23	2.14	0.47
1:3:13:LEU:HB2	1:3:18:ILE:CD1	2.45	0.47
1:3:38:THR:HA	1:3:61:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:73:ASP:OD1	1:3:75:GLU:HB2	2.15	0.47
3:5:100:PHE:HB3	5:Q:4:GLU:OE2	2.14	0.47
1:6:137:MET:HE3	1:6:148:ILE:HG13	1.96	0.47
3:8:100:PHE:O	3:8:104:GLY:N	2.48	0.47
5:H:162:ASN:OD1	5:H:277:THR:HG22	2.15	0.47
3:Z:29:ILE:HG22	3:Z:30:GLU:N	2.28	0.47
1:0:160:VAL:O	1:0:161:GLN:OXT	2.33	0.47
1:0:13:LEU:HB2	1:0:18:ILE:CD1	2.45	0.47
2:1:223:PHE:O	2:1:227:ILE:HG23	2.15	0.47
3:2:29:ILE:CG2	3:2:30:GLU:N	2.77	0.47
3:5:100:PHE:O	3:5:104:GLY:N	2.48	0.47
2:7:207:LYS:HZ2	2:7:208:GLU:CA	2.25	0.47
3:8:29:ILE:HA	1:9:103:ILE:HD11	1.95	0.47
1:9:160:VAL:O	1:9:161:GLN:OXT	2.33	0.47
1:9:13:LEU:HB2	1:9:18:ILE:CD1	2.45	0.47
5:K:162:ASN:OD1	5:K:277:THR:HG22	2.15	0.47
5:N:162:ASN:OD1	5:N:277:THR:HG22	2.15	0.47
5:O:250:ILE:HG23	5:O:253:GLU:HG2	1.96	0.47
5:O:162:ASN:OD1	5:O:277:THR:HG22	2.15	0.47
3:2:100:PHE:O	3:2:104:GLY:N	2.48	0.47
1:3:160:VAL:O	1:3:161:GLN:OXT	2.33	0.47
5:G:299:MET:HE2	5:G:331:ALA:HB2	1.96	0.47
1:3:58:ASP:HB3	5:R:364:GLU:OE2	2.14	0.47
1:0:103:ILE:HD11	3:Z:29:ILE:HA	1.95	0.47
2:1:234:ILE:O	2:1:235:VAL:C	2.53	0.47
1:6:13:LEU:HB2	1:6:18:ILE:CD1	2.45	0.47
5:D:162:ASN:OD1	5:D:277:THR:HG22	2.15	0.47
5:F:162:ASN:OD1	5:F:277:THR:HG22	2.15	0.47
5:I:324:THR:O	5:K:244:ASP:HA	2.09	0.47
5:J:287:ILE:HA	5:L:202:THR:HG21	1.58	0.47
5:S:162:ASN:OD1	5:S:277:THR:HG22	2.15	0.47
3:Z:11:THR:HA	3:Z:14:ARG:HH21	1.80	0.47
3:2:29:ILE:HA	1:3:103:ILE:HD11	1.95	0.47
3:5:29:ILE:CG2	3:5:30:GLU:N	2.77	0.47
3:5:92:LEU:HD12	3:5:93:GLU:N	2.30	0.47
1:9:124:THR:HG23	1:9:126:GLU:N	2.30	0.47
1:9:73:ASP:OD1	1:9:75:GLU:HB2	2.15	0.47
5:E:162:ASN:OD1	5:E:277:THR:HG22	2.15	0.47
5:O:253:GLU:HA	5:O:256:ARG:CG	2.42	0.47
5:P:162:ASN:OD1	5:P:277:THR:HG22	2.15	0.47
3:8:97:GLN:CA	5:S:4:GLU:OE2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:212:TRP:HA	2:Y:212:TRP:CE3	2.50	0.47
1:6:124:THR:HG23	1:6:126:GLU:N	2.30	0.47
5:D:253:GLU:HA	5:D:256:ARG:CG	2.42	0.47
5:J:288:ASP:CA	5:L:204:ALA:HB2	2.32	0.47
2:7:212:TRP:CE3	2:7:212:TRP:HA	2.50	0.47
5:Q:162:ASN:OD1	5:Q:277:THR:HG22	2.15	0.47
5:R:162:ASN:OD1	5:R:277:THR:HG22	2.15	0.47
3:2:92:LEU:HD12	3:2:93:GLU:N	2.30	0.46
5:G:162:ASN:OD1	5:G:277:THR:HG22	2.15	0.46
5:M:162:ASN:OD1	5:M:277:THR:HG22	2.15	0.46
1:3:58:ASP:CG	5:R:364:GLU:OE1	2.54	0.46
2:1:207:LYS:HZ2	2:1:208:GLU:CA	2.26	0.46
1:3:124:THR:HG23	1:3:126:GLU:N	2.30	0.46
2:7:234:ILE:O	2:7:235:VAL:C	2.53	0.46
5:I:162:ASN:OD1	5:I:277:THR:HG22	2.15	0.46
5:K:299:MET:HE2	5:K:331:ALA:HB2	1.96	0.46
2:Y:221:TYR:CE2	3:Z:40:LYS:HG3	2.50	0.46
1:0:124:THR:HG23	1:0:126:GLU:N	2.30	0.46
2:4:234:ILE:O	2:4:235:VAL:C	2.53	0.46
3:8:11:THR:HA	3:8:14:ARG:HH21	1.80	0.46
1:0:131:GLU:OE1	1:0:131:GLU:N	2.49	0.46
2:1:212:TRP:CE3	2:1:212:TRP:HA	2.50	0.46
1:6:73:ASP:OD1	1:6:75:GLU:HB2	2.15	0.46
5:F:299:MET:HE2	5:F:331:ALA:HB2	1.97	0.46
5:H:290:ARG:HH22	5:J:202:THR:CG2	2.18	0.46
5:N:6:THR:HG22	5:N:101:HIS:HA	1.97	0.46
1:0:73:ASP:OD1	1:0:75:GLU:HB2	2.15	0.46
1:3:17:MET:HA	1:3:17:MET:HE2	1.96	0.46
2:4:212:TRP:CE3	2:4:212:TRP:HA	2.50	0.46
3:8:92:LEU:HD12	3:8:93:GLU:N	2.30	0.46
1:6:58:ASP:CB	5:Q:360:GLN:HE21	2.26	0.46
2:1:221:TYR:CE2	3:2:40:LYS:HG3	2.50	0.46
2:4:221:TYR:CE2	3:5:40:LYS:HG3	2.50	0.46
5:I:299:MET:HE2	5:I:331:ALA:HB2	1.96	0.46
5:L:6:THR:HG22	5:L:101:HIS:HA	1.97	0.46
5:Q:6:THR:HG22	5:Q:101:HIS:HA	1.97	0.46
5:R:6:THR:HG22	5:R:101:HIS:HA	1.98	0.46
3:5:133:ASN:ND2	3:5:133:ASN:N	2.61	0.46
2:7:221:TYR:CE2	3:8:40:LYS:HG3	2.50	0.46
5:F:253:GLU:HA	5:F:256:ARG:CG	2.42	0.46
5:F:366:GLY:O	5:F:369:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:6:THR:HG22	5:F:101:HIS:HA	1.97	0.46
5:L:366:GLY:O	5:L:369:ILE:HG22	2.16	0.46
2:Y:234:ILE:O	2:Y:235:VAL:C	2.53	0.46
1:9:105:ASP:OD1	1:9:107:ASN:OD1	2.33	0.46
5:H:6:THR:HG22	5:H:101:HIS:HA	1.98	0.46
5:H:190:MET:O	5:H:194:THR:HG23	2.16	0.46
5:I:253:GLU:HA	5:I:256:ARG:CG	2.42	0.46
5:J:190:MET:O	5:J:194:THR:HG23	2.16	0.46
5:J:366:GLY:O	5:J:369:ILE:HG22	2.16	0.46
5:J:6:THR:HG22	5:J:101:HIS:HA	1.98	0.46
5:R:366:GLY:O	5:R:369:ILE:HG22	2.16	0.46
3:2:11:THR:HA	3:2:14:ARG:HH21	1.80	0.46
1:6:131:GLU:N	1:6:131:GLU:OE1	2.49	0.46
5:H:366:GLY:O	5:H:369:ILE:HG22	2.16	0.46
5:Q:299:MET:HE2	5:Q:331:ALA:HB2	1.98	0.46
1:6:55:GLU:CA	5:Q:360:GLN:CD	2.77	0.46
3:Z:92:LEU:HD12	3:Z:93:GLU:N	2.30	0.46
3:2:87:LYS:O	3:2:90:LYS:HB3	2.16	0.46
1:3:131:GLU:N	1:3:131:GLU:OE1	2.49	0.46
2:7:207:LYS:HZ2	2:7:208:GLU:CG	2.28	0.46
1:9:131:GLU:OE1	1:9:131:GLU:N	2.49	0.46
5:D:299:MET:HE2	5:D:331:ALA:HB2	1.96	0.46
5:E:6:THR:HG22	5:E:101:HIS:HA	1.97	0.46
5:N:253:GLU:HA	5:N:256:ARG:CG	2.42	0.46
3:5:87:LYS:O	3:5:90:LYS:HB3	2.16	0.45
1:6:105:ASP:OD1	1:6:107:ASN:OD1	2.33	0.45
5:D:366:GLY:O	5:D:369:ILE:HG22	2.16	0.45
5:L:223:PHE:CD2	5:L:259:GLU:HG3	2.51	0.45
5:N:366:GLY:O	5:N:369:ILE:HG22	2.16	0.45
5:P:366:GLY:O	5:P:369:ILE:HG22	2.16	0.45
5:Q:366:GLY:O	5:Q:369:ILE:HG22	2.16	0.45
5:S:190:MET:O	5:S:194:THR:HG23	2.16	0.45
5:S:366:GLY:O	5:S:369:ILE:HG22	2.16	0.45
2:4:202:LEU:H	2:4:202:LEU:CD2	2.29	0.45
5:D:6:THR:HG22	5:D:101:HIS:HA	1.97	0.45
5:M:6:THR:HG22	5:M:101:HIS:HA	1.97	0.45
5:R:190:MET:O	5:R:194:THR:HG23	2.16	0.45
3:2:100:PHE:CG	5:R:4:GLU:OE2	2.68	0.45
5:O:290:ARG:HH22	5:S:202:THR:CG2	2.18	0.45
5:S:223:PHE:CD2	5:S:259:GLU:HG3	2.51	0.45
1:0:137:MET:HE3	1:0:148:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:202:LEU:H	2:1:202:LEU:CD2	2.29	0.45
2:7:202:LEU:H	2:7:202:LEU:CD2	2.29	0.45
5:I:190:MET:O	5:I:194:THR:HG23	2.16	0.45
5:J:223:PHE:CD2	5:J:259:GLU:HG3	2.52	0.45
5:K:6:THR:HG22	5:K:101:HIS:HA	1.98	0.45
5:L:190:MET:O	5:L:194:THR:HG23	2.16	0.45
5:M:32:PRO:HB2	5:M:34:ILE:HD11	1.98	0.45
5:N:32:PRO:HB2	5:N:34:ILE:HD11	1.98	0.45
5:O:190:MET:O	5:O:194:THR:HG23	2.16	0.45
5:O:32:PRO:HB2	5:O:34:ILE:HD11	1.98	0.45
5:Q:223:PHE:CD2	5:Q:259:GLU:HG3	2.52	0.45
2:Y:246:LYS:C	2:Y:248:SER:H	2.20	0.45
3:5:11:THR:HA	3:5:14:ARG:HH21	1.80	0.45
5:E:204:ALA:HB2	5:Q:288:ASP:CA	2.32	0.45
5:G:6:THR:HG22	5:G:101:HIS:HA	1.97	0.45
5:L:299:MET:HE2	5:L:331:ALA:HB2	1.98	0.45
5:N:299:MET:HE2	5:N:331:ALA:HB2	1.99	0.45
3:5:97:GLN:NE2	5:Q:4:GLU:OE1	2.46	0.45
5:D:32:PRO:HB2	5:D:34:ILE:HD11	1.98	0.45
5:E:223:PHE:CD2	5:E:259:GLU:HG3	2.51	0.45
5:G:366:GLY:O	5:G:369:ILE:HG22	2.16	0.45
5:K:190:MET:O	5:K:194:THR:HG23	2.16	0.45
5:K:32:PRO:HB2	5:K:34:ILE:HD11	1.98	0.45
5:N:223:PHE:CD2	5:N:259:GLU:HG3	2.51	0.45
5:O:6:THR:HG22	5:O:101:HIS:HA	1.98	0.45
5:P:32:PRO:HB2	5:P:34:ILE:HD11	1.98	0.45
5:S:32:PRO:HB2	5:S:34:ILE:HD11	1.98	0.45
5:S:6:THR:HG22	5:S:101:HIS:HA	1.98	0.45
3:Z:24:LEU:HD23	3:Z:24:LEU:O	2.17	0.45
3:Z:87:LYS:O	3:Z:90:LYS:HB3	2.16	0.45
1:0:105:ASP:OD1	1:0:107:ASN:OD1	2.33	0.45
5:D:223:PHE:CD2	5:D:259:GLU:HG3	2.52	0.45
5:F:32:PRO:HB2	5:F:34:ILE:HD11	1.98	0.45
5:G:190:MET:O	5:G:194:THR:HG23	2.16	0.45
5:H:223:PHE:CD2	5:H:259:GLU:HG3	2.52	0.45
5:I:6:THR:HG22	5:I:101:HIS:HA	1.98	0.45
5:I:223:PHE:CD2	5:I:259:GLU:HG3	2.51	0.45
5:M:190:MET:O	5:M:194:THR:HG23	2.16	0.45
5:O:223:PHE:CD2	5:O:259:GLU:HG3	2.52	0.45
5:O:366:GLY:O	5:O:369:ILE:HG22	2.16	0.45
3:2:100:PHE:CD2	5:R:5:THR:HG22	2.08	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:105:ASP:O	1:0:106:LYS:O	2.35	0.45
1:3:107:ASN:HD21	1:3:109:ASP:CG	2.20	0.45
1:3:105:ASP:OD1	1:3:107:ASN:OD1	2.33	0.45
1:9:105:ASP:O	1:9:106:LYS:O	2.35	0.45
5:E:366:GLY:O	5:E:369:ILE:HG22	2.16	0.45
5:F:190:MET:O	5:F:194:THR:HG23	2.16	0.45
5:F:223:PHE:CD2	5:F:259:GLU:HG3	2.52	0.45
5:K:223:PHE:CD2	5:K:259:GLU:HG3	2.52	0.45
5:K:324:THR:O	5:M:244:ASP:HA	2.10	0.45
5:L:253:GLU:HA	5:L:256:ARG:CG	2.42	0.45
5:P:223:PHE:CD2	5:P:259:GLU:HG3	2.52	0.45
5:Q:190:MET:O	5:Q:194:THR:HG23	2.16	0.45
3:5:24:LEU:HD23	3:5:24:LEU:O	2.17	0.45
5:H:299:MET:HE2	5:H:331:ALA:HB2	1.98	0.45
5:P:6:THR:HG22	5:P:101:HIS:HA	1.98	0.45
5:Q:253:GLU:HA	5:Q:256:ARG:CG	2.42	0.45
5:Q:32:PRO:HB2	5:Q:34:ILE:HD11	1.98	0.45
5:R:32:PRO:HB2	5:R:34:ILE:HD11	1.98	0.45
2:Y:202:LEU:H	2:Y:202:LEU:CD2	2.29	0.45
3:2:129:LYS:NZ	3:2:129:LYS:HA	2.32	0.45
5:E:299:MET:HE2	5:E:331:ALA:HB2	1.99	0.45
5:E:32:PRO:HB2	5:E:34:ILE:HD11	1.98	0.45
5:G:223:PHE:CD2	5:G:259:GLU:HG3	2.51	0.45
5:M:171:LEU:HA	5:M:172:PRO:HD2	1.84	0.45
5:M:223:PHE:CD2	5:M:259:GLU:HG3	2.52	0.45
5:R:299:MET:HE2	5:R:331:ALA:HB2	1.99	0.45
2:4:246:LYS:C	2:4:248:SER:H	2.20	0.45
1:6:112:ILE:HA	1:6:116:GLU:OE2	2.17	0.45
3:8:11:THR:HG22	3:8:14:ARG:HH21	1.82	0.45
5:I:32:PRO:HB2	5:I:34:ILE:HD11	1.98	0.45
5:H:324:THR:N	5:J:245:GLY:CA	2.71	0.45
5:K:366:GLY:O	5:K:369:ILE:HG22	2.16	0.45
5:L:32:PRO:HB2	5:L:34:ILE:HD11	1.98	0.45
3:Z:11:THR:HG22	3:Z:14:ARG:HH21	1.82	0.45
3:2:137:ARG:H	3:2:137:ARG:HG2	1.49	0.44
3:2:142:GLN:HG2	3:2:143:VAL:N	2.32	0.44
2:4:227:ILE:HD12	2:4:228:LYS:N	2.32	0.44
1:6:105:ASP:O	1:6:106:LYS:O	2.35	0.44
5:N:190:MET:O	5:N:194:THR:HG23	2.16	0.44
5:R:223:PHE:HB3	5:R:259:GLU:OE2	2.18	0.44
3:8:97:GLN:CA	5:S:4:GLU:CD	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:123:ARG:NH1	3:Z:123:ARG:HG3	2.28	0.44
2:1:227:ILE:HD12	2:1:228:LYS:N	2.33	0.44
2:7:227:ILE:HG22	3:8:85:LEU:HG	1.99	0.44
5:E:190:MET:O	5:E:194:THR:HG23	2.16	0.44
5:G:32:PRO:HB2	5:G:34:ILE:HD11	1.98	0.44
5:J:223:PHE:HB3	5:J:259:GLU:OE2	2.18	0.44
5:K:253:GLU:HA	5:K:256:ARG:CG	2.42	0.44
5:R:223:PHE:CD2	5:R:259:GLU:HG3	2.52	0.44
2:Y:227:ILE:HD12	2:Y:231:LYS:HD3	2.00	0.44
3:2:24:LEU:HD23	3:2:24:LEU:O	2.17	0.44
1:6:107:ASN:HD21	1:6:109:ASP:CG	2.20	0.44
3:8:24:LEU:O	3:8:24:LEU:HD23	2.17	0.44
5:E:223:PHE:HB3	5:E:259:GLU:OE2	2.18	0.44
5:H:287:ILE:HA	5:J:202:THR:HG21	1.58	0.44
5:H:32:PRO:HB2	5:H:34:ILE:HD11	1.98	0.44
2:Y:227:ILE:HG22	3:Z:85:LEU:HG	2.00	0.44
5:D:190:MET:O	5:D:194:THR:HG23	2.16	0.44
5:M:220:ALA:HB3	5:M:223:PHE:CD1	2.53	0.44
5:M:366:GLY:O	5:M:369:ILE:HG22	2.16	0.44
5:P:190:MET:O	5:P:194:THR:HG23	2.16	0.44
5:Q:223:PHE:HB3	5:Q:259:GLU:OE2	2.18	0.44
2:1:227:ILE:HD12	2:1:231:LYS:HD3	1.99	0.44
2:1:246:LYS:C	2:1:248:SER:H	2.20	0.44
1:3:112:ILE:HA	1:3:116:GLU:OE2	2.17	0.44
3:8:28:GLU:HB3	1:9:103:ILE:HD13	2.00	0.44
5:G:223:PHE:HB3	5:G:259:GLU:OE2	2.18	0.44
5:J:32:PRO:HB2	5:J:34:ILE:HD11	1.98	0.44
5:K:220:ALA:HB3	5:K:223:PHE:CD1	2.53	0.44
5:L:223:PHE:HB3	5:L:259:GLU:OE2	2.18	0.44
1:0:103:ILE:HD13	3:Z:28:GLU:HB3	2.00	0.44
1:3:105:ASP:O	1:3:106:LYS:O	2.35	0.44
2:4:226:GLN:O	2:4:227:ILE:C	2.56	0.44
2:4:227:ILE:HG22	3:5:85:LEU:HG	2.00	0.44
3:8:123:ARG:NH1	3:8:123:ARG:HG3	2.29	0.44
3:8:53:LEU:H	3:8:53:LEU:CD1	2.10	0.44
5:D:193:LEU:O	5:D:198:TYR:HD2	2.01	0.44
5:E:193:LEU:O	5:E:198:TYR:HD2	2.01	0.44
5:I:223:PHE:HB3	5:I:259:GLU:OE2	2.18	0.44
5:J:299:MET:HE2	5:J:331:ALA:HB2	2.00	0.44
5:N:223:PHE:HB3	5:N:259:GLU:OE2	2.18	0.44
5:O:220:ALA:HB3	5:O:223:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:227:ILE:HD12	2:Y:228:LYS:N	2.32	0.44
3:Z:137:ARG:HG2	3:Z:137:ARG:H	1.49	0.44
1:0:112:ILE:HA	1:0:116:GLU:OE2	2.17	0.44
2:1:226:GLN:O	2:1:227:ILE:C	2.56	0.44
3:5:129:LYS:HA	3:5:129:LYS:NZ	2.32	0.44
1:6:59:ALA:H	5:Q:360:GLN:HG3	1.81	0.44
2:7:246:LYS:C	2:7:248:SER:H	2.20	0.44
3:8:87:LYS:O	3:8:90:LYS:HB3	2.16	0.44
1:9:107:ASN:HD21	1:9:109:ASP:CG	2.20	0.44
5:H:223:PHE:HB3	5:H:259:GLU:OE2	2.18	0.44
5:I:220:ALA:HB3	5:I:223:PHE:CD1	2.53	0.44
5:I:290:ARG:HH22	5:K:202:THR:CG2	2.18	0.44
5:K:223:PHE:HB3	5:K:259:GLU:OE2	2.17	0.44
3:Z:142:GLN:HG2	3:Z:143:VAL:N	2.32	0.44
3:2:18:LYS:O	3:2:21:MET:HB2	2.18	0.44
5:F:223:PHE:HB3	5:F:259:GLU:OE2	2.18	0.44
5:G:193:LEU:O	5:G:198:TYR:HD2	2.01	0.44
5:I:366:GLY:O	5:I:369:ILE:HG22	2.16	0.44
5:S:223:PHE:HB3	5:S:259:GLU:OE2	2.18	0.44
3:Z:129:LYS:HA	3:Z:129:LYS:NZ	2.32	0.44
3:2:11:THR:HG22	3:2:14:ARG:HH21	1.82	0.44
2:1:221:TYR:CD2	3:2:40:LYS:HG3	2.53	0.44
2:1:227:ILE:HG22	3:2:85:LEU:HG	1.99	0.44
3:5:114:VAL:HG22	3:5:115:ARG:O	2.18	0.44
2:4:221:TYR:CD2	3:5:40:LYS:HG3	2.53	0.44
2:7:227:ILE:HD12	2:7:228:LYS:N	2.32	0.44
2:7:227:ILE:HD12	2:7:231:LYS:HD3	2.00	0.44
3:8:129:LYS:HA	3:8:129:LYS:NZ	2.32	0.44
3:8:142:GLN:HG2	3:8:143:VAL:N	2.32	0.44
5:J:205:GLU:O	5:J:208:ILE:HG22	2.18	0.44
5:M:324:THR:O	5:O:244:ASP:HA	2.09	0.44
5:N:205:GLU:O	5:N:208:ILE:HG22	2.18	0.44
5:O:223:PHE:HB3	5:O:259:GLU:OE2	2.18	0.44
5:P:193:LEU:O	5:P:198:TYR:HD2	2.01	0.44
5:S:193:LEU:O	5:S:198:TYR:HD2	2.01	0.44
5:S:220:ALA:HB3	5:S:223:PHE:CD1	2.53	0.44
2:Y:226:GLN:O	2:Y:227:ILE:C	2.56	0.44
2:1:215:GLN:O	2:1:219:GLU:HG3	2.18	0.43
1:9:112:ILE:HA	1:9:116:GLU:OE2	2.17	0.43
5:D:223:PHE:HB3	5:D:259:GLU:OE2	2.18	0.43
5:E:287:ILE:N	5:G:202:THR:CG2	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:193:LEU:O	5:I:198:TYR:HD2	2.01	0.43
5:M:223:PHE:HB3	5:M:259:GLU:OE2	2.18	0.43
5:O:193:LEU:O	5:O:198:TYR:HD2	2.01	0.43
5:P:223:PHE:HB3	5:P:259:GLU:OE2	2.18	0.43
5:Q:205:GLU:O	5:Q:208:ILE:HG22	2.18	0.43
5:R:205:GLU:O	5:R:208:ILE:HG22	2.18	0.43
2:Y:215:GLN:O	2:Y:219:GLU:HG3	2.18	0.43
2:4:221:TYR:O	2:4:224:ALA:HB3	2.19	0.43
3:5:142:GLN:HG2	3:5:143:VAL:N	2.32	0.43
2:7:187:GLU:O	2:7:189:ARG:N	2.52	0.43
2:7:215:GLN:O	2:7:219:GLU:HG3	2.18	0.43
3:8:68:HIS:HA	3:8:71:ILE:HD12	2.00	0.43
5:G:220:ALA:HB3	5:G:223:PHE:CD1	2.53	0.43
5:L:205:GLU:O	5:L:208:ILE:HG22	2.18	0.43
3:Z:122:LEU:HD23	3:Z:134:MET:HE1	2.00	0.43
1:0:107:ASN:HD21	1:0:109:ASP:CG	2.20	0.43
3:2:63:LEU:O	3:2:66:LYS:HB3	2.18	0.43
3:5:11:THR:HG22	3:5:14:ARG:HH21	1.82	0.43
3:5:18:LYS:O	3:5:21:MET:HB2	2.18	0.43
5:F:193:LEU:O	5:F:198:TYR:HD2	2.01	0.43
3:2:68:HIS:HA	3:2:71:ILE:HD12	2.00	0.43
3:2:28:GLU:HB3	1:3:103:ILE:HD13	2.00	0.43
3:5:141:LYS:CD	3:5:141:LYS:N	2.70	0.43
1:6:10:ARG:HH21	1:6:75:GLU:CD	2.22	0.43
2:7:221:TYR:O	2:7:224:ALA:HB3	2.19	0.43
2:7:230:LYS:NZ	3:8:89:ILE:HG12	2.34	0.43
5:D:204:ALA:H	5:P:287:ILE:CB	2.15	0.43
5:J:149:THR:HA	5:J:165:ILE:O	2.19	0.43
5:J:193:LEU:O	5:J:198:TYR:HD2	2.01	0.43
5:L:149:THR:HA	5:L:165:ILE:O	2.18	0.43
5:L:193:LEU:O	5:L:198:TYR:HD2	2.01	0.43
5:Q:149:THR:HA	5:Q:165:ILE:O	2.19	0.43
5:R:149:THR:HA	5:R:165:ILE:O	2.19	0.43
2:Y:230:LYS:NZ	3:Z:89:ILE:HG12	2.34	0.43
3:Z:85:LEU:CD2	3:Z:89:ILE:HG13	2.48	0.43
2:1:221:TYR:O	2:1:224:ALA:HB3	2.18	0.43
3:2:114:VAL:HG22	3:2:115:ARG:O	2.18	0.43
1:3:10:ARG:HH21	1:3:75:GLU:CD	2.22	0.43
3:5:122:LEU:HD23	3:5:134:MET:HE1	2.00	0.43
3:5:63:LEU:O	3:5:66:LYS:HB3	2.18	0.43
2:7:198:ASN:HD22	2:7:201:LYS:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:149:THR:HA	5:E:165:ILE:O	2.19	0.43
5:E:205:GLU:O	5:E:208:ILE:HG22	2.18	0.43
5:F:149:THR:HA	5:F:165:ILE:O	2.19	0.43
5:M:193:LEU:O	5:M:198:TYR:HD2	2.01	0.43
5:M:324:THR:N	5:O:245:GLY:CA	2.71	0.43
3:5:53:LEU:HA	3:5:54:PRO:HD3	1.83	0.43
3:5:85:LEU:CD2	3:5:89:ILE:HG13	2.48	0.43
3:8:58:GLN:O	3:8:62:GLU:HB2	2.19	0.43
5:D:217:CYS:C	5:D:218:TYR:HD1	2.22	0.43
5:E:220:ALA:HB3	5:E:223:PHE:CD1	2.53	0.43
5:F:205:GLU:O	5:F:208:ILE:HG22	2.18	0.43
5:G:149:THR:HA	5:G:165:ILE:O	2.19	0.43
5:I:149:THR:HA	5:I:165:ILE:O	2.19	0.43
5:L:220:ALA:HB3	5:L:223:PHE:CD1	2.53	0.43
5:N:220:ALA:HB3	5:N:223:PHE:CD1	2.53	0.43
5:Q:193:LEU:O	5:Q:198:TYR:HD2	2.01	0.43
2:Y:198:ASN:HD22	2:Y:201:LYS:HB2	1.83	0.43
1:0:65:ASP:OD1	1:0:69:SER:OG	2.37	0.43
2:1:198:ASN:HD22	2:1:201:LYS:HB2	1.84	0.43
3:8:114:VAL:HG22	3:8:115:ARG:O	2.18	0.43
3:8:18:LYS:O	3:8:21:MET:HB2	2.18	0.43
2:7:221:TYR:CD2	3:8:40:LYS:HG3	2.53	0.43
5:N:149:THR:HA	5:N:165:ILE:O	2.19	0.43
5:O:171:LEU:HA	5:O:172:PRO:HD2	1.84	0.43
2:Y:221:TYR:O	2:Y:224:ALA:HB3	2.19	0.43
3:Z:18:LYS:O	3:Z:21:MET:HB2	2.18	0.43
3:Z:68:HIS:HA	3:Z:71:ILE:HD12	2.00	0.43
1:0:74:PHE:O	1:0:78:LEU:HG	2.19	0.43
3:2:85:LEU:CD2	3:2:89:ILE:HG13	2.48	0.43
2:4:215:GLN:O	2:4:219:GLU:HG3	2.18	0.43
2:4:227:ILE:HD12	2:4:231:LYS:HD3	2.00	0.43
3:5:68:HIS:HA	3:5:71:ILE:HD12	2.00	0.43
5:G:205:GLU:O	5:G:208:ILE:HG22	2.18	0.43
5:H:149:THR:HA	5:H:165:ILE:O	2.19	0.43
5:M:315:LYS:HD2	5:M:315:LYS:HA	1.92	0.43
5:N:193:LEU:O	5:N:198:TYR:HD2	2.01	0.43
2:Y:221:TYR:CD2	3:Z:40:LYS:HG3	2.53	0.43
3:2:58:GLN:O	3:2:62:GLU:HB2	2.18	0.43
1:3:65:ASP:OD1	1:3:69:SER:OG	2.37	0.43
3:5:28:GLU:HB3	1:6:103:ILE:HD13	2.00	0.43
3:5:14:ARG:HG2	1:6:136:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:32:GLU:O	3:8:36:LYS:HB2	2.19	0.43
3:8:85:LEU:CD2	3:8:89:ILE:HG13	2.48	0.43
1:9:74:PHE:O	1:9:78:LEU:HG	2.19	0.43
5:F:217:CYS:C	5:F:218:TYR:HD1	2.22	0.43
5:H:205:GLU:O	5:H:208:ILE:HG22	2.18	0.43
5:P:217:CYS:C	5:P:218:TYR:HD1	2.22	0.43
5:R:217:CYS:C	5:R:218:TYR:HD1	2.22	0.43
5:R:220:ALA:HB3	5:R:223:PHE:CD1	2.53	0.43
1:3:58:ASP:HB3	5:R:360:GLN:HG2	1.57	0.43
3:Z:114:VAL:HG22	3:Z:115:ARG:O	2.17	0.43
1:0:136:LEU:HG	3:Z:14:ARG:HG2	2.01	0.43
3:Z:32:GLU:O	3:Z:36:LYS:HB2	2.19	0.43
3:2:32:GLU:O	3:2:36:LYS:HB2	2.19	0.43
1:6:65:ASP:OD1	1:6:69:SER:OG	2.37	0.43
2:7:226:GLN:O	2:7:227:ILE:C	2.56	0.43
3:8:14:ARG:HG2	1:9:136:LEU:HG	2.01	0.43
5:E:245:GLY:CA	5:Q:324:THR:N	2.71	0.43
5:E:315:LYS:HA	5:E:315:LYS:HD2	1.92	0.43
5:K:193:LEU:O	5:K:198:TYR:HD2	2.01	0.43
5:P:220:ALA:HB3	5:P:223:PHE:CD1	2.53	0.43
3:2:14:ARG:HG2	1:3:136:LEU:HG	2.01	0.42
2:4:198:ASN:HD22	2:4:201:LYS:HB2	1.84	0.42
3:8:63:LEU:O	3:8:66:LYS:HB3	2.18	0.42
1:9:10:ARG:HH21	1:9:75:GLU:CD	2.22	0.42
5:D:149:THR:HA	5:D:165:ILE:O	2.19	0.42
5:J:220:ALA:HB3	5:J:223:PHE:CD1	2.53	0.42
5:L:180:LEU:HD11	5:L:261:LEU:HD23	2.01	0.42
5:M:222:ASP:OD1	5:M:224:GLU:HB3	2.20	0.42
5:N:180:LEU:HD11	5:N:261:LEU:HD23	2.01	0.42
5:O:149:THR:HA	5:O:165:ILE:O	2.19	0.42
5:Q:171:LEU:HA	5:Q:172:PRO:HD2	1.84	0.42
5:Q:180:LEU:HD11	5:Q:261:LEU:HD23	2.01	0.42
5:R:180:LEU:HD11	5:R:261:LEU:HD23	2.01	0.42
1:9:65:ASP:OD1	1:9:69:SER:OG	2.37	0.42
5:H:220:ALA:HB3	5:H:223:PHE:CD1	2.53	0.42
5:I:180:LEU:HD11	5:I:261:LEU:HD23	2.01	0.42
5:J:180:LEU:HD11	5:J:261:LEU:HD23	2.01	0.42
5:K:149:THR:HA	5:K:165:ILE:O	2.19	0.42
5:I:324:THR:N	5:K:245:GLY:CA	2.71	0.42
5:Q:220:ALA:HB3	5:Q:223:PHE:CD1	2.53	0.42
3:Z:58:GLN:O	3:Z:62:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:8:GLU:HA	1:3:11:ALA:HB3	2.01	0.42
3:5:58:GLN:O	3:5:62:GLU:HB2	2.19	0.42
2:7:234:ILE:HG12	3:8:92:LEU:HB3	2.02	0.42
5:E:180:LEU:HD11	5:E:261:LEU:HD23	2.01	0.42
5:F:206:ARG:O	5:F:209:VAL:HG12	2.20	0.42
5:H:206:ARG:O	5:H:209:VAL:HG12	2.20	0.42
5:H:180:LEU:HD11	5:H:261:LEU:HD23	2.01	0.42
5:I:217:CYS:C	5:I:218:TYR:HD1	2.22	0.42
5:K:217:CYS:C	5:K:218:TYR:HD1	2.22	0.42
5:K:180:LEU:HD11	5:K:261:LEU:HD23	2.01	0.42
5:M:217:CYS:C	5:M:218:TYR:HD1	2.22	0.42
2:Y:234:ILE:HG12	3:Z:92:LEU:HB3	2.02	0.42
2:4:234:ILE:HG12	3:5:92:LEU:HB3	2.02	0.42
3:5:32:GLU:O	3:5:36:LYS:HB2	2.19	0.42
3:5:53:LEU:H	3:5:53:LEU:CD1	2.10	0.42
1:6:8:GLU:HA	1:6:11:ALA:HB3	2.01	0.42
1:6:46:ARG:NH1	1:6:51:ASN:ND2	2.59	0.42
5:D:180:LEU:HD11	5:D:261:LEU:HD23	2.01	0.42
5:E:206:ARG:O	5:E:209:VAL:HG12	2.20	0.42
5:F:180:LEU:HD11	5:F:261:LEU:HD23	2.01	0.42
5:I:206:ARG:O	5:I:209:VAL:HG12	2.20	0.42
5:K:222:ASP:OD1	5:K:224:GLU:HB3	2.19	0.42
5:M:180:LEU:HD11	5:M:261:LEU:HD23	2.01	0.42
5:O:324:THR:O	5:S:244:ASP:HA	2.10	0.42
5:P:180:LEU:HD11	5:P:261:LEU:HD23	2.01	0.42
5:R:206:ARG:O	5:R:209:VAL:HG12	2.20	0.42
5:S:180:LEU:HD11	5:S:261:LEU:HD23	2.01	0.42
3:Z:130:HIS:HE1	3:Z:134:MET:CE	2.32	0.42
3:2:130:HIS:CE1	3:2:134:MET:HE3	2.51	0.42
1:3:13:LEU:HB2	1:3:18:ILE:HD11	2.01	0.42
5:D:202:THR:CG2	5:P:287:ILE:N	2.76	0.42
5:D:220:ALA:HB3	5:D:223:PHE:CD1	2.53	0.42
5:G:180:LEU:HD11	5:G:261:LEU:HD23	2.01	0.42
5:H:193:LEU:O	5:H:198:TYR:HD2	2.01	0.42
5:I:205:GLU:O	5:I:208:ILE:HG22	2.18	0.42
5:J:206:ARG:O	5:J:209:VAL:HG12	2.19	0.42
5:K:206:ARG:O	5:K:209:VAL:HG12	2.20	0.42
5:M:206:ARG:O	5:M:209:VAL:HG12	2.19	0.42
5:M:196:ARG:HH21	5:M:249:THR:HG23	1.85	0.42
5:N:217:CYS:C	5:N:218:TYR:HD1	2.22	0.42
5:O:180:LEU:HD11	5:O:261:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:206:ARG:O	5:O:209:VAL:HG12	2.20	0.42
5:P:149:THR:HA	5:P:165:ILE:O	2.19	0.42
5:R:193:LEU:O	5:R:198:TYR:HD2	2.01	0.42
3:2:100:PHE:HB3	5:R:4:GLU:OE2	2.16	0.42
2:1:230:LYS:NZ	3:2:89:ILE:HG12	2.34	0.42
1:3:74:PHE:O	1:3:78:LEU:HG	2.19	0.42
1:6:74:PHE:O	1:6:78:LEU:HG	2.19	0.42
2:7:207:LYS:HG3	2:7:208:GLU:N	2.35	0.42
5:E:222:ASP:OD1	5:E:224:GLU:HB3	2.19	0.42
5:G:196:ARG:HH21	5:G:249:THR:HG23	1.85	0.42
5:F:290:ARG:HH22	5:H:202:THR:CG2	2.18	0.42
5:K:287:ILE:N	5:M:202:THR:CG2	2.76	0.42
5:O:205:GLU:O	5:O:208:ILE:HG22	2.18	0.42
5:Q:196:ARG:HH21	5:Q:249:THR:HG23	1.85	0.42
5:Q:193:LEU:HD11	5:Q:250:ILE:HG13	2.02	0.42
3:Z:63:LEU:O	3:Z:66:LYS:HB3	2.18	0.42
1:0:10:ARG:HH21	1:0:75:GLU:CD	2.22	0.42
2:1:234:ILE:HG12	3:2:92:LEU:HB3	2.02	0.42
3:2:53:LEU:HA	3:2:54:PRO:HD3	1.83	0.42
5:D:193:LEU:HD11	5:D:250:ILE:HG13	2.02	0.42
5:H:217:CYS:C	5:H:218:TYR:HD1	2.22	0.42
5:I:196:ARG:HH21	5:I:249:THR:HG23	1.85	0.42
5:K:205:GLU:O	5:K:208:ILE:HG22	2.18	0.42
5:M:149:THR:HA	5:M:165:ILE:O	2.19	0.42
5:N:222:ASP:OD1	5:N:224:GLU:HB3	2.19	0.42
5:O:217:CYS:C	5:O:218:TYR:HD1	2.23	0.42
5:D:244:ASP:HA	5:P:324:THR:O	2.09	0.42
5:N:287:ILE:HA	5:R:202:THR:HG21	1.58	0.42
5:S:193:LEU:HD11	5:S:250:ILE:HG13	2.02	0.42
3:Z:46:GLU:HA	3:Z:49:PRO:HG3	2.02	0.42
3:Z:7:ARG:HG2	3:Z:7:ARG:O	2.20	0.42
2:4:190:LYS:HA	2:4:191:PRO:HD2	1.80	0.42
2:4:230:LYS:NZ	3:5:89:ILE:HG12	2.34	0.42
1:9:59:ALA:HB2	5:S:360:GLN:HG3	2.02	0.42
5:D:205:GLU:O	5:D:208:ILE:HG22	2.19	0.42
5:D:206:ARG:O	5:D:209:VAL:HG12	2.20	0.42
5:F:220:ALA:HB3	5:F:223:PHE:CD1	2.53	0.42
5:F:222:ASP:OD1	5:F:224:GLU:HB3	2.20	0.42
5:F:196:ARG:HH21	5:F:249:THR:HG23	1.85	0.42
5:G:217:CYS:C	5:G:218:TYR:HD1	2.22	0.42
5:L:217:CYS:C	5:L:218:TYR:HD1	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:193:LEU:HD11	5:O:250:ILE:HG13	2.02	0.42
5:O:222:ASP:OD1	5:O:224:GLU:HB3	2.20	0.42
5:O:196:ARG:HH21	5:O:249:THR:HG23	1.85	0.42
5:O:369:ILE:HG23	5:O:370:VAL:N	2.35	0.42
5:P:171:LEU:HA	5:P:172:PRO:HD2	1.84	0.42
5:Q:217:CYS:C	5:Q:218:TYR:HD1	2.22	0.42
5:R:222:ASP:OD1	5:R:224:GLU:HB3	2.19	0.42
5:S:149:THR:HA	5:S:165:ILE:O	2.19	0.42
5:S:206:ARG:O	5:S:209:VAL:HG12	2.20	0.42
1:O:13:LEU:HB2	1:O:18:ILE:HD11	2.01	0.42
3:2:46:GLU:HA	3:2:49:PRO:HG3	2.02	0.42
2:7:202:LEU:N	2:7:202:LEU:HD22	2.35	0.42
3:8:7:ARG:HG2	3:8:7:ARG:O	2.20	0.42
5:D:196:ARG:HH21	5:D:249:THR:HG23	1.85	0.42
5:D:369:ILE:HG23	5:D:370:VAL:N	2.35	0.42
5:F:287:ILE:N	5:H:202:THR:CG2	2.76	0.42
5:F:369:ILE:HG23	5:F:370:VAL:N	2.35	0.42
5:G:193:LEU:HD11	5:G:250:ILE:HG13	2.02	0.42
5:H:369:ILE:HG23	5:H:370:VAL:N	2.35	0.42
5:J:221:LEU:HA	5:J:312:ARG:HG2	2.02	0.42
5:J:369:ILE:HG23	5:J:370:VAL:N	2.35	0.42
5:K:369:ILE:HG23	5:K:370:VAL:N	2.35	0.42
5:N:206:ARG:O	5:N:209:VAL:HG12	2.20	0.42
5:P:205:GLU:O	5:P:208:ILE:HG22	2.18	0.42
5:Q:206:ARG:O	5:Q:209:VAL:HG12	2.20	0.42
5:Q:222:ASP:OD1	5:Q:224:GLU:HB3	2.19	0.42
5:R:193:LEU:HD11	5:R:250:ILE:HG13	2.02	0.42
5:S:217:CYS:C	5:S:218:TYR:HD1	2.22	0.42
3:Z:53:LEU:CD1	3:Z:53:LEU:H	2.10	0.42
2:1:207:LYS:HG3	2:1:208:GLU:N	2.35	0.42
1:3:137:MET:HE3	1:3:148:ILE:HG13	1.99	0.42
1:3:82:VAL:O	1:3:83:ARG:C	2.59	0.42
2:4:207:LYS:HG3	2:4:208:GLU:N	2.35	0.42
3:5:46:GLU:HA	3:5:49:PRO:HG3	2.02	0.42
1:6:150:PHE:O	1:6:154:LEU:HD22	2.20	0.42
3:8:130:HIS:HE1	3:8:134:MET:CE	2.32	0.42
5:D:221:LEU:HA	5:D:312:ARG:HG2	2.02	0.42
5:G:222:ASP:OD1	5:G:224:GLU:HB3	2.20	0.42
5:G:369:ILE:HG23	5:G:370:VAL:N	2.35	0.42
5:H:221:LEU:HA	5:H:312:ARG:HG2	2.02	0.42
5:J:222:ASP:OD1	5:J:224:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:315:LYS:HD2	5:K:315:LYS:HA	1.92	0.42
5:L:193:LEU:HD11	5:L:250:ILE:HG13	2.02	0.42
5:L:222:ASP:OD1	5:L:224:GLU:HB3	2.20	0.42
5:L:221:LEU:HA	5:L:312:ARG:HG2	2.02	0.42
5:M:193:LEU:HD11	5:M:250:ILE:HG13	2.02	0.42
5:P:222:ASP:OD1	5:P:224:GLU:HB3	2.19	0.42
5:P:369:ILE:HG23	5:P:370:VAL:N	2.35	0.42
5:R:196:ARG:HH21	5:R:249:THR:HG23	1.85	0.42
5:S:221:LEU:HA	5:S:312:ARG:HG2	2.02	0.42
3:5:140:LEU:HD12	3:5:140:LEU:HA	1.73	0.41
3:8:46:GLU:HA	3:8:49:PRO:HG3	2.02	0.41
1:9:13:LEU:HB2	1:9:18:ILE:HD11	2.01	0.41
5:E:193:LEU:HD11	5:E:250:ILE:HG13	2.02	0.41
5:E:217:CYS:C	5:E:218:TYR:HD1	2.22	0.41
5:F:221:LEU:HA	5:F:312:ARG:HG2	2.02	0.41
5:F:287:ILE:HA	5:H:202:THR:HG21	1.58	0.41
5:H:222:ASP:OD1	5:H:224:GLU:HB3	2.20	0.41
5:I:193:LEU:HD11	5:I:250:ILE:HG13	2.02	0.41
5:I:226:GLU:HG3	5:I:255:PHE:CE2	2.55	0.41
5:L:369:ILE:HG23	5:L:370:VAL:N	2.35	0.41
5:M:205:GLU:O	5:M:208:ILE:HG22	2.18	0.41
5:M:369:ILE:HG23	5:M:370:VAL:N	2.35	0.41
5:N:221:LEU:HA	5:N:312:ARG:HG2	2.02	0.41
5:O:287:ILE:N	5:S:202:THR:CG2	2.76	0.41
5:P:206:ARG:O	5:P:209:VAL:HG12	2.20	0.41
5:P:221:LEU:HA	5:P:312:ARG:HG2	2.02	0.41
5:R:171:LEU:HA	5:R:172:PRO:HD2	1.84	0.41
5:R:369:ILE:HG23	5:R:370:VAL:N	2.35	0.41
5:S:369:ILE:HG23	5:S:370:VAL:N	2.35	0.41
3:2:7:ARG:O	3:2:7:ARG:HG2	2.20	0.41
2:4:245:GLN:O	2:4:246:LYS:C	2.59	0.41
3:5:130:HIS:HE1	3:5:134:MET:CE	2.32	0.41
1:6:13:LEU:HB2	1:6:18:ILE:HD11	2.01	0.41
1:9:8:GLU:HA	1:9:11:ALA:HB3	2.01	0.41
5:D:222:ASP:OD1	5:D:224:GLU:HB3	2.20	0.41
5:E:204:ALA:H	5:Q:287:ILE:CB	2.15	0.41
5:F:193:LEU:HD11	5:F:250:ILE:HG13	2.02	0.41
5:I:369:ILE:HG23	5:I:370:VAL:N	2.35	0.41
5:J:217:CYS:C	5:J:218:TYR:HD1	2.22	0.41
5:K:193:LEU:HD11	5:K:250:ILE:HG13	2.02	0.41
5:N:369:ILE:HG23	5:N:370:VAL:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:226:GLU:HG3	5:O:255:PHE:CE2	2.55	0.41
2:Y:212:TRP:HA	2:Y:212:TRP:HE3	1.85	0.41
3:5:105:LYS:HG3	5:Q:1:ASP:OD1	2.20	0.41
1:9:82:VAL:O	1:9:83:ARG:C	2.58	0.41
5:E:369:ILE:HG23	5:E:370:VAL:N	2.35	0.41
5:G:226:GLU:HG3	5:G:255:PHE:CE2	2.56	0.41
5:E:324:THR:N	5:G:245:GLY:CA	2.71	0.41
5:H:193:LEU:HD11	5:H:250:ILE:HG13	2.02	0.41
5:N:193:LEU:HD11	5:N:250:ILE:HG13	2.02	0.41
5:O:221:LEU:HA	5:O:312:ARG:HG2	2.02	0.41
5:P:196:ARG:HH21	5:P:249:THR:HG23	1.85	0.41
5:P:193:LEU:HD11	5:P:250:ILE:HG13	2.02	0.41
5:Q:369:ILE:HG23	5:Q:370:VAL:N	2.35	0.41
5:N:290:ARG:HH22	5:R:202:THR:CG2	2.18	0.41
1:3:58:ASP:CG	5:R:364:GLU:OE2	2.58	0.41
3:Z:82:GLU:O	3:Z:86:GLN:HG3	2.20	0.41
5:E:196:ARG:HH21	5:E:249:THR:HG23	1.85	0.41
5:H:226:GLU:HG3	5:H:255:PHE:CE2	2.55	0.41
5:J:226:GLU:HG3	5:J:255:PHE:CE2	2.55	0.41
5:J:196:ARG:HH21	5:J:249:THR:HG23	1.85	0.41
5:J:193:LEU:HD11	5:J:250:ILE:HG13	2.02	0.41
5:J:315:LYS:HA	5:J:315:LYS:HD2	1.92	0.41
5:N:227:MET:O	5:N:230:ALA:HB3	2.21	0.41
5:N:288:ASP:CA	5:R:204:ALA:HB2	2.32	0.41
2:1:187:GLU:O	2:1:189:ARG:N	2.52	0.41
2:1:190:LYS:HA	2:1:191:PRO:HD2	1.80	0.41
3:2:66:LYS:HE2	3:2:66:LYS:HB2	1.90	0.41
1:6:82:VAL:O	1:6:83:ARG:C	2.59	0.41
2:7:212:TRP:HE3	2:7:212:TRP:HA	1.85	0.41
1:9:17:MET:HA	1:9:17:MET:HE2	2.02	0.41
5:G:206:ARG:O	5:G:209:VAL:HG12	2.20	0.41
5:G:315:LYS:HD2	5:G:315:LYS:HA	1.92	0.41
5:L:196:ARG:HH21	5:L:249:THR:HG23	1.85	0.41
5:J:324:THR:N	5:L:245:GLY:CA	2.71	0.41
5:N:287:ILE:HD11	5:R:202:THR:HA	1.64	0.41
5:S:226:GLU:HG3	5:S:255:PHE:CE2	2.55	0.41
1:0:8:GLU:HA	1:0:11:ALA:HB3	2.01	0.41
3:2:105:LYS:HA	5:R:1:ASP:CG	2.41	0.41
1:3:150:PHE:O	1:3:154:LEU:HD22	2.20	0.41
2:4:230:LYS:HA	2:4:233:GLU:HG3	2.02	0.41
3:5:82:GLU:O	3:5:86:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:122:LEU:HD23	3:8:134:MET:HE1	2.03	0.41
1:9:144:ASN:O	1:9:144:ASN:ND2	2.54	0.41
5:D:227:MET:O	5:D:230:ALA:HB3	2.21	0.41
5:D:324:THR:O	5:F:244:ASP:HA	2.10	0.41
5:E:204:ALA:HA	5:Q:288:ASP:OD1	2.21	0.41
5:F:226:GLU:HG3	5:F:255:PHE:CE2	2.55	0.41
5:D:324:THR:N	5:F:245:GLY:CA	2.71	0.41
5:E:288:ASP:OD1	5:G:204:ALA:HA	2.21	0.41
5:I:222:ASP:OD1	5:I:224:GLU:HB3	2.19	0.41
5:L:226:GLU:HG3	5:L:255:PHE:CE2	2.55	0.41
5:M:226:GLU:HG3	5:M:255:PHE:CE2	2.55	0.41
5:M:221:LEU:HA	5:M:312:ARG:HG2	2.02	0.41
5:M:32:PRO:HB2	5:M:34:ILE:CD1	2.51	0.41
5:P:299:MET:HE2	5:P:331:ALA:HB2	2.01	0.41
5:P:144:ALA:HB2	5:P:342:GLY:CA	2.51	0.41
5:Q:227:MET:O	5:Q:230:ALA:HB3	2.21	0.41
5:Q:221:LEU:HA	5:Q:312:ARG:HG2	2.02	0.41
5:R:221:LEU:HA	5:R:312:ARG:HG2	2.02	0.41
5:R:226:GLU:HG3	5:R:255:PHE:CE2	2.55	0.41
5:S:171:LEU:HA	5:S:172:PRO:HD2	1.84	0.41
5:S:222:ASP:OD1	5:S:224:GLU:HB3	2.20	0.41
5:S:196:ARG:HH21	5:S:249:THR:HG23	1.85	0.41
2:Y:207:LYS:HG3	2:Y:208:GLU:N	2.35	0.41
1:0:79:VAL:HG12	1:0:83:ARG:NE	2.36	0.41
2:4:187:GLU:O	2:4:189:ARG:N	2.51	0.41
3:8:82:GLU:O	3:8:86:GLN:HG3	2.20	0.41
1:9:150:PHE:O	1:9:154:LEU:HD22	2.20	0.41
1:9:79:VAL:HG12	1:9:83:ARG:NE	2.36	0.41
5:D:226:GLU:HG3	5:D:255:PHE:CE2	2.55	0.41
5:E:227:MET:O	5:E:230:ALA:HB3	2.21	0.41
5:F:32:PRO:HB2	5:F:34:ILE:CD1	2.51	0.41
5:H:196:ARG:HH21	5:H:249:THR:HG23	1.85	0.41
5:G:288:ASP:OD1	5:I:204:ALA:HA	2.21	0.41
5:I:315:LYS:HA	5:I:315:LYS:HD2	1.92	0.41
5:K:227:MET:O	5:K:230:ALA:HB3	2.21	0.41
5:L:206:ARG:O	5:L:209:VAL:HG12	2.20	0.41
5:L:227:MET:O	5:L:230:ALA:HB3	2.21	0.41
5:M:287:ILE:HD11	5:O:202:THR:HA	1.64	0.41
5:N:196:ARG:HH21	5:N:249:THR:HG23	1.85	0.41
5:O:256:ARG:HD2	5:O:256:ARG:HH11	1.78	0.41
5:O:32:PRO:HB2	5:O:34:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:144:ALA:HB2	5:R:342:GLY:CA	2.51	0.41
5:R:315:LYS:HA	5:R:315:LYS:HD2	1.92	0.41
1:0:5:GLN:C	1:0:7:ALA:N	2.74	0.41
1:0:82:VAL:O	1:0:83:ARG:C	2.59	0.41
3:2:82:GLU:O	3:2:86:GLN:HG3	2.20	0.41
3:5:7:ARG:O	3:5:7:ARG:HG2	2.20	0.41
5:D:32:PRO:HB2	5:D:34:ILE:CD1	2.51	0.41
5:I:227:MET:O	5:I:230:ALA:HB3	2.21	0.41
5:K:32:PRO:HB2	5:K:34:ILE:CD1	2.51	0.41
5:P:32:PRO:HB2	5:P:34:ILE:CD1	2.51	0.41
5:Q:144:ALA:HB2	5:Q:342:GLY:CA	2.51	0.41
5:S:227:MET:O	5:S:230:ALA:HB3	2.21	0.41
5:S:32:PRO:HB2	5:S:34:ILE:CD1	2.51	0.41
3:2:130:HIS:HE1	3:2:134:MET:CE	2.32	0.41
1:6:79:VAL:HG12	1:6:83:ARG:NE	2.36	0.41
3:8:100:PHE:CB	5:S:4:GLU:OE2	2.69	0.41
3:8:140:LEU:HA	3:8:140:LEU:HD12	1.72	0.41
2:7:189:ARG:NE	3:8:72:ASP:OD1	2.47	0.41
1:9:5:GLN:C	1:9:7:ALA:N	2.74	0.41
5:D:144:ALA:HB2	5:D:342:GLY:CA	2.51	0.41
5:E:221:LEU:HA	5:E:312:ARG:HG2	2.02	0.41
5:G:32:PRO:HB2	5:G:34:ILE:CD1	2.51	0.41
5:H:227:MET:O	5:H:230:ALA:HB3	2.21	0.41
5:I:144:ALA:HB2	5:I:342:GLY:CA	2.51	0.41
5:G:287:ILE:CB	5:I:204:ALA:H	2.14	0.41
5:J:144:ALA:HB2	5:J:342:GLY:CA	2.51	0.41
5:I:288:ASP:OD1	5:K:204:ALA:HA	2.21	0.41
5:K:226:GLU:HG3	5:K:255:PHE:CE2	2.55	0.41
5:L:144:ALA:HB2	5:L:342:GLY:CA	2.51	0.41
5:M:227:MET:O	5:M:230:ALA:HB3	2.21	0.41
5:N:226:GLU:HG3	5:N:255:PHE:CE2	2.55	0.41
5:N:315:LYS:HA	5:N:315:LYS:HD2	1.92	0.41
5:N:144:ALA:HB2	5:N:342:GLY:CA	2.51	0.41
5:S:205:GLU:O	5:S:208:ILE:HG22	2.19	0.41
2:Y:198:ASN:CB	2:Y:201:LYS:HB2	2.39	0.41
2:Y:245:GLN:O	2:Y:246:LYS:C	2.59	0.41
2:1:230:LYS:HA	2:1:233:GLU:HG3	2.02	0.41
3:2:53:LEU:H	3:2:53:LEU:CD1	2.10	0.41
1:3:79:VAL:HG12	1:3:83:ARG:NE	2.36	0.41
5:E:144:ALA:HB2	5:E:342:GLY:CA	2.51	0.41
5:H:324:THR:O	5:J:244:ASP:HA	2.10	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:221:LEU:HA	5:I:312:ARG:HG2	2.02	0.41
5:I:32:PRO:HB2	5:I:34:ILE:CD1	2.51	0.41
5:K:221:LEU:HA	5:K:312:ARG:HG2	2.02	0.41
5:K:144:ALA:HB2	5:K:342:GLY:CA	2.51	0.41
5:L:315:LYS:HA	5:L:315:LYS:HD2	1.92	0.41
5:P:227:MET:O	5:P:230:ALA:HB3	2.21	0.41
5:Q:226:GLU:HG3	5:Q:255:PHE:CE2	2.55	0.41
5:S:299:MET:HE2	5:S:331:ALA:HB2	2.02	0.41
1:0:144:ASN:O	1:0:144:ASN:ND2	2.54	0.41
1:0:150:PHE:O	1:0:154:LEU:HD22	2.20	0.41
1:0:155:LYS:O	1:0:158:GLU:HB2	2.21	0.41
1:3:144:ASN:ND2	1:3:144:ASN:O	2.54	0.41
1:3:155:LYS:O	1:3:158:GLU:HB2	2.21	0.41
5:D:288:ASP:OD1	5:F:204:ALA:HA	2.21	0.41
5:E:226:GLU:HG3	5:E:255:PHE:CE2	2.55	0.41
5:F:144:ALA:HB2	5:F:342:GLY:CA	2.51	0.41
5:G:221:LEU:HA	5:G:312:ARG:HG2	2.02	0.41
5:G:144:ALA:HB2	5:G:342:GLY:CA	2.51	0.41
5:H:32:PRO:HB2	5:H:34:ILE:CD1	2.51	0.41
5:I:219:VAL:HG22	5:I:258:PRO:CB	2.51	0.41
5:J:120:THR:HG21	5:J:370:VAL:CG1	2.51	0.41
5:K:196:ARG:HH21	5:K:249:THR:HG23	1.85	0.41
5:N:120:THR:HG21	5:N:370:VAL:CG1	2.51	0.41
5:O:299:MET:HE2	5:O:331:ALA:HB2	2.02	0.41
5:Q:32:PRO:HB2	5:Q:34:ILE:CD1	2.51	0.41
5:N:288:ASP:OD1	5:R:204:ALA:HA	2.21	0.41
5:R:227:MET:O	5:R:230:ALA:HB3	2.21	0.41
5:R:32:PRO:HB2	5:R:34:ILE:CD1	2.51	0.41
2:Y:202:LEU:HD22	2:Y:202:LEU:N	2.35	0.41
2:1:245:GLN:O	2:1:246:LYS:C	2.59	0.40
2:1:199:GLU:OE2	3:2:56:SER:O	2.39	0.40
2:4:202:LEU:N	2:4:202:LEU:HD22	2.35	0.40
5:E:32:PRO:HB2	5:E:34:ILE:CD1	2.51	0.40
5:F:120:THR:HG21	5:F:370:VAL:CG1	2.52	0.40
5:F:324:THR:O	5:H:244:ASP:HA	2.10	0.40
5:H:315:LYS:HA	5:H:315:LYS:HD2	1.92	0.40
5:J:324:THR:O	5:L:244:ASP:HA	2.10	0.40
5:K:219:VAL:HG22	5:K:258:PRO:CB	2.52	0.40
5:L:324:THR:O	5:N:244:ASP:HA	2.10	0.40
5:M:144:ALA:HB2	5:M:342:GLY:CA	2.51	0.40
5:N:32:PRO:HB2	5:N:34:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:219:VAL:HG22	5:S:258:PRO:CB	2.52	0.40
2:4:212:TRP:HE3	2:4:212:TRP:HA	1.85	0.40
2:7:230:LYS:HA	2:7:233:GLU:HG3	2.02	0.40
3:8:4:GLU:OE2	3:8:7:ARG:CZ	2.69	0.40
5:D:287:ILE:N	5:F:202:THR:CG2	2.76	0.40
5:H:144:ALA:HB2	5:H:342:GLY:CA	2.51	0.40
5:H:288:ASP:OD1	5:J:204:ALA:HA	2.21	0.40
5:M:250:ILE:HG22	5:M:254:ARG:HB2	2.04	0.40
5:M:219:VAL:HG22	5:M:258:PRO:CB	2.51	0.40
5:M:299:MET:HE2	5:M:331:ALA:HB2	2.02	0.40
5:N:324:THR:O	5:R:244:ASP:HA	2.09	0.40
5:O:120:THR:HG21	5:O:370:VAL:CG1	2.52	0.40
5:O:287:ILE:H	5:O:287:ILE:CD1	2.31	0.40
5:P:120:THR:HG21	5:P:370:VAL:CG1	2.52	0.40
2:Y:188:ARG:HG3	2:Y:188:ARG:H	1.57	0.40
1:0:121:LEU:HA	1:0:121:LEU:HD12	1.89	0.40
2:4:207:LYS:C	2:4:207:LYS:HD2	2.42	0.40
3:5:49:PRO:O	3:5:50:PRO:C	2.60	0.40
2:4:223:PHE:HB3	3:5:81:THR:HG22	2.03	0.40
1:6:118:GLY:CA	1:6:133:ILE:HD13	2.52	0.40
1:9:155:LYS:O	1:9:158:GLU:HB2	2.21	0.40
5:D:250:ILE:HG22	5:D:254:ARG:HB2	2.04	0.40
5:K:120:THR:HG21	5:K:370:VAL:CG1	2.52	0.40
5:N:171:LEU:HA	5:N:172:PRO:HD2	1.84	0.40
5:O:144:ALA:HB2	5:O:342:GLY:CA	2.51	0.40
5:Q:219:VAL:HG22	5:Q:258:PRO:CB	2.52	0.40
5:Q:315:LYS:HA	5:Q:315:LYS:HD2	1.92	0.40
2:Y:187:GLU:O	2:Y:189:ARG:N	2.51	0.40
1:6:155:LYS:O	1:6:158:GLU:HB2	2.21	0.40
1:6:5:GLN:C	1:6:7:ALA:H	2.25	0.40
3:8:105:LYS:HA	5:S:1:ASP:OD1	2.21	0.40
1:9:53:THR:HG1	1:9:56:GLU:HG3	1.84	0.40
5:F:227:MET:O	5:F:230:ALA:HB3	2.21	0.40
5:J:32:PRO:HB2	5:J:34:ILE:CD1	2.51	0.40
5:M:288:ASP:OD1	5:O:204:ALA:HA	2.21	0.40
5:L:288:ASP:OD1	5:N:204:ALA:HA	2.21	0.40
5:N:250:ILE:HG22	5:N:254:ARG:HB2	2.04	0.40
5:N:287:ILE:N	5:R:202:THR:CG2	2.76	0.40
5:O:227:MET:O	5:O:230:ALA:HB3	2.21	0.40
5:P:219:VAL:HG22	5:P:258:PRO:CB	2.52	0.40
5:P:226:GLU:HG3	5:P:255:PHE:CE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:250:ILE:HG22	5:S:254:ARG:HB2	2.04	0.40
3:2:49:PRO:O	3:2:50:PRO:C	2.60	0.40
3:2:4:GLU:OE2	3:2:7:ARG:CZ	2.70	0.40
1:3:5:GLN:C	1:3:7:ALA:N	2.74	0.40
3:5:137:ARG:H	3:5:137:ARG:HG2	1.49	0.40
1:6:5:GLN:C	1:6:7:ALA:N	2.74	0.40
3:8:130:HIS:CE1	3:8:134:MET:HE3	2.52	0.40
3:8:53:LEU:HA	3:8:54:PRO:HD3	1.83	0.40
5:D:120:THR:HG21	5:D:370:VAL:CG1	2.52	0.40
5:E:219:VAL:HG22	5:E:258:PRO:CB	2.51	0.40
5:E:250:ILE:HG22	5:E:254:ARG:HB2	2.04	0.40
5:G:75:ILE:HG23	5:G:75:ILE:HD12	1.92	0.40
5:H:219:VAL:HG22	5:H:258:PRO:CB	2.52	0.40
5:I:250:ILE:HG22	5:I:254:ARG:HB2	2.04	0.40
5:J:219:VAL:HG22	5:J:258:PRO:CB	2.51	0.40
5:J:250:ILE:HG22	5:J:254:ARG:HB2	2.04	0.40
5:N:237:GLU:HA	5:N:251:GLY:CA	2.43	0.40
5:S:144:ALA:HB2	5:S:342:GLY:CA	2.51	0.40
2:Y:230:LYS:HA	2:Y:233:GLU:HG3	2.02	0.40
3:Z:4:GLU:OE2	3:Z:7:ARG:CZ	2.70	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	0	157/159 (99%)	130 (83%)	20 (13%)	7 (4%)	3	29
1	3	157/159 (99%)	130 (83%)	20 (13%)	7 (4%)	3	29
1	6	157/159 (99%)	130 (83%)	20 (13%)	7 (4%)	3	29
1	9	157/159 (99%)	130 (83%)	20 (13%)	7 (4%)	3	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	88/90 (98%)	66 (75%)	18 (20%)	4 (4%)	3	29
2	4	88/90 (98%)	66 (75%)	18 (20%)	4 (4%)	3	29
2	7	88/90 (98%)	65 (74%)	19 (22%)	4 (4%)	3	29
2	Y	88/90 (98%)	66 (75%)	18 (20%)	4 (4%)	3	29
3	2	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	1	14
3	5	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	1	14
3	8	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	1	14
3	Z	139/141 (99%)	107 (77%)	19 (14%)	13 (9%)	1	14
4	A	275/277 (99%)	266 (97%)	7 (2%)	2 (1%)	25	68
4	B	275/277 (99%)	264 (96%)	11 (4%)	0	100	100
4	C	37/277 (13%)	34 (92%)	3 (8%)	0	100	100
4	T	37/277 (13%)	34 (92%)	3 (8%)	0	100	100
4	U	275/277 (99%)	264 (96%)	11 (4%)	0	100	100
4	V	275/277 (99%)	266 (97%)	7 (2%)	2 (1%)	25	68
4	W	37/277 (13%)	34 (92%)	3 (8%)	0	100	100
4	X	37/277 (13%)	34 (92%)	3 (8%)	0	100	100
5	D	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	E	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	11	51
5	F	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	G	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	11	51
5	H	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	11	51
5	I	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	J	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	K	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	L	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	M	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	N	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
5	O	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	11	51
5	P	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	11	51
5	Q	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	11	51
5	R	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	11	51
All	All	8704/9728 (90%)	7764 (89%)	744 (8%)	196 (2%)	11	43

All (196) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	107	ASN
1	0	126	GLU
3	2	57	MET
3	2	142	GLN
1	3	107	ASN
1	3	126	GLU
3	5	57	MET
3	5	142	GLN
1	6	107	ASN
1	6	126	GLU
3	8	57	MET
3	8	142	GLN
1	9	107	ASN
1	9	126	GLU
5	D	246	GLN
5	E	246	GLN
5	F	246	GLN
5	G	246	GLN
5	H	246	GLN
5	I	246	GLN
5	J	246	GLN
5	K	246	GLN
5	L	246	GLN
5	M	246	GLN
5	N	246	GLN
5	O	246	GLN
5	P	246	GLN
5	Q	246	GLN
5	R	246	GLN
5	S	246	GLN
3	Z	57	MET
3	Z	142	GLN
1	0	30	ALA
1	0	106	LYS
1	0	160	VAL
2	1	188	ARG

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Mol	Chain	Res	Type
3	2	4	GLU
3	2	55	GLY
3	2	112	ARG
3	2	136	LEU
1	3	30	ALA
1	3	106	LYS
1	3	160	VAL
2	4	188	ARG
3	5	4	GLU
3	5	55	GLY
3	5	112	ARG
3	5	136	LEU
1	6	106	LYS
1	6	160	VAL
2	7	188	ARG
3	8	4	GLU
3	8	55	GLY
3	8	112	ARG
3	8	136	LEU
1	9	30	ALA
1	9	106	LYS
1	9	160	VAL
4	A	152	ASP
5	D	274	ILE
5	E	274	ILE
5	F	274	ILE
5	G	274	ILE
5	H	274	ILE
5	I	274	ILE
5	J	274	ILE
5	K	274	ILE
5	L	274	ILE
5	M	274	ILE
5	N	274	ILE
5	O	274	ILE
5	P	274	ILE
5	Q	274	ILE
5	R	274	ILE
5	S	274	ILE
4	V	152	ASP
2	Y	188	ARG
3	Z	4	GLU

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Mol	Chain	Res	Type
3	Z	55	GLY
3	Z	112	ARG
3	Z	136	LEU
2	1	191	PRO
2	1	246	LYS
3	2	7	ARG
3	2	54	PRO
3	2	98	LYS
3	2	102	LEU
2	4	191	PRO
2	4	246	LYS
3	5	7	ARG
3	5	54	PRO
3	5	98	LYS
3	5	102	LEU
1	6	30	ALA
2	7	191	PRO
2	7	246	LYS
3	8	7	ARG
3	8	54	PRO
3	8	98	LYS
3	8	102	LEU
5	D	233	SER
5	E	233	SER
5	F	233	SER
5	G	233	SER
5	H	233	SER
5	I	233	SER
5	J	233	SER
5	K	233	SER
5	L	233	SER
5	M	233	SER
5	N	233	SER
5	O	233	SER
5	P	233	SER
5	Q	233	SER
5	R	233	SER
5	S	233	SER
2	Y	191	PRO
2	Y	246	LYS
3	Z	7	ARG
3	Z	54	PRO

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Mol	Chain	Res	Type
3	Z	98	LYS
3	Z	102	LEU
1	0	62	GLU
3	2	50	PRO
3	2	141	LYS
1	3	62	GLU
3	5	50	PRO
3	5	141	LYS
1	6	62	GLU
3	8	50	PRO
3	8	141	LYS
1	9	62	GLU
4	A	151	ALA
5	D	2	GLU
5	E	2	GLU
5	E	253	GLU
5	F	2	GLU
5	F	253	GLU
5	G	2	GLU
5	H	2	GLU
5	I	2	GLU
5	I	253	GLU
5	J	2	GLU
5	K	2	GLU
5	L	2	GLU
5	L	253	GLU
5	M	2	GLU
5	M	253	GLU
5	N	2	GLU
5	O	2	GLU
5	O	253	GLU
5	P	2	GLU
5	Q	2	GLU
5	R	2	GLU
5	S	2	GLU
5	S	253	GLU
4	V	151	ALA
3	Z	50	PRO
3	Z	141	LYS
5	D	253	GLU
5	G	253	GLU
5	H	253	GLU

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Mol	Chain	Res	Type
5	J	253	GLU
5	K	253	GLU
5	N	253	GLU
5	P	253	GLU
5	Q	253	GLU
5	R	253	GLU
2	1	247	HIS
2	4	247	HIS
2	7	247	HIS
2	Y	247	HIS
1	0	34	GLY
1	3	34	GLY
1	6	34	GLY
1	9	34	GLY
5	D	242	LEU
5	E	242	LEU
5	F	242	LEU
5	G	242	LEU
5	H	242	LEU
5	I	242	LEU
5	J	242	LEU
5	K	242	LEU
5	L	242	LEU
5	M	242	LEU
5	N	242	LEU
5	O	242	LEU
5	P	242	LEU
5	Q	242	LEU
5	R	242	LEU
5	S	242	LEU
3	2	132	VAL
3	5	132	VAL
3	8	132	VAL
3	Z	132	VAL

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	0	134/134 (100%)	115 (86%)	19 (14%)	4	22
1	3	134/134 (100%)	115 (86%)	19 (14%)	4	22
1	6	134/134 (100%)	115 (86%)	19 (14%)	4	22
1	9	134/134 (100%)	115 (86%)	19 (14%)	4	22
2	1	82/82 (100%)	70 (85%)	12 (15%)	3	21
2	4	82/82 (100%)	70 (85%)	12 (15%)	3	21
2	7	82/82 (100%)	70 (85%)	12 (15%)	3	21
2	Y	82/82 (100%)	70 (85%)	12 (15%)	3	21
3	2	124/124 (100%)	108 (87%)	16 (13%)	5	25
3	5	124/124 (100%)	108 (87%)	16 (13%)	5	25
3	8	124/124 (100%)	108 (87%)	16 (13%)	5	25
3	Z	124/124 (100%)	108 (87%)	16 (13%)	5	25
4	A	239/239 (100%)	212 (89%)	27 (11%)	7	29
4	B	239/239 (100%)	206 (86%)	33 (14%)	4	23
4	C	36/239 (15%)	31 (86%)	5 (14%)	4	23
4	T	36/239 (15%)	28 (78%)	8 (22%)	1	7
4	U	239/239 (100%)	206 (86%)	33 (14%)	4	23
4	V	239/239 (100%)	212 (89%)	27 (11%)	7	29
4	W	36/239 (15%)	28 (78%)	8 (22%)	1	7
4	X	36/239 (15%)	31 (86%)	5 (14%)	4	23
5	D	315/315 (100%)	269 (85%)	46 (15%)	3	21
5	E	315/315 (100%)	269 (85%)	46 (15%)	3	21
5	F	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	G	315/315 (100%)	269 (85%)	46 (15%)	3	21
5	H	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	I	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	J	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	K	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	L	315/315 (100%)	269 (85%)	46 (15%)	3	21
5	M	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	N	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	O	315/315 (100%)	268 (85%)	47 (15%)	3	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	P	315/315 (100%)	269 (85%)	46 (15%)	3	21
5	Q	315/315 (100%)	269 (85%)	46 (15%)	3	21
5	R	315/315 (100%)	268 (85%)	47 (15%)	3	20
5	S	315/315 (100%)	269 (85%)	46 (15%)	3	21
All	All	7500/8312 (90%)	6421 (86%)	1079 (14%)	7	22

All (1079) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	12	PHE
1	0	31	ASP
1	0	45	MET
1	0	62	GLU
1	0	64	VAL
1	0	83	ARG
1	0	95	GLU
1	0	103	ILE
1	0	106	LYS
1	0	107	ASN
1	0	126	GLU
1	0	129	THR
1	0	131	GLU
1	0	135	ASP
1	0	136	LEU
1	0	147	ARG
1	0	154	LEU
1	0	155	LYS
1	0	158	GLU
2	1	160	TYR
2	1	185	LEU
2	1	190	LYS
2	1	192	LEU
2	1	199	GLU
2	1	207	LYS
2	1	215	GLN
2	1	218	THR
2	1	227	ILE
2	1	229	ARG
2	1	243	GLN
2	1	248	SER
3	2	4	GLU

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Mol	Chain	Res	Type
3	2	5	LYS
3	2	6	LYS
3	2	13	ARG
3	2	29	ILE
3	2	53	LEU
3	2	58	GLN
3	2	59	GLU
3	2	103	ARG
3	2	112	ARG
3	2	122	LEU
3	2	129	LYS
3	2	131	LYS
3	2	133	ASN
3	2	137	ARG
3	2	141	LYS
1	3	12	PHE
1	3	31	ASP
1	3	45	MET
1	3	62	GLU
1	3	64	VAL
1	3	83	ARG
1	3	95	GLU
1	3	103	ILE
1	3	106	LYS
1	3	107	ASN
1	3	126	GLU
1	3	129	THR
1	3	131	GLU
1	3	135	ASP
1	3	136	LEU
1	3	147	ARG
1	3	154	LEU
1	3	155	LYS
1	3	158	GLU
2	4	160	TYR
2	4	185	LEU
2	4	190	LYS
2	4	192	LEU
2	4	199	GLU
2	4	207	LYS
2	4	215	GLN
2	4	218	THR

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Mol	Chain	Res	Type
2	4	227	ILE
2	4	229	ARG
2	4	243	GLN
2	4	248	SER
3	5	4	GLU
3	5	5	LYS
3	5	6	LYS
3	5	13	ARG
3	5	29	ILE
3	5	53	LEU
3	5	58	GLN
3	5	59	GLU
3	5	103	ARG
3	5	112	ARG
3	5	122	LEU
3	5	129	LYS
3	5	131	LYS
3	5	133	ASN
3	5	137	ARG
3	5	141	LYS
1	6	12	PHE
1	6	31	ASP
1	6	45	MET
1	6	62	GLU
1	6	64	VAL
1	6	83	ARG
1	6	95	GLU
1	6	103	ILE
1	6	106	LYS
1	6	107	ASN
1	6	126	GLU
1	6	129	THR
1	6	131	GLU
1	6	135	ASP
1	6	136	LEU
1	6	147	ARG
1	6	154	LEU
1	6	155	LYS
1	6	158	GLU
2	7	160	TYR
2	7	185	LEU
2	7	190	LYS

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Mol	Chain	Res	Type
2	7	192	LEU
2	7	199	GLU
2	7	207	LYS
2	7	215	GLN
2	7	218	THR
2	7	227	ILE
2	7	229	ARG
2	7	243	GLN
2	7	248	SER
3	8	4	GLU
3	8	5	LYS
3	8	6	LYS
3	8	13	ARG
3	8	29	ILE
3	8	53	LEU
3	8	58	GLN
3	8	59	GLU
3	8	103	ARG
3	8	112	ARG
3	8	122	LEU
3	8	129	LYS
3	8	131	LYS
3	8	133	ASN
3	8	137	ARG
3	8	141	LYS
1	9	12	PHE
1	9	31	ASP
1	9	45	MET
1	9	62	GLU
1	9	64	VAL
1	9	83	ARG
1	9	95	GLU
1	9	103	ILE
1	9	106	LYS
1	9	107	ASN
1	9	126	GLU
1	9	129	THR
1	9	131	GLU
1	9	135	ASP
1	9	136	LEU
1	9	147	ARG
1	9	154	LEU

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Mol	Chain	Res	Type
1	9	155	LYS
1	9	158	GLU
4	A	29	SER
4	A	34	ASP
4	A	37	VAL
4	A	53	TYR
4	A	57	LEU
4	A	99	LEU
4	A	106	LEU
4	A	122	VAL
4	A	125	SER
4	A	146	HIS
4	A	158	VAL
4	A	162	LEU
4	A	163	VAL
4	A	164	ILE
4	A	165	ILE
4	A	193	VAL
4	A	195	ASN
4	A	207	TYR
4	A	214	TYR
4	A	220	VAL
4	A	222	SER
4	A	234	PHE
4	A	251	ASP
4	A	254	TYR
4	A	263	ILE
4	A	269	HIS
4	A	274	MET
4	B	29	SER
4	B	34	ASP
4	B	37	VAL
4	B	41	LYS
4	B	53	TYR
4	B	54	SER
4	B	57	LEU
4	B	80	SER
4	B	88	VAL
4	B	99	LEU
4	B	106	LEU
4	B	122	VAL
4	B	146	HIS

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Mol	Chain	Res	Type
4	B	158	VAL
4	B	162	LEU
4	B	163	VAL
4	B	164	ILE
4	B	165	ILE
4	B	193	VAL
4	B	195	ASN
4	B	207	TYR
4	B	214	TYR
4	B	220	VAL
4	B	222	SER
4	B	234	PHE
4	B	241	LYS
4	B	251	ASP
4	B	254	TYR
4	B	263	ILE
4	B	264	SER
4	B	269	HIS
4	B	274	MET
4	B	276	SER
4	C	251	ASP
4	C	254	TYR
4	C	263	ILE
4	C	269	HIS
4	C	274	MET
5	D	33	SER
5	D	34	ILE
5	D	37	ARG
5	D	66	THR
5	D	72	GLU
5	D	80	ASP
5	D	100	GLU
5	D	109	PRO
5	D	116	ARG
5	D	145	SER
5	D	153	LEU
5	D	159	VAL
5	D	180	LEU
5	D	191	LYS
5	D	196	ARG
5	D	199	SER
5	D	201	VAL

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Mol	Chain	Res	Type
5	D	206	ARG
5	D	221	LEU
5	D	223	PHE
5	D	229	THR
5	D	239	SER
5	D	242	LEU
5	D	246	GLN
5	D	263	GLN
5	D	281	SER
5	D	283	MET
5	D	287	ILE
5	D	291	LYS
5	D	293	LEU
5	D	297	ASN
5	D	299	MET
5	D	312	ARG
5	D	315	LYS
5	D	318	THR
5	D	320	LEU
5	D	327	ILE
5	D	334	GLU
5	D	349	LEU
5	D	350	SER
5	D	351	THR
5	D	354	GLN
5	D	359	LYS
5	D	360	GLN
5	D	361	GLU
5	D	368	SER
5	E	33	SER
5	E	34	ILE
5	E	37	ARG
5	E	66	THR
5	E	72	GLU
5	E	80	ASP
5	E	100	GLU
5	E	109	PRO
5	E	116	ARG
5	E	145	SER
5	E	153	LEU
5	E	159	VAL
5	E	180	LEU

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Mol	Chain	Res	Type
5	E	191	LYS
5	E	196	ARG
5	E	199	SER
5	E	201	VAL
5	E	206	ARG
5	E	221	LEU
5	E	223	PHE
5	E	229	THR
5	E	239	SER
5	E	242	LEU
5	E	246	GLN
5	E	263	GLN
5	E	281	SER
5	E	283	MET
5	E	287	ILE
5	E	291	LYS
5	E	293	LEU
5	E	297	ASN
5	E	299	MET
5	E	312	ARG
5	E	315	LYS
5	E	318	THR
5	E	320	LEU
5	E	327	ILE
5	E	334	GLU
5	E	349	LEU
5	E	350	SER
5	E	351	THR
5	E	354	GLN
5	E	359	LYS
5	E	360	GLN
5	E	361	GLU
5	E	368	SER
5	F	16	LEU
5	F	33	SER
5	F	34	ILE
5	F	37	ARG
5	F	66	THR
5	F	72	GLU
5	F	80	ASP
5	F	100	GLU
5	F	109	PRO

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Mol	Chain	Res	Type
5	F	116	ARG
5	F	145	SER
5	F	153	LEU
5	F	159	VAL
5	F	180	LEU
5	F	191	LYS
5	F	196	ARG
5	F	199	SER
5	F	201	VAL
5	F	206	ARG
5	F	221	LEU
5	F	223	PHE
5	F	229	THR
5	F	239	SER
5	F	242	LEU
5	F	246	GLN
5	F	263	GLN
5	F	281	SER
5	F	283	MET
5	F	287	ILE
5	F	291	LYS
5	F	293	LEU
5	F	297	ASN
5	F	299	MET
5	F	312	ARG
5	F	315	LYS
5	F	318	THR
5	F	320	LEU
5	F	327	ILE
5	F	334	GLU
5	F	349	LEU
5	F	350	SER
5	F	351	THR
5	F	354	GLN
5	F	359	LYS
5	F	360	GLN
5	F	361	GLU
5	F	368	SER
5	G	33	SER
5	G	34	ILE
5	G	37	ARG
5	G	66	THR

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Mol	Chain	Res	Type
5	G	72	GLU
5	G	80	ASP
5	G	100	GLU
5	G	109	PRO
5	G	116	ARG
5	G	145	SER
5	G	153	LEU
5	G	159	VAL
5	G	180	LEU
5	G	191	LYS
5	G	196	ARG
5	G	199	SER
5	G	201	VAL
5	G	206	ARG
5	G	221	LEU
5	G	223	PHE
5	G	229	THR
5	G	239	SER
5	G	242	LEU
5	G	246	GLN
5	G	263	GLN
5	G	281	SER
5	G	283	MET
5	G	287	ILE
5	G	291	LYS
5	G	293	LEU
5	G	297	ASN
5	G	299	MET
5	G	312	ARG
5	G	315	LYS
5	G	318	THR
5	G	320	LEU
5	G	327	ILE
5	G	334	GLU
5	G	349	LEU
5	G	350	SER
5	G	351	THR
5	G	354	GLN
5	G	359	LYS
5	G	360	GLN
5	G	361	GLU
5	G	368	SER

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Mol	Chain	Res	Type
5	H	16	LEU
5	H	33	SER
5	H	34	ILE
5	H	37	ARG
5	H	66	THR
5	H	72	GLU
5	H	80	ASP
5	H	100	GLU
5	H	109	PRO
5	H	116	ARG
5	H	145	SER
5	H	153	LEU
5	H	159	VAL
5	H	180	LEU
5	H	191	LYS
5	H	196	ARG
5	H	199	SER
5	H	201	VAL
5	H	206	ARG
5	H	221	LEU
5	H	223	PHE
5	H	229	THR
5	H	239	SER
5	H	242	LEU
5	H	246	GLN
5	H	263	GLN
5	H	281	SER
5	H	283	MET
5	H	287	ILE
5	H	291	LYS
5	H	293	LEU
5	H	297	ASN
5	H	299	MET
5	H	312	ARG
5	H	315	LYS
5	H	318	THR
5	H	320	LEU
5	H	327	ILE
5	H	334	GLU
5	H	349	LEU
5	H	350	SER
5	H	351	THR

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Mol	Chain	Res	Type
5	H	354	GLN
5	H	359	LYS
5	H	360	GLN
5	H	361	GLU
5	H	368	SER
5	I	16	LEU
5	I	33	SER
5	I	34	ILE
5	I	37	ARG
5	I	66	THR
5	I	72	GLU
5	I	80	ASP
5	I	100	GLU
5	I	109	PRO
5	I	116	ARG
5	I	145	SER
5	I	153	LEU
5	I	159	VAL
5	I	180	LEU
5	I	191	LYS
5	I	196	ARG
5	I	199	SER
5	I	201	VAL
5	I	206	ARG
5	I	221	LEU
5	I	223	PHE
5	I	229	THR
5	I	239	SER
5	I	242	LEU
5	I	246	GLN
5	I	263	GLN
5	I	281	SER
5	I	283	MET
5	I	287	ILE
5	I	291	LYS
5	I	293	LEU
5	I	297	ASN
5	I	299	MET
5	I	312	ARG
5	I	315	LYS
5	I	318	THR
5	I	320	LEU

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Mol	Chain	Res	Type
5	I	327	ILE
5	I	334	GLU
5	I	349	LEU
5	I	350	SER
5	I	351	THR
5	I	354	GLN
5	I	359	LYS
5	I	360	GLN
5	I	361	GLU
5	I	368	SER
5	J	16	LEU
5	J	33	SER
5	J	34	ILE
5	J	37	ARG
5	J	66	THR
5	J	72	GLU
5	J	80	ASP
5	J	100	GLU
5	J	109	PRO
5	J	116	ARG
5	J	145	SER
5	J	153	LEU
5	J	159	VAL
5	J	180	LEU
5	J	191	LYS
5	J	196	ARG
5	J	199	SER
5	J	201	VAL
5	J	206	ARG
5	J	221	LEU
5	J	223	PHE
5	J	229	THR
5	J	239	SER
5	J	242	LEU
5	J	246	GLN
5	J	263	GLN
5	J	281	SER
5	J	283	MET
5	J	287	ILE
5	J	291	LYS
5	J	293	LEU
5	J	297	ASN

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Mol	Chain	Res	Type
5	J	299	MET
5	J	312	ARG
5	J	315	LYS
5	J	318	THR
5	J	320	LEU
5	J	327	ILE
5	J	334	GLU
5	J	349	LEU
5	J	350	SER
5	J	351	THR
5	J	354	GLN
5	J	359	LYS
5	J	360	GLN
5	J	361	GLU
5	J	368	SER
5	K	16	LEU
5	K	33	SER
5	K	34	ILE
5	K	37	ARG
5	K	66	THR
5	K	72	GLU
5	K	80	ASP
5	K	100	GLU
5	K	109	PRO
5	K	116	ARG
5	K	145	SER
5	K	153	LEU
5	K	159	VAL
5	K	180	LEU
5	K	191	LYS
5	K	196	ARG
5	K	199	SER
5	K	201	VAL
5	K	206	ARG
5	K	221	LEU
5	K	223	PHE
5	K	229	THR
5	K	239	SER
5	K	242	LEU
5	K	246	GLN
5	K	263	GLN
5	K	281	SER

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Mol	Chain	Res	Type
5	K	283	MET
5	K	287	ILE
5	K	291	LYS
5	K	293	LEU
5	K	297	ASN
5	K	299	MET
5	K	312	ARG
5	K	315	LYS
5	K	318	THR
5	K	320	LEU
5	K	327	ILE
5	K	334	GLU
5	K	349	LEU
5	K	350	SER
5	K	351	THR
5	K	354	GLN
5	K	359	LYS
5	K	360	GLN
5	K	361	GLU
5	K	368	SER
5	L	33	SER
5	L	34	ILE
5	L	37	ARG
5	L	66	THR
5	L	72	GLU
5	L	80	ASP
5	L	100	GLU
5	L	109	PRO
5	L	116	ARG
5	L	145	SER
5	L	153	LEU
5	L	159	VAL
5	L	180	LEU
5	L	191	LYS
5	L	196	ARG
5	L	199	SER
5	L	201	VAL
5	L	206	ARG
5	L	221	LEU
5	L	223	PHE
5	L	229	THR
5	L	239	SER

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Mol	Chain	Res	Type
5	L	242	LEU
5	L	246	GLN
5	L	263	GLN
5	L	281	SER
5	L	283	MET
5	L	287	ILE
5	L	291	LYS
5	L	293	LEU
5	L	297	ASN
5	L	299	MET
5	L	312	ARG
5	L	315	LYS
5	L	318	THR
5	L	320	LEU
5	L	327	ILE
5	L	334	GLU
5	L	349	LEU
5	L	350	SER
5	L	351	THR
5	L	354	GLN
5	L	359	LYS
5	L	360	GLN
5	L	361	GLU
5	L	368	SER
5	M	16	LEU
5	M	33	SER
5	M	34	ILE
5	M	37	ARG
5	M	66	THR
5	M	72	GLU
5	M	80	ASP
5	M	100	GLU
5	M	109	PRO
5	M	116	ARG
5	M	145	SER
5	M	153	LEU
5	M	159	VAL
5	M	180	LEU
5	M	191	LYS
5	M	196	ARG
5	M	199	SER
5	M	201	VAL

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Mol	Chain	Res	Type
5	M	206	ARG
5	M	221	LEU
5	M	223	PHE
5	M	229	THR
5	M	239	SER
5	M	242	LEU
5	M	246	GLN
5	M	263	GLN
5	M	281	SER
5	M	283	MET
5	M	287	ILE
5	M	291	LYS
5	M	293	LEU
5	M	297	ASN
5	M	299	MET
5	M	312	ARG
5	M	315	LYS
5	M	318	THR
5	M	320	LEU
5	M	327	ILE
5	M	334	GLU
5	M	349	LEU
5	M	350	SER
5	M	351	THR
5	M	354	GLN
5	M	359	LYS
5	M	360	GLN
5	M	361	GLU
5	M	368	SER
5	N	16	LEU
5	N	33	SER
5	N	34	ILE
5	N	37	ARG
5	N	66	THR
5	N	72	GLU
5	N	80	ASP
5	N	100	GLU
5	N	109	PRO
5	N	116	ARG
5	N	145	SER
5	N	153	LEU
5	N	159	VAL

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Mol	Chain	Res	Type
5	N	180	LEU
5	N	191	LYS
5	N	196	ARG
5	N	199	SER
5	N	201	VAL
5	N	206	ARG
5	N	221	LEU
5	N	223	PHE
5	N	229	THR
5	N	239	SER
5	N	242	LEU
5	N	246	GLN
5	N	263	GLN
5	N	281	SER
5	N	283	MET
5	N	287	ILE
5	N	291	LYS
5	N	293	LEU
5	N	297	ASN
5	N	299	MET
5	N	312	ARG
5	N	315	LYS
5	N	318	THR
5	N	320	LEU
5	N	327	ILE
5	N	334	GLU
5	N	349	LEU
5	N	350	SER
5	N	351	THR
5	N	354	GLN
5	N	359	LYS
5	N	360	GLN
5	N	361	GLU
5	N	368	SER
5	O	16	LEU
5	O	33	SER
5	O	34	ILE
5	O	37	ARG
5	O	66	THR
5	O	72	GLU
5	O	80	ASP
5	O	100	GLU

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Mol	Chain	Res	Type
5	O	109	PRO
5	O	116	ARG
5	O	145	SER
5	O	153	LEU
5	O	159	VAL
5	O	180	LEU
5	O	191	LYS
5	O	196	ARG
5	O	199	SER
5	O	201	VAL
5	O	206	ARG
5	O	221	LEU
5	O	223	PHE
5	O	229	THR
5	O	239	SER
5	O	242	LEU
5	O	246	GLN
5	O	263	GLN
5	O	281	SER
5	O	283	MET
5	O	287	ILE
5	O	291	LYS
5	O	293	LEU
5	O	297	ASN
5	O	299	MET
5	O	312	ARG
5	O	315	LYS
5	O	318	THR
5	O	320	LEU
5	O	327	ILE
5	O	334	GLU
5	O	349	LEU
5	O	350	SER
5	O	351	THR
5	O	354	GLN
5	O	359	LYS
5	O	360	GLN
5	O	361	GLU
5	O	368	SER
5	P	33	SER
5	P	34	ILE
5	P	37	ARG

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Mol	Chain	Res	Type
5	P	66	THR
5	P	72	GLU
5	P	80	ASP
5	P	100	GLU
5	P	109	PRO
5	P	116	ARG
5	P	145	SER
5	P	153	LEU
5	P	159	VAL
5	P	180	LEU
5	P	191	LYS
5	P	196	ARG
5	P	199	SER
5	P	201	VAL
5	P	206	ARG
5	P	221	LEU
5	P	223	PHE
5	P	229	THR
5	P	239	SER
5	P	242	LEU
5	P	246	GLN
5	P	263	GLN
5	P	281	SER
5	P	283	MET
5	P	287	ILE
5	P	291	LYS
5	P	293	LEU
5	P	297	ASN
5	P	299	MET
5	P	312	ARG
5	P	315	LYS
5	P	318	THR
5	P	320	LEU
5	P	327	ILE
5	P	334	GLU
5	P	349	LEU
5	P	350	SER
5	P	351	THR
5	P	354	GLN
5	P	359	LYS
5	P	360	GLN
5	P	361	GLU

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Mol	Chain	Res	Type
5	P	368	SER
5	Q	33	SER
5	Q	34	ILE
5	Q	37	ARG
5	Q	66	THR
5	Q	72	GLU
5	Q	80	ASP
5	Q	100	GLU
5	Q	109	PRO
5	Q	116	ARG
5	Q	145	SER
5	Q	153	LEU
5	Q	159	VAL
5	Q	180	LEU
5	Q	191	LYS
5	Q	196	ARG
5	Q	199	SER
5	Q	201	VAL
5	Q	206	ARG
5	Q	221	LEU
5	Q	223	PHE
5	Q	229	THR
5	Q	239	SER
5	Q	242	LEU
5	Q	246	GLN
5	Q	263	GLN
5	Q	281	SER
5	Q	283	MET
5	Q	287	ILE
5	Q	291	LYS
5	Q	293	LEU
5	Q	297	ASN
5	Q	299	MET
5	Q	312	ARG
5	Q	315	LYS
5	Q	318	THR
5	Q	320	LEU
5	Q	327	ILE
5	Q	334	GLU
5	Q	349	LEU
5	Q	350	SER
5	Q	351	THR

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Mol	Chain	Res	Type
5	Q	354	GLN
5	Q	359	LYS
5	Q	360	GLN
5	Q	361	GLU
5	Q	368	SER
5	R	16	LEU
5	R	33	SER
5	R	34	ILE
5	R	37	ARG
5	R	66	THR
5	R	72	GLU
5	R	80	ASP
5	R	100	GLU
5	R	109	PRO
5	R	116	ARG
5	R	145	SER
5	R	153	LEU
5	R	159	VAL
5	R	180	LEU
5	R	191	LYS
5	R	196	ARG
5	R	199	SER
5	R	201	VAL
5	R	206	ARG
5	R	221	LEU
5	R	223	PHE
5	R	229	THR
5	R	239	SER
5	R	242	LEU
5	R	246	GLN
5	R	263	GLN
5	R	281	SER
5	R	283	MET
5	R	287	ILE
5	R	291	LYS
5	R	293	LEU
5	R	297	ASN
5	R	299	MET
5	R	312	ARG
5	R	315	LYS
5	R	318	THR
5	R	320	LEU

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Mol	Chain	Res	Type
5	R	327	ILE
5	R	334	GLU
5	R	349	LEU
5	R	350	SER
5	R	351	THR
5	R	354	GLN
5	R	359	LYS
5	R	360	GLN
5	R	361	GLU
5	R	368	SER
5	S	33	SER
5	S	34	ILE
5	S	37	ARG
5	S	66	THR
5	S	72	GLU
5	S	80	ASP
5	S	100	GLU
5	S	109	PRO
5	S	116	ARG
5	S	145	SER
5	S	153	LEU
5	S	159	VAL
5	S	180	LEU
5	S	191	LYS
5	S	196	ARG
5	S	199	SER
5	S	201	VAL
5	S	206	ARG
5	S	221	LEU
5	S	223	PHE
5	S	229	THR
5	S	239	SER
5	S	242	LEU
5	S	246	GLN
5	S	263	GLN
5	S	281	SER
5	S	283	MET
5	S	287	ILE
5	S	291	LYS
5	S	293	LEU
5	S	297	ASN
5	S	299	MET

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Mol	Chain	Res	Type
5	S	312	ARG
5	S	315	LYS
5	S	318	THR
5	S	320	LEU
5	S	327	ILE
5	S	334	GLU
5	S	349	LEU
5	S	350	SER
5	S	351	THR
5	S	354	GLN
5	S	359	LYS
5	S	360	GLN
5	S	361	GLU
5	S	368	SER
4	T	241	LYS
4	T	251	ASP
4	T	254	TYR
4	T	263	ILE
4	T	264	SER
4	T	269	HIS
4	T	274	MET
4	T	276	SER
4	U	29	SER
4	U	34	ASP
4	U	37	VAL
4	U	41	LYS
4	U	53	TYR
4	U	54	SER
4	U	57	LEU
4	U	80	SER
4	U	88	VAL
4	U	99	LEU
4	U	106	LEU
4	U	122	VAL
4	U	146	HIS
4	U	158	VAL
4	U	162	LEU
4	U	163	VAL
4	U	164	ILE
4	U	165	ILE
4	U	193	VAL
4	U	195	ASN

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Mol	Chain	Res	Type
4	U	207	TYR
4	U	214	TYR
4	U	220	VAL
4	U	222	SER
4	U	234	PHE
4	U	241	LYS
4	U	251	ASP
4	U	254	TYR
4	U	263	ILE
4	U	264	SER
4	U	269	HIS
4	U	274	MET
4	U	276	SER
4	V	29	SER
4	V	34	ASP
4	V	37	VAL
4	V	53	TYR
4	V	57	LEU
4	V	99	LEU
4	V	106	LEU
4	V	122	VAL
4	V	125	SER
4	V	146	HIS
4	V	158	VAL
4	V	162	LEU
4	V	163	VAL
4	V	164	ILE
4	V	165	ILE
4	V	193	VAL
4	V	195	ASN
4	V	207	TYR
4	V	214	TYR
4	V	220	VAL
4	V	222	SER
4	V	234	PHE
4	V	251	ASP
4	V	254	TYR
4	V	263	ILE
4	V	269	HIS
4	V	274	MET
4	W	241	LYS
4	W	251	ASP

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Mol	Chain	Res	Type
4	W	254	TYR
4	W	263	ILE
4	W	264	SER
4	W	269	HIS
4	W	274	MET
4	W	276	SER
4	X	251	ASP
4	X	254	TYR
4	X	263	ILE
4	X	269	HIS
4	X	274	MET
2	Y	160	TYR
2	Y	185	LEU
2	Y	190	LYS
2	Y	192	LEU
2	Y	199	GLU
2	Y	207	LYS
2	Y	215	GLN
2	Y	218	THR
2	Y	227	ILE
2	Y	229	ARG
2	Y	243	GLN
2	Y	248	SER
3	Z	4	GLU
3	Z	5	LYS
3	Z	6	LYS
3	Z	13	ARG
3	Z	29	ILE
3	Z	53	LEU
3	Z	58	GLN
3	Z	59	GLU
3	Z	103	ARG
3	Z	112	ARG
3	Z	122	LEU
3	Z	129	LYS
3	Z	131	LYS
3	Z	133	ASN
3	Z	137	ARG
3	Z	141	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	50	GLN
1	0	51	ASN
1	0	84	GLN
1	0	144	ASN
2	1	175	GLN
2	1	198	ASN
2	1	243	GLN
2	1	245	GLN
3	2	42	ASN
3	2	47	HIS
3	2	58	GLN
3	2	61	GLN
3	2	86	GLN
3	2	97	GLN
3	2	130	HIS
3	2	133	ASN
3	2	142	GLN
1	3	50	GLN
1	3	51	ASN
1	3	84	GLN
1	3	144	ASN
2	4	175	GLN
2	4	198	ASN
2	4	243	GLN
2	4	245	GLN
3	5	42	ASN
3	5	47	HIS
3	5	58	GLN
3	5	61	GLN
3	5	86	GLN
3	5	97	GLN
3	5	130	HIS
3	5	133	ASN
3	5	142	GLN
1	6	50	GLN
1	6	51	ASN
1	6	84	GLN
1	6	144	ASN
2	7	175	GLN
2	7	198	ASN
2	7	243	GLN
2	7	245	GLN
3	8	42	ASN

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Mol	Chain	Res	Type
3	8	47	HIS
3	8	58	GLN
3	8	61	GLN
3	8	86	GLN
3	8	130	HIS
3	8	133	ASN
3	8	142	GLN
1	9	50	GLN
1	9	51	ASN
1	9	84	GLN
1	9	144	ASN
5	D	41	GLN
5	D	92	ASN
5	D	137	GLN
5	D	252	ASN
5	D	263	GLN
5	D	354	GLN
5	E	41	GLN
5	E	92	ASN
5	E	137	GLN
5	E	252	ASN
5	E	263	GLN
5	E	354	GLN
5	F	41	GLN
5	F	92	ASN
5	F	137	GLN
5	F	252	ASN
5	F	263	GLN
5	F	354	GLN
5	G	41	GLN
5	G	92	ASN
5	G	137	GLN
5	G	252	ASN
5	G	263	GLN
5	G	354	GLN
5	H	41	GLN
5	H	92	ASN
5	H	137	GLN
5	H	252	ASN
5	H	263	GLN
5	H	354	GLN
5	I	41	GLN

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Mol	Chain	Res	Type
5	I	92	ASN
5	I	137	GLN
5	I	252	ASN
5	I	263	GLN
5	I	354	GLN
5	J	41	GLN
5	J	92	ASN
5	J	137	GLN
5	J	252	ASN
5	J	263	GLN
5	J	354	GLN
5	K	41	GLN
5	K	92	ASN
5	K	137	GLN
5	K	252	ASN
5	K	263	GLN
5	K	354	GLN
5	L	41	GLN
5	L	87	HIS
5	L	92	ASN
5	L	137	GLN
5	L	252	ASN
5	L	263	GLN
5	L	354	GLN
5	M	41	GLN
5	M	92	ASN
5	M	137	GLN
5	M	252	ASN
5	M	263	GLN
5	M	354	GLN
5	N	41	GLN
5	N	92	ASN
5	N	137	GLN
5	N	252	ASN
5	N	263	GLN
5	N	354	GLN
5	O	41	GLN
5	O	92	ASN
5	O	137	GLN
5	O	252	ASN
5	O	263	GLN
5	O	354	GLN

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Mol	Chain	Res	Type
5	P	41	GLN
5	P	92	ASN
5	P	137	GLN
5	P	252	ASN
5	P	263	GLN
5	P	354	GLN
5	Q	41	GLN
5	Q	92	ASN
5	Q	137	GLN
5	Q	252	ASN
5	Q	263	GLN
5	Q	354	GLN
5	Q	360	GLN
5	R	41	GLN
5	R	92	ASN
5	R	137	GLN
5	R	252	ASN
5	R	263	GLN
5	R	354	GLN
5	S	41	GLN
5	S	92	ASN
5	S	137	GLN
5	S	252	ASN
5	S	263	GLN
5	S	354	GLN
2	Y	175	GLN
2	Y	198	ASN
2	Y	243	GLN
2	Y	245	GLN
3	Z	42	ASN
3	Z	47	HIS
3	Z	58	GLN
3	Z	61	GLN
3	Z	86	GLN
3	Z	97	GLN
3	Z	130	HIS
3	Z	133	ASN
3	Z	142	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.