



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 03:02 AM UTC

PDB ID : 2W4U / pdb_00002w4u
EMDB ID : EMD-1584
Title : Isometrically contracting insect asynchronous flight muscle quick frozen after a length step
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 : 2008-12-02
Resolution : 35.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

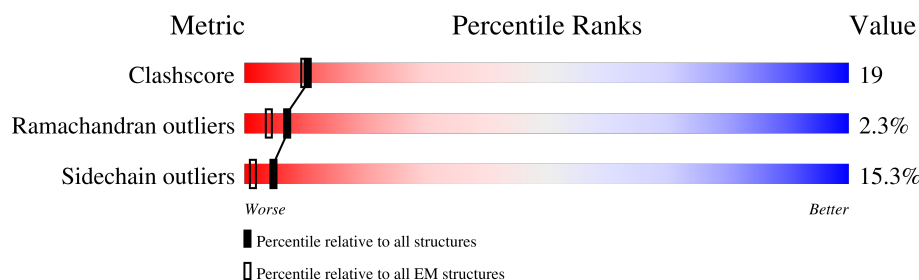
1 Overall quality at a glance

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.



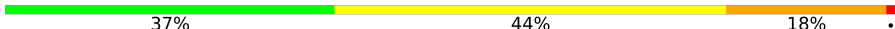
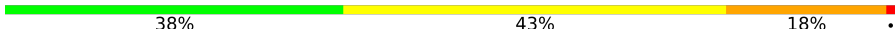
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	0	159	43% 47% 8% .
1	3	159	44% 47% 8% .
1	6	159	42% 48% 8% .
1	9	159	43% 48% 8% .
2	1	90	51% 37% 12%
2	4	90	51% 36% 13%
2	7	90	51% 36% 13%
2	Y	90	51% 37% 12%
3	2	141	36% 44% 20%

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Mol	Chain	Length	Quality of chain
3	5	141	
3	8	141	
3	Z	141	
4	A	277	
4	B	277	
4	C	277	
4	T	277	
4	U	277	
4	V	277	
4	W	277	
4	X	277	
5	D	372	
5	E	372	
5	F	372	
5	G	372	
5	H	372	
5	I	372	
5	J	372	
5	K	372	
5	L	372	
5	M	372	
5	N	372	
5	O	372	
5	P	372	
5	Q	372	

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Mol	Chain	Length	Quality of chain
5	R	372	55% 34% 10%
5	S	372	56% 33% 9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 69221 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	260	Total	C	N	O	S	0	0
			2091	1278	353	456	4		
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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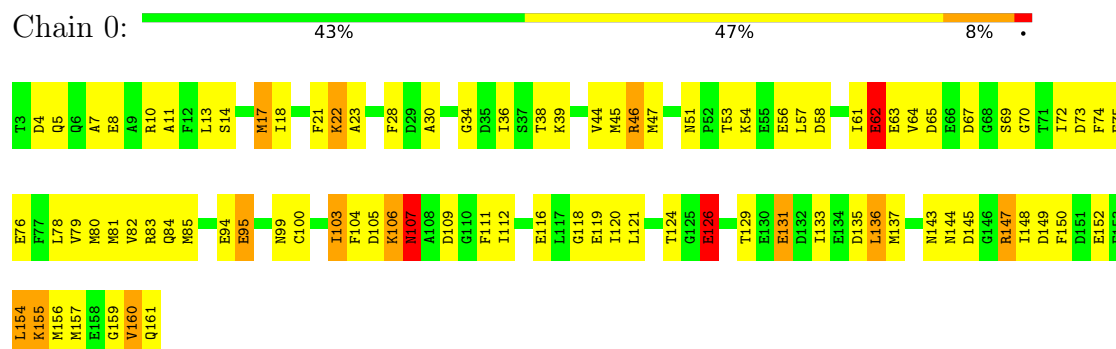
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	372	Total 2907	C 1836	N 489	O 562	S 20	0	0
5	I	372	Total 2907	C 1836	N 489	O 562	S 20	0	0
5	J	372	Total 2907	C 1836	N 489	O 562	S 20	0	0
5	K	372	Total 2907	C 1836	N 489	O 562	S 20	0	0
5	L	372	Total 2907	C 1836	N 489	O 562	S 20	0	0
5	M	372	Total 2907	C 1836	N 489	O 562	S 20	0	0
5	N	372	Total 2907	C 1836	N 489	O 562	S 20	0	0
5	O	372	Total 2907	C 1836	N 489	O 562	S 20	0	0
5	P	372	Total 2907	C 1836	N 489	O 562	S 20	0	0
5	Q	372	Total 2907	C 1836	N 489	O 562	S 20	0	0
5	R	372	Total 2907	C 1836	N 489	O 562	S 20	0	0
5	S	372	Total 2907	C 1836	N 489	O 562	S 20	0	0

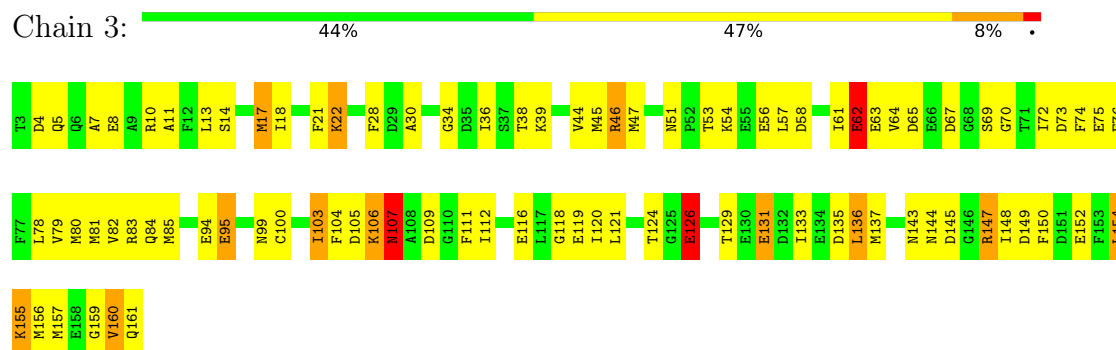
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

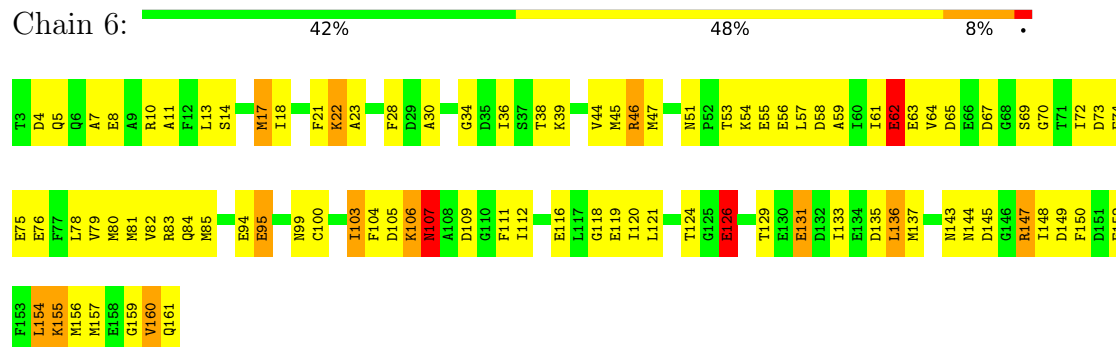
• Molecule 1: TROPONIN C, SKELETAL MUSCLE



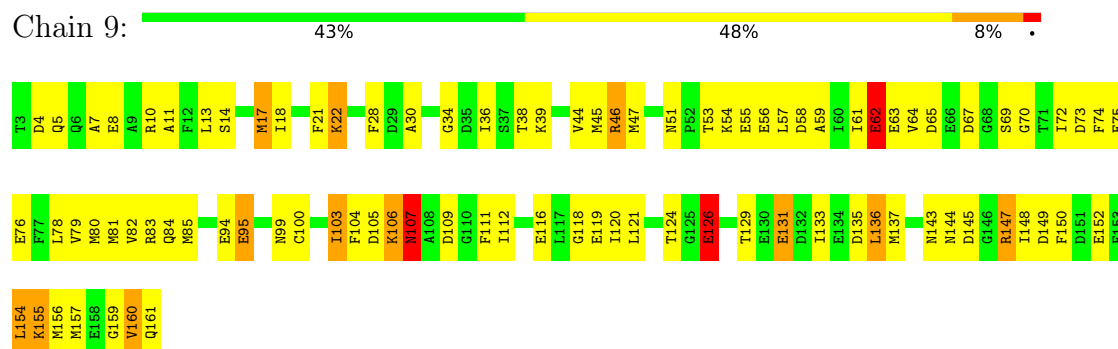
• Molecule 1: TROPONIN C, SKELETAL MUSCLE



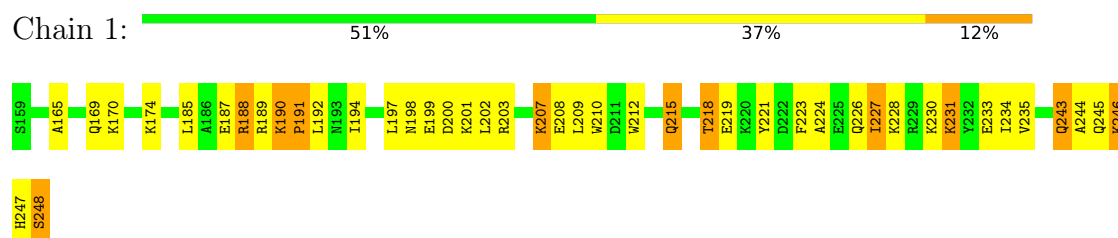
• Molecule 1: TROPONIN C, SKELETAL MUSCLE



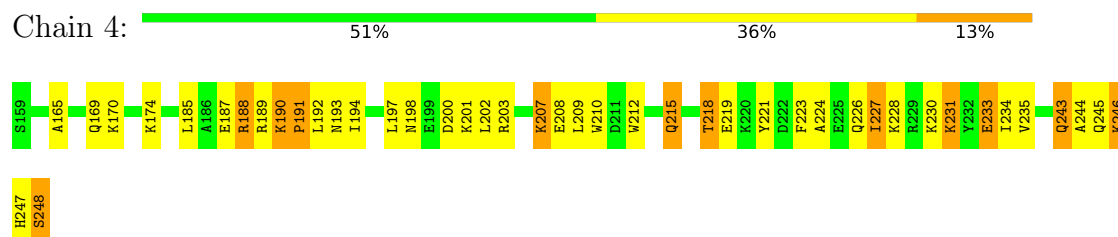
• Molecule 1: TROPONIN C, SKELETAL MUSCLE



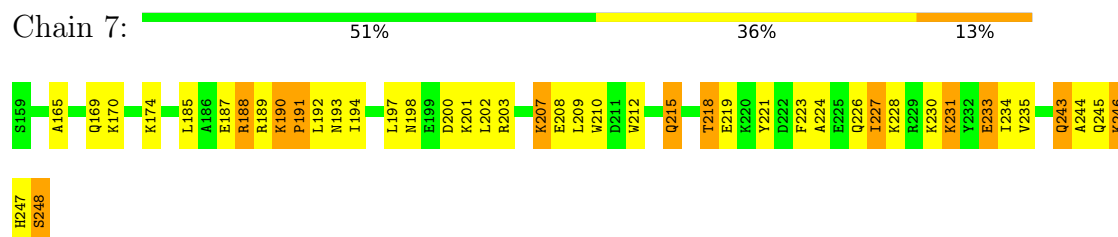
- Molecule 2: TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS



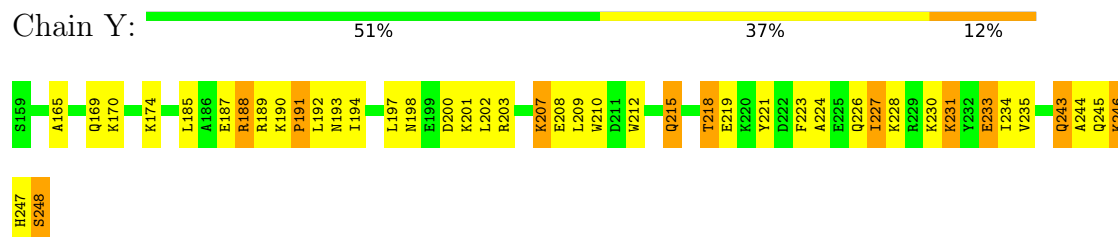
- Molecule 2: TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS



- Molecule 2: TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS

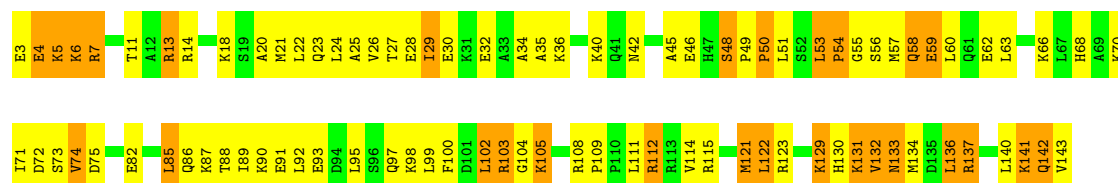


- Molecule 2: TROPONIN T, FAST SKELETAL MUSCLE ISOFORMS



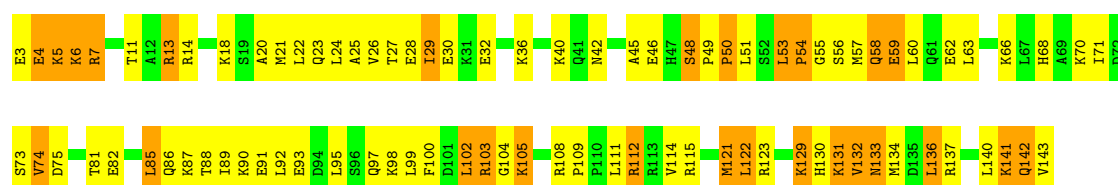
- Molecule 3: TROPONIN I, FAST SKELETAL MUSCLE

Chain 2: 



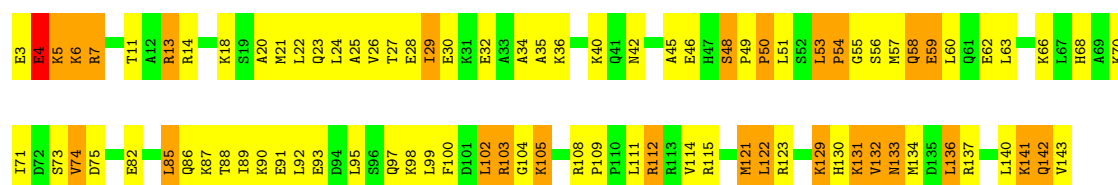
- Molecule 3: TROPONIN I, FAST SKELETAL MUSCLE

Chain 5: 



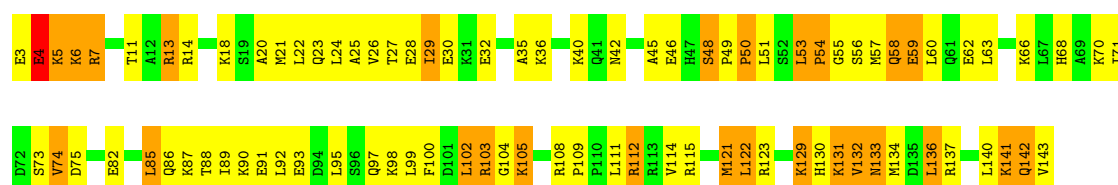
- Molecule 3: TROPONIN I, FAST SKELETAL MUSCLE

Chain 8: 



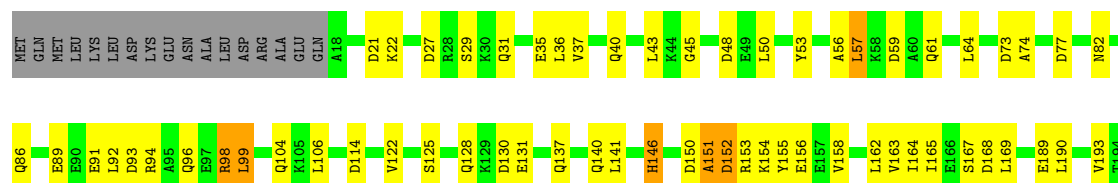
- Molecule 3: TROPONIN I, FAST SKELETAL MUSCLE

Chain Z: 



- Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

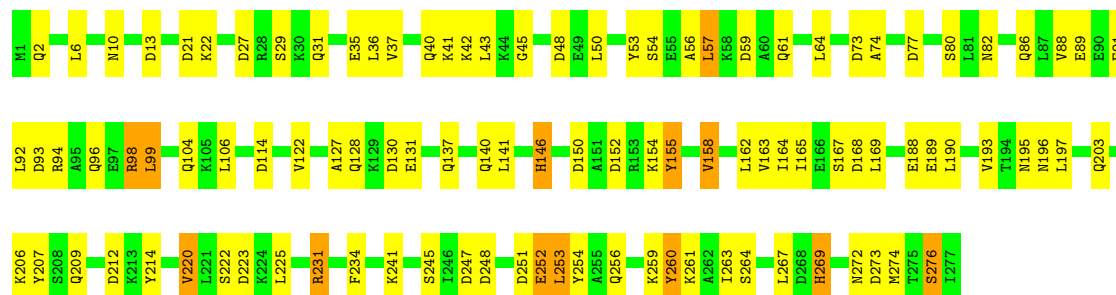
Chain A: 





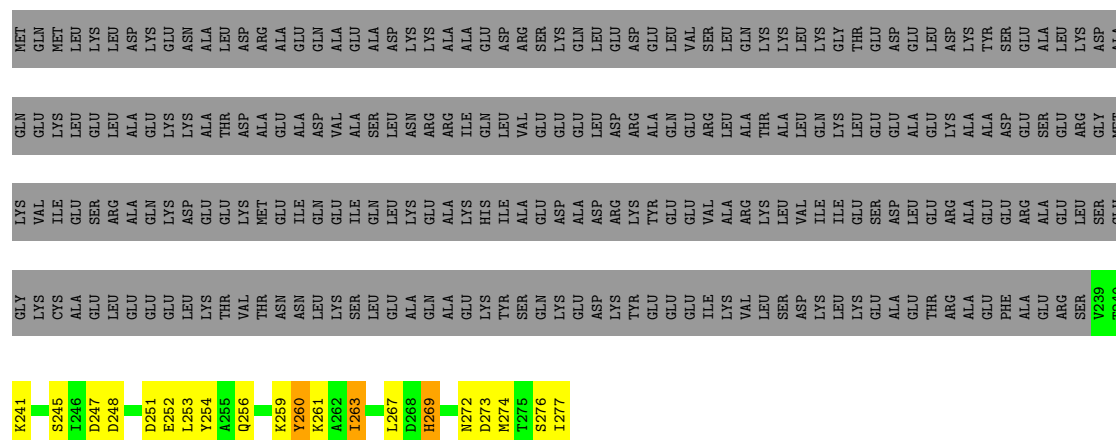
• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain B: 62% 33% 5%



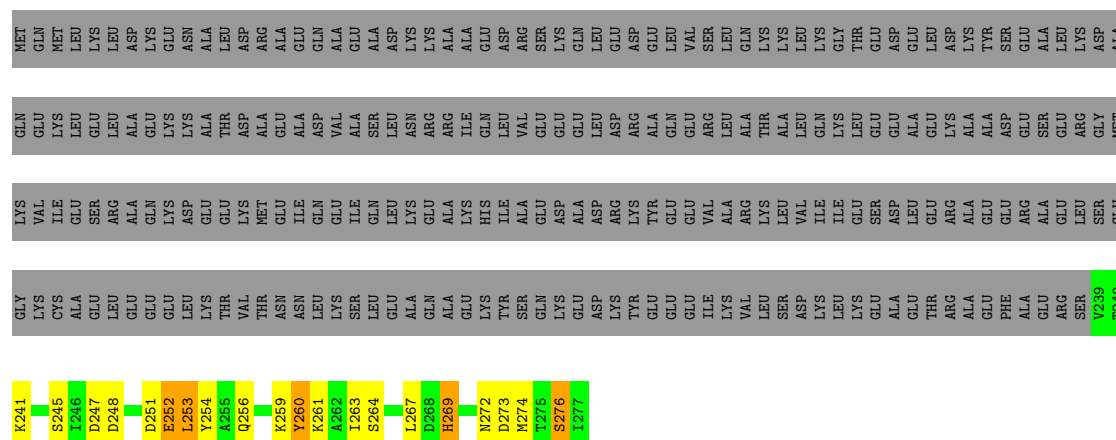
• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

Chain C: 7% 6% 86%

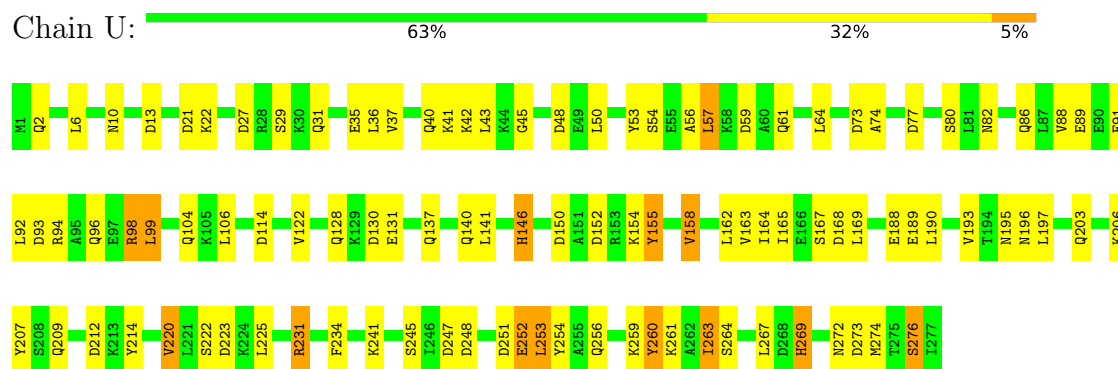


• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

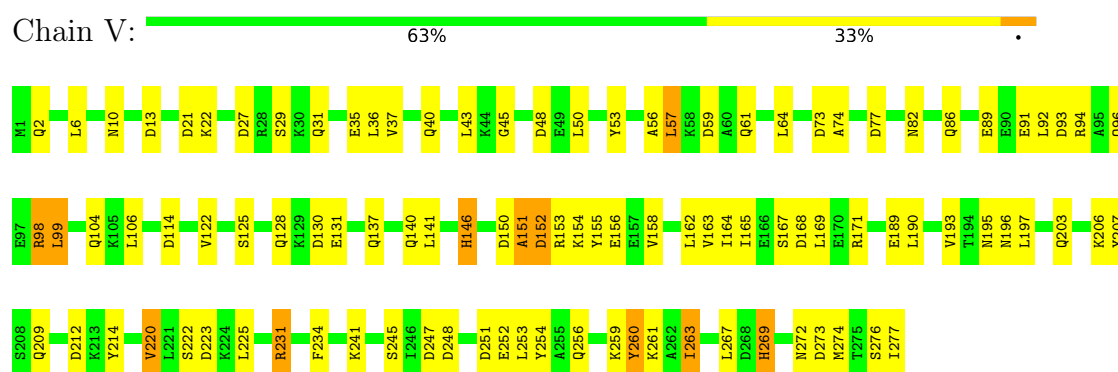
Chain T: 7% 5% 86%



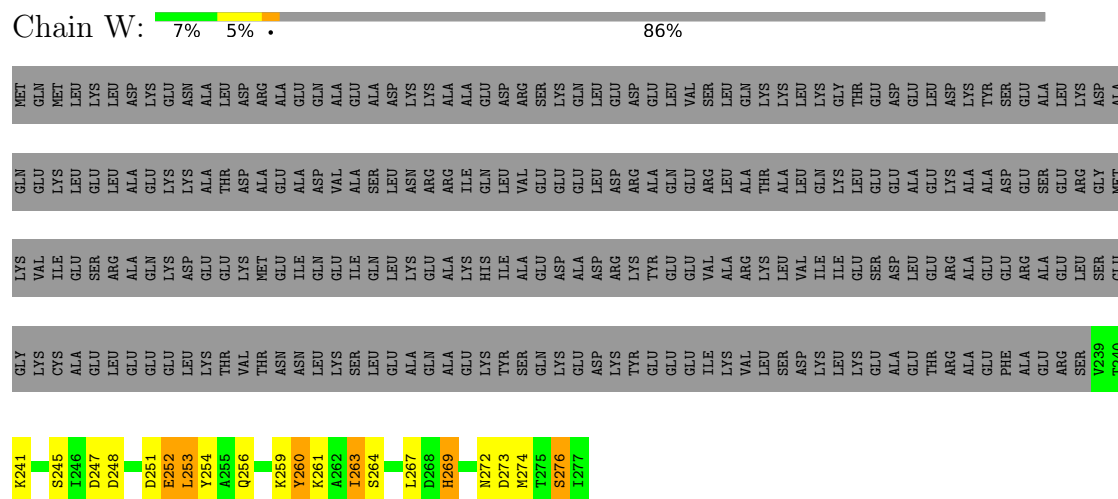
• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN



• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

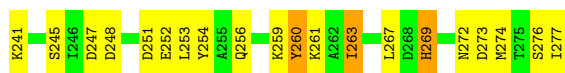


• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

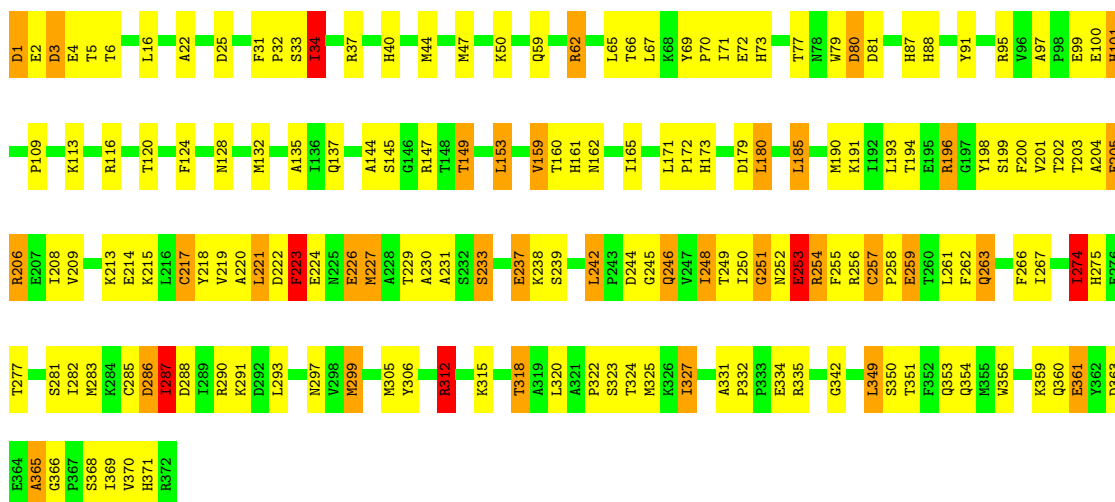


• Molecule 4: TROPOMYOSIN ALPHA-1 CHAIN

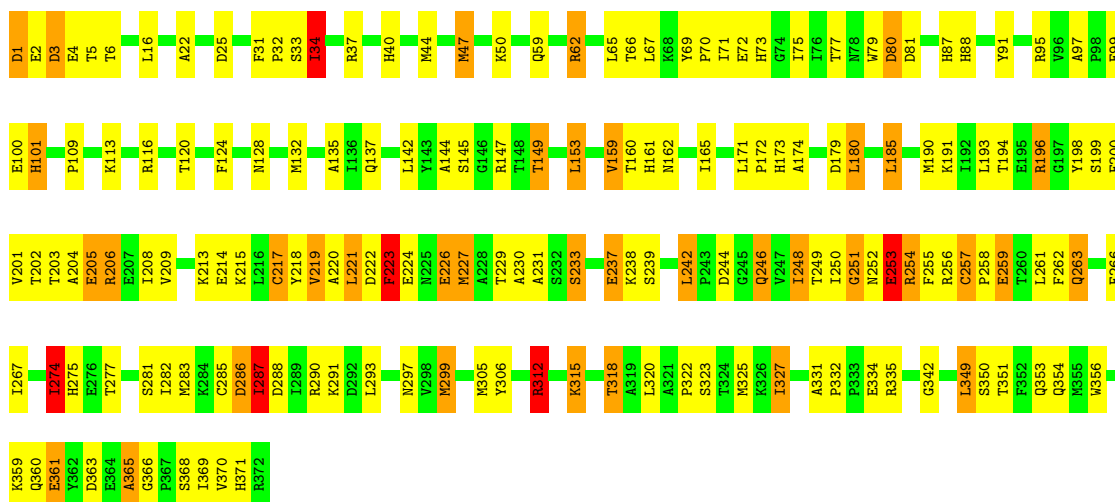




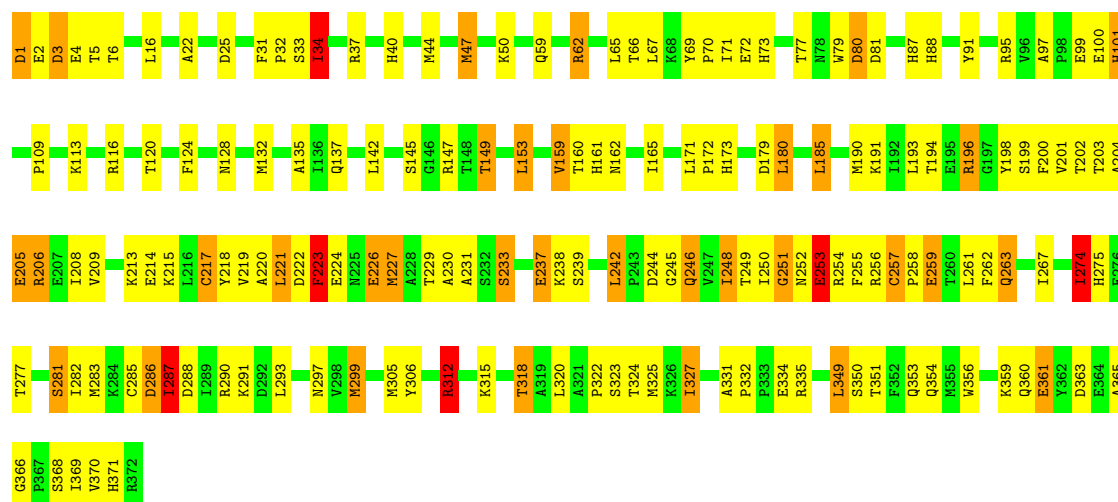
Chain D: 55% 35% 9%



Chain E: 54% 34% 10%

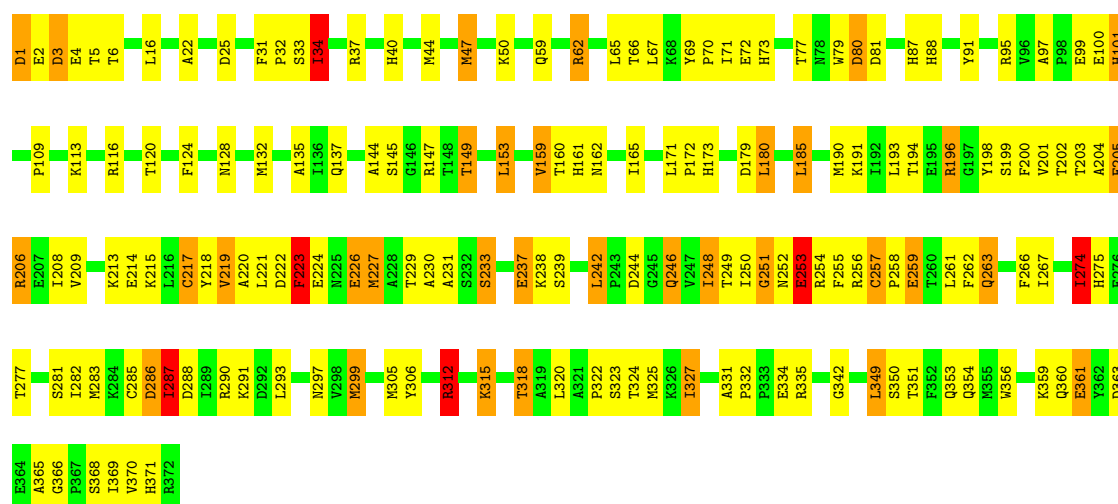


Chain F:  55% 34% 9% .



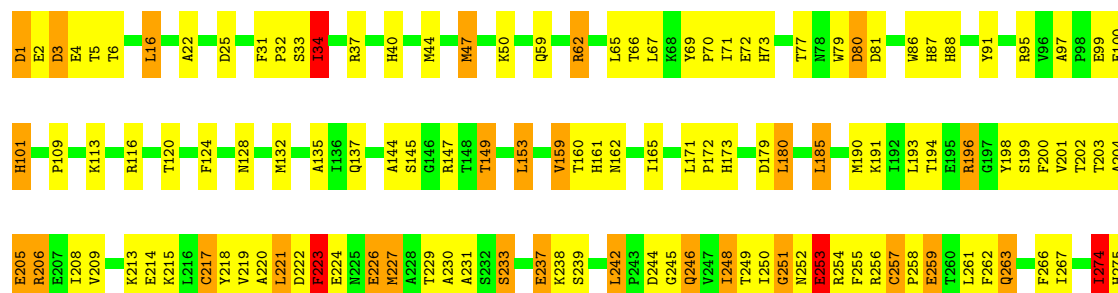
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

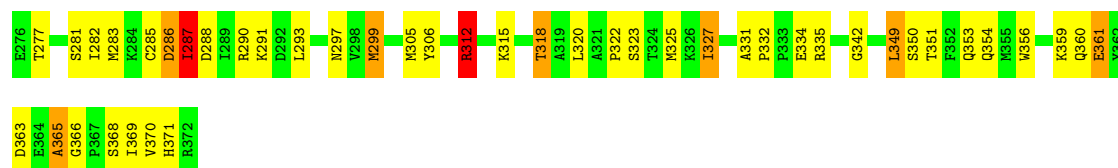
Chain G:  55% 34% 9% .



• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

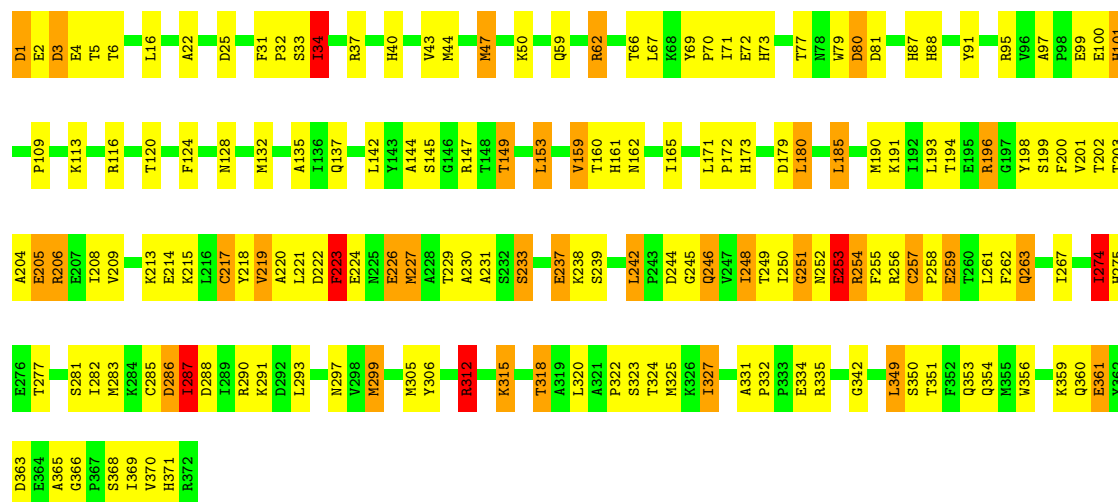
Chain H:  55% 34% 9% .





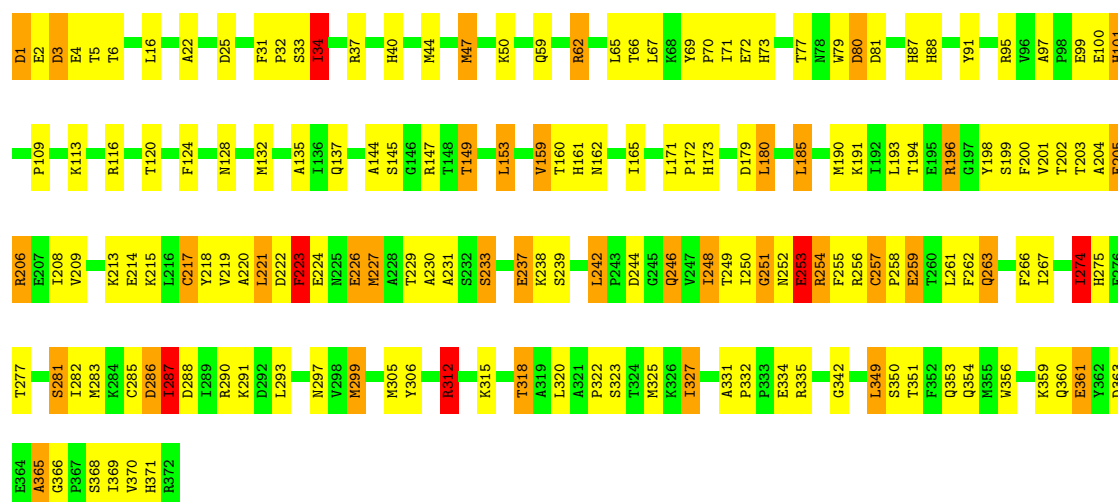
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain I: 55% 34% 9%



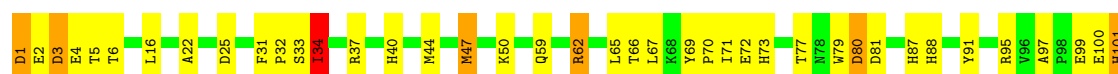
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

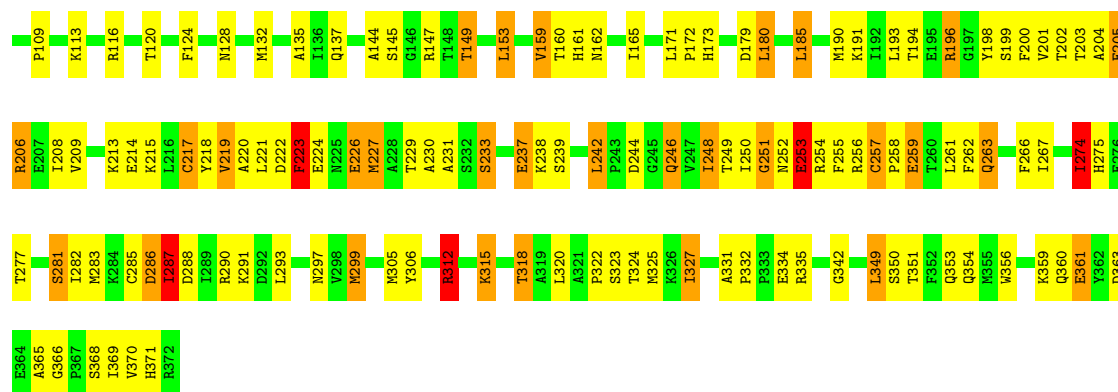
Chain J: 55% 34% 10%



• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

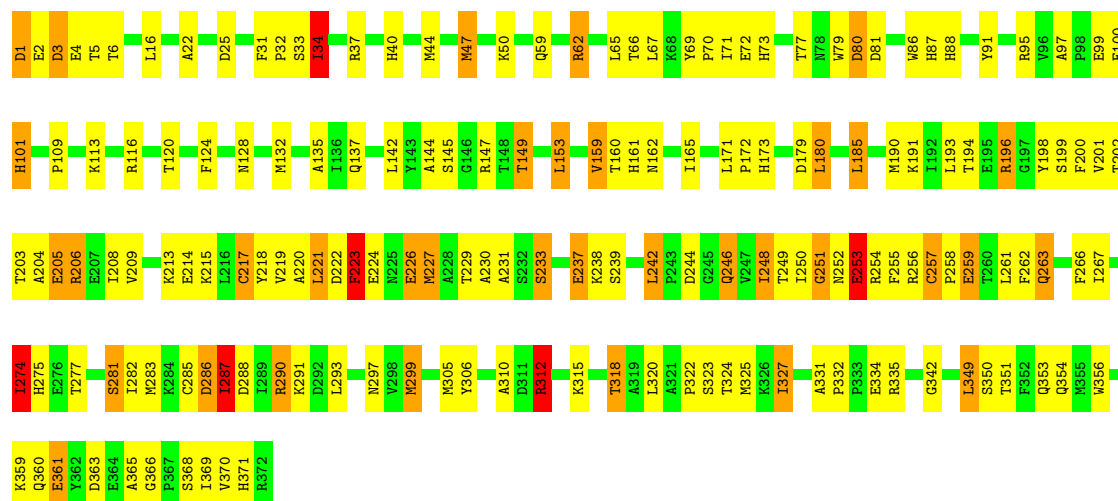
Chain K: 55% 34% 9%





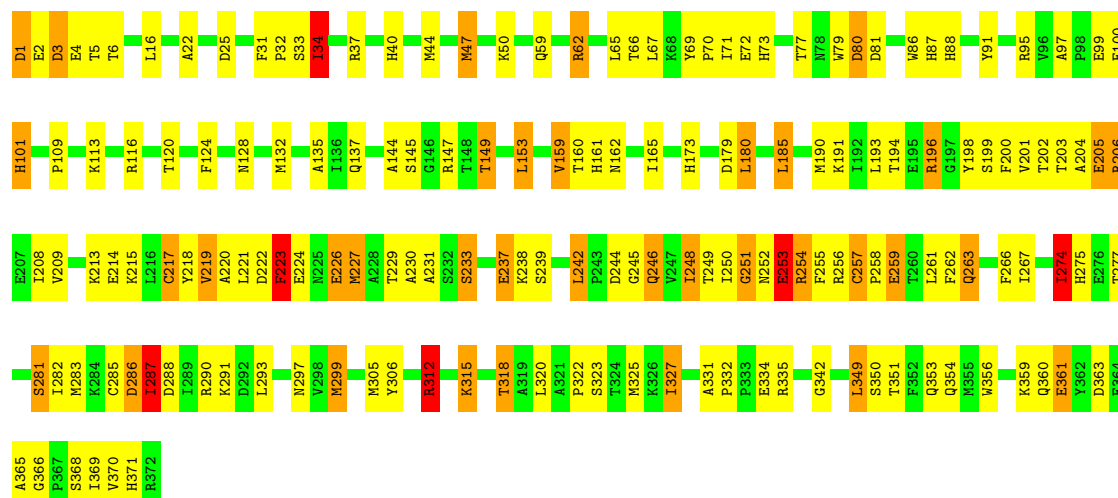
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain L: 54% 35% 9% .

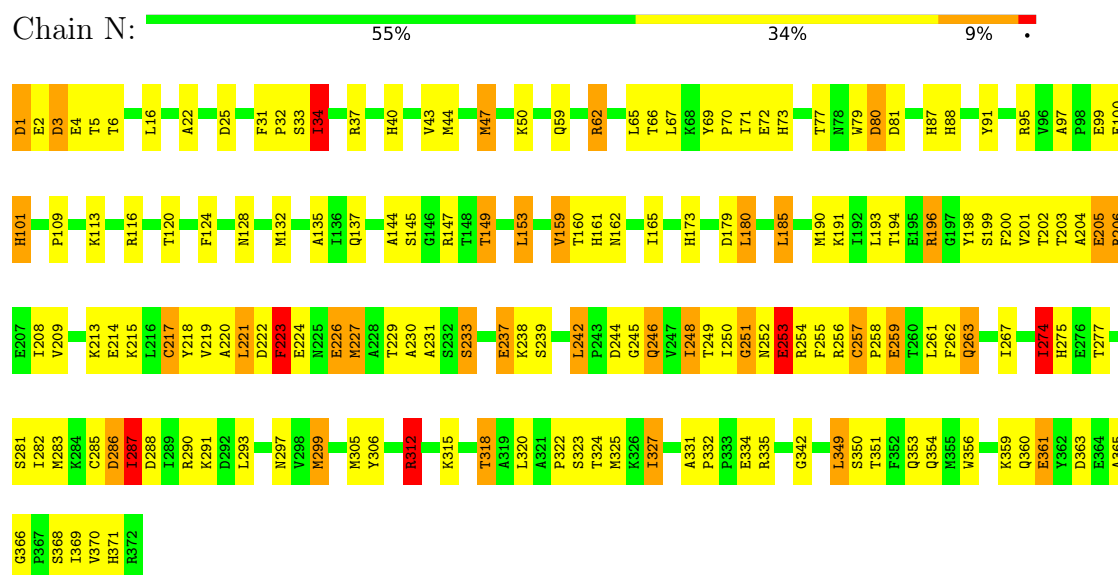


• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

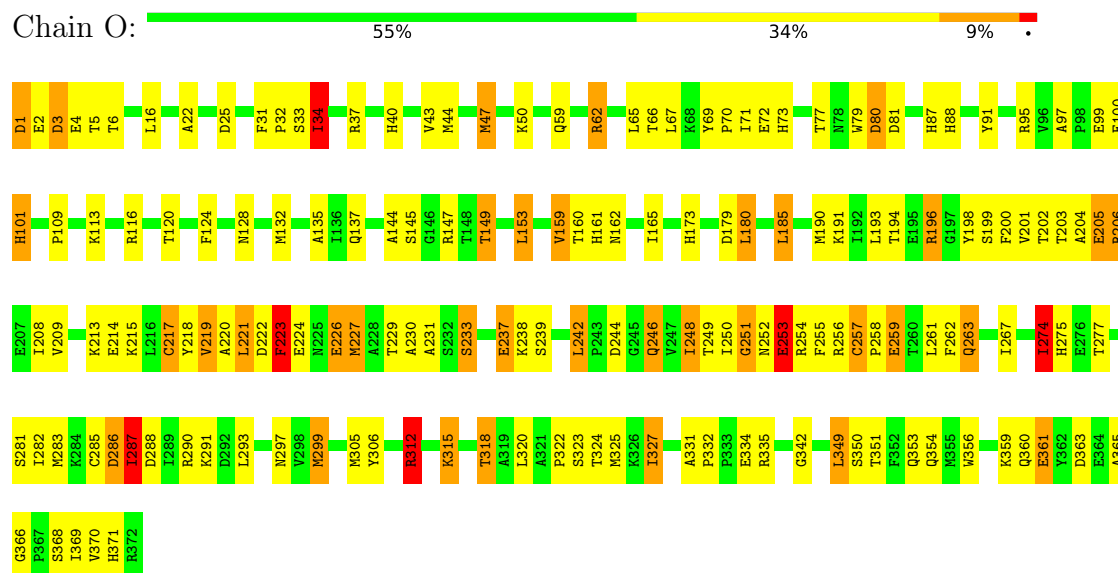
Chain M: 55% 34% 10% .



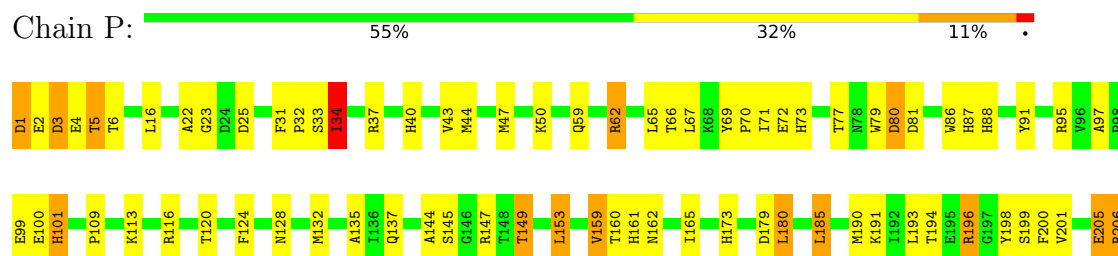
- Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

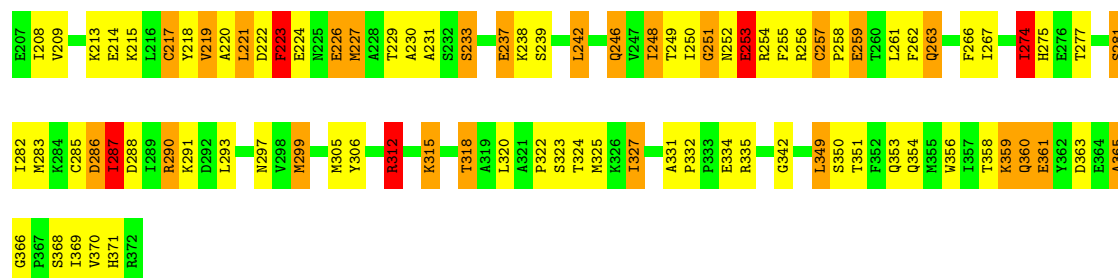


- Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE



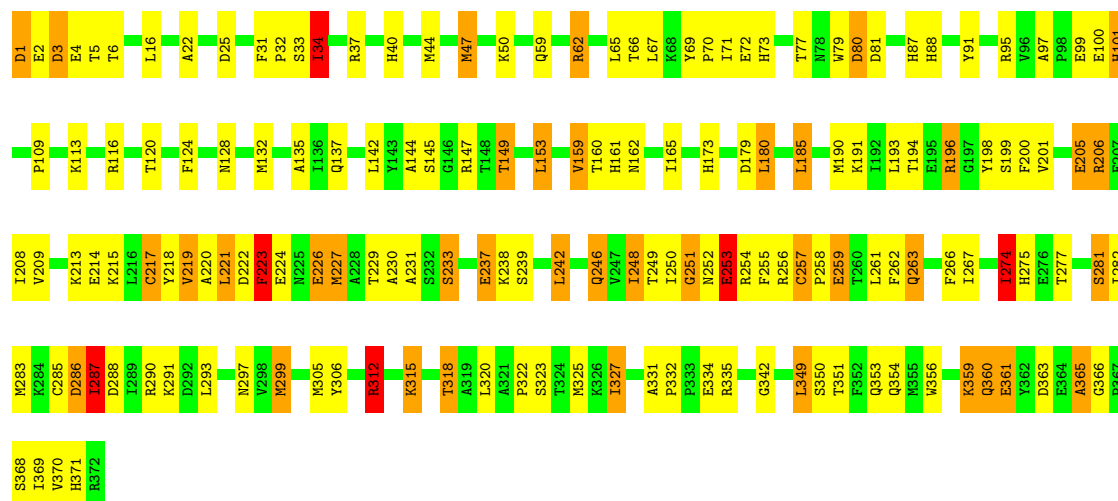
- Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE





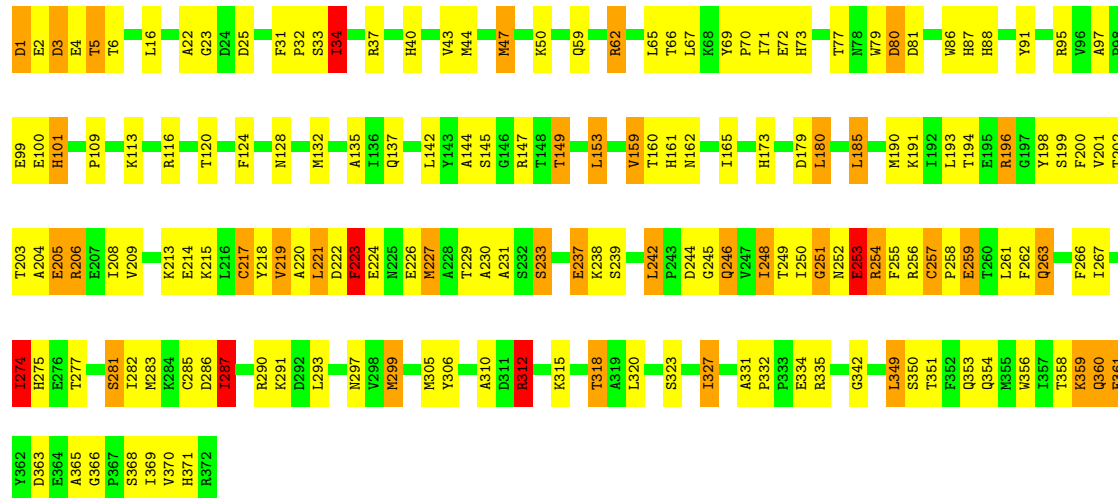
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain Q: 56% 31% 10% .



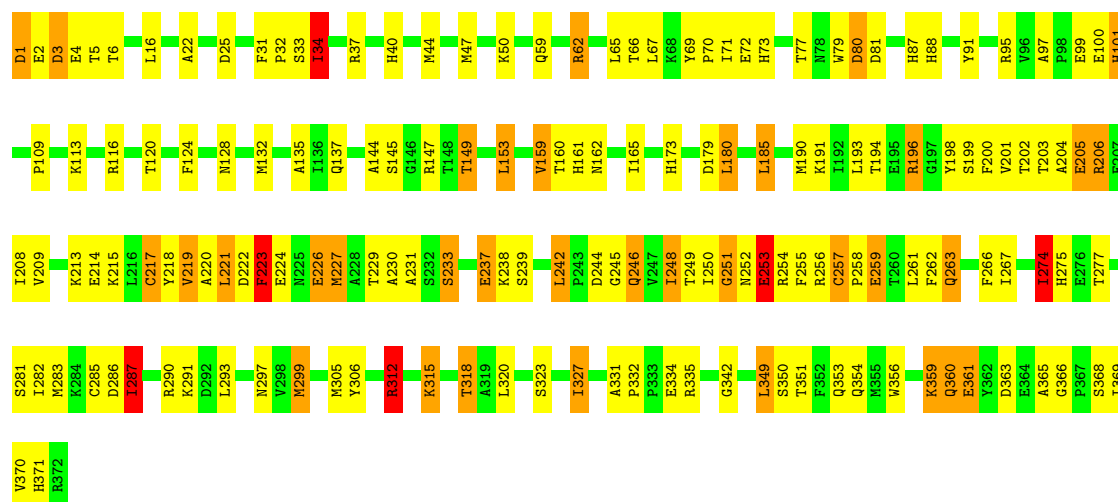
• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Chain R: 55% 34% 10% .



• Molecule 5: ACTIN, ALPHA SKELETAL MUSCLE

Response	Percentage
Yes	56%
No	33%
Don't know	9%



4 Experimental information

Property	Value	Source
EM 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	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F224 (2k x 2k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.69	0/1264	0.96	2/1687 (0.1%)
1	3	0.69	0/1264	0.96	2/1687 (0.1%)
1	6	0.69	0/1264	0.96	2/1687 (0.1%)
1	9	0.69	0/1264	0.96	2/1687 (0.1%)
2	1	0.69	0/786	0.94	3/1046 (0.3%)
2	4	0.69	0/786	0.94	3/1046 (0.3%)
2	7	0.69	0/786	0.94	3/1046 (0.3%)
2	Y	0.69	0/786	0.94	3/1046 (0.3%)
3	2	0.70	1/1152 (0.1%)	1.13	7/1535 (0.5%)
3	5	0.70	1/1152 (0.1%)	1.13	7/1535 (0.5%)
3	8	0.70	1/1152 (0.1%)	1.13	7/1535 (0.5%)
3	Z	0.70	1/1152 (0.1%)	1.13	7/1535 (0.5%)
4	A	3.67	26/2099 (1.2%)	2.48	109/2799 (3.9%)
4	B	4.62	18/2238 (0.8%)	2.41	109/2983 (3.7%)
4	C	8.94	10/318 (3.1%)	2.86	23/425 (5.4%)
4	T	8.96	9/318 (2.8%)	2.85	23/425 (5.4%)
4	U	4.62	18/2238 (0.8%)	2.41	112/2983 (3.8%)
4	V	3.56	26/2238 (1.2%)	2.45	115/2983 (3.9%)
4	W	8.96	9/318 (2.8%)	2.84	24/425 (5.6%)
4	X	8.93	10/318 (3.1%)	2.86	23/425 (5.4%)
5	D	1.17	13/2969 (0.4%)	2.00	100/4023 (2.5%)
5	E	1.17	13/2969 (0.4%)	2.00	102/4023 (2.5%)
5	F	1.17	13/2969 (0.4%)	2.00	100/4023 (2.5%)
5	G	1.17	13/2969 (0.4%)	2.00	99/4023 (2.5%)
5	H	1.17	13/2969 (0.4%)	2.00	102/4023 (2.5%)
5	I	1.17	12/2969 (0.4%)	2.00	100/4023 (2.5%)
5	J	1.17	13/2969 (0.4%)	2.00	100/4023 (2.5%)
5	K	1.17	13/2969 (0.4%)	2.00	100/4023 (2.5%)
5	L	1.17	13/2969 (0.4%)	2.00	106/4023 (2.6%)
5	M	1.17	13/2969 (0.4%)	2.00	102/4023 (2.5%)
5	N	1.17	12/2969 (0.4%)	2.01	101/4023 (2.5%)
5	O	1.17	13/2969 (0.4%)	2.00	99/4023 (2.5%)
5	P	1.17	13/2969 (0.4%)	2.01	103/4023 (2.6%)
5	Q	1.17	13/2969 (0.4%)	2.01	102/4023 (2.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	R	1.17	13/2969 (0.4%)	2.00	104/4023 (2.6%)
5	S	1.17	13/2969 (0.4%)	2.00	100/4023 (2.5%)
All	All	2.15	336/70397 (0.5%)	1.95	2206/94888 (2.3%)

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 (336) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	260	TYR	CA-CB	155.18	3.97	1.53
4	W	260	TYR	CA-CB	155.10	3.97	1.53
4	B	260	TYR	CA-CB	155.08	3.97	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	260	TYR	CA-CB	155.07	3.97	1.53
4	C	260	TYR	CA-CB	154.66	3.96	1.53
4	V	260	TYR	CA-CB	154.64	3.96	1.53
4	A	260	TYR	CA-CB	154.63	3.96	1.53
4	X	260	TYR	CA-CB	154.58	3.96	1.53
4	B	155	TYR	CA-CB	142.76	3.94	1.53
4	U	155	TYR	CA-CB	142.75	3.94	1.53
4	C	260	TYR	CG-CD1	19.54	1.80	1.39
4	A	260	TYR	CG-CD1	19.54	1.80	1.39
4	X	260	TYR	CG-CD1	19.48	1.80	1.39
4	W	260	TYR	CG-CD1	19.48	1.80	1.39
4	B	260	TYR	CG-CD1	19.46	1.80	1.39
4	V	260	TYR	CG-CD1	19.46	1.80	1.39
4	T	260	TYR	CG-CD1	19.43	1.80	1.39
4	U	260	TYR	CG-CD1	19.43	1.80	1.39
4	A	155	TYR	CG-CD2	16.11	1.73	1.39
4	V	155	TYR	CG-CD2	16.08	1.73	1.39
4	U	260	TYR	CE1-CZ	14.06	1.72	1.38
4	W	260	TYR	CE1-CZ	14.05	1.72	1.38
4	B	260	TYR	CE1-CZ	14.01	1.71	1.38
4	T	260	TYR	CE1-CZ	13.99	1.71	1.38
4	A	155	TYR	CE2-CZ	13.96	1.71	1.38
4	V	155	TYR	CE2-CZ	13.95	1.71	1.38
4	X	260	TYR	CE1-CZ	13.79	1.71	1.38
4	A	260	TYR	CE1-CZ	13.77	1.71	1.38
4	C	260	TYR	CE1-CZ	13.77	1.71	1.38
4	V	260	TYR	CE1-CZ	13.77	1.71	1.38
4	A	155	TYR	CE1-CZ	13.62	1.71	1.38
4	V	155	TYR	CE1-CZ	13.58	1.70	1.38
4	A	155	TYR	CG-CD1	13.29	1.67	1.39
4	V	155	TYR	CG-CD1	13.26	1.67	1.39
4	W	260	TYR	CG-CD2	13.13	1.67	1.39
4	T	260	TYR	CG-CD2	13.12	1.66	1.39
4	U	260	TYR	CG-CD2	13.11	1.66	1.39
4	B	260	TYR	CG-CD2	13.11	1.66	1.39
4	X	260	TYR	CG-CD2	12.88	1.66	1.39
4	V	260	TYR	CG-CD2	12.86	1.66	1.39
4	C	260	TYR	CG-CD2	12.85	1.66	1.39
4	A	260	TYR	CG-CD2	12.83	1.66	1.39
4	A	155	TYR	CD2-CE2	11.99	1.74	1.38
4	V	155	TYR	CD2-CE2	11.94	1.74	1.38
4	W	260	TYR	CE2-CZ	11.51	1.65	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	260	TYR	CE2-CZ	11.50	1.65	1.38
4	B	260	TYR	CE2-CZ	11.47	1.65	1.38
4	T	260	TYR	CE2-CZ	11.47	1.65	1.38
4	T	260	TYR	CD1-CE1	11.35	1.72	1.38
4	U	260	TYR	CD1-CE1	11.31	1.72	1.38
4	W	260	TYR	CD1-CE1	11.29	1.72	1.38
4	B	260	TYR	CD1-CE1	11.29	1.72	1.38
4	V	260	TYR	CD1-CE1	11.22	1.72	1.38
4	A	260	TYR	CE2-CZ	11.19	1.65	1.38
4	V	260	TYR	CE2-CZ	11.18	1.65	1.38
4	X	260	TYR	CE2-CZ	11.18	1.65	1.38
4	C	260	TYR	CE2-CZ	11.18	1.65	1.38
4	X	260	TYR	CD1-CE1	11.17	1.72	1.38
4	A	260	TYR	CD1-CE1	11.15	1.72	1.38
4	C	260	TYR	CD1-CE1	11.15	1.72	1.38
4	A	155	TYR	CD1-CE1	9.97	1.68	1.38
4	V	155	TYR	CD1-CE1	9.96	1.68	1.38
4	V	155	TYR	CA-CB	9.17	1.69	1.54
4	A	155	TYR	CA-CB	9.12	1.69	1.54
4	B	260	TYR	CD2-CE2	8.69	1.64	1.38
4	T	260	TYR	CD2-CE2	8.69	1.64	1.38
4	U	260	TYR	CD2-CE2	8.67	1.64	1.38
4	W	260	TYR	CD2-CE2	8.64	1.64	1.38
4	V	260	TYR	CD2-CE2	8.52	1.64	1.38
4	X	260	TYR	CD2-CE2	8.51	1.64	1.38
4	A	260	TYR	CD2-CE2	8.49	1.64	1.38
4	C	260	TYR	CD2-CE2	8.49	1.64	1.38
5	K	101	HIS	CD2-NE2	-7.45	1.29	1.37
5	O	101	HIS	CD2-NE2	-7.44	1.29	1.37
5	E	101	HIS	CD2-NE2	-7.43	1.29	1.37
5	R	101	HIS	CD2-NE2	-7.42	1.29	1.37
5	E	87	HIS	CD2-NE2	-7.39	1.29	1.37
5	M	88	HIS	CD2-NE2	-7.38	1.29	1.37
5	E	88	HIS	CD2-NE2	-7.37	1.29	1.37
5	L	101	HIS	CD2-NE2	-7.37	1.29	1.37
5	N	87	HIS	CD2-NE2	-7.37	1.29	1.37
5	S	88	HIS	CD2-NE2	-7.35	1.29	1.37
5	D	87	HIS	CD2-NE2	-7.34	1.29	1.37
5	R	88	HIS	CD2-NE2	-7.34	1.29	1.37
5	O	87	HIS	CD2-NE2	-7.34	1.29	1.37
5	G	101	HIS	CD2-NE2	-7.34	1.29	1.37
5	M	87	HIS	CD2-NE2	-7.34	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	101	HIS	CD2-NE2	-7.34	1.29	1.37
5	M	101	HIS	CD2-NE2	-7.34	1.29	1.37
5	F	101	HIS	CD2-NE2	-7.33	1.29	1.37
5	G	88	HIS	CD2-NE2	-7.33	1.29	1.37
5	Q	88	HIS	CD2-NE2	-7.33	1.29	1.37
5	J	88	HIS	CD2-NE2	-7.32	1.29	1.37
5	P	101	HIS	CD2-NE2	-7.32	1.29	1.37
5	G	87	HIS	CD2-NE2	-7.32	1.29	1.37
5	S	87	HIS	CD2-NE2	-7.32	1.29	1.37
5	F	88	HIS	CD2-NE2	-7.32	1.29	1.37
5	O	88	HIS	CD2-NE2	-7.32	1.29	1.37
5	J	101	HIS	CD2-NE2	-7.31	1.29	1.37
5	H	101	HIS	CD2-NE2	-7.29	1.29	1.37
5	Q	101	HIS	CD2-NE2	-7.29	1.29	1.37
5	L	88	HIS	CD2-NE2	-7.28	1.29	1.37
5	H	88	HIS	CD2-NE2	-7.28	1.29	1.37
5	I	101	HIS	CD2-NE2	-7.28	1.29	1.37
5	O	275	HIS	CD2-NE2	-7.27	1.29	1.37
5	Q	275	HIS	CD2-NE2	-7.26	1.29	1.37
5	K	88	HIS	CD2-NE2	-7.25	1.29	1.37
5	K	87	HIS	CD2-NE2	-7.25	1.29	1.37
5	P	88	HIS	CD2-NE2	-7.25	1.29	1.37
5	N	88	HIS	CD2-NE2	-7.23	1.29	1.37
5	L	275	HIS	CD2-NE2	-7.22	1.29	1.37
5	E	275	HIS	CD2-NE2	-7.22	1.29	1.37
5	I	88	HIS	CD2-NE2	-7.22	1.29	1.37
5	Q	87	HIS	CD2-NE2	-7.22	1.29	1.37
5	H	275	HIS	CD2-NE2	-7.21	1.29	1.37
5	R	275	HIS	CD2-NE2	-7.21	1.29	1.37
5	J	40	HIS	CD2-NE2	-7.21	1.29	1.37
5	P	275	HIS	CD2-NE2	-7.20	1.29	1.37
5	P	87	HIS	CD2-NE2	-7.20	1.29	1.37
5	R	87	HIS	CD2-NE2	-7.20	1.29	1.37
5	F	275	HIS	CD2-NE2	-7.20	1.29	1.37
5	J	87	HIS	CD2-NE2	-7.18	1.29	1.37
5	M	40	HIS	CD2-NE2	-7.18	1.29	1.37
5	L	87	HIS	CD2-NE2	-7.18	1.29	1.37
5	H	87	HIS	CD2-NE2	-7.17	1.29	1.37
5	N	101	HIS	CD2-NE2	-7.16	1.29	1.37
5	I	275	HIS	CD2-NE2	-7.16	1.29	1.37
5	S	40	HIS	CD2-NE2	-7.16	1.29	1.37
5	F	87	HIS	CD2-NE2	-7.16	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	275	HIS	CD2-NE2	-7.15	1.29	1.37
5	D	101	HIS	CD2-NE2	-7.15	1.29	1.37
5	D	40	HIS	CD2-NE2	-7.15	1.29	1.37
5	R	40	HIS	CD2-NE2	-7.14	1.29	1.37
5	D	275	HIS	CD2-NE2	-7.14	1.29	1.37
5	K	275	HIS	CD2-NE2	-7.14	1.29	1.37
5	I	87	HIS	CD2-NE2	-7.13	1.30	1.37
5	J	275	HIS	CD2-NE2	-7.13	1.30	1.37
5	K	40	HIS	CD2-NE2	-7.12	1.30	1.37
5	D	88	HIS	CD2-NE2	-7.10	1.30	1.37
5	E	40	HIS	CD2-NE2	-7.10	1.30	1.37
5	L	40	HIS	CD2-NE2	-7.10	1.30	1.37
5	S	275	HIS	CD2-NE2	-7.09	1.30	1.37
5	O	40	HIS	CD2-NE2	-7.08	1.30	1.37
5	N	40	HIS	CD2-NE2	-7.07	1.30	1.37
5	M	275	HIS	CD2-NE2	-7.07	1.30	1.37
5	G	275	HIS	CD2-NE2	-7.06	1.30	1.37
5	F	40	HIS	CD2-NE2	-7.03	1.30	1.37
5	P	40	HIS	CD2-NE2	-7.02	1.30	1.37
5	H	40	HIS	CD2-NE2	-6.99	1.30	1.37
5	G	40	HIS	CD2-NE2	-6.98	1.30	1.37
5	Q	40	HIS	CD2-NE2	-6.96	1.30	1.37
5	I	40	HIS	CD2-NE2	-6.91	1.30	1.37
5	E	371	HIS	CD2-NE2	-6.80	1.30	1.37
5	I	371	HIS	CD2-NE2	-6.75	1.30	1.37
5	R	371	HIS	CD2-NE2	-6.70	1.30	1.37
5	L	371	HIS	CD2-NE2	-6.69	1.30	1.37
5	O	371	HIS	CD2-NE2	-6.67	1.30	1.37
5	J	371	HIS	CD2-NE2	-6.65	1.30	1.37
5	S	371	HIS	CD2-NE2	-6.65	1.30	1.37
5	G	371	HIS	CD2-NE2	-6.64	1.30	1.37
5	N	371	HIS	CD2-NE2	-6.64	1.30	1.37
5	H	371	HIS	CD2-NE2	-6.61	1.30	1.37
5	F	371	HIS	CD2-NE2	-6.57	1.30	1.37
5	M	371	HIS	CD2-NE2	-6.57	1.30	1.37
5	P	371	HIS	CD2-NE2	-6.55	1.30	1.37
5	D	371	HIS	CD2-NE2	-6.55	1.30	1.37
5	K	371	HIS	CD2-NE2	-6.55	1.30	1.37
5	R	88	HIS	CG-ND1	-6.53	1.31	1.38
5	L	88	HIS	CG-ND1	-6.50	1.31	1.38
5	H	101	HIS	CG-ND1	-6.47	1.31	1.38
5	J	101	HIS	CG-ND1	-6.47	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	88	HIS	CG-ND1	-6.46	1.31	1.38
5	Q	88	HIS	CG-ND1	-6.43	1.31	1.38
5	D	101	HIS	CG-ND1	-6.43	1.31	1.38
5	Q	101	HIS	CG-ND1	-6.42	1.31	1.38
5	P	101	HIS	CG-ND1	-6.42	1.31	1.38
5	G	88	HIS	CG-ND1	-6.41	1.31	1.38
5	N	88	HIS	CG-ND1	-6.41	1.31	1.38
5	O	101	HIS	CG-ND1	-6.41	1.31	1.38
5	F	101	HIS	CG-ND1	-6.41	1.31	1.38
5	O	88	HIS	CG-ND1	-6.41	1.31	1.38
5	Q	371	HIS	CD2-NE2	-6.40	1.30	1.37
4	U	146	HIS	CD2-NE2	-6.40	1.30	1.37
5	J	88	HIS	CG-ND1	-6.40	1.31	1.38
5	S	88	HIS	CG-ND1	-6.40	1.31	1.38
5	D	88	HIS	CG-ND1	-6.39	1.31	1.38
5	E	88	HIS	CG-ND1	-6.39	1.31	1.38
5	G	101	HIS	CG-ND1	-6.38	1.31	1.38
5	I	88	HIS	CG-ND1	-6.38	1.31	1.38
5	I	101	HIS	CG-ND1	-6.38	1.31	1.38
5	M	88	HIS	CG-ND1	-6.38	1.31	1.38
5	P	88	HIS	CG-ND1	-6.37	1.31	1.38
4	V	146	HIS	CD2-NE2	-6.37	1.30	1.37
5	H	88	HIS	CG-ND1	-6.36	1.31	1.38
5	F	88	HIS	CG-ND1	-6.33	1.31	1.38
5	N	101	HIS	CG-ND1	-6.33	1.31	1.38
5	E	101	HIS	CG-ND1	-6.33	1.31	1.38
5	K	101	HIS	CG-ND1	-6.33	1.31	1.38
4	B	146	HIS	CD2-NE2	-6.30	1.30	1.37
3	2	74	VAL	CA-CB	-6.29	1.46	1.54
3	Z	74	VAL	CA-CB	-6.29	1.46	1.54
5	L	101	HIS	CG-ND1	-6.29	1.31	1.38
5	R	101	HIS	CG-ND1	-6.27	1.31	1.38
4	A	146	HIS	CD2-NE2	-6.26	1.30	1.37
3	5	74	VAL	CA-CB	-6.26	1.46	1.54
3	8	74	VAL	CA-CB	-6.26	1.46	1.54
5	S	101	HIS	CG-ND1	-6.24	1.31	1.38
5	M	101	HIS	CG-ND1	-6.20	1.31	1.38
4	W	269	HIS	CD2-NE2	-6.19	1.31	1.37
4	X	253	LEU	CA-CB	-6.18	1.43	1.53
4	U	269	HIS	CD2-NE2	-6.18	1.31	1.37
4	U	169	LEU	CB-CG	-6.16	1.41	1.53
4	T	269	HIS	CD2-NE2	-6.15	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	253	LEU	CA-CB	-6.14	1.43	1.53
4	V	253	LEU	CA-CB	-6.14	1.43	1.53
4	A	269	HIS	CD2-NE2	-6.13	1.31	1.37
4	B	169	LEU	CB-CG	-6.12	1.41	1.53
4	V	269	HIS	CD2-NE2	-6.12	1.31	1.37
4	C	253	LEU	CA-CB	-6.11	1.43	1.53
4	X	269	HIS	CD2-NE2	-6.11	1.31	1.37
5	Q	161	HIS	CD2-NE2	-6.10	1.31	1.37
4	B	269	HIS	CD2-NE2	-6.09	1.31	1.37
4	C	269	HIS	CD2-NE2	-6.08	1.31	1.37
5	F	161	HIS	CD2-NE2	-6.08	1.31	1.37
4	A	169	LEU	CB-CG	-6.01	1.41	1.53
5	G	161	HIS	CD2-NE2	-6.01	1.31	1.37
5	O	173	HIS	CD2-NE2	-5.99	1.31	1.37
4	V	169	LEU	CB-CG	-5.97	1.41	1.53
5	J	161	HIS	CD2-NE2	-5.96	1.31	1.37
5	S	173	HIS	CD2-NE2	-5.96	1.31	1.37
5	G	173	HIS	CD2-NE2	-5.96	1.31	1.37
5	M	173	HIS	CD2-NE2	-5.93	1.31	1.37
5	D	161	HIS	CD2-NE2	-5.92	1.31	1.37
5	I	161	HIS	CD2-NE2	-5.90	1.31	1.37
5	P	161	HIS	CD2-NE2	-5.90	1.31	1.37
5	H	173	HIS	CD2-NE2	-5.89	1.31	1.37
5	M	161	HIS	CD2-NE2	-5.89	1.31	1.37
5	F	173	HIS	CD2-NE2	-5.88	1.31	1.37
5	L	161	HIS	CD2-NE2	-5.88	1.31	1.37
5	S	161	HIS	CD2-NE2	-5.88	1.31	1.37
5	K	173	HIS	CD2-NE2	-5.87	1.31	1.37
5	H	161	HIS	CD2-NE2	-5.87	1.31	1.37
5	K	161	HIS	CD2-NE2	-5.86	1.31	1.37
5	E	173	HIS	CD2-NE2	-5.86	1.31	1.37
5	I	173	HIS	CD2-NE2	-5.85	1.31	1.37
5	N	173	HIS	CD2-NE2	-5.84	1.31	1.37
5	O	161	HIS	CD2-NE2	-5.84	1.31	1.37
5	N	161	HIS	CD2-NE2	-5.83	1.31	1.37
5	E	161	HIS	CD2-NE2	-5.83	1.31	1.37
5	R	161	HIS	CD2-NE2	-5.82	1.31	1.37
5	P	173	HIS	CD2-NE2	-5.81	1.31	1.37
5	L	173	HIS	CD2-NE2	-5.79	1.31	1.37
4	V	197	LEU	CB-CG	-5.79	1.41	1.53
5	D	173	HIS	CD2-NE2	-5.76	1.31	1.37
5	J	173	HIS	CD2-NE2	-5.75	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	173	HIS	CD2-NE2	-5.74	1.31	1.37
4	A	197	LEU	CB-CG	-5.73	1.42	1.53
5	Q	173	HIS	CD2-NE2	-5.72	1.31	1.37
5	E	275	HIS	CG-ND1	-5.69	1.31	1.38
4	X	253	LEU	CB-CG	-5.66	1.42	1.53
4	A	253	LEU	CB-CG	-5.64	1.42	1.53
4	V	253	LEU	CB-CG	-5.62	1.42	1.53
5	H	275	HIS	CG-ND1	-5.61	1.32	1.38
4	C	253	LEU	CB-CG	-5.61	1.42	1.53
5	O	275	HIS	CG-ND1	-5.59	1.32	1.38
4	B	92	LEU	CB-CG	-5.58	1.42	1.53
5	J	275	HIS	CG-ND1	-5.58	1.32	1.38
5	F	275	HIS	CG-ND1	-5.58	1.32	1.38
5	K	275	HIS	CG-ND1	-5.57	1.32	1.38
4	U	92	LEU	CB-CG	-5.56	1.42	1.53
5	I	275	HIS	CG-ND1	-5.56	1.32	1.38
5	G	275	HIS	CG-ND1	-5.55	1.32	1.38
5	R	275	HIS	CG-ND1	-5.55	1.32	1.38
5	N	275	HIS	CG-ND1	-5.54	1.32	1.38
5	M	275	HIS	CG-ND1	-5.53	1.32	1.38
5	P	275	HIS	CG-ND1	-5.53	1.32	1.38
5	L	275	HIS	CG-ND1	-5.53	1.32	1.38
5	S	275	HIS	CG-ND1	-5.51	1.32	1.38
4	A	197	LEU	CA-C	-5.47	1.46	1.52
4	B	197	LEU	CA-C	-5.46	1.46	1.52
5	D	275	HIS	CG-ND1	-5.46	1.32	1.38
5	Q	275	HIS	CG-ND1	-5.45	1.32	1.38
4	U	253	LEU	CA-C	-5.45	1.46	1.52
4	V	197	LEU	CA-C	-5.44	1.46	1.52
4	W	253	LEU	CA-C	-5.44	1.46	1.52
4	V	197	LEU	CA-CB	-5.43	1.45	1.53
4	B	169	LEU	CA-CB	-5.40	1.45	1.53
4	A	197	LEU	CA-CB	-5.39	1.45	1.53
4	U	197	LEU	CA-C	-5.38	1.46	1.52
4	V	169	LEU	CA-CB	-5.35	1.45	1.53
4	U	92	LEU	CA-CB	-5.34	1.45	1.53
4	B	92	LEU	CA-CB	-5.32	1.45	1.53
4	U	169	LEU	CA-CB	-5.31	1.45	1.53
4	A	169	LEU	CA-CB	-5.29	1.45	1.53
5	J	259	GLU	CA-CB	5.24	1.62	1.53
5	F	259	GLU	CA-CB	5.23	1.62	1.53
4	T	253	LEU	CA-C	-5.23	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	253	LEU	CA-C	-5.22	1.46	1.52
4	A	154	LYS	CA-C	5.21	1.59	1.52
5	D	259	GLU	CA-CB	5.20	1.62	1.53
5	H	259	GLU	CA-CB	5.20	1.62	1.53
5	I	259	GLU	CA-CB	5.19	1.62	1.53
5	P	259	GLU	CA-CB	5.19	1.62	1.53
4	U	92	LEU	CA-C	-5.19	1.46	1.52
5	E	259	GLU	CA-CB	5.18	1.62	1.53
5	K	259	GLU	CA-CB	5.17	1.62	1.53
5	N	259	GLU	CA-CB	5.17	1.62	1.53
5	O	259	GLU	CA-CB	5.17	1.62	1.53
4	A	169	LEU	CA-C	-5.17	1.46	1.52
4	A	92	LEU	CB-CG	-5.16	1.43	1.53
4	V	154	LYS	CA-C	5.15	1.59	1.52
5	M	259	GLU	CA-CB	5.13	1.62	1.53
5	Q	214	GLU	CA-CB	5.13	1.61	1.53
5	L	259	GLU	CA-CB	5.13	1.62	1.53
5	G	259	GLU	CA-CB	5.12	1.62	1.53
4	V	92	LEU	CB-CG	-5.12	1.43	1.53
5	S	259	GLU	CA-CB	5.12	1.62	1.53
4	B	92	LEU	CA-C	-5.11	1.46	1.52
5	J	214	GLU	CA-CB	5.10	1.61	1.53
5	M	214	GLU	CA-CB	5.10	1.61	1.53
5	Q	259	GLU	CA-CB	5.10	1.62	1.53
5	L	214	GLU	CA-CB	5.09	1.61	1.53
5	F	214	GLU	CA-CB	5.09	1.61	1.53
5	P	214	GLU	CA-CB	5.09	1.61	1.53
5	D	214	GLU	CA-CB	5.08	1.61	1.53
4	V	169	LEU	CA-C	-5.08	1.46	1.52
4	U	169	LEU	CA-C	-5.08	1.46	1.52
5	H	214	GLU	CA-CB	5.06	1.61	1.53
5	O	214	GLU	CA-CB	5.06	1.61	1.53
5	S	214	GLU	CA-CB	5.06	1.61	1.53
5	R	214	GLU	CA-CB	5.05	1.61	1.53
5	R	259	GLU	CA-CB	5.05	1.62	1.53
5	E	214	GLU	CA-CB	5.04	1.61	1.53
4	B	169	LEU	CA-C	-5.04	1.46	1.52
5	K	214	GLU	CA-CB	5.03	1.61	1.53
5	G	214	GLU	CA-CB	5.01	1.61	1.53

All (2206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	253	LEU	N-CA-C	25.38	138.55	111.14
4	B	253	LEU	N-CA-C	25.26	138.42	111.14
4	W	253	LEU	N-CA-C	24.73	138.49	111.03
4	U	253	LEU	N-CA-C	24.69	138.44	111.03
4	C	253	LEU	N-CA-C	24.36	137.52	110.97
4	V	253	LEU	N-CA-C	24.34	137.50	110.97
4	A	253	LEU	N-CA-C	24.29	137.45	110.97
4	X	253	LEU	N-CA-C	24.28	137.43	110.97
4	V	92	LEU	N-CA-C	19.19	134.82	111.40
4	A	92	LEU	N-CA-C	19.18	134.80	111.40
4	B	92	LEU	N-CA-C	18.78	135.47	111.24
4	U	92	LEU	N-CA-C	18.77	135.45	111.24
4	A	197	LEU	N-CA-C	17.52	130.48	111.03
4	V	197	LEU	N-CA-C	17.47	130.43	111.03
4	U	169	LEU	N-CA-C	17.16	130.08	111.03
4	B	169	LEU	N-CA-C	17.08	129.99	111.03
4	V	169	LEU	N-CA-C	16.81	129.69	111.03
4	A	169	LEU	N-CA-C	16.72	129.59	111.03
4	B	197	LEU	N-CA-C	15.78	128.18	111.14
4	U	197	LEU	N-CA-C	15.69	128.08	111.14
4	C	274	MET	CA-CB-CG	13.55	141.20	114.10
4	A	274	MET	CA-CB-CG	13.53	141.16	114.10
4	X	274	MET	CA-CB-CG	13.53	141.16	114.10
4	V	274	MET	CA-CB-CG	13.52	141.13	114.10
4	T	267	LEU	N-CA-C	13.45	125.96	111.03
4	B	267	LEU	N-CA-C	13.45	125.95	111.03
4	V	155	TYR	N-CA-C	-13.43	97.39	114.04
4	U	267	LEU	N-CA-C	13.40	125.91	111.03
4	A	155	TYR	N-CA-C	-13.39	97.43	114.04
4	W	267	LEU	N-CA-C	13.37	125.87	111.03
4	V	73	ASP	CA-CB-CG	12.82	125.42	112.60
4	A	73	ASP	CA-CB-CG	12.79	125.39	112.60
4	U	73	ASP	CA-CB-CG	12.73	125.33	112.60
4	B	73	ASP	CA-CB-CG	12.68	125.28	112.60
4	W	274	MET	CA-CB-CG	12.66	139.42	114.10
4	T	274	MET	CA-CB-CG	12.66	139.41	114.10
4	B	274	MET	CA-CB-CG	12.65	139.41	114.10
4	U	274	MET	CA-CB-CG	12.65	139.41	114.10
4	V	64	LEU	N-CA-C	12.57	124.68	110.97
4	X	267	LEU	N-CA-C	12.54	124.94	111.03
4	V	267	LEU	N-CA-C	12.53	124.94	111.03
4	A	64	LEU	N-CA-C	12.53	124.63	110.97
4	A	267	LEU	N-CA-C	12.53	124.93	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	267	LEU	N-CA-C	12.47	124.87	111.03
4	W	248	ASP	CA-CB-CG	12.27	124.87	112.60
4	U	248	ASP	CA-CB-CG	12.23	124.83	112.60
4	B	248	ASP	CA-CB-CG	12.20	124.80	112.60
4	T	248	ASP	CA-CB-CG	12.20	124.80	112.60
4	U	50	LEU	N-CA-C	12.16	124.53	111.03
4	V	231	ARG	CD-NE-CZ	-12.16	107.37	124.40
4	B	50	LEU	N-CA-C	12.16	124.53	111.03
4	A	231	ARG	CD-NE-CZ	-12.11	107.44	124.40
4	U	64	LEU	N-CA-C	11.83	123.86	110.97
4	B	64	LEU	N-CA-C	11.78	123.81	110.97
4	X	248	ASP	CA-CB-CG	11.73	124.33	112.60
4	A	50	LEU	N-CA-C	11.67	123.99	111.03
4	A	248	ASP	CA-CB-CG	11.65	124.25	112.60
4	V	248	ASP	CA-CB-CG	11.64	124.24	112.60
4	V	50	LEU	N-CA-C	11.63	123.94	111.03
4	C	248	ASP	CA-CB-CG	11.61	124.21	112.60
4	B	260	TYR	CA-C-O	-11.45	108.78	120.80
4	B	77	ASP	CA-CB-CG	11.38	123.98	112.60
4	T	260	TYR	CA-C-O	-11.37	108.86	120.80
4	W	260	TYR	CA-C-O	-11.36	108.87	120.80
4	V	27	ASP	CA-CB-CG	11.36	123.96	112.60
4	U	77	ASP	CA-CB-CG	11.35	123.95	112.60
4	U	260	TYR	CA-C-O	-11.34	108.90	120.80
4	C	260	TYR	CA-C-O	-11.31	108.93	120.80
4	A	27	ASP	CA-CB-CG	11.29	123.89	112.60
4	V	260	TYR	CA-C-O	-11.28	108.95	120.80
4	A	260	TYR	CA-C-O	-11.27	108.96	120.80
4	X	260	TYR	CA-C-O	-11.27	108.97	120.80
4	U	27	ASP	CA-CB-CG	11.18	123.78	112.60
4	B	27	ASP	CA-CB-CG	11.14	123.75	112.60
4	A	114	ASP	CA-CB-CG	11.13	123.73	112.60
4	A	197	LEU	CD1-CG-CD2	11.11	135.24	110.80
4	A	36	LEU	CD1-CG-CD2	11.11	135.24	110.80
4	V	36	LEU	CD1-CG-CD2	11.10	135.21	110.80
4	V	197	LEU	CD1-CG-CD2	11.08	135.18	110.80
4	V	114	ASP	CA-CB-CG	11.06	123.66	112.60
4	U	223	ASP	CA-CB-CG	11.06	123.66	112.60
4	B	223	ASP	CA-CB-CG	10.98	123.58	112.60
4	V	59	ASP	CA-CB-CG	10.92	123.52	112.60
4	A	59	ASP	CA-CB-CG	10.88	123.47	112.60
4	A	77	ASP	CA-CB-CG	10.87	123.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	150	ASP	CA-CB-CG	10.86	123.46	112.60
4	V	77	ASP	CA-CB-CG	10.81	123.42	112.60
4	B	150	ASP	CA-CB-CG	10.79	123.39	112.60
4	U	150	ASP	CA-CB-CG	10.76	123.36	112.60
4	C	256	GLN	OE1-CD-NE2	-10.76	111.84	122.60
4	A	154	LYS	N-CA-C	10.76	125.92	113.01
4	V	256	GLN	OE1-CD-NE2	-10.75	111.85	122.60
4	A	223	ASP	CA-CB-CG	10.73	123.33	112.60
4	V	150	ASP	CA-CB-CG	10.73	123.33	112.60
4	V	154	LYS	N-CA-C	10.73	125.88	113.01
4	A	48	ASP	CA-CB-CG	10.72	123.33	112.60
4	A	256	GLN	OE1-CD-NE2	-10.72	111.88	122.60
4	V	48	ASP	CA-CB-CG	10.72	123.32	112.60
4	X	256	GLN	OE1-CD-NE2	-10.70	111.90	122.60
4	B	36	LEU	N-CA-C	10.70	124.45	111.40
4	V	223	ASP	CA-CB-CG	10.68	123.28	112.60
4	W	256	GLN	OE1-CD-NE2	-10.67	111.93	122.60
4	B	59	ASP	CA-CB-CG	10.65	123.25	112.60
4	B	256	GLN	OE1-CD-NE2	-10.61	111.99	122.60
4	B	36	LEU	CD1-CG-CD2	10.60	134.12	110.80
4	T	256	GLN	OE1-CD-NE2	-10.60	112.00	122.60
4	U	36	LEU	N-CA-C	10.60	124.33	111.40
4	U	256	GLN	OE1-CD-NE2	-10.59	112.01	122.60
4	B	155	TYR	CB-CG-CD1	-10.58	104.93	120.80
4	U	59	ASP	CA-CB-CG	10.58	123.18	112.60
4	U	36	LEU	CD1-CG-CD2	10.57	134.05	110.80
4	V	225	LEU	N-CA-C	10.57	122.49	110.97
4	A	225	LEU	N-CA-C	10.54	122.46	110.97
4	U	169	LEU	CD1-CG-CD2	10.54	133.99	110.80
4	B	169	LEU	CD1-CG-CD2	10.53	133.96	110.80
4	U	155	TYR	CB-CG-CD1	-10.53	105.01	120.80
4	U	114	ASP	CA-CB-CG	10.50	123.10	112.60
4	U	48	ASP	CA-CB-CG	10.47	123.07	112.60
4	B	114	ASP	CA-CB-CG	10.45	123.05	112.60
4	V	190	LEU	CD1-CG-CD2	10.44	133.77	110.80
4	A	190	LEU	CD1-CG-CD2	10.44	133.77	110.80
4	B	92	LEU	CD1-CG-CD2	10.42	133.73	110.80
4	U	92	LEU	CD1-CG-CD2	10.40	133.69	110.80
4	B	48	ASP	CA-CB-CG	10.38	122.98	112.60
4	A	155	TYR	CA-CB-CG	10.38	132.58	113.90
4	V	155	TYR	CA-CB-CG	10.35	132.54	113.90
4	B	13	ASP	CA-CB-CG	10.34	122.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	169	LEU	CD1-CG-CD2	10.29	133.44	110.80
4	U	13	ASP	CA-CB-CG	10.26	122.86	112.60
4	A	169	LEU	CD1-CG-CD2	10.26	133.37	110.80
4	U	212	ASP	CA-CB-CG	10.21	122.81	112.60
4	B	212	ASP	CA-CB-CG	10.19	122.79	112.60
4	C	247	ASP	CA-CB-CG	10.04	122.64	112.60
4	X	247	ASP	CA-CB-CG	10.04	122.64	112.60
4	A	247	ASP	CA-CB-CG	10.03	122.63	112.60
4	V	36	LEU	N-CA-C	10.02	123.63	111.40
4	A	92	LEU	CD1-CG-CD2	10.02	132.85	110.80
4	A	212	ASP	CA-CB-CG	10.01	122.61	112.60
4	A	36	LEU	N-CA-C	10.00	123.60	111.40
4	V	92	LEU	CD1-CG-CD2	9.99	132.78	110.80
4	V	247	ASP	CA-CB-CG	9.99	122.59	112.60
4	V	212	ASP	CA-CB-CG	9.98	122.58	112.60
4	B	197	LEU	CD1-CG-CD2	9.93	132.65	110.80
4	U	197	LEU	CD1-CG-CD2	9.93	132.65	110.80
4	W	247	ASP	CA-CB-CG	9.93	122.53	112.60
4	B	247	ASP	CA-CB-CG	9.92	122.52	112.60
4	U	247	ASP	CA-CB-CG	9.89	122.49	112.60
4	T	247	ASP	CA-CB-CG	9.86	122.46	112.60
4	V	13	ASP	CA-CB-CG	9.84	122.44	112.60
4	B	141	LEU	CD1-CG-CD2	9.77	132.29	110.80
3	Z	48	SER	CA-C-N	9.77	126.69	119.66
3	Z	48	SER	C-N-CA	9.77	126.69	119.66
4	U	141	LEU	CD1-CG-CD2	9.75	132.26	110.80
4	B	225	LEU	N-CA-C	9.72	121.57	110.97
3	2	48	SER	CA-C-N	9.72	126.66	119.66
3	2	48	SER	C-N-CA	9.72	126.66	119.66
4	U	225	LEU	N-CA-C	9.68	121.52	110.97
4	A	43	LEU	CD1-CG-CD2	9.66	132.06	110.80
4	U	10	ASN	OD1-CG-ND2	-9.66	112.94	122.60
4	V	43	LEU	CD1-CG-CD2	9.66	132.05	110.80
4	B	10	ASN	OD1-CG-ND2	-9.65	112.95	122.60
4	V	155	TYR	N-CA-CB	9.62	125.05	110.81
4	A	155	TYR	N-CA-CB	9.60	125.01	110.81
3	5	48	SER	CA-C-N	9.59	126.56	119.66
3	5	48	SER	C-N-CA	9.59	126.56	119.66
4	B	43	LEU	CD1-CG-CD2	9.53	131.76	110.80
4	V	141	LEU	CD1-CG-CD2	9.51	131.73	110.80
4	A	141	LEU	CD1-CG-CD2	9.50	131.71	110.80
4	U	43	LEU	CD1-CG-CD2	9.50	131.70	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	8	48	SER	CA-C-N	9.49	126.49	119.66
3	8	48	SER	C-N-CA	9.49	126.49	119.66
5	K	147	ARG	N-CA-C	9.43	123.36	110.35
4	B	190	LEU	CD1-CG-CD2	9.43	131.53	110.80
4	U	190	LEU	CD1-CG-CD2	9.42	131.53	110.80
5	G	147	ARG	N-CA-C	9.40	123.33	110.35
5	N	147	ARG	N-CA-C	9.39	123.31	110.35
5	I	147	ARG	N-CA-C	9.39	123.30	110.35
5	S	147	ARG	N-CA-C	9.39	123.30	110.35
5	M	147	ARG	N-CA-C	9.37	123.29	110.35
5	Q	147	ARG	N-CA-C	9.37	123.29	110.35
5	P	147	ARG	N-CA-C	9.37	123.28	110.35
5	F	147	ARG	N-CA-C	9.36	123.27	110.35
5	J	147	ARG	N-CA-C	9.36	123.27	110.35
5	H	147	ARG	N-CA-C	9.35	123.26	110.35
5	R	147	ARG	N-CA-C	9.34	123.23	110.35
5	E	147	ARG	N-CA-C	9.33	123.22	110.35
5	D	147	ARG	N-CA-C	9.32	123.22	110.35
5	L	147	ARG	N-CA-C	9.32	123.21	110.35
5	O	147	ARG	N-CA-C	9.32	123.21	110.35
4	B	152	ASP	CA-CB-CG	9.29	121.89	112.60
5	M	3	ASP	CA-CB-CG	9.29	121.89	112.60
4	U	152	ASP	CA-CB-CG	9.29	121.89	112.60
5	F	3	ASP	CA-CB-CG	9.27	121.87	112.60
5	S	3	ASP	CA-CB-CG	9.26	121.86	112.60
4	V	10	ASN	OD1-CG-ND2	-9.25	113.35	122.60
5	K	3	ASP	CA-CB-CG	9.25	121.85	112.60
5	L	3	ASP	CA-CB-CG	9.24	121.84	112.60
5	G	3	ASP	CA-CB-CG	9.24	121.84	112.60
5	R	3	ASP	CA-CB-CG	9.23	121.83	112.60
5	O	3	ASP	CA-CB-CG	9.22	121.82	112.60
5	P	3	ASP	CA-CB-CG	9.20	121.80	112.60
5	D	3	ASP	CA-CB-CG	9.19	121.79	112.60
5	H	3	ASP	CA-CB-CG	9.19	121.79	112.60
5	N	3	ASP	CA-CB-CG	9.19	121.78	112.60
5	E	3	ASP	CA-CB-CG	9.18	121.78	112.60
5	I	3	ASP	CA-CB-CG	9.17	121.77	112.60
5	Q	3	ASP	CA-CB-CG	9.17	121.77	112.60
5	J	3	ASP	CA-CB-CG	9.12	121.72	112.60
4	A	57	LEU	N-CA-C	9.01	120.87	111.14
4	V	57	LEU	N-CA-C	8.97	120.83	111.14
4	V	130	ASP	CA-C-O	-8.92	111.72	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	130	ASP	CA-C-O	-8.89	111.74	120.90
5	P	179	ASP	CA-CB-CG	8.87	121.47	112.60
5	Q	179	ASP	CA-CB-CG	8.86	121.46	112.60
4	B	57	LEU	N-CA-C	8.86	120.70	111.14
5	K	179	ASP	CA-CB-CG	8.83	121.43	112.60
4	U	57	LEU	N-CA-C	8.83	120.68	111.14
5	L	179	ASP	CA-CB-CG	8.81	121.41	112.60
5	D	179	ASP	CA-CB-CG	8.80	121.40	112.60
5	O	179	ASP	CA-CB-CG	8.80	121.40	112.60
5	R	179	ASP	CA-CB-CG	8.79	121.39	112.60
5	I	179	ASP	CA-CB-CG	8.78	121.38	112.60
5	S	179	ASP	CA-CB-CG	8.78	121.38	112.60
5	G	179	ASP	CA-CB-CG	8.77	121.37	112.60
5	M	179	ASP	CA-CB-CG	8.77	121.37	112.60
5	E	179	ASP	CA-CB-CG	8.76	121.36	112.60
5	J	179	ASP	CA-CB-CG	8.76	121.36	112.60
5	N	179	ASP	CA-CB-CG	8.75	121.35	112.60
5	H	179	ASP	CA-CB-CG	8.74	121.34	112.60
5	F	179	ASP	CA-CB-CG	8.70	121.30	112.60
4	U	272	ASN	OD1-CG-ND2	-8.66	113.94	122.60
4	B	272	ASN	OD1-CG-ND2	-8.65	113.95	122.60
4	W	272	ASN	OD1-CG-ND2	-8.65	113.95	122.60
4	T	272	ASN	OD1-CG-ND2	-8.60	114.00	122.60
4	V	153	ARG	N-CA-C	8.57	121.86	111.40
4	B	130	ASP	CA-C-O	-8.54	112.10	120.90
4	U	130	ASP	CA-C-O	-8.53	112.12	120.90
4	A	153	ARG	N-CA-C	8.52	121.80	111.40
4	V	272	ASN	OD1-CG-ND2	-8.50	114.10	122.60
4	A	272	ASN	OD1-CG-ND2	-8.46	114.14	122.60
4	X	272	ASN	OD1-CG-ND2	-8.46	114.14	122.60
4	C	272	ASN	OD1-CG-ND2	-8.45	114.15	122.60
4	X	276	SER	N-CA-C	8.43	122.06	111.69
4	V	82	ASN	OD1-CG-ND2	-8.42	114.18	122.60
4	V	276	SER	N-CA-C	8.41	122.04	111.69
4	A	276	SER	N-CA-C	8.41	122.04	111.69
4	A	82	ASN	OD1-CG-ND2	-8.38	114.22	122.60
4	C	276	SER	N-CA-C	8.38	121.99	111.69
4	V	260	TYR	CB-CG-CD2	-8.33	108.31	120.80
4	X	260	TYR	CB-CG-CD2	-8.32	108.32	120.80
4	U	154	LYS	CA-C-N	8.31	137.41	121.54
4	U	154	LYS	C-N-CA	8.31	137.41	121.54
4	C	260	TYR	CB-CG-CD2	-8.30	108.35	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	82	ASN	OD1-CG-ND2	-8.29	114.31	122.60
4	A	260	TYR	CB-CG-CD2	-8.29	108.37	120.80
4	B	154	LYS	CA-C-N	8.27	137.34	121.54
4	B	154	LYS	C-N-CA	8.27	137.34	121.54
4	B	231	ARG	NE-CZ-NH2	-8.27	111.76	119.20
4	U	82	ASN	OD1-CG-ND2	-8.24	114.36	122.60
4	U	196	ASN	OD1-CG-ND2	-8.21	114.39	122.60
4	U	231	ARG	NE-CZ-NH2	-8.19	111.83	119.20
4	A	154	LYS	CA-C-N	8.15	136.85	122.42
4	A	154	LYS	C-N-CA	8.15	136.85	122.42
4	B	196	ASN	OD1-CG-ND2	-8.15	114.45	122.60
4	V	154	LYS	CA-C-N	8.13	136.81	122.42
4	V	154	LYS	C-N-CA	8.13	136.81	122.42
5	R	363	ASP	CA-CB-CG	8.06	120.66	112.60
5	M	286	ASP	CA-CB-CG	8.05	120.65	112.60
4	B	273	ASP	CA-CB-CG	8.04	120.64	112.60
4	T	273	ASP	CA-CB-CG	8.03	120.63	112.60
4	W	273	ASP	CA-CB-CG	8.03	120.63	112.60
4	U	273	ASP	CA-CB-CG	8.02	120.62	112.60
5	L	363	ASP	CA-CB-CG	8.01	120.61	112.60
4	U	40	GLN	OE1-CD-NE2	-8.01	114.59	122.60
4	U	260	TYR	CB-CG-CD2	-8.00	108.80	120.80
5	P	363	ASP	CA-CB-CG	8.00	120.59	112.60
4	B	40	GLN	OE1-CD-NE2	-7.99	114.61	122.60
5	S	286	ASP	CA-CB-CG	7.98	120.58	112.60
4	W	260	TYR	CB-CG-CD2	-7.98	108.83	120.80
4	B	260	TYR	CB-CG-CD2	-7.97	108.84	120.80
4	T	260	TYR	CB-CG-CD2	-7.97	108.84	120.80
5	M	363	ASP	CA-CB-CG	7.97	120.57	112.60
5	I	363	ASP	CA-CB-CG	7.95	120.55	112.60
5	Q	363	ASP	CA-CB-CG	7.95	120.55	112.60
5	D	363	ASP	CA-CB-CG	7.95	120.55	112.60
5	S	363	ASP	CA-CB-CG	7.95	120.55	112.60
5	O	363	ASP	CA-CB-CG	7.95	120.55	112.60
4	V	40	GLN	OE1-CD-NE2	-7.95	114.65	122.60
5	G	363	ASP	CA-CB-CG	7.94	120.54	112.60
5	P	286	ASP	CA-CB-CG	7.94	120.54	112.60
4	V	43	LEU	N-CA-C	7.93	121.45	111.69
5	H	363	ASP	CA-CB-CG	7.93	120.53	112.60
4	A	196	ASN	OD1-CG-ND2	-7.93	114.67	122.60
5	N	128	ASN	CA-CB-CG	7.93	120.53	112.60
5	E	128	ASN	CA-CB-CG	7.92	120.53	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	363	ASP	CA-CB-CG	7.92	120.52	112.60
4	V	196	ASN	OD1-CG-ND2	-7.92	114.68	122.60
5	D	128	ASN	CA-CB-CG	7.92	120.52	112.60
5	S	128	ASN	CA-CB-CG	7.92	120.52	112.60
5	J	363	ASP	CA-CB-CG	7.91	120.51	112.60
5	E	363	ASP	CA-CB-CG	7.91	120.51	112.60
5	F	363	ASP	CA-CB-CG	7.91	120.51	112.60
5	K	363	ASP	CA-CB-CG	7.91	120.51	112.60
5	K	128	ASN	CA-CB-CG	7.90	120.50	112.60
5	F	286	ASP	CA-CB-CG	7.89	120.49	112.60
5	G	286	ASP	CA-CB-CG	7.88	120.48	112.60
5	J	286	ASP	CA-CB-CG	7.88	120.48	112.60
4	A	40	GLN	OE1-CD-NE2	-7.88	114.72	122.60
5	H	286	ASP	CA-CB-CG	7.88	120.48	112.60
5	R	128	ASN	CA-CB-CG	7.88	120.48	112.60
5	H	128	ASN	CA-CB-CG	7.88	120.48	112.60
5	P	128	ASN	CA-CB-CG	7.88	120.48	112.60
5	K	286	ASP	CA-CB-CG	7.87	120.47	112.60
5	M	128	ASN	CA-CB-CG	7.87	120.47	112.60
5	F	128	ASN	CA-CB-CG	7.86	120.46	112.60
5	G	128	ASN	CA-CB-CG	7.86	120.46	112.60
5	I	128	ASN	CA-CB-CG	7.86	120.45	112.60
5	O	286	ASP	CA-CB-CG	7.86	120.45	112.60
5	L	286	ASP	CA-CB-CG	7.85	120.45	112.60
5	N	286	ASP	CA-CB-CG	7.85	120.45	112.60
5	O	128	ASN	CA-CB-CG	7.84	120.44	112.60
5	R	286	ASP	CA-CB-CG	7.84	120.44	112.60
5	E	286	ASP	CA-CB-CG	7.84	120.44	112.60
5	D	286	ASP	CA-CB-CG	7.83	120.43	112.60
5	L	128	ASN	CA-CB-CG	7.83	120.43	112.60
5	Q	286	ASP	CA-CB-CG	7.83	120.43	112.60
5	J	128	ASN	CA-CB-CG	7.83	120.43	112.60
5	I	286	ASP	CA-CB-CG	7.81	120.41	112.60
5	Q	128	ASN	CA-CB-CG	7.80	120.40	112.60
4	A	43	LEU	N-CA-C	7.80	121.28	111.69
4	U	61	GLN	OE1-CD-NE2	-7.78	114.82	122.60
5	Q	25	ASP	CA-CB-CG	7.73	120.33	112.60
4	A	203	GLN	OE1-CD-NE2	-7.72	114.88	122.60
4	W	253	LEU	CD1-CG-CD2	7.71	127.77	110.80
4	B	253	LEU	CD1-CG-CD2	7.70	127.73	110.80
4	T	253	LEU	CD1-CG-CD2	7.69	127.73	110.80
4	U	253	LEU	CD1-CG-CD2	7.69	127.73	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	25	ASP	CA-CB-CG	7.68	120.28	112.60
5	J	25	ASP	CA-CB-CG	7.68	120.28	112.60
5	H	25	ASP	CA-CB-CG	7.67	120.27	112.60
5	K	360	GLN	N-CA-C	-7.67	102.61	110.97
5	S	223	PHE	CA-CB-CG	7.67	121.47	113.80
5	D	25	ASP	CA-CB-CG	7.66	120.26	112.60
5	E	25	ASP	CA-CB-CG	7.66	120.26	112.60
5	H	223	PHE	CA-CB-CG	7.66	121.46	113.80
5	L	25	ASP	CA-CB-CG	7.66	120.26	112.60
5	M	223	PHE	CA-CB-CG	7.66	121.46	113.80
5	J	360	GLN	N-CA-C	-7.65	102.63	110.97
2	7	197	LEU	N-CA-C	-7.65	105.11	114.75
5	H	360	GLN	N-CA-C	-7.65	102.63	110.97
4	B	61	GLN	OE1-CD-NE2	-7.65	114.95	122.60
5	R	25	ASP	CA-CB-CG	7.65	120.25	112.60
4	V	61	GLN	OE1-CD-NE2	-7.65	114.95	122.60
5	Q	215	LYS	N-CA-C	7.64	119.40	111.14
5	S	25	ASP	CA-CB-CG	7.64	120.24	112.60
4	V	156	GLU	N-CA-C	-7.64	103.03	111.36
5	E	360	GLN	N-CA-C	-7.64	102.64	110.97
4	V	203	GLN	OE1-CD-NE2	-7.64	114.96	122.60
2	1	197	LEU	N-CA-C	-7.63	105.13	114.75
5	F	360	GLN	N-CA-C	-7.63	102.65	110.97
5	O	360	GLN	N-CA-C	-7.63	102.65	110.97
5	Q	223	PHE	CA-CB-CG	7.63	121.43	113.80
5	M	25	ASP	CA-CB-CG	7.63	120.23	112.60
4	A	156	GLU	N-CA-C	-7.63	103.05	111.36
2	Y	197	LEU	N-CA-C	-7.62	105.15	114.75
2	4	197	LEU	N-CA-C	-7.62	105.15	114.75
5	I	252	ASN	OD1-CG-ND2	-7.62	114.98	122.60
5	N	223	PHE	CA-CB-CG	7.62	121.42	113.80
5	N	252	ASN	OD1-CG-ND2	-7.62	114.98	122.60
5	G	360	GLN	N-CA-C	-7.61	102.67	110.97
5	E	252	ASN	OD1-CG-ND2	-7.61	114.99	122.60
5	K	25	ASP	CA-CB-CG	7.61	120.21	112.60
5	I	25	ASP	CA-CB-CG	7.60	120.20	112.60
5	H	252	ASN	OD1-CG-ND2	-7.60	115.00	122.60
5	P	223	PHE	CA-CB-CG	7.59	121.39	113.80
5	P	360	GLN	N-CA-C	-7.59	102.69	110.97
5	F	25	ASP	CA-CB-CG	7.59	120.19	112.60
5	N	360	GLN	N-CA-C	-7.59	102.70	110.97
5	P	25	ASP	CA-CB-CG	7.59	120.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	152	ASP	CA-CB-CG	7.59	120.19	112.60
5	O	252	ASN	OD1-CG-ND2	-7.59	115.01	122.60
5	D	360	GLN	N-CA-C	-7.58	102.71	110.97
5	N	25	ASP	CA-CB-CG	7.58	120.18	112.60
5	S	252	ASN	OD1-CG-ND2	-7.58	115.02	122.60
4	B	203	GLN	OE1-CD-NE2	-7.58	115.02	122.60
5	L	360	GLN	N-CA-C	-7.58	102.71	110.97
5	D	223	PHE	CA-CB-CG	7.57	121.37	113.80
5	O	25	ASP	CA-CB-CG	7.57	120.17	112.60
4	A	61	GLN	OE1-CD-NE2	-7.57	115.03	122.60
5	I	360	GLN	N-CA-C	-7.57	102.72	110.97
4	U	96	GLN	OE1-CD-NE2	-7.57	115.03	122.60
5	I	223	PHE	CA-CB-CG	7.56	121.36	113.80
5	M	252	ASN	OD1-CG-ND2	-7.56	115.04	122.60
5	R	223	PHE	CA-CB-CG	7.56	121.36	113.80
5	L	173	HIS	CA-CB-CG	-7.56	106.24	113.80
5	D	215	LYS	N-CA-C	7.55	119.30	111.14
5	N	215	LYS	N-CA-C	7.55	119.30	111.14
5	R	173	HIS	CA-CB-CG	-7.55	106.25	113.80
5	O	215	LYS	N-CA-C	7.55	119.29	111.14
5	F	223	PHE	CA-CB-CG	7.54	121.34	113.80
5	K	223	PHE	CA-CB-CG	7.54	121.34	113.80
5	P	252	ASN	OD1-CG-ND2	-7.54	115.06	122.60
5	J	223	PHE	CA-CB-CG	7.54	121.34	113.80
4	A	152	ASP	CA-CB-CG	7.54	120.14	112.60
5	J	252	ASN	OD1-CG-ND2	-7.54	115.06	122.60
5	Q	360	GLN	N-CA-C	-7.54	102.75	110.97
4	U	203	GLN	OE1-CD-NE2	-7.54	115.06	122.60
5	L	223	PHE	CA-CB-CG	7.53	121.33	113.80
5	J	215	LYS	N-CA-C	7.53	119.27	111.14
5	E	62	ARG	N-CA-C	7.53	120.36	111.71
5	J	173	HIS	CA-CB-CG	-7.52	106.28	113.80
5	G	223	PHE	CA-CB-CG	7.52	121.32	113.80
5	R	360	GLN	N-CA-C	-7.52	102.78	110.97
4	V	86	GLN	OE1-CD-NE2	-7.52	115.08	122.60
4	B	96	GLN	OE1-CD-NE2	-7.51	115.09	122.60
5	E	173	HIS	CA-CB-CG	-7.51	106.29	113.80
5	E	223	PHE	CA-CB-CG	7.51	121.31	113.80
5	S	215	LYS	N-CA-C	7.51	119.25	111.14
5	L	252	ASN	OD1-CG-ND2	-7.51	115.09	122.60
5	G	215	LYS	N-CA-C	7.50	119.24	111.14
5	I	215	LYS	N-CA-C	7.50	119.24	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	62	ARG	N-CA-C	7.50	120.33	111.71
5	K	62	ARG	N-CA-C	7.50	120.33	111.71
5	M	173	HIS	CA-CB-CG	-7.50	106.30	113.80
5	M	360	GLN	N-CA-C	-7.50	102.80	110.97
5	O	62	ARG	N-CA-C	7.50	120.33	111.71
5	F	252	ASN	OD1-CG-ND2	-7.50	115.11	122.60
5	H	62	ARG	N-CA-C	7.50	120.33	111.71
5	S	173	HIS	CA-CB-CG	-7.49	106.31	113.80
5	M	62	ARG	N-CA-C	7.49	120.33	111.71
5	J	62	ARG	N-CA-C	7.49	120.32	111.71
5	O	223	PHE	CA-CB-CG	7.49	121.29	113.80
5	Q	252	ASN	OD1-CG-ND2	-7.49	115.11	122.60
5	R	215	LYS	N-CA-C	7.49	119.23	111.14
5	E	215	LYS	N-CA-C	7.49	119.23	111.14
5	K	173	HIS	CA-CB-CG	-7.49	106.31	113.80
5	L	62	ARG	N-CA-C	7.49	120.32	111.71
4	V	104	GLN	OE1-CD-NE2	-7.49	115.11	122.60
5	D	62	ARG	N-CA-C	7.48	120.32	111.71
5	I	62	ARG	N-CA-C	7.48	120.31	111.71
5	F	173	HIS	CA-CB-CG	-7.48	106.32	113.80
5	N	62	ARG	N-CA-C	7.48	120.31	111.71
5	S	62	ARG	N-CA-C	7.48	120.31	111.71
5	G	62	ARG	N-CA-C	7.48	120.31	111.71
5	G	252	ASN	OD1-CG-ND2	-7.48	115.12	122.60
5	K	252	ASN	OD1-CG-ND2	-7.47	115.12	122.60
5	P	62	ARG	N-CA-C	7.47	120.31	111.71
5	I	173	HIS	CA-CB-CG	-7.47	106.33	113.80
5	S	360	GLN	N-CA-C	-7.47	102.83	110.97
5	P	215	LYS	N-CA-C	7.47	119.20	111.14
5	G	173	HIS	CA-CB-CG	-7.47	106.33	113.80
5	R	62	ARG	N-CA-C	7.47	120.30	111.71
5	K	215	LYS	N-CA-C	7.46	119.20	111.14
5	R	252	ASN	OD1-CG-ND2	-7.46	115.14	122.60
5	H	173	HIS	CA-CB-CG	-7.46	106.34	113.80
4	A	104	GLN	OE1-CD-NE2	-7.45	115.15	122.60
4	U	86	GLN	OE1-CD-NE2	-7.45	115.15	122.60
5	N	173	HIS	CA-CB-CG	-7.45	106.36	113.80
5	O	173	HIS	CA-CB-CG	-7.44	106.36	113.80
5	M	215	LYS	N-CA-C	7.44	119.17	111.14
4	A	96	GLN	OE1-CD-NE2	-7.44	115.16	122.60
5	F	215	LYS	N-CA-C	7.44	119.17	111.14
4	B	86	GLN	OE1-CD-NE2	-7.44	115.16	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	173	HIS	CA-CB-CG	-7.44	106.36	113.80
5	Q	62	ARG	N-CA-C	7.43	120.26	111.71
5	H	215	LYS	N-CA-C	7.43	119.16	111.14
4	V	96	GLN	OE1-CD-NE2	-7.42	115.18	122.60
5	L	215	LYS	N-CA-C	7.42	119.15	111.14
4	A	167	SER	N-CA-C	7.40	119.42	111.36
4	V	2	GLN	OE1-CD-NE2	-7.39	115.20	122.60
4	A	86	GLN	OE1-CD-NE2	-7.38	115.22	122.60
4	C	273	ASP	CA-CB-CG	7.38	119.97	112.60
5	Q	173	HIS	CA-CB-CG	-7.37	106.43	113.80
4	V	167	SER	N-CA-C	7.37	119.39	111.36
5	H	34	ILE	CA-CB-CG2	-7.37	97.97	110.50
5	P	173	HIS	CA-CB-CG	-7.37	106.43	113.80
5	D	252	ASN	OD1-CG-ND2	-7.36	115.24	122.60
4	B	167	SER	N-CA-C	7.35	119.08	111.14
4	U	104	GLN	OE1-CD-NE2	-7.35	115.25	122.60
4	V	273	ASP	CA-CB-CG	7.35	119.95	112.60
4	U	167	SER	N-CA-C	7.34	119.06	111.14
5	I	34	ILE	CA-CB-CG2	-7.33	98.04	110.50
4	B	104	GLN	OE1-CD-NE2	-7.33	115.28	122.60
5	P	34	ILE	CA-CB-CG2	-7.33	98.05	110.50
1	9	107	ASN	N-CA-C	-7.32	95.20	110.80
1	0	107	ASN	N-CA-C	-7.32	95.21	110.80
1	3	107	ASN	N-CA-C	-7.32	95.21	110.80
1	6	107	ASN	N-CA-C	-7.32	95.20	110.80
5	J	34	ILE	CA-CB-CG2	-7.32	98.06	110.50
4	A	273	ASP	CA-CB-CG	7.31	119.91	112.60
4	X	273	ASP	CA-CB-CG	7.31	119.91	112.60
5	L	34	ILE	CA-CB-CG2	-7.30	98.08	110.50
5	N	34	ILE	CA-CB-CG2	-7.30	98.08	110.50
4	B	2	GLN	OE1-CD-NE2	-7.30	115.30	122.60
5	R	34	ILE	CA-CB-CG2	-7.30	98.10	110.50
5	Q	34	ILE	CA-CB-CG2	-7.29	98.10	110.50
5	D	34	ILE	CA-CB-CG2	-7.29	98.11	110.50
5	E	34	ILE	CA-CB-CG2	-7.29	98.11	110.50
5	F	34	ILE	CA-CB-CG2	-7.29	98.11	110.50
5	G	34	ILE	CA-CB-CG2	-7.28	98.12	110.50
4	U	2	GLN	OE1-CD-NE2	-7.28	115.32	122.60
5	S	34	ILE	CA-CB-CG2	-7.28	98.13	110.50
5	M	34	ILE	CA-CB-CG2	-7.28	98.13	110.50
5	K	34	ILE	CA-CB-CG2	-7.27	98.14	110.50
5	G	159	VAL	CB-CA-C	-7.26	99.08	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	159	VAL	CB-CA-C	-7.25	99.09	110.69
5	D	159	VAL	CB-CA-C	-7.25	99.09	110.69
5	F	159	VAL	CB-CA-C	-7.25	99.10	110.69
5	H	159	VAL	CB-CA-C	-7.24	99.10	110.69
5	O	34	ILE	CA-CB-CG2	-7.24	98.19	110.50
5	J	159	VAL	CB-CA-C	-7.24	99.11	110.69
5	O	323	SER	N-CA-C	7.24	121.75	112.34
5	N	159	VAL	CB-CA-C	-7.23	99.13	110.69
5	M	159	VAL	CB-CA-C	-7.22	99.13	110.69
5	K	159	VAL	CB-CA-C	-7.22	99.13	110.69
5	R	159	VAL	CB-CA-C	-7.22	99.13	110.69
5	Q	159	VAL	CB-CA-C	-7.22	99.14	110.69
5	S	159	VAL	CB-CA-C	-7.22	99.14	110.69
5	L	159	VAL	CB-CA-C	-7.21	99.15	110.69
5	O	159	VAL	CB-CA-C	-7.20	99.17	110.69
5	I	159	VAL	CB-CA-C	-7.20	99.17	110.69
4	U	209	GLN	OE1-CD-NE2	-7.19	115.41	122.60
5	G	323	SER	N-CA-C	7.19	121.68	112.34
4	A	209	GLN	OE1-CD-NE2	-7.18	115.42	122.60
4	B	209	GLN	OE1-CD-NE2	-7.18	115.42	122.60
5	R	323	SER	N-CA-C	7.18	121.68	112.34
4	V	209	GLN	OE1-CD-NE2	-7.18	115.42	122.60
4	X	253	LEU	CD1-CG-CD2	7.18	126.61	110.80
5	M	259	GLU	CB-CG-CD	7.18	124.80	112.60
5	S	259	GLU	CB-CG-CD	7.18	124.81	112.60
4	C	253	LEU	CD1-CG-CD2	7.18	126.59	110.80
5	G	259	GLU	CB-CG-CD	7.17	124.80	112.60
5	E	159	VAL	CB-CA-C	-7.17	99.21	110.69
5	R	259	GLU	CB-CG-CD	7.17	124.79	112.60
4	V	253	LEU	CD1-CG-CD2	7.17	126.58	110.80
5	N	323	SER	N-CA-C	7.17	121.66	112.34
5	K	259	GLU	CB-CG-CD	7.16	124.78	112.60
5	L	259	GLU	CB-CG-CD	7.16	124.78	112.60
5	O	259	GLU	CB-CG-CD	7.16	124.78	112.60
5	H	259	GLU	CB-CG-CD	7.16	124.76	112.60
5	E	259	GLU	CB-CG-CD	7.15	124.76	112.60
5	K	323	SER	N-CA-C	7.15	121.64	112.34
5	Q	259	GLU	CB-CG-CD	7.15	124.75	112.60
4	V	128	GLN	OE1-CD-NE2	-7.15	115.45	122.60
5	P	259	GLU	CB-CG-CD	7.14	124.74	112.60
5	O	69	TYR	CA-C-N	7.14	126.84	119.56
5	O	69	TYR	C-N-CA	7.14	126.84	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	323	SER	N-CA-C	7.14	121.62	112.34
5	F	259	GLU	CB-CG-CD	7.14	124.74	112.60
5	J	323	SER	N-CA-C	7.14	121.62	112.34
4	U	128	GLN	OE1-CD-NE2	-7.14	115.46	122.60
5	N	259	GLU	CB-CG-CD	7.14	124.73	112.60
4	A	253	LEU	CD1-CG-CD2	7.14	126.50	110.80
5	D	259	GLU	CB-CG-CD	7.13	124.73	112.60
5	D	323	SER	N-CA-C	7.13	121.61	112.34
5	L	323	SER	N-CA-C	7.13	121.62	112.34
5	S	323	SER	N-CA-C	7.13	121.62	112.34
5	I	259	GLU	CB-CG-CD	7.13	124.72	112.60
5	P	323	SER	N-CA-C	7.13	121.61	112.34
5	H	323	SER	N-CA-C	7.13	121.61	112.34
5	M	323	SER	N-CA-C	7.13	121.61	112.34
5	G	69	TYR	CA-C-N	7.12	126.82	119.56
5	G	69	TYR	C-N-CA	7.12	126.82	119.56
5	I	323	SER	N-CA-C	7.12	121.59	112.34
4	U	169	LEU	CB-CA-C	-7.11	99.93	110.95
5	J	259	GLU	CB-CG-CD	7.11	124.69	112.60
4	B	169	LEU	CB-CA-C	-7.11	99.93	110.95
4	B	168	ASP	CA-CB-CG	7.11	119.71	112.60
5	N	69	TYR	CA-C-N	7.10	126.80	119.56
5	N	69	TYR	C-N-CA	7.10	126.80	119.56
5	H	69	TYR	CA-C-N	7.09	126.80	119.56
5	H	69	TYR	C-N-CA	7.09	126.80	119.56
4	A	128	GLN	OE1-CD-NE2	-7.09	115.51	122.60
4	T	276	SER	N-CA-C	7.09	120.41	111.69
5	E	323	SER	N-CA-C	7.09	121.56	112.34
5	E	69	TYR	CA-C-N	7.09	126.79	119.56
5	E	69	TYR	C-N-CA	7.09	126.79	119.56
5	I	69	TYR	CA-C-N	7.09	126.79	119.56
5	I	69	TYR	C-N-CA	7.09	126.79	119.56
5	D	69	TYR	CA-C-N	7.08	126.78	119.56
5	D	69	TYR	C-N-CA	7.08	126.78	119.56
4	B	276	SER	N-CA-C	7.08	120.40	111.69
4	U	276	SER	N-CA-C	7.08	120.40	111.69
4	U	168	ASP	CA-CB-CG	7.07	119.67	112.60
4	B	128	GLN	OE1-CD-NE2	-7.07	115.53	122.60
5	F	323	SER	N-CA-C	7.07	121.53	112.34
4	W	276	SER	N-CA-C	7.06	120.38	111.69
4	C	274	MET	N-CA-CB	7.05	121.20	110.28
5	J	73	HIS	CA-CB-CG	-7.04	106.76	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	69	TYR	CA-C-N	7.04	126.74	119.56
5	F	69	TYR	C-N-CA	7.04	126.74	119.56
5	P	69	TYR	CA-C-N	7.04	126.74	119.56
5	P	69	TYR	C-N-CA	7.04	126.74	119.56
4	A	274	MET	N-CA-CB	7.04	121.18	110.28
5	G	73	HIS	CA-CB-CG	-7.03	106.77	113.80
4	X	274	MET	N-CA-CB	7.03	121.18	110.28
5	S	69	TYR	CA-C-N	7.03	126.73	119.56
5	S	69	TYR	C-N-CA	7.03	126.73	119.56
4	V	169	LEU	CB-CA-C	-7.03	100.06	110.95
5	M	69	TYR	CA-C-N	7.02	126.72	119.56
5	M	69	TYR	C-N-CA	7.02	126.72	119.56
5	P	73	HIS	CA-CB-CG	-7.02	106.78	113.80
4	V	274	MET	N-CA-CB	7.02	121.16	110.28
5	N	73	HIS	CA-CB-CG	-7.01	106.79	113.80
4	A	169	LEU	CB-CA-C	-7.01	100.08	110.95
5	H	73	HIS	CA-CB-CG	-7.00	106.80	113.80
5	K	69	TYR	CA-C-N	7.00	126.70	119.56
5	K	69	TYR	C-N-CA	7.00	126.70	119.56
5	I	73	HIS	CA-CB-CG	-6.99	106.81	113.80
5	R	69	TYR	CA-C-N	6.99	126.69	119.56
5	R	69	TYR	C-N-CA	6.99	126.69	119.56
5	D	73	HIS	CA-CB-CG	-6.99	106.81	113.80
5	Q	69	TYR	CA-C-N	6.99	126.69	119.56
5	Q	69	TYR	C-N-CA	6.99	126.69	119.56
5	F	73	HIS	CA-CB-CG	-6.98	106.82	113.80
5	S	287	ILE	CB-CA-C	-6.98	102.71	112.14
5	L	69	TYR	CA-C-N	6.98	126.68	119.56
5	L	69	TYR	C-N-CA	6.98	126.68	119.56
5	O	73	HIS	CA-CB-CG	-6.97	106.83	113.80
5	J	287	ILE	CB-CA-C	-6.97	102.73	112.14
5	S	73	HIS	CA-CB-CG	-6.97	106.83	113.80
5	D	287	ILE	CB-CA-C	-6.97	102.73	112.14
5	M	73	HIS	CA-CB-CG	-6.97	106.83	113.80
5	Q	73	HIS	CA-CB-CG	-6.96	106.84	113.80
5	Q	287	ILE	CB-CA-C	-6.96	102.75	112.14
5	H	287	ILE	CB-CA-C	-6.95	102.76	112.14
5	M	287	ILE	CB-CA-C	-6.95	102.76	112.14
5	E	287	ILE	N-CA-C	6.94	117.70	110.62
5	R	287	ILE	N-CA-C	6.94	117.70	110.62
5	I	287	ILE	CB-CA-C	-6.94	102.77	112.14
5	K	73	HIS	CA-CB-CG	-6.94	106.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	191	LYS	CA-C-O	-6.94	113.55	120.70
5	O	287	ILE	CB-CA-C	-6.93	102.78	112.14
5	J	69	TYR	CA-C-N	6.93	126.63	119.56
5	J	69	TYR	C-N-CA	6.93	126.63	119.56
5	N	287	ILE	CB-CA-C	-6.93	102.79	112.14
4	B	31	GLN	OE1-CD-NE2	-6.92	115.68	122.60
5	F	287	ILE	CB-CA-C	-6.92	102.80	112.14
5	E	73	HIS	CA-CB-CG	-6.92	106.88	113.80
5	R	73	HIS	CA-CB-CG	-6.92	106.88	113.80
5	L	73	HIS	CA-CB-CG	-6.91	106.89	113.80
5	L	287	ILE	N-CA-C	6.91	117.67	110.62
5	R	191	LYS	CA-C-O	-6.91	113.58	120.70
4	V	269	HIS	CA-CB-CG	-6.91	106.89	113.80
5	K	287	ILE	CB-CA-C	-6.91	102.82	112.14
4	U	31	GLN	OE1-CD-NE2	-6.91	115.69	122.60
4	V	140	GLN	OE1-CD-NE2	-6.90	115.70	122.60
5	E	287	ILE	CB-CA-C	-6.90	102.82	112.14
5	L	287	ILE	CB-CA-C	-6.90	102.82	112.14
5	P	287	ILE	CB-CA-C	-6.90	102.82	112.14
4	C	252	GLU	CA-C-O	6.90	127.93	120.20
5	L	191	LYS	CA-C-O	-6.90	113.59	120.70
4	V	252	GLU	CA-C-O	6.90	127.93	120.20
4	X	269	HIS	CA-CB-CG	-6.90	106.90	113.80
5	G	287	ILE	CB-CA-C	-6.89	102.84	112.14
5	I	191	LYS	CA-C-O	-6.89	113.61	120.70
5	F	287	ILE	N-CA-C	6.88	117.64	110.62
5	K	191	LYS	CA-C-O	-6.88	113.61	120.70
5	R	287	ILE	CB-CA-C	-6.88	102.84	112.14
5	O	191	LYS	CA-C-O	-6.88	113.61	120.70
5	Q	287	ILE	N-CA-C	6.88	117.64	110.62
4	A	269	HIS	CA-CB-CG	-6.88	106.92	113.80
4	A	140	GLN	OE1-CD-NE2	-6.87	115.73	122.60
5	D	287	ILE	N-CA-C	6.87	117.63	110.62
5	E	191	LYS	CA-C-O	-6.87	113.63	120.70
4	C	269	HIS	CA-CB-CG	-6.87	106.93	113.80
5	F	191	LYS	CA-C-O	-6.86	113.63	120.70
5	O	287	ILE	N-CA-C	6.86	117.62	110.62
4	A	252	GLU	CA-C-O	6.86	127.88	120.20
5	N	191	LYS	CA-C-O	-6.86	113.64	120.70
4	X	252	GLU	CA-C-O	6.86	127.88	120.20
5	H	191	LYS	CA-C-O	-6.86	113.64	120.70
5	P	287	ILE	N-CA-C	6.85	117.60	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	287	ILE	N-CA-C	6.83	117.59	110.62
4	A	31	GLN	OE1-CD-NE2	-6.83	115.77	122.60
5	J	191	LYS	CA-C-O	-6.83	113.66	120.70
5	M	191	LYS	CA-C-O	-6.83	113.67	120.70
5	G	191	LYS	CA-C-O	-6.83	113.67	120.70
5	R	259	GLU	N-CA-C	-6.83	104.05	112.38
5	S	191	LYS	CA-C-O	-6.82	113.67	120.70
5	J	287	ILE	N-CA-C	6.82	117.57	110.62
5	Q	191	LYS	CA-C-O	-6.82	113.68	120.70
5	S	287	ILE	N-CA-C	6.81	117.57	110.62
5	M	287	ILE	N-CA-C	6.81	117.56	110.62
4	B	140	GLN	OE1-CD-NE2	-6.80	115.80	122.60
5	G	287	ILE	N-CA-C	6.80	117.56	110.62
5	L	259	GLU	N-CA-C	-6.80	104.08	112.38
4	B	269	HIS	CA-CB-CG	-6.80	107.00	113.80
4	V	31	GLN	OE1-CD-NE2	-6.80	115.80	122.60
4	U	140	GLN	OE1-CD-NE2	-6.79	115.81	122.60
5	J	214	GLU	CB-CG-CD	6.79	124.14	112.60
5	S	259	GLU	N-CA-C	-6.79	104.10	112.38
4	V	231	ARG	NE-CZ-NH1	6.79	128.29	121.50
5	M	259	GLU	N-CA-C	-6.78	104.10	112.38
5	G	214	GLU	CB-CG-CD	6.78	124.12	112.60
4	W	269	HIS	CA-CB-CG	-6.77	107.03	113.80
5	D	191	LYS	CA-C-O	-6.77	113.72	120.70
5	I	287	ILE	N-CA-C	6.77	117.53	110.62
5	K	259	GLU	N-CA-C	-6.77	104.12	112.38
4	A	152	ASP	N-CA-C	6.77	125.21	110.80
5	K	287	ILE	N-CA-C	6.76	117.52	110.62
4	U	43	LEU	N-CA-C	6.76	121.78	112.04
4	U	146	HIS	CB-CG-CD2	-6.75	122.42	131.20
5	N	287	ILE	N-CA-C	6.75	117.50	110.62
4	A	231	ARG	NE-CZ-NH1	6.75	128.25	121.50
4	B	43	LEU	N-CA-C	6.75	121.76	112.04
5	N	214	GLU	CB-CG-CD	6.74	124.06	112.60
5	N	259	GLU	N-CA-C	-6.74	104.15	112.38
5	H	214	GLU	CB-CG-CD	6.74	124.06	112.60
4	V	152	ASP	N-CA-C	6.74	125.16	110.80
5	E	214	GLU	CB-CG-CD	6.74	124.06	112.60
5	I	214	GLU	CB-CG-CD	6.74	124.06	112.60
5	O	214	GLU	CB-CG-CD	6.74	124.06	112.60
5	P	214	GLU	CB-CG-CD	6.73	124.05	112.60
4	U	269	HIS	CA-CB-CG	-6.73	107.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	259	GLU	N-CA-C	-6.73	104.17	112.38
5	E	259	GLU	N-CA-C	-6.73	104.17	112.38
5	M	214	GLU	CB-CG-CD	6.73	124.04	112.60
5	P	259	GLU	N-CA-C	-6.72	104.18	112.38
5	S	214	GLU	CB-CG-CD	6.72	124.03	112.60
4	B	146	HIS	CB-CG-CD2	-6.72	122.47	131.20
5	G	259	GLU	N-CA-C	-6.72	104.18	112.38
5	F	214	GLU	CB-CG-CD	6.72	124.02	112.60
4	T	269	HIS	CA-CB-CG	-6.72	107.08	113.80
4	A	154	LYS	CA-CB-CG	6.71	127.52	114.10
5	Q	259	GLU	N-CA-C	-6.71	104.19	112.38
5	Q	214	GLU	CB-CG-CD	6.71	124.00	112.60
5	R	214	GLU	CB-CG-CD	6.70	124.00	112.60
5	L	214	GLU	CB-CG-CD	6.70	123.98	112.60
4	V	154	LYS	CA-CB-CG	6.69	127.48	114.10
5	F	259	GLU	N-CA-C	-6.67	104.24	112.38
5	D	214	GLU	CB-CG-CD	6.67	123.94	112.60
5	K	214	GLU	CB-CG-CD	6.67	123.94	112.60
5	J	259	GLU	N-CA-C	-6.66	104.26	112.38
5	O	259	GLU	N-CA-C	-6.66	104.26	112.38
5	D	259	GLU	N-CA-C	-6.65	104.27	112.38
5	H	259	GLU	N-CA-C	-6.65	104.27	112.38
4	A	146	HIS	CB-CG-CD2	-6.62	122.59	131.20
4	V	146	HIS	CB-CG-CD2	-6.61	122.60	131.20
4	U	274	MET	N-CA-CB	6.59	120.50	110.28
5	E	371	HIS	CA-CB-CG	-6.59	107.21	113.80
5	Q	371	HIS	CA-CB-CG	-6.58	107.22	113.80
5	H	371	HIS	CA-CB-CG	-6.57	107.23	113.80
4	W	274	MET	N-CA-CB	6.57	120.46	110.28
5	S	286	ASP	CA-C-N	6.56	129.44	120.46
5	S	286	ASP	C-N-CA	6.56	129.44	120.46
5	I	371	HIS	CA-CB-CG	-6.56	107.24	113.80
4	B	158	VAL	N-CA-C	6.55	117.24	110.36
4	U	158	VAL	N-CA-C	6.55	117.24	110.36
4	V	168	ASP	CA-CB-CG	6.55	119.16	112.60
5	P	371	HIS	CA-CB-CG	-6.55	107.25	113.80
4	A	168	ASP	CA-CB-CG	6.54	119.14	112.60
4	B	274	MET	N-CA-CB	6.54	120.42	110.28
4	T	274	MET	N-CA-CB	6.54	120.41	110.28
5	F	286	ASP	CA-C-N	6.53	129.41	120.46
5	F	286	ASP	C-N-CA	6.53	129.41	120.46
5	M	286	ASP	CA-C-N	6.53	129.41	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	286	ASP	C-N-CA	6.53	129.41	120.46
5	K	286	ASP	CA-C-N	6.53	129.41	120.46
5	K	286	ASP	C-N-CA	6.53	129.41	120.46
5	D	80	ASP	CA-CB-CG	6.50	119.10	112.60
5	Q	286	ASP	CA-C-N	6.50	129.37	120.46
5	Q	286	ASP	C-N-CA	6.50	129.37	120.46
5	N	286	ASP	CA-C-N	6.50	129.36	120.46
5	N	286	ASP	C-N-CA	6.50	129.36	120.46
5	S	371	HIS	CA-CB-CG	-6.50	107.30	113.80
4	U	22	LYS	CB-CG-CD	-6.50	96.36	111.30
4	B	22	LYS	CB-CG-CD	-6.49	96.37	111.30
5	G	101	HIS	CB-CG-CD2	-6.49	122.76	131.20
5	N	80	ASP	CA-CB-CG	6.49	119.09	112.60
5	F	371	HIS	CA-CB-CG	-6.49	107.31	113.80
5	G	371	HIS	CA-CB-CG	-6.49	107.31	113.80
5	J	101	HIS	CB-CG-CD2	-6.48	122.77	131.20
5	M	371	HIS	CA-CB-CG	-6.48	107.32	113.80
5	D	101	HIS	CB-CG-CD2	-6.48	122.78	131.20
5	D	286	ASP	CA-C-N	6.48	129.33	120.46
5	D	286	ASP	C-N-CA	6.48	129.33	120.46
5	I	286	ASP	CA-C-N	6.48	129.33	120.46
5	I	286	ASP	C-N-CA	6.48	129.33	120.46
5	G	80	ASP	CA-CB-CG	6.47	119.07	112.60
5	K	371	HIS	CA-CB-CG	-6.47	107.33	113.80
5	N	371	HIS	CA-CB-CG	-6.47	107.33	113.80
5	R	371	HIS	CA-CB-CG	-6.47	107.33	113.80
5	G	286	ASP	CA-C-N	6.46	129.31	120.46
5	G	286	ASP	C-N-CA	6.46	129.31	120.46
5	J	286	ASP	CA-C-N	6.46	129.31	120.46
5	J	286	ASP	C-N-CA	6.46	129.31	120.46
5	O	371	HIS	CA-CB-CG	-6.45	107.35	113.80
5	H	286	ASP	CA-C-N	6.45	129.30	120.46
5	H	286	ASP	C-N-CA	6.45	129.30	120.46
5	L	371	HIS	CA-CB-CG	-6.45	107.35	113.80
5	O	286	ASP	CA-C-N	6.45	129.30	120.46
5	O	286	ASP	C-N-CA	6.45	129.30	120.46
5	I	101	HIS	CB-CG-CD2	-6.45	122.82	131.20
5	Q	101	HIS	CB-CG-CD2	-6.44	122.83	131.20
5	P	286	ASP	CA-C-N	6.44	129.28	120.46
5	P	286	ASP	C-N-CA	6.44	129.28	120.46
5	H	101	HIS	CB-CG-CD2	-6.43	122.85	131.20
5	N	101	HIS	CB-CG-CD2	-6.42	122.85	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	80	ASP	CA-CB-CG	6.42	119.02	112.60
5	K	101	HIS	CB-CG-CD2	-6.41	122.86	131.20
4	T	252	GLU	CA-C-O	6.41	127.38	120.20
5	F	259	GLU	CA-CB-CG	6.41	126.92	114.10
5	P	101	HIS	CB-CG-CD2	-6.41	122.87	131.20
5	R	259	GLU	CA-CB-CG	6.41	126.92	114.10
5	E	282	ILE	CA-C-O	-6.40	113.94	121.05
5	E	286	ASP	CA-C-N	6.40	129.23	120.46
5	E	286	ASP	C-N-CA	6.40	129.23	120.46
5	L	259	GLU	CA-CB-CG	6.40	126.90	114.10
5	D	371	HIS	CA-CB-CG	-6.40	107.40	113.80
5	F	80	ASP	CA-CB-CG	6.40	119.00	112.60
5	J	47	MET	CA-CB-CG	-6.39	101.31	114.10
5	K	259	GLU	CA-CB-CG	6.39	126.89	114.10
5	L	286	ASP	CA-C-N	6.39	129.22	120.46
5	L	286	ASP	C-N-CA	6.39	129.22	120.46
5	O	101	HIS	CB-CG-CD2	-6.39	122.89	131.20
5	S	259	GLU	CA-CB-CG	6.39	126.89	114.10
4	B	98	ARG	NE-CZ-NH2	-6.39	113.45	119.20
5	D	259	GLU	CA-CB-CG	6.39	126.89	114.10
5	G	259	GLU	CA-CB-CG	6.39	126.89	114.10
5	M	80	ASP	CA-CB-CG	6.39	118.99	112.60
5	M	259	GLU	CA-CB-CG	6.39	126.89	114.10
5	D	47	MET	CA-CB-CG	-6.39	101.32	114.10
5	F	101	HIS	CB-CG-CD2	-6.39	122.89	131.20
5	J	259	GLU	CA-CB-CG	6.39	126.88	114.10
5	N	259	GLU	CA-CB-CG	6.39	126.88	114.10
5	O	259	GLU	CA-CB-CG	6.39	126.88	114.10
5	E	47	MET	CA-CB-CG	-6.39	101.33	114.10
5	L	217	CYS	N-CA-C	6.39	119.73	110.28
5	P	259	GLU	CA-CB-CG	6.39	126.87	114.10
5	P	47	MET	CA-CB-CG	-6.38	101.33	114.10
5	Q	259	GLU	CA-CB-CG	6.38	126.87	114.10
5	E	101	HIS	CB-CG-CD2	-6.38	122.90	131.20
5	S	80	ASP	CA-CB-CG	6.38	118.98	112.60
4	A	154	LYS	N-CA-CB	-6.38	99.23	110.39
4	B	189	GLU	CA-C-O	6.38	127.13	119.61
5	O	47	MET	CA-CB-CG	-6.38	101.35	114.10
5	S	101	HIS	CB-CG-CD2	-6.38	122.91	131.20
5	D	282	ILE	CA-C-O	-6.37	113.98	121.05
5	R	47	MET	CA-CB-CG	-6.37	101.35	114.10
5	H	259	GLU	CA-CB-CG	6.37	126.84	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	47	MET	CA-CB-CG	-6.37	101.36	114.10
5	I	259	GLU	CA-CB-CG	6.37	126.84	114.10
5	L	282	ILE	CA-C-O	-6.37	113.98	121.05
5	K	47	MET	CA-CB-CG	-6.37	101.36	114.10
5	S	47	MET	CA-CB-CG	-6.37	101.36	114.10
5	L	47	MET	CA-CB-CG	-6.37	101.36	114.10
4	B	252	GLU	CA-C-O	6.37	127.33	120.20
5	E	259	GLU	CA-CB-CG	6.36	126.83	114.10
4	V	154	LYS	N-CA-CB	-6.36	99.26	110.39
5	P	282	ILE	CA-C-O	-6.36	113.99	121.05
5	L	101	HIS	CB-CG-CD2	-6.36	122.94	131.20
5	H	80	ASP	CA-CB-CG	6.35	118.95	112.60
5	J	80	ASP	CA-CB-CG	6.35	118.95	112.60
5	Q	80	ASP	CA-CB-CG	6.35	118.95	112.60
5	H	47	MET	CA-CB-CG	-6.35	101.40	114.10
5	Q	47	MET	CA-CB-CG	-6.35	101.40	114.10
5	M	101	HIS	CB-CG-CD2	-6.35	122.95	131.20
5	R	282	ILE	CA-C-O	-6.35	114.01	121.05
5	M	47	MET	CA-CB-CG	-6.34	101.41	114.10
5	F	47	MET	CA-CB-CG	-6.34	101.42	114.10
5	F	217	CYS	N-CA-C	6.34	119.67	110.28
5	R	217	CYS	N-CA-C	6.34	119.67	110.28
5	R	286	ASP	CA-C-N	6.34	129.15	120.46
5	R	286	ASP	C-N-CA	6.34	129.15	120.46
5	N	47	MET	CA-CB-CG	-6.33	101.43	114.10
5	G	47	MET	CA-CB-CG	-6.33	101.44	114.10
5	I	80	ASP	CA-CB-CG	6.33	118.93	112.60
5	J	371	HIS	CA-CB-CG	-6.33	107.47	113.80
4	U	189	GLU	CA-C-O	6.33	127.08	119.61
5	R	101	HIS	CB-CG-CD2	-6.33	122.97	131.20
5	F	282	ILE	CA-C-O	-6.33	114.03	121.05
5	P	80	ASP	CA-CB-CG	6.32	118.92	112.60
4	W	252	GLU	CA-C-O	6.32	127.28	120.20
4	U	98	ARG	NE-CZ-NH2	-6.32	113.51	119.20
5	M	282	ILE	CA-C-O	-6.32	114.04	121.05
4	A	197	LEU	CB-CA-C	-6.31	101.17	110.95
5	L	80	ASP	CA-CB-CG	6.30	118.90	112.60
5	S	282	ILE	CA-C-O	-6.30	114.06	121.05
4	U	252	GLU	CA-C-O	6.30	127.25	120.20
5	N	282	ILE	CA-C-O	-6.30	114.06	121.05
5	O	282	ILE	CA-C-O	-6.30	114.06	121.05
5	Q	282	ILE	CA-C-O	-6.30	114.06	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	98	ARG	NE-CZ-NH2	-6.29	113.54	119.20
5	H	217	CYS	N-CA-C	6.28	119.58	110.28
5	J	1	ASP	CA-CB-CG	6.28	118.88	112.60
5	O	80	ASP	CA-CB-CG	6.27	118.87	112.60
4	A	137	GLN	CA-CB-CG	-6.27	101.56	114.10
5	J	282	ILE	CA-C-O	-6.27	114.09	121.05
5	M	217	CYS	N-CA-C	6.27	119.56	110.28
5	O	217	CYS	N-CA-C	6.27	119.56	110.28
5	K	217	CYS	N-CA-C	6.26	119.55	110.28
5	E	80	ASP	CA-CB-CG	6.26	118.86	112.60
4	B	92	LEU	CB-CA-C	-6.26	100.54	110.86
5	S	217	CYS	N-CA-C	6.26	119.54	110.28
5	L	1	ASP	CA-CB-CG	6.25	118.86	112.60
5	Q	217	CYS	N-CA-C	6.25	119.54	110.28
4	V	197	LEU	CB-CA-C	-6.25	101.26	110.95
5	J	217	CYS	N-CA-C	6.24	119.52	110.28
5	E	217	CYS	N-CA-C	6.24	119.51	110.28
5	P	1	ASP	CA-CB-CG	6.24	118.84	112.60
4	U	92	LEU	CB-CA-C	-6.24	100.57	110.86
5	I	217	CYS	N-CA-C	6.24	119.51	110.28
5	K	1	ASP	CA-CB-CG	6.24	118.83	112.60
5	I	1	ASP	CA-CB-CG	6.23	118.83	112.60
5	S	1	ASP	CA-CB-CG	6.23	118.83	112.60
5	R	80	ASP	CA-CB-CG	6.23	118.83	112.60
5	R	1	ASP	CA-CB-CG	6.23	118.83	112.60
5	K	282	ILE	CA-C-O	-6.22	114.14	121.05
4	V	137	GLN	CA-CB-CG	-6.22	101.66	114.10
5	H	282	ILE	CA-C-O	-6.22	114.15	121.05
5	P	217	CYS	N-CA-C	6.22	119.48	110.28
5	G	217	CYS	N-CA-C	6.21	119.48	110.28
5	D	217	CYS	N-CA-C	6.21	119.47	110.28
4	B	195	ASN	OD1-CG-ND2	-6.21	116.39	122.60
4	U	195	ASN	OD1-CG-ND2	-6.21	116.39	122.60
5	Q	1	ASP	CA-CB-CG	6.21	118.81	112.60
4	V	98	ARG	NE-CZ-NH2	-6.21	113.62	119.20
5	S	219	VAL	CB-CA-C	-6.20	102.92	110.99
5	G	282	ILE	CA-C-O	-6.20	114.17	121.05
5	I	282	ILE	CA-C-O	-6.20	114.17	121.05
5	M	219	VAL	CB-CA-C	-6.20	102.94	110.99
5	K	219	VAL	CB-CA-C	-6.19	102.94	110.99
5	M	1	ASP	CA-CB-CG	6.19	118.79	112.60
4	V	189	GLU	CA-C-O	6.18	126.91	119.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	1	ASP	CA-CB-CG	6.18	118.78	112.60
4	U	155	TYR	CA-CB-CG	6.18	125.02	113.90
5	I	205	GLU	N-CA-C	-6.18	104.47	112.68
5	P	219	VAL	CB-CA-C	-6.18	102.96	110.99
5	Q	219	VAL	CB-CA-C	-6.17	102.96	110.99
4	C	274	MET	CB-CA-C	-6.17	98.82	110.67
5	F	1	ASP	CA-CB-CG	6.17	118.77	112.60
4	B	155	TYR	CA-CB-CG	6.17	125.00	113.90
5	G	205	GLU	N-CA-C	-6.17	104.47	112.68
5	H	1	ASP	CA-CB-CG	6.17	118.77	112.60
5	I	219	VAL	N-CA-CB	6.16	119.67	111.90
4	A	274	MET	CB-CA-C	-6.16	98.84	110.67
5	O	219	VAL	CB-CA-C	-6.16	102.98	110.99
5	D	1	ASP	CA-CB-CG	6.15	118.75	112.60
5	F	219	VAL	CB-CA-C	-6.15	102.99	110.99
5	D	219	VAL	CB-CA-C	-6.15	103.00	110.99
5	I	219	VAL	CB-CA-C	-6.15	103.00	110.99
5	E	1	ASP	CA-CB-CG	6.15	118.75	112.60
5	H	219	VAL	CB-CA-C	-6.14	103.00	110.99
5	N	217	CYS	N-CA-C	6.14	119.38	110.28
5	N	219	VAL	CB-CA-C	-6.14	103.00	110.99
4	U	137	GLN	CA-CB-CG	-6.14	101.81	114.10
5	O	1	ASP	CA-CB-CG	6.14	118.74	112.60
5	R	219	VAL	CB-CA-C	-6.14	103.01	110.99
4	V	274	MET	CB-CA-C	-6.14	98.89	110.67
4	B	137	GLN	CA-CB-CG	-6.13	101.83	114.10
5	L	219	VAL	CB-CA-C	-6.13	103.02	110.99
5	I	128	ASN	N-CA-CB	-6.13	102.59	111.91
5	P	128	ASN	N-CA-CB	-6.13	102.59	111.91
4	A	189	GLU	CA-C-O	6.13	126.84	119.61
5	D	59	GLN	OE1-CD-NE2	-6.13	116.47	122.60
5	G	219	VAL	N-CA-CB	6.13	119.62	111.90
5	O	219	VAL	N-CA-CB	6.13	119.62	111.90
5	F	128	ASN	N-CA-CB	-6.12	102.60	111.91
5	J	128	ASN	N-CA-CB	-6.12	102.60	111.91
5	J	219	VAL	CB-CA-C	-6.12	103.03	110.99
5	P	205	GLU	N-CA-C	-6.12	104.54	112.68
5	M	219	VAL	N-CA-CB	6.12	119.61	111.90
4	X	274	MET	CB-CA-C	-6.12	98.92	110.67
5	G	1	ASP	CA-CB-CG	6.12	118.72	112.60
5	Q	128	ASN	N-CA-CB	-6.12	102.61	111.91
5	E	219	VAL	N-CA-CB	6.12	119.61	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	59	GLN	OE1-CD-NE2	-6.11	116.49	122.60
5	S	219	VAL	N-CA-CB	6.11	119.59	111.90
5	O	128	ASN	N-CA-CB	-6.10	102.63	111.91
5	H	205	GLU	N-CA-C	-6.10	104.57	112.68
5	M	128	ASN	N-CA-CB	-6.10	102.64	111.91
5	O	205	GLU	N-CA-C	-6.10	104.57	112.68
5	Q	205	GLU	N-CA-C	-6.10	104.57	112.68
5	G	128	ASN	N-CA-CB	-6.10	102.64	111.91
4	B	94	ARG	N-CA-C	6.09	117.59	111.07
5	M	205	GLU	N-CA-C	-6.09	104.57	112.68
5	S	128	ASN	N-CA-CB	-6.09	102.65	111.91
5	J	219	VAL	N-CA-CB	6.09	119.58	111.90
5	N	205	GLU	N-CA-C	-6.09	104.58	112.68
5	L	59	GLN	OE1-CD-NE2	-6.09	116.51	122.60
5	L	128	ASN	N-CA-CB	-6.09	102.65	111.91
5	J	205	GLU	N-CA-C	-6.09	104.58	112.68
5	E	95	ARG	CA-CB-CG	6.08	126.27	114.10
5	P	219	VAL	N-CA-CB	6.08	119.57	111.90
5	E	219	VAL	CB-CA-C	-6.08	103.08	110.99
5	G	219	VAL	CB-CA-C	-6.08	103.08	110.99
5	R	128	ASN	N-CA-CB	-6.08	102.67	111.91
5	S	205	GLU	N-CA-C	-6.08	104.59	112.68
5	E	5	THR	CA-C-N	6.07	130.86	120.72
5	E	5	THR	C-N-CA	6.07	130.86	120.72
5	F	219	VAL	N-CA-CB	6.07	119.55	111.90
5	D	128	ASN	N-CA-CB	-6.07	102.69	111.91
5	G	59	GLN	OE1-CD-NE2	-6.07	116.53	122.60
5	H	128	ASN	N-CA-CB	-6.07	102.69	111.91
5	K	128	ASN	N-CA-CB	-6.07	102.69	111.91
5	O	252	ASN	CA-CB-CG	6.07	118.67	112.60
4	U	94	ARG	N-CA-C	6.06	117.56	111.07
5	D	219	VAL	N-CA-CB	6.06	119.53	111.90
5	L	205	GLU	N-CA-C	-6.06	104.62	112.68
5	K	219	VAL	N-CA-CB	6.05	119.53	111.90
4	V	22	LYS	CB-CG-CD	-6.05	97.38	111.30
4	U	35	GLU	CA-C-O	6.05	126.75	119.61
5	E	205	GLU	N-CA-C	-6.05	104.64	112.68
5	R	95	ARG	CA-CB-CG	6.05	126.20	114.10
5	L	95	ARG	CA-CB-CG	6.05	126.20	114.10
5	R	205	GLU	N-CA-C	-6.05	104.64	112.68
5	Q	219	VAL	N-CA-CB	6.04	119.52	111.90
5	M	95	ARG	CA-CB-CG	6.04	126.18	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	205	GLU	N-CA-C	-6.04	104.65	112.68
5	R	5	THR	CA-C-N	6.04	130.80	120.72
5	R	5	THR	C-N-CA	6.04	130.80	120.72
5	S	95	ARG	CA-CB-CG	6.04	126.18	114.10
4	A	273	ASP	O-C-N	-6.04	115.72	122.12
5	L	219	VAL	N-CA-CB	6.04	119.51	111.90
5	K	205	GLU	N-CA-C	-6.03	104.66	112.68
5	N	128	ASN	N-CA-CB	-6.03	102.74	111.91
5	P	231	ALA	N-CA-C	6.03	117.53	111.07
4	B	35	GLU	CA-C-O	6.03	126.72	119.61
4	A	22	LYS	CB-CG-CD	-6.03	97.44	111.30
5	E	128	ASN	N-CA-CB	-6.03	102.75	111.91
5	J	95	ARG	CA-CB-CG	6.03	126.15	114.10
5	N	95	ARG	CA-CB-CG	6.03	126.15	114.10
5	I	95	ARG	CA-CB-CG	6.02	126.15	114.10
5	N	231	ALA	N-CA-C	6.02	117.51	111.07
5	D	95	ARG	CA-CB-CG	6.02	126.13	114.10
5	D	5	THR	CA-C-N	6.01	130.76	120.72
5	D	5	THR	C-N-CA	6.01	130.76	120.72
5	F	252	ASN	CA-CB-CG	6.01	118.61	112.60
5	Q	95	ARG	CA-CB-CG	6.01	126.12	114.10
5	K	231	ALA	N-CA-C	6.01	117.50	111.07
5	N	59	GLN	OE1-CD-NE2	-6.01	116.59	122.60
5	L	5	THR	CA-C-N	6.01	130.75	120.72
5	L	5	THR	C-N-CA	6.01	130.75	120.72
5	S	231	ALA	N-CA-C	6.01	117.50	111.07
5	K	95	ARG	CA-CB-CG	6.00	126.11	114.10
5	N	219	VAL	N-CA-CB	6.00	119.47	111.90
5	Q	5	THR	CA-C-N	6.00	130.75	120.72
5	Q	5	THR	C-N-CA	6.00	130.75	120.72
5	H	219	VAL	N-CA-CB	6.00	119.46	111.90
5	E	59	GLN	OE1-CD-NE2	-6.00	116.60	122.60
5	F	95	ARG	CA-CB-CG	6.00	126.10	114.10
5	K	252	ASN	CA-CB-CG	6.00	118.60	112.60
5	S	5	THR	CA-C-N	6.00	130.74	120.72
5	S	5	THR	C-N-CA	6.00	130.74	120.72
5	N	252	ASN	CA-CB-CG	6.00	118.60	112.60
5	I	5	THR	CA-C-N	5.99	130.73	120.72
5	I	5	THR	C-N-CA	5.99	130.73	120.72
5	J	59	GLN	OE1-CD-NE2	-5.99	116.61	122.60
5	M	5	THR	CA-C-N	5.99	130.73	120.72
5	M	5	THR	C-N-CA	5.99	130.73	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	59	GLN	OE1-CD-NE2	-5.99	116.61	122.60
5	F	5	THR	CA-C-N	5.99	130.73	120.72
5	F	5	THR	C-N-CA	5.99	130.73	120.72
5	G	95	ARG	CA-CB-CG	5.99	126.08	114.10
5	O	95	ARG	CA-CB-CG	5.99	126.08	114.10
5	J	252	ASN	CA-CB-CG	5.99	118.59	112.60
5	P	95	ARG	CA-CB-CG	5.99	126.08	114.10
4	A	195	ASN	OD1-CG-ND2	-5.99	116.61	122.60
4	C	273	ASP	O-C-N	-5.99	115.77	122.12
5	O	5	THR	CA-C-N	5.98	130.71	120.72
5	O	5	THR	C-N-CA	5.98	130.71	120.72
5	M	252	ASN	CA-CB-CG	5.98	118.58	112.60
5	F	205	GLU	N-CA-C	-5.98	104.73	112.68
5	R	219	VAL	N-CA-CB	5.98	119.43	111.90
4	U	158	VAL	O-C-N	-5.97	115.97	121.94
5	N	5	THR	CA-C-N	5.97	130.69	120.72
5	N	5	THR	C-N-CA	5.97	130.69	120.72
5	M	231	ALA	N-CA-C	5.97	117.46	111.07
5	Q	59	GLN	OE1-CD-NE2	-5.97	116.63	122.60
5	J	233	SER	CA-C-O	5.97	129.04	120.51
5	K	5	THR	CA-C-N	5.96	130.68	120.72
5	K	5	THR	C-N-CA	5.96	130.68	120.72
5	G	5	THR	CA-C-N	5.96	130.67	120.72
5	G	5	THR	C-N-CA	5.96	130.67	120.72
5	K	59	GLN	OE1-CD-NE2	-5.96	116.64	122.60
5	S	233	SER	CA-C-O	5.96	129.03	120.51
4	V	94	ARG	N-CA-C	5.96	117.45	111.07
4	V	153	ARG	O-C-N	-5.96	114.96	122.17
5	I	97	ALA	N-CA-C	-5.96	102.27	109.72
5	N	97	ALA	N-CA-C	-5.96	102.27	109.72
5	J	231	ALA	N-CA-C	5.96	117.45	111.07
5	N	233	SER	CA-C-O	5.96	129.03	120.51
5	H	95	ARG	CA-CB-CG	5.95	126.01	114.10
5	O	231	ALA	N-CA-C	5.95	117.44	111.07
5	S	252	ASN	CA-CB-CG	5.95	118.55	112.60
4	X	273	ASP	O-C-N	-5.95	115.81	122.12
4	A	94	ARG	N-CA-C	5.95	117.44	111.07
4	V	273	ASP	O-C-N	-5.95	115.81	122.12
5	K	335	ARG	CA-CB-CG	5.95	126.00	114.10
5	D	252	ASN	CA-CB-CG	5.95	118.55	112.60
5	H	231	ALA	N-CA-C	5.95	117.43	111.07
5	P	335	ARG	CA-CB-CG	5.95	125.99	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	5	THR	CA-C-N	5.95	130.65	120.72
5	H	5	THR	C-N-CA	5.95	130.65	120.72
5	I	335	ARG	CA-CB-CG	5.95	125.99	114.10
5	P	5	THR	CA-C-N	5.95	130.65	120.72
5	P	5	THR	C-N-CA	5.95	130.65	120.72
5	R	97	ALA	N-CA-C	-5.95	102.29	109.72
5	F	231	ALA	N-CA-C	5.94	117.43	111.07
5	J	5	THR	CA-C-N	5.94	130.64	120.72
5	J	5	THR	C-N-CA	5.94	130.64	120.72
5	Q	335	ARG	CA-CB-CG	5.94	125.98	114.10
5	P	233	SER	CA-C-O	5.94	129.00	120.51
5	R	252	ASN	CA-CB-CG	5.94	118.54	112.60
4	V	6	LEU	N-CA-C	5.93	117.42	111.07
5	D	335	ARG	CA-CB-CG	5.93	125.96	114.10
5	S	335	ARG	CA-CB-CG	5.93	125.96	114.10
5	K	233	SER	CA-C-O	5.93	128.99	120.51
5	Q	231	ALA	N-CA-C	5.93	117.42	111.07
5	L	97	ALA	N-CA-C	-5.93	102.31	109.72
5	O	59	GLN	OE1-CD-NE2	-5.93	116.67	122.60
5	H	97	ALA	N-CA-C	-5.93	102.31	109.72
5	J	335	ARG	CA-CB-CG	5.93	125.95	114.10
5	K	34	ILE	CB-CA-C	-5.93	102.37	110.90
5	L	252	ASN	CA-CB-CG	5.93	118.53	112.60
4	V	92	LEU	CB-CA-C	-5.93	100.83	110.79
4	V	195	ASN	OD1-CG-ND2	-5.93	116.67	122.60
4	A	153	ARG	O-C-N	-5.92	115.00	122.17
5	F	97	ALA	N-CA-C	-5.92	102.31	109.72
5	M	233	SER	CA-C-O	5.92	128.98	120.51
5	P	97	ALA	N-CA-C	-5.92	102.32	109.72
5	P	34	ILE	CB-CA-C	-5.92	102.37	110.90
5	D	97	ALA	N-CA-C	-5.92	102.32	109.72
5	G	231	ALA	N-CA-C	5.92	117.41	111.07
5	O	335	ARG	CA-CB-CG	5.92	125.94	114.10
5	M	59	GLN	OE1-CD-NE2	-5.92	116.68	122.60
5	M	335	ARG	CA-CB-CG	5.92	125.94	114.10
5	N	335	ARG	CA-CB-CG	5.92	125.94	114.10
5	F	34	ILE	CB-CA-C	-5.92	102.38	110.90
5	Q	252	ASN	CA-CB-CG	5.92	118.52	112.60
5	S	59	GLN	OE1-CD-NE2	-5.92	116.68	122.60
5	F	335	ARG	CA-CB-CG	5.92	125.93	114.10
5	E	252	ASN	CA-CB-CG	5.91	118.51	112.60
5	H	59	GLN	OE1-CD-NE2	-5.91	116.69	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	85	LEU	N-CA-C	-5.91	104.76	111.14
5	Q	97	ALA	N-CA-C	-5.91	102.33	109.72
5	K	97	ALA	N-CA-C	-5.91	102.33	109.72
4	V	130	ASP	CA-CB-CG	5.91	118.51	112.60
5	Q	263	GLN	CA-C-N	5.91	125.52	119.56
5	Q	263	GLN	C-N-CA	5.91	125.52	119.56
5	I	257	CYS	O-C-N	-5.90	116.20	120.27
4	B	158	VAL	O-C-N	-5.90	116.04	121.94
5	E	335	ARG	CA-CB-CG	5.90	125.90	114.10
5	H	335	ARG	CA-CB-CG	5.90	125.90	114.10
5	E	34	ILE	CB-CA-C	-5.90	102.40	110.90
5	G	335	ARG	CA-CB-CG	5.90	125.90	114.10
5	I	252	ASN	CA-CB-CG	5.90	118.50	112.60
5	R	335	ARG	CA-CB-CG	5.90	125.90	114.10
5	I	233	SER	CA-C-O	5.90	128.94	120.51
3	8	85	LEU	N-CA-C	-5.89	104.77	111.14
5	H	34	ILE	CB-CA-C	-5.89	102.42	110.90
5	H	263	GLN	CA-C-N	5.89	125.51	119.56
5	H	263	GLN	C-N-CA	5.89	125.51	119.56
5	O	233	SER	CA-C-O	5.89	128.94	120.51
5	Q	34	ILE	CB-CA-C	-5.89	102.42	110.90
4	A	92	LEU	CB-CA-C	-5.89	100.90	110.79
5	D	34	ILE	CB-CA-C	-5.89	102.42	110.90
5	F	233	SER	CA-C-O	5.89	128.93	120.51
5	L	335	ARG	CA-CB-CG	5.89	125.88	114.10
5	S	257	CYS	O-C-N	-5.89	116.21	120.27
5	E	231	ALA	N-CA-C	5.89	117.37	111.07
5	H	252	ASN	CA-CB-CG	5.89	118.49	112.60
5	E	263	GLN	CA-C-N	5.88	125.50	119.56
5	E	263	GLN	C-N-CA	5.88	125.50	119.56
5	G	34	ILE	CB-CA-C	-5.88	102.43	110.90
5	J	263	GLN	CA-C-N	5.88	125.50	119.56
5	J	263	GLN	C-N-CA	5.88	125.50	119.56
5	L	231	ALA	N-CA-C	5.88	117.37	111.07
5	M	97	ALA	N-CA-C	-5.88	102.36	109.72
5	M	257	CYS	O-C-N	-5.88	116.21	120.27
3	2	85	LEU	N-CA-C	-5.88	104.79	111.14
5	E	233	SER	CA-C-O	5.88	128.92	120.51
5	K	263	GLN	CA-C-N	5.88	125.50	119.56
5	K	263	GLN	C-N-CA	5.88	125.50	119.56
5	Q	233	SER	CA-C-O	5.88	128.92	120.51
5	R	34	ILE	CB-CA-C	-5.88	102.43	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	97	ALA	N-CA-C	-5.88	102.37	109.72
5	O	34	ILE	CB-CA-C	-5.88	102.44	110.90
5	O	97	ALA	N-CA-C	-5.88	102.37	109.72
5	J	34	ILE	CB-CA-C	-5.88	102.44	110.90
4	U	231	ARG	NE-CZ-NH1	5.88	127.38	121.50
3	Z	85	LEU	N-CA-C	-5.88	104.79	111.14
5	G	97	ALA	N-CA-C	-5.87	102.38	109.72
5	G	233	SER	CA-C-O	5.87	128.91	120.51
5	M	34	ILE	CB-CA-C	-5.87	102.44	110.90
5	S	97	ALA	N-CA-C	-5.87	102.38	109.72
5	F	59	GLN	OE1-CD-NE2	-5.87	116.73	122.60
5	L	233	SER	CA-C-O	5.87	128.91	120.51
5	L	263	GLN	CA-C-N	5.87	125.49	119.56
5	L	263	GLN	C-N-CA	5.87	125.49	119.56
5	R	263	GLN	CA-C-N	5.87	125.49	119.56
5	R	263	GLN	C-N-CA	5.87	125.49	119.56
5	N	263	GLN	CA-C-N	5.87	125.49	119.56
5	N	263	GLN	C-N-CA	5.87	125.49	119.56
5	L	34	ILE	CB-CA-C	-5.87	102.45	110.90
5	Q	257	CYS	O-C-N	-5.87	116.22	120.27
5	F	263	GLN	CA-C-N	5.86	125.48	119.56
5	F	263	GLN	C-N-CA	5.86	125.48	119.56
5	K	263	GLN	OE1-CD-NE2	-5.86	116.74	122.60
5	E	97	ALA	N-CA-C	-5.86	102.39	109.72
4	V	36	LEU	CB-CA-C	-5.86	100.95	110.79
5	I	59	GLN	OE1-CD-NE2	-5.86	116.74	122.60
5	J	257	CYS	O-C-N	-5.86	116.23	120.27
5	D	254	ARG	N-CA-CB	-5.86	100.59	110.49
4	U	99	LEU	N-CA-C	5.86	117.46	111.14
5	R	231	ALA	N-CA-C	5.85	117.33	111.07
5	I	263	GLN	CA-C-N	5.85	125.47	119.56
5	I	263	GLN	C-N-CA	5.85	125.47	119.56
5	N	34	ILE	CB-CA-C	-5.85	102.47	110.90
5	G	263	GLN	CA-C-N	5.85	125.47	119.56
5	G	263	GLN	C-N-CA	5.85	125.47	119.56
5	O	263	GLN	CA-C-N	5.85	125.47	119.56
5	O	263	GLN	C-N-CA	5.85	125.47	119.56
3	Z	20	ALA	N-CA-C	-5.85	105.03	111.82
3	8	20	ALA	N-CA-C	-5.85	105.04	111.82
5	R	113	LYS	CA-CB-CG	5.85	125.80	114.10
5	S	254	ARG	N-CA-CB	-5.85	100.61	110.49
4	X	263	ILE	N-CA-C	5.85	116.58	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	99	LEU	N-CA-C	5.85	117.45	111.14
5	K	254	ARG	N-CA-CB	-5.84	100.61	110.49
5	N	254	ARG	N-CA-CB	-5.84	100.61	110.49
3	2	20	ALA	N-CA-C	-5.84	105.04	111.82
4	A	130	ASP	CA-CB-CG	5.84	118.44	112.60
5	H	185	LEU	N-CA-C	5.84	118.43	111.71
5	I	231	ALA	N-CA-C	5.84	117.32	111.07
5	J	254	ARG	N-CA-CB	-5.84	100.62	110.49
5	P	252	ASN	CA-CB-CG	5.84	118.44	112.60
5	O	254	ARG	N-CA-CB	-5.84	100.62	110.49
5	M	254	ARG	N-CA-CB	-5.84	100.62	110.49
5	E	257	CYS	O-C-N	-5.84	116.24	120.27
5	S	34	ILE	CB-CA-C	-5.84	102.50	110.90
4	C	263	ILE	N-CA-C	5.83	116.57	110.62
5	F	254	ARG	N-CA-CB	-5.83	100.63	110.49
4	V	263	ILE	N-CA-C	5.83	116.57	110.62
4	B	231	ARG	NE-CZ-NH1	5.83	127.33	121.50
5	I	185	LEU	N-CA-C	5.83	118.42	111.71
5	G	254	ARG	N-CA-CB	-5.83	100.63	110.49
5	I	34	ILE	CB-CA-C	-5.83	102.50	110.90
5	M	113	LYS	CA-CB-CG	5.83	125.76	114.10
5	E	254	ARG	N-CA-CB	-5.83	100.64	110.49
3	5	20	ALA	N-CA-C	-5.83	105.06	111.82
5	L	113	LYS	CA-CB-CG	5.83	125.75	114.10
5	M	263	GLN	CA-C-N	5.83	125.44	119.56
5	M	263	GLN	C-N-CA	5.83	125.44	119.56
4	A	263	ILE	N-CA-C	5.82	116.56	110.62
5	F	113	LYS	CA-CB-CG	5.82	125.75	114.10
5	G	252	ASN	CA-CB-CG	5.82	118.42	112.60
5	H	233	SER	CA-C-O	5.82	128.84	120.51
5	P	263	GLN	CA-C-N	5.82	125.44	119.56
5	P	263	GLN	C-N-CA	5.82	125.44	119.56
5	I	254	ARG	N-CA-CB	-5.82	100.65	110.49
5	P	254	ARG	N-CA-CB	-5.82	100.65	110.49
5	Q	254	ARG	N-CA-CB	-5.82	100.65	110.49
4	U	274	MET	CB-CA-C	-5.82	99.50	110.67
4	A	151	ALA	CA-C-O	-5.81	112.20	120.51
5	D	231	ALA	N-CA-C	5.81	117.29	111.07
5	G	257	CYS	O-C-N	-5.81	116.26	120.27
5	R	233	SER	CA-C-O	5.81	128.82	120.51
5	S	263	GLN	CA-C-N	5.81	125.43	119.56
5	S	263	GLN	C-N-CA	5.81	125.43	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	21	ASP	CA-CB-CG	5.81	118.41	112.60
5	R	254	ARG	N-CA-CB	-5.81	100.67	110.49
4	T	274	MET	CB-CA-C	-5.81	99.51	110.67
5	O	257	CYS	O-C-N	-5.81	116.26	120.27
5	R	257	CYS	O-C-N	-5.81	116.26	120.27
5	H	113	LYS	CA-CB-CG	5.81	125.72	114.10
5	K	257	CYS	O-C-N	-5.81	116.26	120.27
4	A	140	GLN	CA-C-O	5.80	126.46	119.61
5	G	113	LYS	CA-CB-CG	5.80	125.71	114.10
4	V	21	ASP	CA-CB-CG	5.80	118.40	112.60
5	Q	113	LYS	CA-CB-CG	5.80	125.71	114.10
4	W	274	MET	CB-CA-C	-5.80	99.53	110.67
4	B	274	MET	CB-CA-C	-5.80	99.53	110.67
5	J	263	GLN	OE1-CD-NE2	-5.80	116.80	122.60
5	L	254	ARG	N-CA-CB	-5.80	100.69	110.49
5	H	254	ARG	N-CA-CB	-5.80	100.69	110.49
5	K	161	HIS	CB-CG-CD2	-5.80	123.66	131.20
4	U	196	ASN	CA-C-O	5.80	126.69	120.20
4	V	151	ALA	CA-C-O	-5.80	112.22	120.51
5	J	113	LYS	CA-CB-CG	5.79	125.69	114.10
5	S	113	LYS	CA-CB-CG	5.79	125.69	114.10
4	A	36	LEU	CB-CA-C	-5.79	101.06	110.79
5	D	257	CYS	O-C-N	-5.79	116.28	120.27
5	L	257	CYS	O-C-N	-5.79	116.28	120.27
5	P	161	HIS	CB-CG-CD2	-5.79	123.68	131.20
5	P	113	LYS	CA-CB-CG	5.79	125.67	114.10
5	M	135	ALA	O-C-N	-5.79	116.58	123.06
5	S	335	ARG	N-CA-C	5.79	123.12	110.80
5	I	113	LYS	CA-CB-CG	5.78	125.67	114.10
5	M	335	ARG	N-CA-C	5.78	123.12	110.80
5	H	257	CYS	O-C-N	-5.78	116.28	120.27
5	N	257	CYS	O-C-N	-5.78	116.28	120.27
4	T	273	ASP	O-C-N	-5.78	115.99	122.12
5	D	263	GLN	CA-C-N	5.78	125.40	119.56
5	D	263	GLN	C-N-CA	5.78	125.40	119.56
4	A	21	ASP	CA-CB-CG	5.78	118.38	112.60
5	F	335	ARG	N-CA-C	5.78	123.10	110.80
5	K	113	LYS	CA-CB-CG	5.78	125.65	114.10
5	K	335	ARG	N-CA-C	5.78	123.10	110.80
5	D	233	SER	CA-C-O	5.77	128.77	120.51
5	N	113	LYS	CA-CB-CG	5.77	125.65	114.10
5	O	113	LYS	CA-CB-CG	5.77	125.63	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	263	GLN	OE1-CD-NE2	-5.77	116.83	122.60
4	X	260	TYR	N-CA-CB	5.76	118.54	110.07
4	V	140	GLN	CA-C-O	5.76	126.41	119.61
5	P	335	ARG	N-CA-C	5.76	123.07	110.80
5	E	335	ARG	N-CA-C	5.76	123.06	110.80
5	L	335	ARG	N-CA-C	5.76	123.06	110.80
5	Q	263	GLN	OE1-CD-NE2	-5.76	116.84	122.60
5	S	135	ALA	O-C-N	-5.76	116.61	123.06
5	D	135	ALA	O-C-N	-5.75	116.62	123.06
5	D	161	HIS	CB-CG-CD2	-5.75	123.72	131.20
5	E	113	LYS	CA-CB-CG	5.75	125.60	114.10
5	P	257	CYS	O-C-N	-5.75	116.30	120.27
5	G	263	GLN	OE1-CD-NE2	-5.75	116.85	122.60
5	H	263	GLN	OE1-CD-NE2	-5.75	116.85	122.60
5	H	335	ARG	N-CA-C	5.75	123.04	110.80
5	M	161	HIS	CB-CG-CD2	-5.75	123.73	131.20
5	Q	335	ARG	N-CA-C	5.75	123.04	110.80
5	R	335	ARG	N-CA-C	5.75	123.04	110.80
4	V	260	TYR	N-CA-CB	5.75	118.52	110.07
4	A	260	TYR	N-CA-CB	5.74	118.51	110.07
4	B	196	ASN	CA-C-O	5.74	126.63	120.20
4	C	260	TYR	N-CA-CB	5.74	118.51	110.07
5	D	335	ARG	N-CA-C	5.74	123.02	110.80
5	I	335	ARG	N-CA-C	5.74	123.02	110.80
5	J	135	ALA	O-C-N	-5.74	116.63	123.06
5	J	335	ARG	N-CA-C	5.74	123.02	110.80
5	N	335	ARG	N-CA-C	5.74	123.02	110.80
5	D	113	LYS	CA-CB-CG	5.74	125.58	114.10
5	R	161	HIS	CB-CG-CD2	-5.74	123.74	131.20
5	F	161	HIS	CB-CG-CD2	-5.74	123.74	131.20
5	L	161	HIS	CB-CG-CD2	-5.74	123.75	131.20
5	O	161	HIS	CB-CG-CD2	-5.74	123.74	131.20
5	S	161	HIS	CB-CG-CD2	-5.74	123.74	131.20
5	E	161	HIS	CB-CG-CD2	-5.73	123.75	131.20
5	H	161	HIS	CB-CG-CD2	-5.73	123.75	131.20
4	B	21	ASP	CA-CB-CG	5.73	118.33	112.60
5	O	335	ARG	N-CA-C	5.73	123.00	110.80
5	D	263	GLN	OE1-CD-NE2	-5.73	116.87	122.60
5	G	335	ARG	N-CA-C	5.72	122.99	110.80
5	I	161	HIS	CB-CG-CD2	-5.72	123.76	131.20
5	G	135	ALA	O-C-N	-5.72	116.66	123.06
5	N	263	GLN	OE1-CD-NE2	-5.72	116.88	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	2	GLN	N-CA-C	5.71	117.97	111.11
4	V	253	LEU	CB-CA-C	-5.71	102.17	110.96
5	J	161	HIS	CB-CG-CD2	-5.71	123.78	131.20
4	B	273	ASP	O-C-N	-5.71	116.07	122.12
5	M	263	GLN	OE1-CD-NE2	-5.71	116.89	122.60
5	O	263	GLN	OE1-CD-NE2	-5.70	116.90	122.60
5	G	161	HIS	CB-CG-CD2	-5.70	123.79	131.20
4	C	253	LEU	CB-CA-C	-5.70	102.18	110.96
4	B	130	ASP	CA-CB-CG	5.70	118.30	112.60
5	F	263	GLN	OE1-CD-NE2	-5.70	116.90	122.60
5	Q	135	ALA	O-C-N	-5.70	116.68	123.06
5	E	135	ALA	O-C-N	-5.69	116.69	123.06
5	N	161	HIS	CB-CG-CD2	-5.69	123.80	131.20
5	O	185	LEU	N-CA-C	5.69	118.42	111.82
5	Q	262	PHE	CA-CB-CG	-5.69	108.11	113.80
5	F	185	LEU	N-CA-C	5.68	118.41	111.82
5	O	135	ALA	O-C-N	-5.68	116.69	123.06
5	R	135	ALA	O-C-N	-5.68	116.69	123.06
5	K	135	ALA	O-C-N	-5.68	116.70	123.06
4	U	158	VAL	N-CA-CB	-5.68	104.21	110.51
5	Q	161	HIS	CB-CG-CD2	-5.68	123.82	131.20
4	A	253	LEU	CB-CA-C	-5.67	102.22	110.96
5	F	257	CYS	O-C-N	-5.67	116.35	120.27
4	X	253	LEU	CB-CA-C	-5.67	102.22	110.96
4	A	141	LEU	N-CA-C	5.67	120.33	112.45
5	S	263	GLN	OE1-CD-NE2	-5.67	116.93	122.60
2	4	209	LEU	N-CA-C	-5.67	105.01	111.07
5	H	135	ALA	O-C-N	-5.67	116.71	123.06
5	E	185	LEU	N-CA-C	5.67	118.39	111.82
5	L	135	ALA	O-C-N	-5.66	116.72	123.06
5	I	263	GLN	OE1-CD-NE2	-5.66	116.94	122.60
4	A	220	VAL	O-C-N	-5.66	116.38	121.87
5	G	185	LEU	N-CA-C	5.66	118.38	111.82
4	B	158	VAL	N-CA-CB	-5.65	104.23	110.51
5	F	262	PHE	CA-CB-CG	-5.65	108.15	113.80
4	U	130	ASP	CA-CB-CG	5.65	118.25	112.60
5	F	135	ALA	O-C-N	-5.65	116.73	123.06
5	L	185	LEU	N-CA-C	5.65	118.37	111.82
5	K	185	LEU	N-CA-C	5.64	118.37	111.82
5	R	185	LEU	N-CA-C	5.64	118.36	111.82
5	P	185	LEU	N-CA-C	5.64	118.36	111.82
5	P	135	ALA	O-C-N	-5.64	116.74	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	262	PHE	CA-CB-CG	-5.64	108.16	113.80
5	J	262	PHE	CA-CB-CG	-5.64	108.16	113.80
4	U	273	ASP	O-C-N	-5.64	116.15	122.12
5	K	262	PHE	CA-CB-CG	-5.63	108.17	113.80
5	N	185	LEU	N-CA-C	5.63	118.35	111.82
2	7	209	LEU	N-CA-C	-5.62	105.05	111.07
5	E	263	GLN	OE1-CD-NE2	-5.62	116.98	122.60
5	Q	185	LEU	N-CA-C	5.62	118.34	111.82
4	U	220	VAL	O-C-N	-5.62	116.42	121.87
5	S	44	MET	N-CA-C	-5.62	102.20	110.52
4	B	220	VAL	N-CA-C	5.62	116.35	110.62
5	M	185	LEU	N-CA-C	5.62	118.33	111.82
5	P	262	PHE	CA-CB-CG	-5.62	108.19	113.80
5	S	185	LEU	N-CA-C	5.61	118.33	111.82
4	V	141	LEU	N-CA-C	5.61	120.25	112.45
5	M	44	MET	N-CA-C	-5.61	102.22	110.52
4	W	273	ASP	O-C-N	-5.60	116.18	122.12
4	U	74	ALA	O-C-N	-5.60	116.18	122.12
5	I	135	ALA	O-C-N	-5.60	116.79	123.06
5	J	137	GLN	CA-C-O	-5.60	115.12	121.00
2	Y	209	LEU	N-CA-C	-5.60	105.08	111.07
5	E	262	PHE	CA-CB-CG	-5.60	108.20	113.80
5	D	262	PHE	CA-CB-CG	-5.59	108.20	113.80
5	Q	349	LEU	CA-C-N	5.59	127.77	120.28
5	Q	349	LEU	C-N-CA	5.59	127.77	120.28
5	E	275	HIS	CB-CG-CD2	-5.59	123.94	131.20
5	N	262	PHE	CA-CB-CG	-5.59	108.21	113.80
4	B	272	ASN	N-CA-C	5.59	117.05	111.07
4	V	220	VAL	O-C-N	-5.59	116.45	121.87
5	O	262	PHE	CA-CB-CG	-5.58	108.22	113.80
5	J	312	ARG	NE-CZ-NH2	5.58	124.22	119.20
2	1	209	LEU	N-CA-C	-5.58	105.10	111.07
5	D	185	LEU	N-CA-C	5.58	118.29	111.82
5	N	349	LEU	CA-C-N	5.58	127.75	120.28
5	N	349	LEU	C-N-CA	5.58	127.75	120.28
4	B	74	ALA	O-C-N	-5.58	116.21	122.12
5	P	137	GLN	CA-C-O	-5.57	115.15	121.00
5	I	262	PHE	CA-CB-CG	-5.57	108.23	113.80
5	L	263	GLN	OE1-CD-NE2	-5.57	117.03	122.60
4	U	272	ASN	N-CA-C	5.57	117.03	111.07
4	W	272	ASN	N-CA-C	5.56	117.02	111.07
5	J	185	LEU	N-CA-C	5.56	118.27	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	140	GLN	CA-C-O	5.56	126.17	119.61
5	D	349	LEU	CA-C-N	5.56	127.73	120.28
5	D	349	LEU	C-N-CA	5.56	127.73	120.28
5	M	349	LEU	CA-C-N	5.56	127.73	120.28
5	M	349	LEU	C-N-CA	5.56	127.73	120.28
5	J	275	HIS	CB-CG-CD2	-5.56	123.97	131.20
4	U	190	LEU	N-CA-C	5.55	120.04	112.04
5	G	262	PHE	CA-CB-CG	-5.55	108.25	113.80
5	O	44	MET	N-CA-C	-5.55	102.31	110.52
3	Z	105	LYS	N-CA-C	-5.55	100.94	109.76
5	N	135	ALA	O-C-N	-5.55	116.85	123.06
5	K	275	HIS	CB-CG-CD2	-5.55	123.99	131.20
5	P	116	ARG	N-CA-C	-5.54	105.24	111.28
5	S	349	LEU	CA-C-N	5.54	127.70	120.28
5	S	349	LEU	C-N-CA	5.54	127.70	120.28
4	B	220	VAL	O-C-N	-5.54	116.50	121.87
5	E	44	MET	N-CA-C	-5.54	102.32	110.52
5	R	263	GLN	OE1-CD-NE2	-5.54	117.06	122.60
5	S	262	PHE	CA-CB-CG	-5.54	108.26	113.80
5	E	349	LEU	CA-C-N	5.54	127.70	120.28
5	E	349	LEU	C-N-CA	5.54	127.70	120.28
5	F	312	ARG	NE-CZ-NH2	5.53	124.18	119.20
5	F	44	MET	N-CA-C	-5.53	102.33	110.52
5	R	275	HIS	CB-CG-CD2	-5.53	124.01	131.20
5	R	312	ARG	NE-CZ-NH2	5.53	124.18	119.20
4	U	140	GLN	CA-C-O	5.53	126.14	119.61
5	Q	226	GLU	N-CA-C	-5.53	107.18	114.04
4	A	190	LEU	N-CA-C	5.53	120.00	112.04
4	B	190	LEU	N-CA-C	5.53	120.00	112.04
5	K	44	MET	N-CA-C	-5.53	102.34	110.52
4	U	220	VAL	N-CA-C	5.52	116.25	110.62
3	2	105	LYS	N-CA-C	-5.52	100.98	109.76
5	L	275	HIS	CB-CG-CD2	-5.52	124.02	131.20
5	S	312	ARG	NE-CZ-NH2	5.52	124.17	119.20
5	F	275	HIS	CB-CG-CD2	-5.52	124.02	131.20
5	G	44	MET	N-CA-C	-5.52	102.35	110.52
5	I	44	MET	N-CA-C	-5.52	102.35	110.52
5	Q	44	MET	N-CA-C	-5.52	102.35	110.52
5	R	31	PHE	CA-CB-CG	5.52	119.32	113.80
5	N	44	MET	N-CA-C	-5.51	102.36	110.52
5	N	200	PHE	CA-C-O	5.51	127.89	121.11
5	Q	312	ARG	NE-CZ-NH2	5.51	124.16	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	272	ASN	N-CA-C	5.51	116.97	111.07
3	5	105	LYS	N-CA-C	-5.51	101.00	109.76
3	8	105	LYS	N-CA-C	-5.51	101.00	109.76
5	I	312	ARG	NE-CZ-NH2	5.51	124.16	119.20
5	M	262	PHE	CA-CB-CG	-5.51	108.29	113.80
5	O	349	LEU	CA-C-N	5.51	127.66	120.28
5	O	349	LEU	C-N-CA	5.51	127.66	120.28
5	Q	200	PHE	CA-C-O	5.51	127.89	121.11
5	D	31	PHE	CA-CB-CG	5.51	119.31	113.80
5	M	275	HIS	CB-CG-CD2	-5.51	124.04	131.20
5	S	275	HIS	CB-CG-CD2	-5.51	124.04	131.20
5	L	44	MET	N-CA-C	-5.51	102.37	110.52
5	G	349	LEU	CA-C-N	5.50	127.66	120.28
5	G	349	LEU	C-N-CA	5.50	127.66	120.28
5	H	44	MET	N-CA-C	-5.50	102.37	110.52
5	I	226	GLU	N-CA-C	-5.50	107.22	114.04
5	O	312	ARG	NE-CZ-NH2	5.50	124.15	119.20
5	E	312	ARG	NE-CZ-NH2	5.50	124.15	119.20
5	K	137	GLN	CA-C-O	-5.50	115.22	121.00
5	D	44	MET	N-CA-C	-5.50	102.38	110.52
5	K	200	PHE	CA-C-O	5.50	127.88	121.11
5	D	275	HIS	CB-CG-CD2	-5.50	124.05	131.20
5	F	116	ARG	N-CA-C	-5.50	105.29	111.28
5	F	349	LEU	CA-C-N	5.50	127.65	120.28
5	F	349	LEU	C-N-CA	5.50	127.65	120.28
5	M	312	ARG	NE-CZ-NH2	5.50	124.15	119.20
5	I	275	HIS	CB-CG-CD2	-5.50	124.05	131.20
5	N	275	HIS	CB-CG-CD2	-5.50	124.05	131.20
5	D	200	PHE	CA-C-O	5.49	127.87	121.11
5	H	226	GLU	N-CA-C	-5.49	107.23	114.04
5	L	31	PHE	CA-CB-CG	5.49	119.29	113.80
4	V	190	LEU	N-CA-C	5.49	119.95	112.04
5	R	44	MET	N-CA-C	-5.49	102.39	110.52
5	O	275	HIS	CB-CG-CD2	-5.49	124.06	131.20
5	H	137	GLN	CA-C-O	-5.49	115.24	121.00
5	P	44	MET	N-CA-C	-5.49	102.40	110.52
5	Q	137	GLN	CA-C-O	-5.49	115.24	121.00
5	E	137	GLN	CA-C-O	-5.49	115.24	121.00
5	N	226	GLU	N-CA-C	-5.49	107.24	114.04
5	H	275	HIS	CB-CG-CD2	-5.49	124.07	131.20
5	K	312	ARG	NE-CZ-NH2	5.49	124.14	119.20
5	N	312	ARG	NE-CZ-NH2	5.48	124.14	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	44	MET	N-CA-C	-5.48	102.41	110.52
5	P	275	HIS	CB-CG-CD2	-5.48	124.07	131.20
5	F	137	GLN	CA-C-O	-5.48	115.25	121.00
5	K	226	GLU	N-CA-C	-5.48	107.25	114.04
5	I	200	PHE	CA-C-O	5.48	127.85	121.11
4	U	56	ALA	CA-C-O	5.48	126.33	120.20
5	J	200	PHE	CA-C-O	5.47	127.84	121.11
5	S	200	PHE	CA-C-O	5.47	127.84	121.11
5	L	257	CYS	N-CA-CB	-5.47	105.19	110.39
5	M	200	PHE	CA-C-O	5.47	127.84	121.11
5	P	312	ARG	NE-CZ-NH2	5.47	124.12	119.20
5	F	31	PHE	CA-CB-CG	5.47	119.27	113.80
4	U	42	LYS	CA-C-O	5.47	126.06	119.61
5	G	275	HIS	CB-CG-CD2	-5.47	124.09	131.20
5	M	137	GLN	CA-C-O	-5.47	115.26	121.00
5	H	312	ARG	NE-CZ-NH2	5.46	124.12	119.20
5	O	137	GLN	CA-C-O	-5.46	115.26	121.00
5	S	137	GLN	CA-C-O	-5.46	115.26	121.00
5	F	200	PHE	CA-C-O	5.46	127.83	121.11
5	R	200	PHE	CA-C-O	5.46	127.83	121.11
4	V	220	VAL	N-CA-C	5.46	116.19	110.62
5	E	200	PHE	CA-C-O	5.46	127.82	121.11
5	G	137	GLN	CA-C-O	-5.46	115.27	121.00
5	H	200	PHE	CA-C-O	5.46	127.82	121.11
5	I	349	LEU	CA-C-N	5.46	127.59	120.28
5	I	349	LEU	C-N-CA	5.46	127.59	120.28
5	L	312	ARG	NE-CZ-NH2	5.46	124.11	119.20
5	D	312	ARG	NE-CZ-NH2	5.45	124.11	119.20
5	F	226	GLU	N-CA-C	-5.45	107.28	114.04
5	K	257	CYS	N-CA-CB	-5.45	105.21	110.39
5	S	226	GLU	N-CA-C	-5.45	107.28	114.04
4	B	36	LEU	CB-CA-C	-5.45	101.63	110.79
4	B	56	ALA	CA-C-O	5.45	126.31	120.20
5	G	200	PHE	CA-C-O	5.45	127.81	121.11
5	J	349	LEU	CA-C-N	5.45	127.58	120.28
5	J	349	LEU	C-N-CA	5.45	127.58	120.28
5	P	200	PHE	CA-C-O	5.45	127.81	121.11
4	V	45	GLY	O-C-N	-5.45	115.61	122.70
4	A	45	GLY	O-C-N	-5.45	115.62	122.70
5	D	226	GLU	N-CA-C	-5.45	107.28	114.04
5	H	116	ARG	N-CA-C	-5.45	105.34	111.28
5	P	77	THR	N-CA-CB	-5.45	102.52	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	226	GLU	N-CA-C	-5.45	107.28	114.04
5	Q	275	HIS	CB-CG-CD2	-5.45	124.12	131.20
5	R	262	PHE	CA-CB-CG	-5.45	108.35	113.80
4	A	220	VAL	N-CA-C	5.45	116.18	110.62
5	D	137	GLN	CA-C-O	-5.45	115.28	121.00
5	L	226	GLU	N-CA-C	-5.44	107.29	114.04
4	U	6	LEU	N-CA-C	5.44	116.89	111.07
4	B	42	LYS	CA-C-O	5.44	126.03	119.61
5	K	349	LEU	CA-C-N	5.44	127.57	120.28
5	K	349	LEU	C-N-CA	5.44	127.57	120.28
5	P	79	TRP	CG-CD2-CE3	5.44	139.34	133.90
5	L	200	PHE	CA-C-O	5.44	127.80	121.11
5	L	262	PHE	CA-CB-CG	-5.44	108.36	113.80
5	O	237	GLU	N-CA-C	5.44	117.31	110.24
5	O	226	GLU	N-CA-C	-5.44	107.30	114.04
5	R	226	GLU	N-CA-C	-5.44	107.30	114.04
5	I	116	ARG	N-CA-C	-5.43	105.36	111.28
5	K	116	ARG	N-CA-C	-5.43	105.36	111.28
5	O	31	PHE	CA-CB-CG	5.43	119.23	113.80
4	B	260	TYR	N-CA-CB	5.43	118.06	110.07
5	D	116	ARG	N-CA-C	-5.43	105.36	111.28
5	N	79	TRP	CG-CD2-CE3	5.43	139.33	133.90
5	P	257	CYS	N-CA-CB	-5.43	105.23	110.39
5	O	116	ARG	N-CA-C	-5.43	105.36	111.28
4	A	168	ASP	CA-C-O	5.43	126.06	119.49
5	E	226	GLU	N-CA-C	-5.43	107.31	114.04
5	F	237	GLU	N-CA-C	5.43	117.29	110.24
4	U	36	LEU	CB-CA-C	-5.43	101.67	110.79
5	J	116	ARG	N-CA-C	-5.42	105.37	111.28
5	J	237	GLU	N-CA-C	5.42	117.29	110.24
5	M	226	GLU	N-CA-C	-5.42	107.31	114.04
5	N	137	GLN	CA-C-O	-5.42	115.30	121.00
5	Q	79	TRP	CG-CD2-CE3	5.42	139.32	133.90
5	E	237	GLU	N-CA-C	5.42	117.29	110.24
5	F	257	CYS	N-CA-CB	-5.42	105.24	110.39
4	A	91	GLU	CA-C-O	5.42	126.05	119.49
5	J	226	GLU	N-CA-C	-5.42	107.32	114.04
5	G	116	ARG	N-CA-C	-5.42	105.37	111.28
5	H	349	LEU	CA-C-N	5.42	127.54	120.28
5	H	349	LEU	C-N-CA	5.42	127.54	120.28
5	M	237	GLU	N-CA-C	5.42	117.28	110.24
4	U	260	TYR	N-CA-CB	5.42	118.03	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	260	TYR	N-CA-CB	5.42	118.03	110.07
5	G	226	GLU	N-CA-C	-5.42	107.33	114.04
5	E	31	PHE	CA-CB-CG	5.41	119.21	113.80
5	J	257	CYS	N-CA-CB	-5.41	105.25	110.39
5	R	237	GLU	N-CA-C	5.41	117.28	110.24
5	E	116	ARG	N-CA-C	-5.41	105.38	111.28
5	G	312	ARG	NE-CZ-NH2	5.41	124.07	119.20
5	K	79	TRP	CG-CD2-CE3	5.41	139.31	133.90
5	S	116	ARG	N-CA-C	-5.41	105.38	111.28
5	Q	116	ARG	N-CA-C	-5.41	105.38	111.28
5	H	31	PHE	CA-CB-CG	5.41	119.21	113.80
5	L	349	LEU	CA-C-N	5.41	127.53	120.28
5	L	349	LEU	C-N-CA	5.41	127.53	120.28
5	I	31	PHE	CA-CB-CG	5.41	119.21	113.80
5	K	31	PHE	CA-CB-CG	5.41	119.21	113.80
5	O	200	PHE	CA-C-O	5.41	127.76	121.11
5	S	237	GLU	N-CA-C	5.41	117.27	110.24
5	N	116	ARG	N-CA-C	-5.40	105.39	111.28
5	O	79	TRP	CG-CD2-CE3	5.40	139.30	133.90
5	G	31	PHE	CA-CB-CG	5.40	119.20	113.80
5	R	257	CYS	N-CA-CB	-5.40	105.26	110.39
5	L	91	TYR	N-CA-C	5.40	119.03	112.23
5	L	237	GLU	N-CA-C	5.40	117.26	110.24
5	N	237	GLU	N-CA-C	5.40	117.26	110.24
5	P	31	PHE	CA-CB-CG	5.40	119.20	113.80
5	P	349	LEU	CA-C-N	5.40	127.52	120.28
5	P	349	LEU	C-N-CA	5.40	127.52	120.28
5	I	137	GLN	CA-C-O	-5.40	115.33	121.00
5	I	257	CYS	N-CA-CB	-5.40	105.26	110.39
4	A	74	ALA	O-C-N	-5.40	116.40	122.12
5	K	237	GLU	N-CA-C	5.40	117.26	110.24
5	R	91	TYR	N-CA-C	5.39	119.02	112.23
4	T	260	TYR	N-CA-CB	5.39	118.00	110.07
5	L	137	GLN	CA-C-O	-5.39	115.34	121.00
5	R	349	LEU	CA-C-N	5.39	127.50	120.28
5	R	349	LEU	C-N-CA	5.39	127.50	120.28
5	J	31	PHE	CA-CB-CG	5.39	119.19	113.80
5	O	257	CYS	N-CA-CB	-5.39	105.27	110.39
5	M	257	CYS	N-CA-CB	-5.38	105.28	110.39
5	H	77	THR	N-CA-CB	-5.38	102.61	110.47
5	S	79	TRP	CG-CD2-CE3	5.38	139.28	133.90
4	B	6	LEU	N-CA-C	5.38	116.82	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	79	TRP	CG-CD2-CE3	5.38	139.28	133.90
5	H	237	GLU	N-CA-C	5.38	117.23	110.24
5	I	77	THR	N-CA-CB	-5.38	102.62	110.47
4	V	91	GLU	CA-C-O	5.38	126.00	119.49
5	S	257	CYS	N-CA-CB	-5.37	105.28	110.39
4	U	245	SER	O-C-N	-5.37	115.66	122.27
5	M	79	TRP	CG-CD2-CE3	5.37	139.27	133.90
4	B	231	ARG	CB-CG-CD	-5.37	98.95	111.30
5	M	31	PHE	CA-CB-CG	5.37	119.17	113.80
5	N	31	PHE	CA-CB-CG	5.37	119.17	113.80
4	W	245	SER	O-C-N	-5.37	115.67	122.27
4	B	155	TYR	CG-CD1-CE1	-5.37	113.15	121.20
5	N	257	CYS	N-CA-CB	-5.37	105.29	110.39
5	Q	91	TYR	N-CA-C	5.37	118.99	112.23
5	G	77	THR	N-CA-CB	-5.36	102.64	110.47
5	G	79	TRP	CG-CD2-CE3	5.36	139.26	133.90
5	O	77	THR	N-CA-CB	-5.36	102.64	110.47
5	R	137	GLN	CA-C-O	-5.36	115.37	121.00
5	E	77	THR	N-CA-CB	-5.36	102.64	110.47
5	F	77	THR	N-CA-CB	-5.36	102.64	110.47
5	J	91	TYR	N-CA-C	5.36	118.98	112.23
5	Q	31	PHE	CA-CB-CG	5.36	119.16	113.80
5	K	349	LEU	O-C-N	5.36	129.46	122.87
5	N	77	THR	N-CA-CB	-5.36	102.65	110.47
4	U	45	GLY	O-C-N	-5.36	115.73	122.70
4	A	93	ASP	N-CA-C	-5.36	104.85	111.33
5	H	349	LEU	O-C-N	5.35	129.46	122.87
5	G	91	TYR	N-CA-C	5.35	118.97	112.23
5	L	77	THR	N-CA-CB	-5.35	102.66	110.47
5	Q	77	THR	N-CA-CB	-5.35	102.66	110.47
4	B	197	LEU	CB-CA-C	-5.35	102.45	110.90
5	D	237	GLU	N-CA-C	5.35	117.19	110.24
5	H	251	GLY	O-C-N	5.35	129.65	122.70
4	V	99	LEU	N-CA-C	5.35	116.92	111.14
4	U	155	TYR	CG-CD1-CE1	-5.35	113.18	121.20
4	V	168	ASP	CA-C-O	5.35	125.96	119.49
5	M	91	TYR	N-CA-C	5.35	118.97	112.23
5	R	116	ARG	N-CA-C	-5.35	105.45	111.28
5	P	91	TYR	N-CA-C	5.34	118.97	112.23
5	R	349	LEU	O-C-N	5.34	129.44	122.87
5	M	116	ARG	N-CA-C	-5.34	105.46	111.28
5	P	349	LEU	O-C-N	5.34	129.44	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	237	GLU	N-CA-C	5.34	117.19	110.24
5	Q	251	GLY	O-C-N	5.34	129.65	122.70
5	G	349	LEU	O-C-N	5.34	129.44	122.87
5	P	237	GLU	N-CA-C	5.34	117.18	110.24
4	B	93	ASP	N-CA-C	-5.34	104.87	111.33
4	U	197	LEU	CB-CA-C	-5.34	102.46	110.90
5	I	91	TYR	N-CA-C	5.34	118.96	112.23
4	B	245	SER	O-C-N	-5.34	115.70	122.27
5	Q	257	CYS	N-CA-CB	-5.34	105.32	110.39
5	R	79	TRP	CG-CD2-CE3	5.34	139.24	133.90
5	N	332	PRO	CA-C-N	5.33	124.67	118.85
5	N	332	PRO	C-N-CA	5.33	124.67	118.85
5	R	77	THR	N-CA-CB	-5.33	102.69	110.47
5	L	116	ARG	N-CA-C	-5.33	105.47	111.28
5	N	356	TRP	CE2-CD2-CG	-5.33	100.81	107.20
5	K	77	THR	N-CA-CB	-5.33	102.69	110.47
4	A	99	LEU	N-CA-C	5.33	116.89	111.14
5	M	356	TRP	CE2-CD2-CG	-5.33	100.81	107.20
5	P	332	PRO	CA-C-N	5.33	124.65	118.85
5	P	332	PRO	C-N-CA	5.33	124.65	118.85
5	S	31	PHE	CA-CB-CG	5.33	119.12	113.80
5	S	91	TYR	N-CA-C	5.33	118.94	112.23
5	G	332	PRO	CA-C-N	5.32	124.65	118.85
5	G	332	PRO	C-N-CA	5.32	124.65	118.85
5	O	91	TYR	N-CA-C	5.32	118.93	112.23
4	U	231	ARG	CB-CG-CD	-5.32	99.06	111.30
5	I	237	GLU	N-CA-C	5.32	117.15	110.24
5	I	349	LEU	O-C-N	5.32	129.41	122.87
5	L	349	LEU	O-C-N	5.32	129.41	122.87
5	J	251	GLY	O-C-N	5.32	129.61	122.70
5	N	251	GLY	O-C-N	5.32	129.61	122.70
5	R	251	GLY	O-C-N	5.32	129.61	122.70
5	J	79	TRP	CG-CD2-CE3	5.31	139.21	133.90
5	M	77	THR	N-CA-CB	-5.31	102.71	110.47
5	D	91	TYR	N-CA-C	5.31	118.92	112.23
5	E	332	PRO	CA-C-N	5.31	124.64	118.85
5	E	332	PRO	C-N-CA	5.31	124.64	118.85
5	H	257	CYS	N-CA-CB	-5.31	105.34	110.39
5	I	79	TRP	CG-CD2-CE3	5.31	139.21	133.90
5	J	77	THR	N-CA-CB	-5.31	102.72	110.47
5	L	332	PRO	CA-C-N	5.31	124.64	118.85
5	L	332	PRO	C-N-CA	5.31	124.64	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	251	GLY	O-C-N	5.31	129.60	122.70
5	L	79	TRP	CG-CD2-CE3	5.31	139.21	133.90
5	R	332	PRO	CA-C-N	5.31	124.64	118.85
5	R	332	PRO	C-N-CA	5.31	124.64	118.85
4	V	93	ASP	N-CA-C	-5.31	104.91	111.33
4	V	74	ALA	O-C-N	-5.31	116.50	122.12
5	G	237	GLU	N-CA-C	5.30	117.14	110.24
4	U	155	TYR	CB-CA-C	5.30	120.97	110.42
5	H	79	TRP	CG-CD2-CE3	5.30	139.20	133.90
5	D	251	GLY	O-C-N	5.30	129.59	122.70
4	A	155	TYR	O-C-N	-5.30	115.89	122.25
4	B	155	TYR	CB-CA-C	5.30	120.96	110.42
5	F	79	TRP	CG-CD2-CE3	5.30	139.20	133.90
5	S	356	TRP	CE2-CD2-CG	-5.30	100.84	107.20
5	J	101	HIS	CA-C-O	-5.29	114.78	119.86
5	M	251	GLY	O-C-N	5.29	129.58	122.70
4	T	245	SER	O-C-N	-5.29	115.76	122.27
5	D	101	HIS	CA-C-O	-5.29	114.78	119.86
5	G	257	CYS	N-CA-CB	-5.29	105.36	110.39
5	L	251	GLY	O-C-N	5.29	129.58	122.70
5	G	251	GLY	O-C-N	5.29	129.57	122.70
5	J	349	LEU	O-C-N	5.29	129.37	122.87
5	S	77	THR	N-CA-CB	-5.29	102.75	110.47
4	V	56	ALA	CA-C-O	5.29	126.12	120.20
5	D	77	THR	N-CA-CB	-5.28	102.75	110.47
5	O	349	LEU	O-C-N	5.28	129.37	122.87
5	Q	332	PRO	CA-C-N	5.28	124.61	118.85
5	Q	332	PRO	C-N-CA	5.28	124.61	118.85
5	E	91	TYR	N-CA-C	5.28	118.89	112.23
4	A	56	ALA	CA-C-O	5.28	126.11	120.20
5	N	62	ARG	CA-CB-CG	5.28	124.66	114.10
4	U	93	ASP	N-CA-C	-5.28	104.94	111.33
5	F	91	TYR	N-CA-C	5.28	118.88	112.23
5	S	332	PRO	CA-C-N	5.28	124.61	118.85
5	S	332	PRO	C-N-CA	5.28	124.61	118.85
5	D	356	TRP	CE2-CD2-CG	-5.28	100.87	107.20
5	E	257	CYS	N-CA-CB	-5.28	105.38	110.39
4	V	155	TYR	O-C-N	-5.28	115.92	122.25
5	J	332	PRO	CA-C-N	5.27	124.60	118.85
5	J	332	PRO	C-N-CA	5.27	124.60	118.85
5	O	251	GLY	O-C-N	5.27	129.56	122.70
5	K	91	TYR	N-CA-C	5.27	118.87	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	251	GLY	O-C-N	5.27	129.55	122.70
5	E	349	LEU	O-C-N	5.27	129.35	122.87
5	G	356	TRP	CE2-CD2-CG	-5.27	100.88	107.20
5	M	332	PRO	CA-C-N	5.27	124.59	118.85
5	M	332	PRO	C-N-CA	5.27	124.59	118.85
4	B	45	GLY	O-C-N	-5.26	115.86	122.70
5	F	349	LEU	O-C-N	5.26	129.34	122.87
5	I	251	GLY	O-C-N	5.26	129.54	122.70
5	D	257	CYS	N-CA-CB	-5.26	105.39	110.39
4	V	259	LYS	CA-C-N	-5.25	112.37	120.88
4	V	259	LYS	C-N-CA	-5.25	112.37	120.88
4	X	259	LYS	CA-C-N	-5.25	112.37	120.88
4	X	259	LYS	C-N-CA	-5.25	112.37	120.88
5	D	79	TRP	CG-CD2-CE3	5.25	139.15	133.90
5	L	62	ARG	CA-CB-CG	5.25	124.61	114.10
5	S	251	GLY	O-C-N	5.25	129.53	122.70
5	D	62	ARG	CA-CB-CG	5.25	124.60	114.10
5	E	62	ARG	CA-CB-CG	5.25	124.60	114.10
5	P	252	ASN	CB-CG-ND2	5.25	124.28	116.40
5	R	356	TRP	CE2-CD2-CG	-5.25	100.90	107.20
5	J	62	ARG	CA-CB-CG	5.25	124.60	114.10
5	K	332	PRO	CA-C-N	5.25	124.57	118.85
5	K	332	PRO	C-N-CA	5.25	124.57	118.85
5	R	62	ARG	CA-CB-CG	5.25	124.60	114.10
5	O	332	PRO	CA-C-N	5.25	124.57	118.85
5	O	332	PRO	C-N-CA	5.25	124.57	118.85
5	K	62	ARG	CA-CB-CG	5.24	124.58	114.10
5	L	356	TRP	CE2-CD2-CG	-5.24	100.91	107.20
5	O	62	ARG	CA-CB-CG	5.24	124.58	114.10
5	E	252	ASN	CB-CG-ND2	5.24	124.26	116.40
5	S	62	ARG	CA-CB-CG	5.24	124.58	114.10
5	J	356	TRP	CE2-CD2-CG	-5.24	100.91	107.20
5	M	62	ARG	CA-CB-CG	5.24	124.58	114.10
5	F	62	ARG	CA-CB-CG	5.24	124.58	114.10
5	E	251	GLY	O-C-N	5.24	129.51	122.70
5	Q	101	HIS	CA-C-O	-5.24	114.83	119.86
5	H	332	PRO	CA-C-N	5.24	124.56	118.85
5	H	332	PRO	C-N-CA	5.24	124.56	118.85
5	I	62	ARG	CA-CB-CG	5.24	124.57	114.10
5	N	22	ALA	N-CA-C	-5.24	102.30	110.10
5	P	101	HIS	CA-C-O	-5.24	114.83	119.86
5	Q	62	ARG	CA-CB-CG	5.24	124.57	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	259	LYS	CA-C-N	-5.24	112.40	120.88
4	U	259	LYS	C-N-CA	-5.24	112.40	120.88
5	F	356	TRP	CE2-CD2-CG	-5.23	100.92	107.20
5	H	252	ASN	CB-CG-ND2	5.23	124.25	116.40
5	I	332	PRO	CA-C-N	5.23	124.55	118.85
5	I	332	PRO	C-N-CA	5.23	124.55	118.85
5	P	62	ARG	CA-CB-CG	5.23	124.56	114.10
5	Q	356	TRP	CE2-CD2-CG	-5.23	100.92	107.20
5	D	349	LEU	O-C-N	5.23	129.30	122.87
5	I	101	HIS	CA-C-O	-5.23	114.84	119.86
4	B	91	GLU	CA-C-O	5.23	125.82	119.49
5	I	252	ASN	CB-CG-ND2	5.23	124.24	116.40
4	W	259	LYS	CA-C-N	-5.23	112.41	120.88
4	W	259	LYS	C-N-CA	-5.23	112.41	120.88
5	G	62	ARG	CA-CB-CG	5.22	124.55	114.10
5	H	91	TYR	N-CA-C	5.22	118.81	112.23
5	Q	22	ALA	N-CA-C	-5.22	102.32	110.10
5	D	332	PRO	CA-C-N	5.22	124.54	118.85
5	D	332	PRO	C-N-CA	5.22	124.54	118.85
5	E	22	ALA	N-CA-C	-5.22	102.32	110.10
5	I	274	ILE	N-CA-CB	-5.22	102.61	111.23
5	S	252	ASN	CB-CG-ND2	5.22	124.23	116.40
5	Q	252	ASN	CB-CG-ND2	5.22	124.23	116.40
5	F	360	GLN	CB-CG-CD	5.22	121.47	112.60
5	K	356	TRP	CE2-CD2-CG	-5.22	100.94	107.20
5	S	349	LEU	O-C-N	5.22	129.29	122.87
5	K	251	GLY	O-C-N	5.22	129.48	122.70
4	A	259	LYS	CA-C-N	-5.22	112.43	120.88
4	A	259	LYS	C-N-CA	-5.22	112.43	120.88
5	I	22	ALA	N-CA-C	-5.22	102.33	110.10
5	N	40	HIS	CB-CG-CD2	-5.22	124.42	131.20
5	D	233	SER	O-C-N	5.21	129.52	122.59
5	G	252	ASN	CB-CG-ND2	5.21	124.22	116.40
3	5	74	VAL	CB-CA-C	-5.21	105.10	112.14
5	D	22	ALA	N-CA-C	-5.21	102.34	110.10
5	L	252	ASN	CB-CG-ND2	5.21	124.21	116.40
5	M	349	LEU	O-C-N	5.21	129.28	122.87
5	P	360	GLN	CB-CG-CD	5.21	121.45	112.60
4	B	2	GLN	N-CA-C	5.21	117.36	111.11
5	H	62	ARG	CA-CB-CG	5.21	124.51	114.10
5	J	227	MET	N-CA-C	-5.21	105.52	111.14
5	K	22	ALA	N-CA-C	-5.21	102.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	252	ASN	CB-CG-ND2	5.21	124.21	116.40
5	O	356	TRP	CE2-CD2-CG	-5.21	100.95	107.20
5	Q	349	LEU	O-C-N	5.20	129.27	122.87
5	K	274	ILE	N-CA-CB	-5.20	102.65	111.23
5	N	349	LEU	O-C-N	5.20	129.27	122.87
4	C	259	LYS	CA-C-N	-5.20	112.45	120.88
4	C	259	LYS	C-N-CA	-5.20	112.45	120.88
5	H	34	ILE	CA-CB-CG1	5.20	119.24	110.40
5	I	34	ILE	CA-CB-CG1	5.20	119.24	110.40
5	K	101	HIS	CA-C-O	-5.20	114.87	119.86
5	F	22	ALA	N-CA-C	-5.20	102.36	110.10
5	O	274	ILE	N-CA-CB	-5.20	102.65	111.23
5	P	356	TRP	CE2-CD2-CG	-5.20	100.96	107.20
5	D	71	ILE	N-CA-CB	-5.20	105.86	112.15
5	E	356	TRP	CE2-CD2-CG	-5.20	100.97	107.20
5	F	332	PRO	CA-C-N	5.20	124.51	118.85
5	F	332	PRO	C-N-CA	5.20	124.51	118.85
5	R	252	ASN	CB-CG-ND2	5.20	124.19	116.40
5	J	22	ALA	N-CA-C	-5.19	102.36	110.10
5	K	248	ILE	N-CA-CB	-5.19	103.39	110.56
5	Q	34	ILE	CA-CB-CG1	5.19	119.23	110.40
5	R	274	ILE	N-CA-CB	-5.19	102.66	111.23
5	G	50	LYS	CB-CG-CD	-5.19	99.36	111.30
5	I	356	TRP	CE2-CD2-CG	-5.19	100.97	107.20
5	J	34	ILE	CA-CB-CG1	5.19	119.23	110.40
5	L	22	ALA	N-CA-C	-5.19	102.36	110.10
5	N	91	TYR	N-CA-C	5.19	118.77	112.23
5	G	40	HIS	CB-CG-CD2	-5.19	124.45	131.20
5	M	22	ALA	N-CA-C	-5.19	102.37	110.10
3	8	74	VAL	CB-CA-C	-5.19	105.13	112.14
5	N	274	ILE	N-CA-CB	-5.19	102.67	111.23
5	S	248	ILE	N-CA-CB	-5.19	103.40	110.56
4	T	259	LYS	CA-C-N	-5.19	112.47	120.88
4	T	259	LYS	C-N-CA	-5.19	112.47	120.88
5	J	252	ASN	CB-CG-ND2	5.19	124.18	116.40
5	M	274	ILE	N-CA-CB	-5.19	102.67	111.23
5	S	22	ALA	N-CA-C	-5.19	102.37	110.10
5	H	22	ALA	N-CA-C	-5.18	102.37	110.10
5	M	360	GLN	CB-CG-CD	5.18	121.42	112.60
5	P	22	ALA	N-CA-C	-5.18	102.38	110.10
5	R	22	ALA	N-CA-C	-5.18	102.37	110.10
4	U	253	LEU	CB-CA-C	-5.18	102.91	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	274	ILE	N-CA-CB	-5.18	102.68	111.23
5	O	71	ILE	N-CA-CB	-5.18	105.88	112.15
5	F	71	ILE	N-CA-CB	-5.18	105.88	112.15
5	Q	274	ILE	N-CA-CB	-5.18	102.68	111.23
5	S	274	ILE	N-CA-CB	-5.18	102.68	111.23
4	W	253	LEU	CB-CA-C	-5.18	102.92	110.95
5	E	274	ILE	N-CA-CB	-5.18	102.69	111.23
5	F	248	ILE	N-CA-CB	-5.18	103.42	110.56
5	P	274	ILE	N-CA-CB	-5.18	102.69	111.23
5	D	50	LYS	CB-CG-CD	-5.17	99.40	111.30
5	D	274	ILE	N-CA-CB	-5.17	102.69	111.23
5	J	40	HIS	CB-CG-CD2	-5.17	124.47	131.20
5	J	274	ILE	N-CA-CB	-5.17	102.69	111.23
5	S	360	GLN	CB-CG-CD	5.17	121.39	112.60
5	G	274	ILE	N-CA-CB	-5.17	102.70	111.23
5	H	360	GLN	CB-CG-CD	5.17	121.39	112.60
5	J	50	LYS	CB-CG-CD	-5.17	99.41	111.30
5	O	248	ILE	N-CA-CB	-5.17	103.42	110.56
5	L	360	GLN	CB-CG-CD	5.17	121.39	112.60
1	9	70	GLY	N-CA-C	-5.17	107.12	115.08
4	B	259	LYS	CA-C-N	-5.17	112.51	120.88
4	B	259	LYS	C-N-CA	-5.17	112.51	120.88
5	F	274	ILE	N-CA-CB	-5.17	102.70	111.23
5	G	101	HIS	CA-C-O	-5.17	114.90	119.86
5	N	360	GLN	CB-CG-CD	5.17	121.39	112.60
5	R	233	SER	O-C-N	5.17	129.46	122.59
3	2	131	LYS	N-CA-C	5.17	117.03	107.73
5	F	252	ASN	CB-CG-ND2	5.17	124.15	116.40
5	G	22	ALA	N-CA-C	-5.17	102.40	110.10
5	L	34	ILE	CA-CB-CG1	5.17	119.18	110.40
5	L	101	HIS	CA-C-O	-5.17	114.90	119.86
5	M	248	ILE	N-CA-CB	-5.17	103.43	110.56
3	Z	131	LYS	N-CA-C	5.17	117.03	107.73
5	O	22	ALA	N-CA-C	-5.17	102.40	110.10
5	E	50	LYS	CB-CG-CD	-5.16	99.42	111.30
5	F	50	LYS	CB-CG-CD	-5.16	99.42	111.30
5	G	71	ILE	N-CA-CB	-5.16	105.90	112.15
5	H	274	ILE	N-CA-CB	-5.16	102.71	111.23
5	D	360	GLN	CB-CG-CD	5.16	121.38	112.60
5	K	252	ASN	CB-CG-ND2	5.16	124.14	116.40
5	L	266	PHE	CA-CB-CG	5.16	118.96	113.80
5	M	40	HIS	CB-CG-CD2	-5.16	124.49	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	34	ILE	CA-CB-CG1	5.16	119.17	110.40
5	Q	71	ILE	N-CA-CB	-5.16	105.91	112.15
5	H	71	ILE	N-CA-CB	-5.16	105.91	112.15
5	K	34	ILE	CA-CB-CG1	5.16	119.17	110.40
1	3	70	GLY	N-CA-C	-5.16	107.14	115.08
1	6	70	GLY	N-CA-C	-5.16	107.14	115.08
5	D	252	ASN	CB-CG-ND2	5.16	124.13	116.40
5	I	248	ILE	N-CA-CB	-5.16	103.45	110.56
5	S	50	LYS	CB-CG-CD	-5.16	99.44	111.30
4	V	35	GLU	CA-C-O	5.16	125.97	120.20
5	E	360	GLN	CB-CG-CD	5.15	121.36	112.60
3	5	131	LYS	N-CA-C	5.15	117.00	107.73
5	F	149	THR	CA-CB-OG1	-5.15	101.87	109.60
5	H	266	PHE	CA-CB-CG	5.15	118.95	113.80
5	K	50	LYS	CB-CG-CD	-5.15	99.45	111.30
5	N	34	ILE	CA-CB-CG1	5.15	119.16	110.40
5	S	71	ILE	N-CA-CB	-5.15	105.92	112.15
5	N	50	LYS	CB-CG-CD	-5.15	99.46	111.30
5	N	101	HIS	CA-C-O	-5.15	114.92	119.86
5	P	248	ILE	N-CA-CB	-5.15	103.45	110.56
5	E	101	HIS	CA-C-O	-5.15	114.92	119.86
5	H	248	ILE	N-CA-CB	-5.15	103.45	110.56
5	E	71	ILE	N-CA-CB	-5.15	105.92	112.15
5	Q	40	HIS	CB-CG-CD2	-5.15	124.51	131.20
5	R	71	ILE	N-CA-CB	-5.15	105.92	112.15
5	S	40	HIS	CB-CG-CD2	-5.15	124.51	131.20
5	O	40	HIS	CB-CG-CD2	-5.14	124.51	131.20
5	P	40	HIS	CB-CG-CD2	-5.14	124.51	131.20
5	R	34	ILE	CA-CB-CG1	5.14	119.15	110.40
5	F	34	ILE	CA-CB-CG1	5.14	119.14	110.40
5	H	50	LYS	CB-CG-CD	-5.14	99.47	111.30
5	J	71	ILE	N-CA-CB	-5.14	105.93	112.15
5	L	233	SER	O-C-N	5.14	129.43	122.59
5	L	50	LYS	CB-CG-CD	-5.14	99.48	111.30
5	M	149	THR	CA-CB-OG1	-5.14	101.89	109.60
5	O	233	SER	O-C-N	5.14	129.43	122.59
5	O	252	ASN	CB-CG-ND2	5.14	124.11	116.40
5	H	101	HIS	CA-C-O	-5.14	114.93	119.86
5	S	34	ILE	CA-CB-CG1	5.14	119.13	110.40
5	G	34	ILE	CA-CB-CG1	5.14	119.13	110.40
5	K	40	HIS	CB-CG-CD2	-5.14	124.52	131.20
5	O	50	LYS	CB-CG-CD	-5.14	99.48	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	248	ILE	N-CA-CB	-5.14	103.47	110.56
5	R	50	LYS	CB-CG-CD	-5.14	99.49	111.30
5	D	40	HIS	CB-CG-CD2	-5.13	124.53	131.20
5	E	217	CYS	CA-CB-SG	-5.13	102.59	114.40
5	N	252	ASN	CB-CG-ND2	5.13	124.10	116.40
5	Q	371	HIS	CB-CG-CD2	-5.13	124.53	131.20
5	G	233	SER	O-C-N	5.13	129.41	122.59
5	H	356	TRP	CE2-CD2-CG	-5.13	101.04	107.20
5	N	248	ILE	N-CA-CB	-5.13	103.48	110.56
5	P	371	HIS	CB-CG-CD2	-5.13	124.53	131.20
5	Q	360	GLN	CB-CG-CD	5.13	121.32	112.60
5	S	101	HIS	CA-C-O	-5.13	114.94	119.86
5	S	149	THR	CA-CB-OG1	-5.13	101.90	109.60
5	I	227	MET	N-CA-C	-5.13	105.60	111.14
5	K	71	ILE	N-CA-CB	-5.13	105.94	112.15
5	E	248	ILE	N-CA-CB	-5.13	103.48	110.56
5	O	360	GLN	CB-CG-CD	5.13	121.32	112.60
5	P	34	ILE	CA-CB-CG1	5.13	119.12	110.40
5	I	50	LYS	CB-CG-CD	-5.13	99.51	111.30
5	M	50	LYS	CB-CG-CD	-5.13	99.51	111.30
5	M	101	HIS	CA-C-O	-5.13	114.94	119.86
5	Q	50	LYS	CB-CG-CD	-5.13	99.51	111.30
1	0	70	GLY	N-CA-C	-5.12	107.19	115.08
5	G	360	GLN	CB-CG-CD	5.12	121.31	112.60
5	J	360	GLN	CB-CG-CD	5.12	121.31	112.60
5	M	34	ILE	CA-CB-CG1	5.12	119.11	110.40
5	D	217	CYS	CA-CB-SG	-5.12	102.62	114.40
5	F	233	SER	O-C-N	5.12	129.40	122.59
5	I	360	GLN	CB-CG-CD	5.12	121.31	112.60
5	N	227	MET	N-CA-C	-5.12	105.61	111.14
5	O	101	HIS	CA-C-O	-5.12	114.94	119.86
4	U	2	GLN	N-CA-C	5.12	117.25	111.11
4	V	245	SER	O-C-N	-5.12	115.97	122.27
5	E	34	ILE	CA-CB-CG1	5.12	119.10	110.40
5	P	217	CYS	CA-CB-SG	-5.12	102.62	114.40
4	A	245	SER	O-C-N	-5.12	115.97	122.27
5	L	71	ILE	N-CA-CB	-5.12	105.96	112.15
5	R	248	ILE	N-CA-CB	-5.12	103.50	110.56
3	8	131	LYS	N-CA-C	5.12	116.94	107.73
5	H	40	HIS	CB-CG-CD2	-5.12	124.55	131.20
5	N	233	SER	O-C-N	5.12	129.39	122.59
5	R	360	GLN	CB-CG-CD	5.12	121.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	233	SER	O-C-N	5.11	129.39	122.59
4	X	245	SER	O-C-N	-5.11	115.98	122.27
5	N	71	ILE	N-CA-CB	-5.11	105.97	112.15
4	U	91	GLU	CA-C-O	5.11	125.67	119.49
2	Y	233	GLU	N-CA-C	-5.11	105.71	111.28
5	L	40	HIS	CB-CG-CD2	-5.11	124.56	131.20
5	M	356	TRP	CG-CD2-CE3	5.11	139.01	133.90
5	P	50	LYS	CB-CG-CD	-5.11	99.56	111.30
5	S	217	CYS	CA-CB-SG	-5.11	102.66	114.40
5	J	248	ILE	N-CA-CB	-5.11	103.51	110.56
3	2	74	VAL	CB-CA-C	-5.10	105.25	112.14
5	F	40	HIS	CB-CG-CD2	-5.10	124.57	131.20
5	I	71	ILE	N-CA-CB	-5.10	105.97	112.15
5	J	217	CYS	CA-CB-SG	-5.10	102.67	114.40
5	Q	217	CYS	CA-CB-SG	-5.10	102.66	114.40
3	Z	74	VAL	CB-CA-C	-5.10	105.25	112.14
5	G	149	THR	CA-CB-OG1	-5.10	101.95	109.60
5	I	217	CYS	CA-CB-SG	-5.10	102.67	114.40
5	M	71	ILE	N-CA-CB	-5.10	105.98	112.15
5	R	142	LEU	CA-C-O	5.10	126.17	120.82
4	B	141	LEU	N-CA-C	5.10	119.53	112.45
5	D	34	ILE	CA-CB-CG1	5.10	119.06	110.40
5	E	149	THR	CA-CB-OG1	-5.09	101.96	109.60
5	H	217	CYS	CA-CB-SG	-5.09	102.68	114.40
5	I	40	HIS	CB-CG-CD2	-5.09	124.58	131.20
5	M	217	CYS	CA-CB-SG	-5.09	102.68	114.40
5	K	217	CYS	CA-CB-SG	-5.09	102.69	114.40
5	L	142	LEU	CA-C-O	5.09	126.17	120.82
4	C	245	SER	O-C-N	-5.09	116.01	122.27
5	F	227	MET	N-CA-C	-5.09	105.64	111.14
5	M	227	MET	N-CA-C	-5.09	105.64	111.14
5	N	217	CYS	CA-CB-SG	-5.09	102.69	114.40
5	R	40	HIS	CB-CG-CD2	-5.09	124.58	131.20
5	R	266	PHE	CA-CB-CG	5.09	118.89	113.80
5	S	227	MET	N-CA-C	-5.09	105.64	111.14
5	E	356	TRP	CG-CD2-CE3	5.09	138.99	133.90
4	T	253	LEU	CB-CA-C	-5.09	102.86	110.90
5	D	248	ILE	N-CA-CB	-5.09	103.54	110.56
5	I	371	HIS	CB-CG-CD2	-5.09	124.59	131.20
5	N	356	TRP	CG-CD2-CE3	5.09	138.99	133.90
5	P	71	ILE	N-CA-CB	-5.09	106.00	112.15
5	Q	266	PHE	CA-CB-CG	5.09	118.89	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	196	ASN	CA-C-O	5.08	125.89	120.20
5	F	217	CYS	CA-CB-SG	-5.08	102.70	114.40
5	K	371	HIS	CB-CG-CD2	-5.08	124.59	131.20
4	U	263	ILE	N-CA-C	5.08	115.81	110.62
5	G	217	CYS	CA-CB-SG	-5.08	102.71	114.40
5	K	360	GLN	CB-CG-CD	5.08	121.24	112.60
5	H	371	HIS	CB-CG-CD2	-5.08	124.59	131.20
5	L	227	MET	N-CA-C	-5.08	105.65	111.14
5	D	149	THR	CA-CB-OG1	-5.08	101.98	109.60
5	O	217	CYS	CA-CB-SG	-5.08	102.72	114.40
5	P	149	THR	CA-CB-OG1	-5.08	101.98	109.60
4	W	263	ILE	N-CA-C	5.08	115.80	110.62
5	F	101	HIS	CA-C-O	-5.08	114.99	119.86
5	G	248	ILE	N-CA-CB	-5.08	103.56	110.56
5	H	233	SER	O-C-N	5.08	129.34	122.59
5	M	371	HIS	CB-CG-CD2	-5.08	124.60	131.20
5	F	359	LYS	CB-CG-CD	5.07	122.97	111.30
5	I	233	SER	O-C-N	5.07	129.34	122.59
5	E	266	PHE	CA-CB-CG	5.07	118.87	113.80
5	J	359	LYS	CB-CG-CD	5.07	122.97	111.30
5	S	356	TRP	CG-CD2-CE3	5.07	138.97	133.90
5	S	371	HIS	CB-CG-CD2	-5.07	124.61	131.20
4	A	231	ARG	NE-CZ-NH2	-5.07	114.64	119.20
4	B	253	LEU	CB-CA-C	-5.07	102.89	110.90
5	M	233	SER	O-C-N	5.07	129.33	122.59
5	N	371	HIS	CB-CG-CD2	-5.07	124.61	131.20
5	S	233	SER	O-C-N	5.07	129.33	122.59
5	D	88	HIS	CB-CG-CD2	-5.07	124.61	131.20
4	U	141	LEU	N-CA-C	5.07	119.50	112.45
5	D	227	MET	N-CA-C	-5.07	105.67	111.14
5	K	356	TRP	CG-CD2-CE3	5.07	138.97	133.90
5	P	266	PHE	CA-CB-CG	5.07	118.87	113.80
4	V	231	ARG	NE-CZ-NH2	-5.07	114.64	119.20
5	E	40	HIS	CB-CG-CD2	-5.07	124.62	131.20
5	M	281	SER	N-CA-C	-5.07	105.65	111.07
5	O	227	MET	N-CA-C	-5.07	105.67	111.14
5	F	281	SER	N-CA-C	-5.06	105.65	111.07
5	G	359	LYS	CB-CG-CD	5.06	122.94	111.30
5	J	149	THR	CA-CB-OG1	-5.06	102.01	109.60
5	F	371	HIS	CB-CG-CD2	-5.06	124.63	131.20
5	I	43	VAL	N-CA-C	5.06	117.29	108.90
5	L	217	CYS	CA-CB-SG	-5.06	102.77	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	227	MET	N-CA-C	-5.06	105.68	111.14
2	1	233	GLU	N-CA-C	-5.06	105.77	111.28
5	L	88	HIS	CB-CG-CD2	-5.05	124.63	131.20
5	L	248	ILE	N-CA-CB	-5.05	103.58	110.56
5	K	281	SER	N-CA-C	-5.05	105.66	111.07
5	Q	142	LEU	CA-C-O	5.05	126.13	120.82
5	P	43	VAL	N-CA-C	5.05	117.28	108.90
5	R	217	CYS	CA-CB-SG	-5.05	102.78	114.40
5	E	359	LYS	CB-CG-CD	5.05	122.91	111.30
5	H	149	THR	CA-CB-OG1	-5.05	102.03	109.60
5	H	359	LYS	CB-CG-CD	5.05	122.91	111.30
5	L	173	HIS	CB-CG-CD2	-5.05	124.64	131.20
5	Q	233	SER	O-C-N	5.05	129.31	122.59
5	R	88	HIS	CB-CG-CD2	-5.05	124.64	131.20
5	D	349	LEU	CA-C-O	5.05	126.74	121.19
5	G	266	PHE	CA-CB-CG	5.05	118.85	113.80
5	M	266	PHE	CA-CB-CG	5.05	118.85	113.80
5	N	43	VAL	N-CA-C	5.05	117.28	108.90
5	O	149	THR	CA-CB-OG1	-5.05	102.03	109.60
5	L	356	TRP	CG-CD2-CE3	5.04	138.94	133.90
5	N	149	THR	CA-CB-OG1	-5.04	102.03	109.60
5	S	359	LYS	CB-CG-CD	5.04	122.90	111.30
5	M	86	TRP	CE2-CD2-CG	-5.04	101.15	107.20
5	M	359	LYS	CB-CG-CD	5.04	122.90	111.30
5	R	359	LYS	CB-CG-CD	5.04	122.90	111.30
4	A	96	GLN	N-CA-C	5.04	116.78	111.28
5	P	365	ALA	N-CA-C	5.04	120.28	113.72
5	N	359	LYS	CB-CG-CD	5.04	122.89	111.30
5	Q	149	THR	CA-CB-OG1	-5.04	102.04	109.60
5	K	149	THR	CA-CB-OG1	-5.04	102.04	109.60
5	R	173	HIS	CB-CG-CD2	-5.04	124.65	131.20
5	K	227	MET	N-CA-C	-5.04	105.70	111.14
5	P	290	ARG	O-C-N	-5.04	116.33	122.22
5	R	356	TRP	CG-CD2-CE3	5.04	138.94	133.90
5	D	359	LYS	CB-CG-CD	5.03	122.88	111.30
5	K	266	PHE	CA-CB-CG	5.03	118.83	113.80
5	K	359	LYS	CB-CG-CD	5.03	122.88	111.30
4	A	35	GLU	CA-C-O	5.03	125.84	120.20
5	H	88	HIS	CB-CG-CD2	-5.03	124.66	131.20
5	H	227	MET	N-CA-C	-5.03	105.70	111.14
5	P	233	SER	O-C-N	5.03	129.28	122.59
2	4	233	GLU	N-CA-C	-5.03	105.80	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	227	MET	N-CA-C	-5.03	105.71	111.14
5	L	281	SER	N-CA-C	-5.03	105.69	111.07
5	L	371	HIS	CB-CG-CD2	-5.03	124.66	131.20
5	N	88	HIS	CB-CG-CD2	-5.03	124.66	131.20
5	D	266	PHE	CA-CB-CG	5.03	118.83	113.80
5	L	359	LYS	CB-CG-CD	5.03	122.87	111.30
5	O	359	LYS	CB-CG-CD	5.03	122.87	111.30
4	U	146	HIS	CB-CG-ND1	5.03	130.24	122.70
2	7	233	GLU	N-CA-C	-5.03	105.80	111.28
5	F	356	TRP	CG-CD2-CE3	5.03	138.93	133.90
5	J	266	PHE	CA-CB-CG	5.03	118.83	113.80
5	R	149	THR	CA-CB-OG1	-5.03	102.06	109.60
5	R	227	MET	N-CA-C	-5.03	105.71	111.14
5	G	227	MET	N-CA-C	-5.03	105.71	111.14
5	I	359	LYS	CB-CG-CD	5.03	122.86	111.30
5	O	43	VAL	N-CA-C	5.03	117.24	108.90
5	P	281	SER	N-CA-C	-5.03	105.69	111.07
5	P	359	LYS	CB-CG-CD	5.03	122.86	111.30
5	Q	227	MET	N-CA-C	-5.03	105.71	111.14
5	R	43	VAL	N-CA-C	5.03	117.24	108.90
4	V	171	ARG	N-CA-C	5.03	116.45	111.07
5	L	149	THR	CA-CB-OG1	-5.02	102.06	109.60
5	G	356	TRP	CG-CD2-CE3	5.02	138.92	133.90
5	I	149	THR	CA-CB-OG1	-5.02	102.07	109.60
4	V	196	ASN	CA-C-O	5.02	125.83	120.20
5	Q	88	HIS	CB-CG-CD2	-5.02	124.67	131.20
5	E	365	ALA	N-CA-C	5.02	120.25	113.72
5	H	365	ALA	N-CA-C	5.02	120.24	113.72
4	V	96	GLN	N-CA-C	5.02	116.75	111.28
5	F	142	LEU	CA-C-O	5.02	126.09	120.82
5	Q	359	LYS	CB-CG-CD	5.02	122.84	111.30
5	J	88	HIS	CB-CG-CD2	-5.02	124.68	131.20
5	G	371	HIS	CB-CG-CD2	-5.01	124.68	131.20
5	O	88	HIS	CB-CG-CD2	-5.01	124.68	131.20
4	U	197	LEU	O-C-N	5.01	127.51	122.09
4	B	127	ALA	O-C-N	-5.01	116.81	122.12
5	H	86	TRP	CE2-CD2-CG	-5.01	101.18	107.20
5	Q	281	SER	N-CA-C	-5.01	105.71	111.07
5	R	281	SER	N-CA-C	-5.01	105.71	111.07
4	U	50	LEU	CA-C-O	-5.01	115.74	120.90
5	J	233	SER	O-C-N	5.01	129.25	122.59
5	L	310	ALA	CA-C-O	-5.01	115.54	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	174	ALA	CA-C-N	5.01	127.29	120.63
5	E	174	ALA	C-N-CA	5.01	127.29	120.63
5	I	173	HIS	CB-CG-CD2	-5.01	124.69	131.20
5	N	349	LEU	CA-C-O	5.01	126.70	121.19
5	P	86	TRP	CE2-CD2-CG	-5.01	101.19	107.20
5	E	142	LEU	CA-C-O	5.01	126.08	120.82
5	L	86	TRP	CE2-CD2-CG	-5.01	101.19	107.20
5	L	290	ARG	O-C-N	-5.01	116.36	122.22
5	M	88	HIS	CB-CG-CD2	-5.01	124.69	131.20
5	O	371	HIS	CB-CG-CD2	-5.01	124.69	131.20
5	R	310	ALA	CA-C-O	-5.01	115.54	120.70
5	S	88	HIS	CB-CG-CD2	-5.01	124.69	131.20
5	H	16	LEU	N-CA-C	5.00	117.73	109.72
5	J	365	ALA	N-CA-C	5.00	120.22	113.72
5	K	88	HIS	CB-CG-CD2	-5.00	124.69	131.20
5	D	365	ALA	N-CA-C	5.00	120.22	113.72
5	I	142	LEU	CA-C-O	5.00	126.07	120.82
5	J	281	SER	N-CA-C	-5.00	105.72	111.07
5	Q	365	ALA	N-CA-C	5.00	120.22	113.72
5	R	86	TRP	CE2-CD2-CG	-5.00	101.20	107.20
5	S	266	PHE	CA-CB-CG	5.00	118.80	113.80

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
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

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Mol	Chain	Res	Type	Group
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 [i](#)

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	1173	110	0
1	3	1252	0	1173	111	0
1	6	1252	0	1173	103	0
1	9	1252	0	1173	101	0
2	1	774	0	796	49	0
2	4	774	0	796	51	0
2	7	774	0	797	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	774	0	791	48	0
3	2	1140	0	1201	109	0
3	5	1140	0	1201	109	0
3	8	1140	0	1201	108	0
3	Z	1140	0	1201	103	0
4	A	2091	0	2082	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	110	0
5	E	2907	0	2862	114	0
5	F	2907	0	2864	107	0
5	G	2907	0	2864	112	0
5	H	2907	0	2864	106	0
5	I	2907	0	2864	113	0
5	J	2907	0	2864	107	0
5	K	2907	0	2864	109	0
5	L	2907	0	2864	108	0
5	M	2907	0	2864	110	0
5	N	2907	0	2864	107	0
5	O	2907	0	2864	109	0
5	P	2907	0	2860	124	0
5	Q	2907	0	2863	122	0
5	R	2907	0	2861	125	0
5	S	2907	0	2864	122	0
All	All	69221	0	68498	2220	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 19.

All (2220) 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)
3:8:97:GLN:HE22	5:S:4:GLU:CG	1.19	1.53
3:5:97:GLN:HE22	5:Q:4:GLU:CG	1.19	1.51
1:3:62:GLU:CG	5:R:359:LYS:HD2	1.51	1.40
1:0:62:GLU:CG	5:P:360:GLN:HB2	1.52	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:62:GLU:CB	5:R:359:LYS:CD	1.76	1.39
1:0:62:GLU:CB	5:P:359:LYS:CD	1.76	1.39
1:3:62:GLU:CG	5:R:360:GLN:HB2	1.52	1.38
1:0:62:GLU:CG	5:P:359:LYS:HD2	1.52	1.37
3:5:97:GLN:NE2	5:Q:4:GLU:CG	1.85	1.37
3:8:97:GLN:NE2	5:S:4:GLU:CG	1.85	1.36
1:3:62:GLU:OE2	5:R:358:THR:HB	1.21	1.29
3:8:97:GLN:NE2	5:S:4:GLU:HG3	1.45	1.28
1:0:62:GLU:OE1	5:P:359:LYS:CE	1.82	1.27
1:0:62:GLU:HB2	5:P:359:LYS:CD	0.93	1.26
1:3:62:GLU:OE1	5:R:359:LYS:CE	1.82	1.26
3:5:97:GLN:NE2	5:Q:4:GLU:HG3	1.45	1.26
1:0:62:GLU:OE2	5:P:358:THR:HB	1.21	1.25
1:3:62:GLU:HB2	5:R:359:LYS:CD	0.92	1.25
3:8:97:GLN:NE2	5:S:4:GLU:CD	1.95	1.23
3:5:97:GLN:NE2	5:Q:4:GLU:CD	1.95	1.22
5:K:322:PRO:CB	5:M:244:ASP:OD2	1.88	1.22
5:F:322:PRO:CB	5:H:244:ASP:OD2	1.88	1.22
5:H:322:PRO:CB	5:J:244:ASP:OD2	1.88	1.22
5:N:322:PRO:CB	5:R:244:ASP:OD2	1.88	1.22
5:E:322:PRO:CB	5:G:244:ASP:OD2	1.88	1.21
1:0:62:GLU:OE1	5:P:359:LYS:HE3	1.36	1.21
1:0:62:GLU:CD	5:P:359:LYS:HD2	1.65	1.21
5:J:322:PRO:CB	5:L:244:ASP:OD2	1.88	1.21
5:L:322:PRO:CB	5:N:244:ASP:OD2	1.88	1.21
5:E:244:ASP:OD2	5:Q:322:PRO:CB	1.88	1.21
5:F:322:PRO:HB2	5:H:244:ASP:OD2	1.41	1.21
5:G:322:PRO:CB	5:I:244:ASP:OD2	1.88	1.21
5:D:322:PRO:CB	5:F:244:ASP:OD2	1.88	1.20
5:O:322:PRO:CB	5:S:244:ASP:OD2	1.88	1.20
5:M:322:PRO:CB	5:O:244:ASP:OD2	1.88	1.20
5:D:244:ASP:OD2	5:P:322:PRO:CB	1.88	1.20
5:I:322:PRO:HB2	5:K:244:ASP:OD2	1.41	1.20
5:G:322:PRO:HB2	5:I:244:ASP:OD2	1.41	1.19
5:J:322:PRO:HB2	5:L:244:ASP:OD2	1.41	1.19
5:E:322:PRO:HB2	5:G:244:ASP:OD2	1.41	1.19
5:K:322:PRO:HB2	5:M:244:ASP:OD2	1.41	1.19
5:O:322:PRO:HB2	5:S:244:ASP:OD2	1.41	1.19
5:I:322:PRO:CB	5:K:244:ASP:OD2	1.88	1.18
1:3:62:GLU:CD	5:R:359:LYS:HD2	1.65	1.18
5:E:244:ASP:OD2	5:Q:322:PRO:HB2	1.41	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:62:GLU:CB	5:P:359:LYS:HD3	1.47	1.17
5:H:322:PRO:HB2	5:J:244:ASP:OD2	1.41	1.17
5:L:322:PRO:HB2	5:N:244:ASP:OD2	1.41	1.17
1:0:62:GLU:HG2	5:P:360:GLN:CB	1.73	1.17
5:N:322:PRO:HB2	5:R:244:ASP:OD2	1.41	1.17
1:9:55:GLU:O	5:S:360:GLN:NE2	1.78	1.17
5:D:322:PRO:HB2	5:F:244:ASP:OD2	1.41	1.16
1:3:62:GLU:HG2	5:R:360:GLN:CB	1.73	1.16
1:6:55:GLU:O	5:Q:360:GLN:NE2	1.78	1.16
5:D:287:ILE:HG21	5:F:205:GLU:HG2	1.18	1.16
5:M:322:PRO:HB2	5:O:244:ASP:OD2	1.41	1.16
5:D:202:THR:HG23	5:P:290:ARG:NH2	1.61	1.16
5:D:290:ARG:NH2	5:F:202:THR:HG23	1.61	1.16
5:F:287:ILE:HG21	5:H:205:GLU:HG2	1.18	1.16
5:F:290:ARG:NH2	5:H:202:THR:HG23	1.61	1.16
5:N:290:ARG:NH2	5:R:202:THR:HG23	1.61	1.16
5:D:205:GLU:HG2	5:P:287:ILE:HG21	1.18	1.15
5:D:244:ASP:OD2	5:P:322:PRO:HB2	1.41	1.15
5:O:287:ILE:HG21	5:S:205:GLU:HG2	1.18	1.15
5:H:290:ARG:NH2	5:J:202:THR:HG23	1.61	1.15
5:E:290:ARG:NH2	5:G:202:THR:HG23	1.61	1.15
5:H:287:ILE:HG21	5:J:205:GLU:HG2	1.18	1.15
5:G:290:ARG:NH2	5:I:202:THR:HG23	1.61	1.14
5:I:290:ARG:NH2	5:K:202:THR:HG23	1.61	1.14
5:K:290:ARG:NH2	5:M:202:THR:HG23	1.61	1.14
1:3:62:GLU:OE1	5:R:359:LYS:HE3	1.36	1.14
5:J:290:ARG:NH2	5:L:202:THR:HG23	1.61	1.14
5:M:290:ARG:NH2	5:O:202:THR:HG23	1.61	1.14
5:M:287:ILE:HG21	5:O:205:GLU:HG2	1.18	1.13
5:E:202:THR:HG23	5:Q:290:ARG:NH2	1.61	1.13
5:O:290:ARG:NH2	5:S:202:THR:HG23	1.61	1.13
1:3:62:GLU:CB	5:R:359:LYS:HD3	1.47	1.12
5:J:287:ILE:HG21	5:L:205:GLU:HG2	1.18	1.12
5:L:290:ARG:NH2	5:N:202:THR:HG23	1.61	1.12
3:2:105:LYS:HB2	5:R:5:THR:CG2	1.81	1.11
5:K:287:ILE:HG21	5:M:205:GLU:HG2	1.18	1.11
5:E:287:ILE:HG21	5:G:205:GLU:HG2	1.18	1.11
5:P:5:THR:CG2	3:Z:105:LYS:HB2	1.81	1.10
5:E:205:GLU:HG2	5:Q:287:ILE:HG21	1.18	1.10
1:0:62:GLU:CB	5:P:359:LYS:HD2	1.53	1.10
5:G:287:ILE:HG21	5:I:205:GLU:HG2	1.18	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:287:ILE:HG21	5:N:205:GLU:HG2	1.18	1.10
5:I:287:ILE:HG21	5:K:205:GLU:HG2	1.18	1.09
5:I:290:ARG:CZ	5:K:202:THR:HG21	1.83	1.09
5:N:287:ILE:HG21	5:R:205:GLU:HG2	1.19	1.09
5:G:290:ARG:CZ	5:I:202:THR:HG21	1.83	1.09
5:N:290:ARG:CZ	5:R:202:THR:HG21	1.83	1.09
5:H:290:ARG:CZ	5:J:202:THR:HG21	1.83	1.09
5:K:290:ARG:CZ	5:M:202:THR:HG21	1.83	1.09
1:O:62:GLU:HG2	5:P:360:GLN:HB2	1.11	1.08
5:J:290:ARG:CZ	5:L:202:THR:HG21	1.83	1.08
1:3:62:GLU:HG3	5:R:360:GLN:HB2	1.35	1.08
5:F:290:ARG:CZ	5:H:202:THR:HG21	1.83	1.08
1:3:58:ASP:O	5:R:360:GLN:HG3	1.54	1.08
5:E:290:ARG:CZ	5:G:202:THR:HG21	1.83	1.08
5:D:202:THR:HG21	5:P:290:ARG:CZ	1.83	1.08
5:L:290:ARG:CZ	5:N:202:THR:HG21	1.83	1.08
5:M:290:ARG:CZ	5:O:202:THR:HG21	1.83	1.07
5:E:202:THR:HG21	5:Q:290:ARG:CZ	1.83	1.07
5:O:290:ARG:CZ	5:S:202:THR:HG21	1.83	1.07
5:D:3:ASP:HA	5:D:6:THR:HB	1.36	1.07
1:O:58:ASP:O	5:P:360:GLN:HG3	1.54	1.07
5:D:290:ARG:CZ	5:F:202:THR:HG21	1.83	1.07
5:M:3:ASP:HA	5:M:6:THR:HB	1.36	1.07
5:P:3:ASP:HA	5:P:6:THR:HB	1.36	1.07
1:3:58:ASP:C	5:R:360:GLN:HG3	1.80	1.06
5:F:3:ASP:HA	5:F:6:THR:HB	1.36	1.06
5:K:3:ASP:HA	5:K:6:THR:HB	1.36	1.06
1:O:58:ASP:C	5:P:360:GLN:HG3	1.80	1.06
1:3:62:GLU:HG2	5:R:360:GLN:HB2	1.12	1.06
5:H:3:ASP:HA	5:H:6:THR:HB	1.36	1.06
5:I:3:ASP:HA	5:I:6:THR:HB	1.36	1.06
5:O:3:ASP:HA	5:O:6:THR:HB	1.36	1.06
3:Z:141:LYS:H	3:Z:141:LYS:HD2	1.20	1.05
5:S:3:ASP:HA	5:S:6:THR:HB	1.36	1.05
1:3:62:GLU:CB	5:R:359:LYS:HD2	1.53	1.04
3:8:141:LYS:H	3:8:141:LYS:HD2	1.20	1.04
1:3:62:GLU:CD	5:R:359:LYS:CD	2.28	1.04
1:3:62:GLU:HG2	5:R:360:GLN:N	1.72	1.04
5:J:3:ASP:HA	5:J:6:THR:HB	1.36	1.04
5:G:3:ASP:HA	5:G:6:THR:HB	1.36	1.03
5:R:3:ASP:HA	5:R:6:THR:HB	1.36	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:62:GLU:HG3	5:P:360:GLN:HB2	1.35	1.03
5:Q:3:ASP:HA	5:Q:6:THR:HB	1.36	1.03
1:0:62:GLU:HG2	5:P:360:GLN:N	1.72	1.02
5:N:3:ASP:HA	5:N:6:THR:HB	1.36	1.02
1:3:62:GLU:CD	5:R:359:LYS:CE	2.33	1.02
5:I:290:ARG:CZ	5:K:202:THR:CG2	2.38	1.02
5:K:290:ARG:CZ	5:M:202:THR:CG2	2.38	1.02
1:0:62:GLU:CD	5:P:359:LYS:CE	2.33	1.01
5:G:290:ARG:CZ	5:I:202:THR:CG2	2.38	1.01
1:0:62:GLU:OE1	5:P:359:LYS:NZ	1.92	1.01
3:2:100:PHE:HE1	5:R:5:THR:HG22	1.25	1.01
5:E:3:ASP:HA	5:E:6:THR:HB	1.36	1.01
5:P:5:THR:HG22	3:Z:100:PHE:HE1	1.25	1.01
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:M:290:ARG:CZ	5:O:202:THR:CG2	2.38	1.01
1:0:62:GLU:CD	5:P:359:LYS:CD	2.28	1.01
3:5:141:LYS:H	3:5:141:LYS:HD2	1.20	1.01
5:D:287:ILE:HB	5:F:204:ALA:H	1.26	1.01
5:E:290:ARG:CZ	5:G:202:THR:CG2	2.38	1.01
5:L:3:ASP:HA	5:L:6:THR:HB	1.36	1.01
1:3:62:GLU:OE1	5:R:359:LYS:NZ	1.92	1.00
5:I:287:ILE:HB	5:K:204:ALA:H	1.26	1.00
5:L:290:ARG:CZ	5:N:202:THR:CG2	2.38	1.00
5:D:202:THR:CG2	5:P:290:ARG:CZ	2.38	1.00
5:D:290:ARG:CZ	5:F:202:THR:CG2	2.38	1.00
5:F:290:ARG:CZ	5:H:202:THR:CG2	2.38	1.00
5:H:287:ILE:HB	5:J:204:ALA:H	1.26	1.00
5:E:287:ILE:HB	5:G:204:ALA:H	1.26	1.00
5:H:290:ARG:CZ	5:J:202:THR:CG2	2.38	1.00
5:J:290:ARG:CZ	5:L:202:THR:CG2	2.38	1.00
5:N:290:ARG:CZ	5:R:202:THR:CG2	2.38	1.00
5:O:290:ARG:CZ	5:S:202:THR:CG2	2.38	1.00
5:M:287:ILE:HB	5:O:204:ALA:H	1.27	1.00
5:N:287:ILE:HB	5:R:204:ALA:H	1.27	1.00
1:3:62:GLU:HG2	5:R:360:GLN:CA	1.92	0.99
5:G:290:ARG:NH2	5:I:202:THR:CG2	2.25	0.99
5:L:287:ILE:HB	5:N:204:ALA:H	1.27	0.99
3:2:141:LYS:H	3:2:141:LYS:HD2	1.20	0.99
5:I:290:ARG:NH2	5:K:202:THR:CG2	2.25	0.99
5:K:290:ARG:NH2	5:M:202:THR:CG2	2.25	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:290:ARG:NH2	5:G:202:THR:CG2	2.25	0.99
5:M:290:ARG:NH2	5:O:202:THR:CG2	2.25	0.99
5:D:202:THR:CG2	5:P:290:ARG:NH2	2.25	0.99
5:F:290:ARG:NH2	5:H:202:THR:CG2	2.25	0.99
5:D:290:ARG:NH2	5:F:202:THR:CG2	2.25	0.99
5:E:202:THR:CG2	5:Q:290:ARG:NH2	2.25	0.99
5:H:290:ARG:NH2	5:J:202:THR:CG2	2.25	0.99
5:N:290:ARG:NH2	5:R:202:THR:CG2	2.25	0.98
5:O:287:ILE:HB	5:S:204:ALA:H	1.27	0.98
5:O:290:ARG:NH2	5:S:202:THR:CG2	2.25	0.98
3:2:105:LYS:HB2	5:R:5:THR:HG21	1.01	0.98
5:E:203:THR:HG22	5:Q:286:ASP:OD1	1.64	0.98
5:M:286:ASP:OD1	5:O:203:THR:HG22	1.64	0.98
5:J:290:ARG:NH2	5:L:202:THR:CG2	2.25	0.98
5:L:290:ARG:NH2	5:N:202:THR:CG2	2.25	0.98
5:D:286:ASP:OD1	5:F:203:THR:HG22	1.64	0.98
5:H:286:ASP:OD1	5:J:203:THR:HG22	1.64	0.98
5:I:286:ASP:OD1	5:K:203:THR:HG22	1.64	0.98
5:J:286:ASP:OD1	5:L:203:THR:HG22	1.64	0.98
5:G:286:ASP:OD1	5:I:203:THR:HG22	1.64	0.98
5:K:287:ILE:HB	5:M:204:ALA:H	1.27	0.98
5:L:322:PRO:HB3	5:N:244:ASP:OD2	1.64	0.97
5:O:286:ASP:OD1	5:S:203:THR:HG22	1.64	0.97
5:G:287:ILE:HB	5:I:204:ALA:H	1.26	0.97
5:L:286:ASP:OD1	5:N:203:THR:HG22	1.64	0.97
5:N:322:PRO:HB3	5:R:244:ASP:OD2	1.64	0.97
5:E:204:ALA:H	5:Q:287:ILE:HB	1.26	0.97
5:F:286:ASP:OD1	5:H:203:THR:HG22	1.64	0.97
5:E:244:ASP:OD2	5:Q:322:PRO:HB3	1.64	0.97
5:E:322:PRO:HB3	5:G:244:ASP:OD2	1.63	0.97
5:D:204:ALA:H	5:P:287:ILE:HB	1.27	0.97
5:J:322:PRO:HB3	5:L:244:ASP:OD2	1.64	0.97
5:N:286:ASP:OD1	5:R:203:THR:HG22	1.64	0.97
1:0:62:GLU:HB2	5:P:359:LYS:HD2	1.16	0.96
1:6:58:ASP:HB2	5:Q:360:GLN:NE2	1.80	0.96
5:E:286:ASP:OD1	5:G:203:THR:HG22	1.64	0.96
5:F:287:ILE:HB	5:H:204:ALA:H	1.27	0.96
1:0:62:GLU:HG2	5:P:360:GLN:CA	1.93	0.96
5:H:322:PRO:HB3	5:J:244:ASP:OD2	1.64	0.96
5:K:286:ASP:OD1	5:M:203:THR:HG22	1.64	0.96
1:9:58:ASP:HB2	5:S:360:GLN:NE2	1.80	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:203:THR:HG22	5:P:286:ASP:OD1	1.64	0.96
5:G:322:PRO:HB3	5:I:244:ASP:OD2	1.64	0.96
5:J:287:ILE:HB	5:L:204:ALA:H	1.27	0.96
3:2:53:LEU:HD13	3:2:53:LEU:H	1.31	0.95
5:F:322:PRO:HB3	5:H:244:ASP:OD2	1.64	0.95
3:8:53:LEU:HD13	3:8:53:LEU:H	1.31	0.95
5:I:322:PRO:HB3	5:K:244:ASP:OD2	1.64	0.95
3:Z:53:LEU:HD13	3:Z:53:LEU:H	1.31	0.95
3:5:53:LEU:HD13	3:5:53:LEU:H	1.31	0.95
5:M:288:ASP:HA	5:O:204:ALA:HB2	1.49	0.95
5:O:288:ASP:HA	5:S:204:ALA:HB2	1.49	0.95
5:D:322:PRO:HB3	5:F:244:ASP:OD2	1.64	0.94
5:K:288:ASP:HA	5:M:204:ALA:HB2	1.49	0.94
5:D:204:ALA:HB2	5:P:288:ASP:HA	1.49	0.94
5:D:244:ASP:OD2	5:P:322:PRO:HB3	1.64	0.94
5:K:322:PRO:HB3	5:M:244:ASP:OD2	1.64	0.94
1:3:62:GLU:OE2	5:R:358:THR:CB	2.15	0.94
5:M:322:PRO:HB3	5:O:244:ASP:OD2	1.64	0.94
5:O:322:PRO:HB3	5:S:244:ASP:OD2	1.64	0.94
5:P:5:THR:HG21	3:Z:105:LYS:CB	1.97	0.94
1:0:62:GLU:OE2	5:P:358:THR:CB	2.15	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:D:288:ASP:HA	5:F:204:ALA:HB2	1.49	0.94
5:F:288:ASP:HA	5:H:204:ALA:HB2	1.49	0.94
5:H:288:ASP:HA	5:J:204:ALA:HB2	1.49	0.94
5:J:288:ASP:HA	5:L:204:ALA:HB2	1.49	0.94
1:0:62:GLU:CG	5:P:360:GLN:CB	2.38	0.93
5:E:288:ASP:HA	5:G:204:ALA:HB2	1.49	0.93
5:L:288:ASP:HA	5:N:204:ALA:HB2	1.49	0.93
5:N:288:ASP:HA	5:R:204:ALA:HB2	1.49	0.93
5:E:204:ALA:HB2	5:Q:288:ASP:HA	1.49	0.93
1:0:62:GLU:HG2	5:P:360:GLN:H	1.35	0.90
5:J:322:PRO:HB2	5:L:244:ASP:CG	1.96	0.90
5:M:322:PRO:HB2	5:O:244:ASP:CG	1.96	0.90
5:L:322:PRO:HB2	5:N:244:ASP:CG	1.96	0.90
1:6:55:GLU:HA	5:Q:360:GLN:CD	1.97	0.90
5:E:244:ASP:CG	5:Q:322:PRO:HB2	1.96	0.90
1:0:61:ILE:HD12	5:P:360:GLN:HE21	1.35	0.90
1:3:62:GLU:HG2	5:R:360:GLN:H	1.35	0.90
1:6:55:GLU:C	5:Q:360:GLN:NE2	2.30	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:55:GLU:HA	5:S:360:GLN:CD	1.97	0.90
5:D:322:PRO:HB2	5:F:244:ASP:CG	1.96	0.90
1:3:61:ILE:HD12	5:R:360:GLN:HE21	1.35	0.90
5:G:322:PRO:HB2	5:I:244:ASP:CG	1.96	0.90
1:9:55:GLU:C	5:S:360:GLN:NE2	2.30	0.90
5:H:322:PRO:HB2	5:J:244:ASP:CG	1.96	0.90
5:D:244:ASP:CG	5:P:322:PRO:HB2	1.96	0.89
5:I:322:PRO:HB2	5:K:244:ASP:CG	1.96	0.89
5:N:322:PRO:HB2	5:R:244:ASP:CG	1.96	0.89
2:Y:198:ASN:HB3	2:Y:201:LYS:HB2	1.54	0.89
5:E:322:PRO:HB2	5:G:244:ASP:CG	1.96	0.89
1:3:62:GLU:CG	5:R:360:GLN:CB	2.38	0.89
1:9:55:GLU:HA	5:S:360:GLN:NE2	1.88	0.89
5:K:322:PRO:HB2	5:M:244:ASP:CG	1.96	0.89
5:F:322:PRO:HB2	5:H:244:ASP:CG	1.96	0.89
2:4:198:ASN:HB3	2:4:201:LYS:HB2	1.53	0.88
2:7:198:ASN:HB3	2:7:201:LYS:HB2	1.54	0.88
5:O:322:PRO:HB2	5:S:244:ASP:CG	1.96	0.88
3:2:105:LYS:CB	5:R:5:THR:HG21	1.97	0.88
1:6:55:GLU:HA	5:Q:360:GLN:NE2	1.88	0.88
1:3:137:MET:HE1	1:3:148:ILE:HG13	1.55	0.88
1:3:62:GLU:HB2	5:R:359:LYS:HD2	1.16	0.88
2:Y:207:LYS:HZ1	2:Y:208:GLU:HG2	1.39	0.87
2:1:198:ASN:HB3	2:1:201:LYS:HB2	1.54	0.87
1:6:137:MET:HE1	1:6:148:ILE:HG13	1.55	0.87
1:9:137:MET:HE1	1:9:148:ILE:HG13	1.55	0.86
1:0:137:MET:HE1	1:0:148:ILE:HG13	1.56	0.86
1:6:55:GLU:CA	5:Q:360:GLN:NE2	2.40	0.85
1:9:55:GLU:CA	5:S:360:GLN:NE2	2.40	0.84
5:L:287:ILE:CG2	5:N:205:GLU:HG2	2.07	0.84
5:I:287:ILE:CG2	5:K:205:GLU:HG2	2.07	0.84
5:L:237:GLU:HA	5:L:251:GLY:HA2	1.60	0.84
1:9:121:LEU:O	1:9:124:THR:HG22	1.78	0.84
5:N:237:GLU:HA	5:N:251:GLY:HA2	1.60	0.84
3:8:97:GLN:CD	5:S:4:GLU:CG	2.50	0.84
5:J:287:ILE:CG2	5:L:205:GLU:HG2	2.07	0.84
5:R:237:GLU:HA	5:R: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
3:5:97:GLN:CD	5:Q:4:GLU:CG	2.50	0.83
5:J:237:GLU:HA	5:J:251:GLY:HA2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:287:ILE:CG2	5:M:205:GLU:HG2	2.07	0.83
1:3:121:LEU:O	1:3:124:THR:HG22	1.78	0.83
5:H:237:GLU:HA	5:H:251:GLY:HA2	1.60	0.83
5:E:287:ILE:CG2	5:G:205:GLU:HG2	2.07	0.83
5:Q:237:GLU:HA	5:Q:251:GLY:HA2	1.60	0.83
5:D:205:GLU:HG2	5:P:287:ILE:CG2	2.07	0.83
5:D:237:GLU:HA	5:D:251:GLY:HA2	1.60	0.83
1:0:121:LEU:O	1:0:124:THR:HG22	1.78	0.83
1:6:121:LEU:O	1:6:124:THR:HG22	1.78	0.83
5:F:287:ILE:CG2	5:H:205:GLU:HG2	2.07	0.83
5:H:287:ILE:CG2	5:J:205:GLU:HG2	2.07	0.83
5:E:237:GLU:HA	5:E:251:GLY:HA2	1.60	0.82
5:S:237:GLU:HA	5:S:251:GLY:HA2	1.60	0.82
5:P:237:GLU:HA	5:P:251:GLY:HA2	1.60	0.82
5:N:287:ILE:CG2	5:R:205:GLU:HG2	2.07	0.82
5:O:287:ILE:CG2	5:S:205:GLU:HG2	2.07	0.82
5:D:287:ILE:CG2	5:F:205:GLU:HG2	2.07	0.82
5:O:237:GLU:HA	5:O:251:GLY:HA2	1.60	0.82
1:3:58:ASP:C	5:R:360:GLN:CG	2.53	0.82
5:L:286:ASP:OD1	5:N:203:THR:CG2	2.28	0.82
5:E:203:THR:CG2	5:Q:286:ASP:OD1	2.28	0.81
5:J:286:ASP:OD1	5:L:203:THR:CG2	2.28	0.81
5:D:286:ASP:OD1	5:F:203:THR:CG2	2.28	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:N:286:ASP:OD1	5:R:203:THR:CG2	2.28	0.81
5:P:5:THR:HG22	3:Z:100:PHE:CE1	2.13	0.81
5:K:237:GLU:HA	5:K:251:GLY:HA2	1.60	0.81
5:D:203:THR:CG2	5:P:286:ASP:OD1	2.28	0.81
5:O:286:ASP:OD1	5:S:203:THR:CG2	2.28	0.81
5:F:286:ASP:OD1	5:H:203:THR:CG2	2.28	0.81
5:H:286:ASP:OD1	5:J:203:THR:CG2	2.28	0.81
5:I:237:GLU:HA	5:I:251:GLY:HA2	1.60	0.81
5:I:286:ASP:OD1	5:K:203:THR:CG2	2.28	0.81
3:2:141:LYS:H	3:2:141:LYS:CD	1.94	0.81
5:E:286:ASP:OD1	5:G:203:THR:CG2	2.28	0.81
5:K:223:PHE:HE1	5:K:255:PHE:HB2	1.46	0.81
5:M:286:ASP:OD1	5:O:203:THR:CG2	2.28	0.81
3:5:141:LYS:H	3:5:141:LYS:CD	1.94	0.81
5:G:286:ASP:OD1	5:I:203:THR:CG2	2.28	0.81
5:P:223:PHE:HE1	5:P:255:PHE:HB2	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:223:PHE:HE1	5:R:255:PHE:HB2	1.46	0.81
5:H:290:ARG:NH1	5:J:202:THR:HG21	1.96	0.80
5:I:223:PHE:HE1	5:I:255:PHE:HB2	1.46	0.80
5:D:223:PHE:HE1	5:D:255:PHE:HB2	1.46	0.80
5:J:290:ARG:NH1	5:L:202:THR:HG21	1.97	0.80
5:N:223:PHE:HE1	5:N:255:PHE:HB2	1.46	0.80
5:K:286:ASP:OD1	5:M:203:THR:CG2	2.28	0.80
5:O:290:ARG:NH1	5:S:202:THR:HG21	1.97	0.80
5:M:223:PHE:HE1	5:M:255:PHE:HB2	1.46	0.80
5:L:223:PHE:HE1	5:L:255:PHE:HB2	1.46	0.80
5:F:290:ARG:NH1	5:H:202:THR:HG21	1.97	0.80
5:M:290:ARG:NH1	5:O:202:THR:HG21	1.97	0.80
5:G:223:PHE:HE1	5:G:255:PHE:HB2	1.46	0.80
5:G:287:ILE:CG2	5:I:205:GLU:HG2	2.07	0.80
5:J:223:PHE:HE1	5:J:255:PHE:HB2	1.46	0.80
3:2:100:PHE:CE1	5:R:5:THR:HG22	2.13	0.79
1:9:55:GLU:HA	5:S:360:GLN:OE1	1.82	0.79
5:E:202:THR:HG21	5:Q:290:ARG:NH1	1.97	0.79
5:F:223:PHE:HE1	5:F:255:PHE:HB2	1.46	0.79
5:I:290:ARG:NH1	5:K:202:THR:HG21	1.97	0.79
5:K:290:ARG:NH1	5:M:202:THR:HG21	1.97	0.79
3:Z:141:LYS:H	3:Z:141:LYS:CD	1.94	0.79
5:Q:223:PHE:HE1	5:Q:255:PHE:HB2	1.46	0.79
1:0:58:ASP:C	5:P:360:GLN:CG	2.53	0.79
5:D:202:THR:HG21	5:P:290:ARG:NH1	1.97	0.79
5:G:290:ARG:NH1	5:I:202:THR:HG21	1.97	0.79
5:L:290:ARG:NH1	5:N:202:THR:HG21	1.97	0.79
3:Z:142:GLN:HG2	3:Z:143:VAL:HG23	1.65	0.79
3:8:132:VAL:HG11	1:9:17:MET:HE3	1.65	0.79
5:S:223:PHE:HE1	5:S:255:PHE:HB2	1.46	0.79
1:6:55:GLU:HA	5:Q:360:GLN:OE1	1.82	0.79
1:6:58:ASP:HB2	5:Q:360:GLN:CG	2.13	0.79
5:D:290:ARG:NH1	5:F:202:THR:HG21	1.97	0.79
5:N:290:ARG:NH1	5:R:202:THR:HG21	1.97	0.79
3:8:141:LYS:H	3:8:141:LYS:CD	1.94	0.79
1:0:17:MET:HE3	3:Z:132:VAL:HG11	1.65	0.79
5:O:223:PHE:HE1	5:O:255:PHE:HB2	1.46	0.79
3:2:132:VAL:HG11	1:3:17:MET:HE3	1.65	0.79
1:9:58:ASP:HB2	5:S:360:GLN:CD	2.08	0.79
5:E:223:PHE:HE1	5:E:255:PHE:HB2	1.46	0.79
5:E:290:ARG:NH1	5:G:202:THR:HG21	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:142:GLN:HG2	3:8:143:VAL:HG23	1.65	0.78
3:5:142:GLN:HG2	3:5:143:VAL:HG23	1.65	0.78
1:3:61:ILE:HD12	5:R:360:GLN:NE2	1.98	0.78
5:H:223:PHE:HE1	5:H:255:PHE:HB2	1.46	0.78
1:0:61:ILE:HD12	5:P:360:GLN:NE2	1.98	0.78
3:5:97:GLN:HE22	5:Q:4:GLU:HG3	0.61	0.78
3:5:132:VAL:HG11	1:6:17:MET:HE3	1.65	0.78
1:6:58:ASP:HB2	5:Q:360:GLN:CD	2.08	0.78
2:1:207:LYS:HZ2	2:1:208:GLU:HG2	1.48	0.78
3:2:142:GLN:HG2	3:2:143:VAL:HG23	1.65	0.78
5:M:287:ILE:HB	5:O:204:ALA:N	1.99	0.78
5:D:287:ILE:HB	5:F:204:ALA:N	1.99	0.77
5:L:223:PHE:HD2	5:L:312:ARG:HH21	1.32	0.77
5:D:204:ALA:N	5:P:287:ILE:HB	1.99	0.77
5:R:223:PHE:HD2	5:R:312:ARG:HH21	1.33	0.77
5:G:287:ILE:HB	5:I:204:ALA:N	1.99	0.77
5:O:287:ILE:HB	5:S:204:ALA:N	1.99	0.77
3:8:97:GLN:HE22	5:S:4:GLU:HG3	0.61	0.77
5:H:223:PHE:HD2	5:H:312:ARG:HH21	1.33	0.77
5:J:223:PHE:HD2	5:J:312:ARG:HH21	1.33	0.77
5:N:223:PHE:HD2	5:N:312:ARG:HH21	1.33	0.77
3:8:141:LYS:HD2	3:8:141:LYS:N	1.99	0.77
1:9:58:ASP:HB2	5:S:360:GLN:CG	2.13	0.77
2:7:207:LYS:HZ2	2:7:208:GLU:HG2	1.50	0.77
5:G:223:PHE:HD2	5:G:312:ARG:HH21	1.33	0.77
2:4:207:LYS:HZ2	2:4:208:GLU:HG2	1.50	0.77
5:I:287:ILE:HB	5:K:204:ALA:N	1.99	0.77
5:E:223:PHE:HD2	5:E:312:ARG:HH21	1.33	0.77
5:E:287:ILE:HB	5:G:204:ALA:N	1.99	0.77
5:F:223:PHE:HD2	5:F:312:ARG:HH21	1.33	0.77
5:I:223:PHE:HD2	5:I:312:ARG:HH21	1.33	0.77
5:E:205:GLU:HG2	5:Q:287:ILE:CG2	2.07	0.76
5:K:287:ILE:HB	5:M:204:ALA:N	1.99	0.76
5:Q:223:PHE:HD2	5:Q:312:ARG:HH21	1.33	0.76
5:F:287:ILE:HB	5:H:204:ALA:N	1.99	0.76
5:P:5:THR:CG2	3:Z:100:PHE:HE1	1.98	0.76
5:D:223:PHE:HD2	5:D:312:ARG:HH21	1.33	0.76
5:K:223:PHE:HD2	5:K:312:ARG:HH21	1.33	0.76
5:P:223:PHE:HD2	5:P:312:ARG:HH21	1.33	0.76
5:E:204:ALA:N	5:Q:287:ILE:HB	1.99	0.76
5:N:287:ILE:HB	5:R:204:ALA:N	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:223:PHE:HD2	5:O:312:ARG:HH21	1.33	0.76
5:S:223:PHE:HD2	5:S:312:ARG:HH21	1.33	0.76
5:L:287:ILE:HB	5:N:204:ALA:N	1.99	0.75
5:M:223:PHE:HD2	5:M:312:ARG:HH21	1.33	0.75
1:O:65:ASP:HA	1:O:76:GLU:OE2	1.86	0.75
5:J:287:ILE:HB	5:L:204:ALA:N	1.99	0.75
1:9:65:ASP:HA	1:9:76:GLU:OE2	1.86	0.75
3:Z:141:LYS:HD2	3:Z:141:LYS:N	1.99	0.75
5:F:253:GLU:HA	5:F:256:ARG:HG3	1.69	0.75
3:2:100:PHE:HE1	5:R:5:THR:CG2	1.98	0.75
5:H:253:GLU:HA	5:H:256:ARG:HG3	1.69	0.75
5:H:287:ILE:HB	5:J:204:ALA:N	1.99	0.75
5:M:253:GLU:HA	5:M:256:ARG:HG3	1.69	0.74
5:O:290:ARG:HH22	5:S:202:THR:HG23	1.52	0.74
5:S:253:GLU:HA	5:S: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	1.69	0.74
3:8:97:GLN:OE1	5:S:4:GLU:HG2	1.87	0.74
5:D:253:GLU:HA	5:D:256:ARG:HG3	1.70	0.74
5:L:253:GLU:HA	5:L:256:ARG:HG3	1.70	0.74
5:D:290:ARG:HH22	5:F:202:THR:HG23	1.52	0.74
5:K:290:ARG:NH1	5:M:202:THR:CG2	2.51	0.74
5:P:253:GLU:HA	5:P:256:ARG:HG3	1.69	0.74
1:6:53:THR:HG1	1:6:56:GLU:HG3	1.52	0.74
1:6:53:THR:OG1	1:6:56:GLU:HG3	1.88	0.74
1:3:62:GLU:CD	5:R:359:LYS:HE3	2.07	0.74
1:3:155:LYS:HA	1:3:155:LYS:HE3	1.69	0.74
1:6:54:LYS:O	5:Q:360:GLN:NE2	2.21	0.74
5:N:290:ARG:NH1	5:R:202:THR:CG2	2.51	0.74
3:5:97:GLN:OE1	5:Q:4:GLU:HG2	1.87	0.73
5:D:202:THR:CG2	5:P:290:ARG:NH1	2.51	0.73
1:3:53:THR:OG1	1:3:56:GLU:HG3	1.88	0.73
5:I:253:GLU:HA	5:I:256:ARG:HG3	1.69	0.73
5:G:290:ARG:NH1	5:I:202:THR:CG2	2.51	0.73
5:J:290:ARG:NH1	5:L:202:THR:CG2	2.51	0.73
5:N:253:GLU:HA	5:N:256:ARG:HG3	1.69	0.73
1:O:53:THR:HG1	1:O:56:GLU:HG3	1.53	0.73
1:6:155:LYS:HA	1:6:155:LYS:HE3	1.69	0.73
5:D:203:THR:HG22	5:P:288:ASP:H	1.53	0.73
5:G:290:ARG:HH22	5:I:202:THR:HG23	1.52	0.73
5:K:253:GLU:HA	5:K:256:ARG:HG3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:288:ASP:H	5:O:203:THR:HG22	1.53	0.73
1:3:65:ASP:HA	1:3:76:GLU:OE2	1.86	0.73
1:6:62:GLU:OE1	5:Q:359:LYS:NZ	2.21	0.73
5:F:288:ASP:H	5:H:203:THR:HG22	1.53	0.73
5:M:290:ARG:NH1	5:O:202:THR:CG2	2.51	0.73
5:R:253:GLU:HA	5:R:256:ARG:HG3	1.70	0.73
1:6:65:ASP:HA	1:6:76:GLU:OE2	1.86	0.73
5:D:290:ARG:NH1	5:F:202:THR:CG2	2.51	0.73
5:E:203:THR:HG22	5:Q:288:ASP:H	1.53	0.73
5:Q:253:GLU:HA	5:Q:256:ARG:HG3	1.69	0.73
1:0:53:THR:OG1	1:0:56:GLU:HG3	1.88	0.73
5:E:253:GLU:HA	5:E:256:ARG:HG3	1.69	0.73
5:L:288:ASP:H	5:N:203:THR:HG22	1.53	0.73
5:E:290:ARG:NH1	5:G:202:THR:CG2	2.51	0.73
5:E:288:ASP:H	5:G:203:THR:HG22	1.53	0.73
5:N:288:ASP:H	5:R:203:THR:HG22	1.54	0.73
5:R:3:ASP:HA	5:R:6:THR:CB	2.18	0.73
1:0:155:LYS:HA	1:0:155:LYS:HE3	1.69	0.73
5:D:288:ASP:H	5:F:203:THR:HG22	1.53	0.73
5:G:253:GLU:HA	5:G:256:ARG:HG3	1.69	0.73
5:I:288:ASP:H	5:K:203:THR:HG22	1.54	0.73
5:I:290:ARG:NH1	5:K:202:THR:CG2	2.51	0.73
5:G:288:ASP:H	5:I:203:THR:HG22	1.53	0.72
5:M:290:ARG:HH22	5:O:202:THR:HG23	1.52	0.72
5:K:288:ASP:H	5:M:203:THR:HG22	1.54	0.72
5:H:288:ASP:H	5:J:203:THR:HG22	1.54	0.72
1:9:53:THR:OG1	1:9:56:GLU:HG3	1.88	0.72
1:9:155:LYS:HA	1:9:155:LYS:HE3	1.69	0.72
1:0:62:GLU:CG	5:P:359:LYS:CD	2.33	0.72
5:O:288:ASP:H	5:S:203:THR:HG22	1.53	0.72
5:P:3:ASP:HA	5:P:6:THR:CB	2.18	0.72
5:D:3:ASP:HA	5:D:6:THR:CB	2.17	0.72
5:O:3:ASP:HA	5:O:6:THR:CB	2.18	0.72
5:S:3:ASP:HA	5:S:6:THR:CB	2.18	0.72
1:9:58:ASP:HB2	5:S:360:GLN:HE21	1.54	0.72
1:9:62:GLU:OE1	5:S:359:LYS:NZ	2.22	0.72
3:5:141:LYS:HD2	3:5:141:LYS:N	1.99	0.72
5:D:202:THR:HG23	5:P:290:ARG:HH22	1.52	0.72
5:M:3:ASP:HA	5:M:6:THR:CB	2.17	0.72
3:2:141:LYS:HD2	3:2:141:LYS:N	1.99	0.71
5:J:288:ASP:H	5:L:203:THR:HG22	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:L:290:ARG:HH22	5:N:202:THR:HG23	1.52	0.71
1:9:54:LYS:O	5:S:360:GLN:NE2	2.22	0.71
5:E:290:ARG:HH22	5:G:202:THR:HG23	1.52	0.71
5:E:202:THR:CG2	5:Q:290:ARG:NH1	2.51	0.71
5:I:3:ASP:HA	5:I:6:THR:CB	2.17	0.71
5:F:3:ASP:HA	5:F:6:THR:CB	2.18	0.71
5:F:290:ARG:NH1	5:H:202:THR:CG2	2.51	0.71
1:0:116:GLU:O	1:0:120:ILE:HG22	1.91	0.71
2:1:215:GLN:O	2:1:218:THR:HG22	1.91	0.71
1:3:116:GLU:O	1:3:120:ILE:HG22	1.91	0.71
5:K:3:ASP:HA	5:K:6:THR:CB	2.18	0.71
1:9:116:GLU:O	1:9:120:ILE:HG22	1.91	0.71
5:E:202:THR:HG23	5:Q:290:ARG:HH22	1.52	0.71
5:H:290:ARG:NH1	5:J:202:THR:CG2	2.51	0.70
5:H:3:ASP:HA	5:H:6:THR:CB	2.18	0.70
5:L:3:ASP:HA	5:L:6:THR:CB	2.18	0.70
2:Y:215:GLN:O	2:Y:218:THR:HG22	1.91	0.70
2:4:215:GLN:O	2:4:218:THR:HG22	1.91	0.70
1:6:39:LYS:H	1:6:39:LYS:HD2	1.57	0.70
2:7:215:GLN:O	2:7:218:THR:HG22	1.91	0.70
5:O:290:ARG:NH1	5:S:202:THR:CG2	2.51	0.70
1:3:39:LYS:H	1:3:39:LYS:HD2	1.57	0.70
1:6:116:GLU:O	1:6:120:ILE:HG22	1.91	0.70
5:N:3:ASP:HA	5:N:6:THR:CB	2.18	0.70
3:2:70:LYS:O	3:2:74:VAL:HG23	1.92	0.70
3:Z:70:LYS:O	3:Z:74:VAL:HG23	1.92	0.70
3:5:70:LYS:O	3:5:74:VAL:HG23	1.92	0.70
5:J:3:ASP:HA	5:J:6:THR:CB	2.18	0.70
1:6:58:ASP:HB2	5:Q:360:GLN:HE21	1.54	0.69
3:8:70:LYS:O	3:8:74:VAL:HG23	1.92	0.69
3:8:97:GLN:CD	5:S:4:GLU:HG2	2.15	0.69
5:H:1:ASP:HA	5:H:4:GLU:HB3	1.74	0.69
5:H:290:ARG:HH22	5:J:202:THR:HG23	1.52	0.69
5:N:290:ARG:HH22	5:R:202:THR:HG23	1.52	0.69
5:G:3:ASP:HA	5:G:6:THR:CB	2.18	0.69
5:J:1:ASP:HA	5:J:4:GLU:HB3	1.74	0.69
5:S:1:ASP:HA	5:S:4:GLU:HB3	1.74	0.69
5:E:3:ASP:HA	5:E:6:THR:CB	2.17	0.69
5:F:1:ASP:HA	5:F:4:GLU:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1:ASP:HA	5:D:4:GLU:HB3	1.74	0.69
5:L:1:ASP:HA	5:L:4:GLU:HB3	1.74	0.69
1:6:55:GLU:CA	5:Q:360:GLN:HE22	2.05	0.69
5:K:290:ARG:HH22	5:M:202:THR:HG23	1.52	0.69
5:M:1:ASP:HA	5:M:4:GLU:HB3	1.74	0.69
5:O:1:ASP:HA	5:O:4:GLU:HB3	1.74	0.69
5:P:1:ASP:HA	5:P:4:GLU:HB3	1.74	0.69
1:0:62:GLU:CD	5:P:359:LYS:HE3	2.07	0.69
1:9:55:GLU:CA	5:S:360:GLN:HE22	2.05	0.69
5:J:290:ARG:HH22	5:L:202:THR:HG23	1.52	0.69
5:N:1:ASP:HA	5:N:4:GLU:HB3	1.74	0.69
1:0:39:LYS:H	1:0:39:LYS:HD2	1.57	0.68
3:5:97:GLN:CD	5:Q:4:GLU:HG2	2.15	0.68
5:K:1:ASP:HA	5:K:4:GLU:HB3	1.74	0.68
5:G:1:ASP:HA	5:G:4:GLU:HB3	1.73	0.68
5:Q:1:ASP:HA	5:Q:4:GLU:HB3	1.74	0.68
5:R:1:ASP:HA	5:R:4:GLU:HB3	1.74	0.68
1:9:39:LYS:H	1:9:39:LYS:HD2	1.57	0.68
5:I:1:ASP:HA	5:I:4:GLU:HB3	1.74	0.68
1:9:137:MET:CE	1:9:148:ILE:HG13	2.24	0.68
5:E:153:LEU:HD11	5:E:274:ILE:HG13	1.76	0.68
5:Q:153:LEU:HD11	5:Q:274:ILE:HG13	1.76	0.68
3:5:29:ILE:HD11	1:6:99:ASN:HB3	1.76	0.68
5:N:153:LEU:HD11	5:N:274:ILE:HG13	1.76	0.68
5:I:153:LEU:HD11	5:I:274:ILE:HG13	1.76	0.67
5:R:153:LEU:HD11	5:R:274:ILE:HG13	1.76	0.67
2:Y:244:ALA:HB1	3:Z:103:ARG:HD2	1.76	0.67
3:2:29:ILE:HD11	1:3:99:ASN:HB3	1.76	0.67
5:E:1:ASP:HA	5:E:4:GLU:HB3	1.74	0.67
5:G:153:LEU:HD11	5:G:274:ILE:HG13	1.76	0.67
1:0:137:MET:CE	1:0:148:ILE:HG13	2.24	0.67
2:7:244:ALA:HB1	3:8:103:ARG:HD2	1.76	0.67
1:6:62:GLU:CD	5:Q:359:LYS:NZ	2.48	0.67
1:0:94:GLU:HB3	3:Z:108:ARG:HG2	1.76	0.67
3:5:108:ARG:HG2	1:6:94:GLU:HB3	1.76	0.67
5:H:160:THR:HG21	5:H:274:ILE:HD11	1.75	0.67
5:J:160:THR:HG21	5:J:274:ILE:HD11	1.76	0.67
2:1:244:ALA:HB1	3:2:103:ARG:HD2	1.76	0.67
3:8:108:ARG:HG2	1:9:94:GLU:HB3	1.76	0.67
5:J:153:LEU:HD11	5:J:274:ILE:HG13	1.76	0.67
5:L:153:LEU:HD11	5:L:274:ILE:HG13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:160:THR:HG21	5:L:274:ILE:HD11	1.76	0.67
2:4:244:ALA:HB1	3:5:103:ARG:HD2	1.76	0.67
5:K:153:LEU:HD11	5:K:274:ILE:HG13	1.76	0.67
5:D:160:THR:HG21	5:D:274:ILE:HD11	1.75	0.67
5:F:160:THR:HG21	5:F:274:ILE:HD11	1.76	0.67
5:N:160:THR:HG21	5:N:274:ILE:HD11	1.75	0.67
5:F:290:ARG:HH22	5:H:202:THR:HG23	1.52	0.66
5:P:153:LEU:HD11	5:P:274:ILE:HG13	1.76	0.66
5:S:153:LEU:HD11	5:S:274:ILE:HG13	1.76	0.66
5:S:160:THR:HG21	5:S:274:ILE:HD11	1.76	0.66
1:6:137:MET:CE	1:6:148:ILE:HG13	2.24	0.66
5:D:153:LEU:HD11	5:D:274:ILE:HG13	1.76	0.66
5:P:160:THR:HG21	5:P:274:ILE:HD11	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
1:0:99:ASN:HB3	3:Z:29:ILE:HD11	1.76	0.66
5:O:160:THR:HG21	5:O:274:ILE:HD11	1.76	0.66
3:2:108:ARG:HG2	1:3:94:GLU:HB3	1.76	0.66
5:M:160:THR:HG21	5:M:274:ILE:HD11	1.76	0.66
5:R:160:THR:HG21	5:R:274:ILE:HD11	1.75	0.66
1:6:58:ASP:HB2	5:Q:360:GLN:HG2	1.77	0.66
1:9:62:GLU:CD	5:S:359:LYS:HZ3	2.03	0.66
5:I:290:ARG:HH22	5:K:202:THR:HG23	1.52	0.66
2:1:198:ASN:HD21	2:1:200:ASP:CG	2.04	0.66
1:9:58:ASP:HB2	5:S:360:GLN:HG2	1.77	0.66
5:Q:160:THR:HG21	5:Q:274:ILE:HD11	1.76	0.66
3:8:29:ILE:HD11	1:9:99:ASN:HB3	1.76	0.65
5:E:160:THR:HG21	5:E:274:ILE:HD11	1.75	0.65
5:F:153:LEU:HD11	5:F:274:ILE:HG13	1.76	0.65
5:G:160:THR:HG21	5:G:274:ILE:HD11	1.76	0.65
5:K:160:THR:HG21	5:K:274:ILE:HD11	1.75	0.65
1:3:137:MET:CE	1:3:148:ILE:HG13	2.24	0.65
5:I:160:THR:HG21	5:I:274:ILE:HD11	1.76	0.65
2:1:203:ARG:HH21	3:2:53:LEU:HG	1.61	0.65
5:O:153:LEU:HD11	5:O:274:ILE:HG13	1.76	0.65
1:3:62:GLU:CG	5:R:359:LYS:CD	2.33	0.65
2:Y:231:LYS:O	2:Y:235:VAL:HG23	1.97	0.65
2:7:203:ARG:HH21	3:8:53:LEU:HG	1.62	0.65
2:Y:203:ARG:HH21	3:Z:53:LEU:HG	1.61	0.65
2:4:198:ASN:HD21	2:4:200:ASP:CG	2.04	0.65
3:5:5:LYS:HE2	3:5:5:LYS:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:231:LYS:O	2:4:235:VAL:HG23	1.97	0.64
1:6:46:ARG:HH11	1:6:51:ASN:ND2	1.95	0.64
1:9:62:GLU:CD	5:S:359:LYS:NZ	2.48	0.64
1:0:46:ARG:HH11	1:0:51:ASN:ND2	1.95	0.64
3:2:5:LYS:HE2	3:2:5:LYS:N	2.13	0.64
1:9:46:ARG:HH11	1:9:51:ASN:ND2	1.95	0.64
3:Z:42:ASN:O	3:Z:45:ALA:HB3	1.98	0.64
2:1:231:LYS:O	2:1:235:VAL:HG23	1.97	0.64
2:4:203:ARG:HH21	3:5:53:LEU:HG	1.62	0.64
3:2:42:ASN:O	3:2:45:ALA:HB3	1.98	0.64
3:8:42:ASN:O	3:8:45:ALA:HB3	1.98	0.64
2:7:231:LYS:O	2:7:235:VAL:HG23	1.97	0.64
5:Q:190:MET:SD	5:Q:209:VAL:HG11	2.38	0.64
3:Z:54:PRO:HB2	3:Z:59:GLU:HB2	1.79	0.64
3:2:54:PRO:HB2	3:2:59:GLU:HB2	1.79	0.64
1:3:21:PHE:CD1	1:3:81:MET:HG3	2.33	0.64
1:3:46:ARG:HH11	1:3:51:ASN:ND2	1.95	0.64
3:5:42:ASN:O	3:5:45:ALA:HB3	1.98	0.64
5:J:190:MET:SD	5:J:209:VAL:HG11	2.38	0.64
2:7:198:ASN:HD21	2:7:200:ASP:CG	2.04	0.64
5:N:190:MET:SD	5:N:209:VAL:HG11	2.38	0.64
3:8:54:PRO:HB2	3:8:59:GLU:HB2	1.79	0.63
5:E:190:MET:SD	5:E:209:VAL:HG11	2.38	0.63
5:G:190:MET:SD	5:G:209:VAL:HG11	2.38	0.63
5:I:190:MET:SD	5:I:209:VAL:HG11	2.38	0.63
5:L:190:MET:SD	5:L:209:VAL:HG11	2.38	0.63
3:2:70:LYS:O	3:2:73:SER:HB3	1.99	0.63
3:8:5:LYS:HE2	3:8:5:LYS:N	2.12	0.63
5:R:190:MET:SD	5:R:209:VAL:HG11	2.38	0.63
5:R:257:CYS:HB3	5:R:258:PRO:HD3	1.81	0.63
2:Y:198:ASN:HD21	2:Y:200:ASP:CG	2.04	0.63
3:Z:70:LYS:O	3:Z:73:SER:HB3	1.99	0.63
1:9:21:PHE:CD1	1:9:81:MET:HG3	2.33	0.63
5:N:257:CYS:HB3	5:N:258:PRO:HD3	1.81	0.63
1:0:21:PHE:CD1	1:0:81:MET:HG3	2.33	0.63
1:6:55:GLU:HA	5:Q:360:GLN:HE22	1.61	0.63
5:G:257:CYS:HB3	5:G:258:PRO:HD3	1.81	0.63
1:6:21:PHE:CD1	1:6:81:MET:HG3	2.33	0.63
3:8:45:ALA:O	3:8:49:PRO:HG3	1.99	0.63
5:H:257:CYS:HB3	5:H:258:PRO:HD3	1.81	0.63
5:L:257:CYS:HB3	5:L:258:PRO:HD3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:4:ASP:O	1:0:7:ALA:HB3	1.99	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
1:6:4:ASP:O	1:6:7:ALA:HB3	1.99	0.63
5:E:257:CYS:HB3	5:E:258:PRO:HD3	1.81	0.63
5:J:257:CYS:HB3	5:J:258:PRO:HD3	1.81	0.63
5:Q:257:CYS:HB3	5:Q:258:PRO:HD3	1.81	0.63
3:Z:45:ALA:O	3:Z:49:PRO:HG3	1.99	0.63
5:S:190:MET:SD	5:S:209:VAL:HG11	2.38	0.63
3:Z:24:LEU:O	3:Z:27:THR:HG22	1.99	0.63
3:2:45:ALA:O	3:2:49:PRO:HG3	1.99	0.62
1:3:57:LEU:O	1:3:61:ILE:HG13	1.99	0.62
3:5:45:ALA:O	3:5:49:PRO:HG3	1.99	0.62
1:6:57:LEU:O	1:6:61:ILE:HG13	1.99	0.62
1:9:4:ASP:O	1:9:7:ALA:HB3	1.99	0.62
5:D:190:MET:SD	5:D:209:VAL:HG11	2.38	0.62
3:5:54:PRO:HB2	3:5:59:GLU:HB2	1.79	0.62
5:F:257:CYS:HB3	5:F:258:PRO:HD3	1.81	0.62
5:P:190:MET:SD	5:P:209:VAL:HG11	2.38	0.62
1:0:58:ASP:O	1:0:62:GLU:HG3	1.99	0.62
1:3:155:LYS:HE3	1:3:155:LYS:CA	2.30	0.62
1:9:57:LEU:O	1:9:61:ILE:HG13	1.99	0.62
1:9:58:ASP:O	1:9:62:GLU:HG3	2.00	0.62
1:9:155:LYS:HE3	1:9:155:LYS:CA	2.30	0.62
5:H:190:MET:SD	5:H:209:VAL:HG11	2.38	0.62
5:M:190:MET:SD	5:M:209:VAL:HG11	2.38	0.62
1:0:57:LEU:O	1:0:61:ILE:HG13	1.99	0.62
3:2:100:PHE:CD1	5:R:4:GLU:OE2	2.53	0.62
5:D:257:CYS:HB3	5:D:258:PRO:HD3	1.81	0.62
3:Z:5:LYS:HE2	3:Z:5:LYS:N	2.12	0.62
1:3:58:ASP:O	1:3:62:GLU:HG3	2.00	0.62
1:6:121:LEU:HD23	1:6:133:ILE:HG12	1.81	0.62
1:6:155:LYS:HE3	1:6:155:LYS:CA	2.30	0.62
5:K:190:MET:SD	5:K:209:VAL:HG11	2.38	0.62
5:O:190:MET:SD	5:O:209:VAL:HG11	2.38	0.62
5:P:4:GLU:OE2	3:Z:100:PHE:CD1	2.53	0.62
5:S:257:CYS:HB3	5:S:258:PRO:HD3	1.81	0.62
3:8:70:LYS:O	3:8:73:SER:HB3	1.99	0.62
3:8:123:ARG:HH11	3:8:123:ARG:HG3	1.65	0.62
5:F:190:MET:SD	5:F:209:VAL:HG11	2.38	0.62
5:K:257:CYS:HB3	5:K:258:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:123:ARG:HG3	3:Z:123:ARG:HH11	1.65	0.62
3:5:108:ARG:NH1	1:6:95:GLU:OE1	2.33	0.62
3:5:24:LEU:O	3:5:27:THR:HG22	1.99	0.62
5:I:257:CYS:HB3	5:I:258:PRO:HD3	1.81	0.62
3:2:24:LEU:O	3:2:27:THR:HG22	1.99	0.62
1:0:95:GLU:OE1	3:Z:108:ARG:NH1	2.33	0.62
1:0:155:LYS:HE3	1:0:155:LYS:CA	2.30	0.62
1:6:59:ALA:HA	5:Q:359:LYS:HZ2	1.65	0.62
3:8:24:LEU:O	3:8:27:THR:HG22	1.99	0.62
5:O:257:CYS:HB3	5:O:258:PRO:HD3	1.81	0.62
5:P:257:CYS:HB3	5:P:258:PRO:HD3	1.81	0.62
3:2:108:ARG:NH1	1:3:95:GLU:OE1	2.33	0.61
5:K:361:GLU:HB3	5:K:369:ILE:HG12	1.82	0.61
1:0:14:SER:H	1:0:17:MET:HG3	1.65	0.61
1:3:121:LEU:HD23	1:3:133:ILE:HG12	1.81	0.61
3:5:123:ARG:HH11	3:5:123:ARG:HG3	1.65	0.61
3:8:108:ARG:NH1	1:9:95:GLU:OE1	2.33	0.61
5:I:361:GLU:HB3	5:I:369:ILE:HG12	1.82	0.61
5:M:257:CYS:HB3	5:M:258:PRO:HD3	1.81	0.61
1:0:143:ASN:ND2	1:0:145:ASP:CG	2.59	0.61
1:3:143:ASN:ND2	1:3:145:ASP:CG	2.59	0.61
1:9:121:LEU:HD23	1:9:133:ILE:HG12	1.81	0.61
5:K:190:MET:HE1	5:K:206:ARG:HA	1.83	0.61
3:2:123:ARG:HH11	3:2:123:ARG:HG3	1.65	0.61
1:0:121:LEU:HD23	1:0:133:ILE:HG12	1.81	0.61
3:5:48:SER:N	3:5:49:PRO:HD3	2.16	0.61
1:6:143:ASN:ND2	1:6:145:ASP:CG	2.59	0.61
3:8:14:ARG:O	3:8:18:LYS:HG3	2.01	0.61
5:E:361:GLU:HB3	5:E:369:ILE:HG12	1.82	0.61
5:G:361:GLU:HB3	5:G:369:ILE:HG12	1.82	0.61
5:H:190:MET:HE1	5:H:206:ARG:HA	1.83	0.61
5:I:190:MET:HE1	5:I:206:ARG:HA	1.83	0.61
3:2:48:SER:N	3:2:49:PRO:HD3	2.16	0.61
5:D:190:MET:HE1	5:D:206:ARG:HA	1.83	0.61
5:F:190:MET:HE1	5:F:206:ARG:HA	1.83	0.61
5:J:190:MET:HE1	5:J:206:ARG:HA	1.83	0.61
5:M:190:MET:HE1	5:M:206:ARG:HA	1.83	0.61
5:M:361:GLU:HB3	5:M:369:ILE:HG12	1.82	0.61
5:O:190:MET:HE1	5:O:206:ARG:HA	1.83	0.61
1:3:14:SER:H	1:3:17:MET:HG3	1.65	0.61
1:6:14:SER:H	1:6:17:MET:HG3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:190:MET:HE1	5:G:206:ARG:HA	1.83	0.61
5:L:190:MET:HE1	5:L:206:ARG:HA	1.83	0.61
5:N:190:MET:HE1	5:N:206:ARG:HA	1.83	0.61
5:Q:361:GLU:HB3	5:Q:369:ILE:HG12	1.82	0.61
5:E:223:PHE:HD2	5:E:312:ARG:NH2	1.99	0.61
5:P:5:THR:HA	3:Z:100:PHE:CZ	2.35	0.61
5:P:361:GLU:HB3	5:P:369:ILE:HG12	1.82	0.61
5:S:190:MET:HE1	5:S:206:ARG:HA	1.83	0.61
1:6:58:ASP:O	1:6:62:GLU:HG3	1.99	0.61
3:8:97:GLN:HA	5:S:4:GLU:OE2	2.00	0.61
5:E:190:MET:HE1	5:E:206:ARG:HA	1.83	0.61
5:F:223:PHE:HD2	5:F:312:ARG:NH2	1.99	0.61
5:P:190:MET:HE1	5:P:206:ARG:HA	1.83	0.61
5:R:361:GLU:HB3	5:R:369:ILE:HG12	1.82	0.61
3:Z:14:ARG:O	3:Z:18:LYS:HG3	2.01	0.61
3:5:14:ARG:O	3:5:18:LYS:HG3	2.01	0.60
1:6:58:ASP:CB	5:Q:360:GLN:NE2	2.62	0.60
5:H:223:PHE:HD2	5:H:312:ARG:NH2	1.99	0.60
5:J:361:GLU:HB3	5:J:369:ILE:HG12	1.82	0.60
5:L:361:GLU:HB3	5:L:369:ILE:HG12	1.82	0.60
5:O:361:GLU:HB3	5:O:369:ILE:HG12	1.82	0.60
5:S:361:GLU:HB3	5:S:369:ILE:HG12	1.82	0.60
1:9:159:GLY:O	1:9:160:VAL:C	2.44	0.60
5:H:361:GLU:HB3	5:H:369:ILE:HG12	1.82	0.60
5:N:361:GLU:HB3	5:N:369:ILE:HG12	1.82	0.60
3:Z:48:SER:N	3:Z:49:PRO:HD3	2.16	0.60
3:Z:132:VAL:HB	3:Z:134:MET:HE2	1.83	0.60
1:0:159:GLY:O	1:0:160:VAL:C	2.44	0.60
1:9:14:SER:H	1:9:17:MET:HG3	1.65	0.60
5:D:361:GLU:HB3	5:D:369:ILE:HG12	1.82	0.60
5:N:223:PHE:HD2	5:N:312:ARG:NH2	1.99	0.60
5:O:223:PHE:HD2	5:O:312:ARG:NH2	1.99	0.60
5:Q:190:MET:HE1	5:Q:206:ARG:HA	1.83	0.60
5:Q:223:PHE:HD2	5:Q:312:ARG:NH2	1.99	0.60
3:2:14:ARG:O	3:2:18:LYS:HG3	2.01	0.60
3:2:100:PHE:HZ	5:R:5:THR:HA	1.67	0.60
1:9:143:ASN:ND2	1:9:145:ASP:CG	2.59	0.60
5:F:361:GLU:HB3	5:F:369:ILE:HG12	1.82	0.60
2:1:227:ILE:C	2:1:227:ILE:HD12	2.27	0.60
3:2:97:GLN:C	3:2:99:LEU:H	2.09	0.60
3:5:97:GLN:HA	5:Q:4:GLU:OE2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:287:ILE:H	5:P:287:ILE:HD12	1.67	0.60
5:R:190:MET:HE1	5:R:206:ARG:HA	1.83	0.60
5:S:223:PHE:HD2	5:S:312:ARG:NH2	2.00	0.60
3:2:100:PHE:CZ	5:R:5:THR:HA	2.35	0.60
3:5:132:VAL:HB	3:5:134:MET:HE2	1.83	0.60
3:8:5:LYS:HE2	3:8:6:LYS:H	1.67	0.60
5:M:223:PHE:HD2	5:M:312:ARG:NH2	1.99	0.60
2:Y:227:ILE:C	2:Y:227:ILE:HD12	2.27	0.60
3:5:97:GLN:C	3:5:99:LEU:H	2.10	0.60
3:8:48:SER:N	3:8:49:PRO:HD3	2.16	0.60
3:8:132:VAL:HB	3:8:134:MET:HE2	1.83	0.60
2:Y:202:LEU:HB3	3:Z:60:LEU:HB3	1.83	0.60
3:Z:97:GLN:C	3:Z:99:LEU:H	2.10	0.60
5:D:223:PHE:HD2	5:D:312:ARG:NH2	2.00	0.60
5:L:223:PHE:HD2	5:L:312:ARG:NH2	1.99	0.60
5:R:287:ILE:HD12	5:R:287:ILE:H	1.67	0.60
5:D:287:ILE:H	5:D:287:ILE:HD12	1.67	0.60
5:K:223:PHE:HD2	5:K:312:ARG:NH2	1.99	0.60
5:K:287:ILE:H	5:K:287:ILE:HD12	1.67	0.60
2:1:202:LEU:HB3	3:2:60:LEU:HB3	1.83	0.59
3:2:5:LYS:HE2	3:2:6:LYS:H	1.67	0.59
3:5:5:LYS:HE2	3:5:6:LYS:H	1.67	0.59
1:9:55:GLU:O	5:S:360:GLN:CD	2.45	0.59
5:P:5:THR:HA	3:Z:100:PHE:HZ	1.67	0.59
2:4:202:LEU:HB3	3:5:60:LEU:HB3	1.83	0.59
1:6:105:ASP:O	1:6:106:LYS:C	2.45	0.59
2:7:202:LEU:HB3	3:8:60:LEU:HB3	1.83	0.59
3:8:97:GLN:C	3:8:99:LEU:H	2.10	0.59
5:I:287:ILE:H	5:I:287:ILE:HD12	1.67	0.59
5:N:287:ILE:H	5:N:287:ILE:HD12	1.67	0.59
1:3:105:ASP:O	1:3:106:LYS:C	2.45	0.59
1:9:59:ALA:HA	5:S:359:LYS:HZ2	1.67	0.59
3:2:132:VAL:HB	3:2:134:MET:HE2	1.83	0.59
1:3:159:GLY:O	1:3:160:VAL:C	2.44	0.59
2:4:207:LYS:HZ2	2:4:208:GLU:CG	2.16	0.59
1:0:105:ASP:O	1:0:106:LYS:C	2.45	0.59
1:6:159:GLY:O	1:6:160:VAL:C	2.44	0.59
5:G:287:ILE:HD12	5:G:287:ILE:H	1.67	0.59
1:6:67:ASP:OD2	1:6:69:SER:HB3	2.03	0.59
5:M:287:ILE:H	5:M:287:ILE:HD12	1.67	0.59
2:4:227:ILE:C	2:4:227:ILE:HD12	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:287:ILE:H	5:F:287:ILE:HD12	1.67	0.59
5:P:223:PHE:HD2	5:P:312:ARG:NH2	2.00	0.59
5:Q:287:ILE:H	5:Q:287:ILE:HD12	1.67	0.59
5:S:287:ILE:H	5:S:287:ILE:HD12	1.67	0.59
2:7:207:LYS:HZ2	2:7:208:GLU:CG	2.16	0.59
5:L:287:ILE:H	5:L:287:ILE:HD12	1.67	0.59
2:1:207:LYS:HZ2	2:1:208:GLU:CG	2.15	0.59
5:I:223:PHE:HD2	5:I:312:ARG:NH2	1.99	0.59
2:7:170:LYS:O	2:7:174:LYS:HG2	2.03	0.58
1:9:67:ASP:OD2	1:9:69:SER:HB3	2.03	0.58
5:J:287:ILE:HD12	5:J:287:ILE:H	1.67	0.58
2:Y:170:LYS:O	2:Y:174:LYS:HG2	2.03	0.58
3:Z:5:LYS:HE2	3:Z:6:LYS:H	1.67	0.58
3:2:130:HIS:HE1	3:2:134:MET:HE3	1.68	0.58
2:7:227:ILE:HD12	2:7:227:ILE:C	2.27	0.58
1:9:105:ASP:O	1:9:106:LYS:C	2.45	0.58
1:3:62:GLU:CG	5:R:360:GLN:H	2.13	0.58
5:H:287:ILE:H	5:H:287:ILE:HD12	1.67	0.58
1:3:150:PHE:CE2	1:3:154:LEU:HD21	2.39	0.58
1:6:84:GLN:O	1:6:85:MET:C	2.47	0.58
5:J:223:PHE:HD2	5:J:312:ARG:NH2	1.99	0.58
3:8:130:HIS:HE1	3:8:134:MET:HE3	1.68	0.58
1:0:67:ASP:OD2	1:0:69:SER:HB3	2.03	0.58
3:2:54:PRO:CB	3:2:59:GLU:HB2	2.34	0.58
1:3:84:GLN:O	1:3:85:MET:C	2.47	0.58
1:9:55:GLU:HA	5:S:360:GLN:HE22	1.61	0.58
1:9:150:PHE:CE2	1:9:154:LEU:HD21	2.39	0.58
1:0:62:GLU:CG	5:P:360:GLN:H	2.13	0.58
1:6:55:GLU:O	5:Q:360:GLN:CD	2.45	0.58
5:E:287:ILE:H	5:E:287:ILE:HD12	1.67	0.58
3:5:130:HIS:HE1	3:5:134:MET:HE3	1.68	0.58
1:6:150:PHE:CE2	1:6:154:LEU:HD21	2.39	0.58
5:O:287:ILE:HD12	5:O:287:ILE:H	1.67	0.58
3:Z:54:PRO:CB	3:Z:59:GLU:HB2	2.34	0.58
2:7:210:TRP:CE2	3:8:51:LEU:HB2	2.39	0.57
2:1:170:LYS:O	2:1:174:LYS:HG2	2.03	0.57
2:1:210:TRP:CE2	3:2:51:LEU:HB2	2.39	0.57
3:5:54:PRO:CB	3:5:59:GLU:HB2	2.34	0.57
1:0:150:PHE:CE2	1:0:154:LEU:HD21	2.39	0.57
1:3:62:GLU:CG	5:R:360:GLN:N	2.59	0.57
5:G:223:PHE:HD2	5:G:312:ARG:NH2	1.99	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:210:TRP:CE2	3:Z:51:LEU:HB2	2.39	0.57
1:3:62:GLU:HB2	5:R:359:LYS:HD3	0.57	0.57
1:3:67:ASP:OD2	1:3:69:SER:HB3	2.03	0.57
2:4:170:LYS:O	2:4:174:LYS:HG2	2.03	0.57
2:4:210:TRP:CE2	3:5:51:LEU:HB2	2.39	0.57
3:5:133:ASN:HD22	3:5:133:ASN:N	2.02	0.57
3:8:54:PRO:CB	3:8:59:GLU:HB2	2.34	0.57
2:Y:194:ILE:HG21	2:Y:201:LYS:HE2	1.86	0.57
1:0:62:GLU:HB2	5:P:359:LYS:HD3	0.57	0.57
2:4:194:ILE:HG21	2:4:201:LYS:HE2	1.86	0.57
2:7:194:ILE:HG21	2:7:201:LYS:HE2	1.86	0.57
1:9:28:PHE:HA	1:9:44:VAL:HG21	1.87	0.57
1:0:28:PHE:HA	1:0:44:VAL:HG21	1.87	0.57
3:Z:130:HIS:HE1	3:Z:134:MET:HE3	1.68	0.57
2:1:194:ILE:HG21	2:1:201:LYS:HE2	1.86	0.57
1:3:28:PHE:HA	1:3:44:VAL:HG21	1.87	0.57
3:2:133:ASN:N	3:2:133:ASN:HD22	2.02	0.56
5:R:223:PHE:HD2	5:R:312:ARG:NH2	1.99	0.56
3:Z:133:ASN:HD22	3:Z:133:ASN:N	2.02	0.56
1:3:143:ASN:HD21	1:3:145:ASP:CG	2.14	0.56
5:J:299:MET:HE2	5:J:331:ALA:HB2	1.87	0.56
1:3:62:GLU:HG3	5:R:360:GLN:CB	2.21	0.56
1:6:143:ASN:HD21	1:6:145:ASP:CG	2.14	0.56
1:6:28:PHE:HA	1:6:44:VAL:HG21	1.87	0.56
5:L:299:MET:HE2	5:L:331:ALA:HB2	1.88	0.56
5:N:299:MET:HE2	5:N:331:ALA:HB2	1.88	0.56
1:0:143:ASN:HD21	1:0:145:ASP:CG	2.14	0.56
5:O:365:ALA:HB3	5:O:369:ILE:HB	1.88	0.56
5:R:299:MET:HE2	5:R:331:ALA:HB2	1.88	0.56
1:3:39:LYS:HD2	1:3:39:LYS:N	2.21	0.56
5:S:365:ALA:HB3	5:S:369:ILE:HB	1.88	0.56
1:3:143:ASN:ND2	1:3:145:ASP:OD1	2.39	0.56
1:6:39:LYS:HD2	1:6:39:LYS:N	2.21	0.56
1:9:143:ASN:ND2	1:9:145:ASP:OD1	2.39	0.56
5:F:299:MET:HE2	5:F:331:ALA:HB2	1.88	0.56
5:F:365:ALA:HB3	5:F:369:ILE:HB	1.88	0.56
5:H:299:MET:HE2	5:H:331:ALA:HB2	1.88	0.56
1:9:84:GLN:O	1:9:85:MET:C	2.47	0.56
5:D:365:ALA:HB3	5:D:369:ILE:HB	1.88	0.56
5:M:365:ALA:HB3	5:M:369:ILE:HB	1.88	0.56
5:Q:299:MET:HE2	5:Q:331:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:133:ASN:HD22	3:8:133:ASN:N	2.02	0.56
5:H:365:ALA:HB3	5:H:369:ILE:HB	1.88	0.56
5:P:365:ALA:HB3	5:P:369:ILE:HB	1.88	0.56
1:0:39:LYS:HD2	1:0:39:LYS:N	2.21	0.55
1:0:84:GLN:O	1:0:85:MET:C	2.47	0.55
5:E:299:MET:HE2	5:E:331:ALA:HB2	1.88	0.55
5:J:365:ALA:HB3	5:J:369:ILE:HB	1.88	0.55
1:9:39:LYS:HD2	1:9:39:LYS:N	2.21	0.55
5:L:365:ALA:HB3	5:L:369:ILE:HB	1.88	0.55
1:3:44:VAL:HA	1:3:47:MET:HE3	1.88	0.55
1:9:143:ASN:HD21	1:9:145:ASP:CG	2.14	0.55
5:K:365:ALA:HB3	5:K:369:ILE:HB	1.88	0.55
5:D:299:MET:HE2	5:D:331:ALA:HB2	1.88	0.55
1:0:62:GLU:CG	5:P:360:GLN:N	2.59	0.55
1:6:44:VAL:HA	1:6:47:MET:HE3	1.88	0.55
5:I:365:ALA:HB3	5:I:369:ILE:HB	1.88	0.55
5:R:365:ALA:HB3	5:R:369:ILE:HB	1.88	0.55
1:0:143:ASN:ND2	1:0:145:ASP:OD1	2.39	0.55
2:4:207:LYS:O	2:4:210:TRP:HB3	2.07	0.55
2:7:243:GLN:HE21	1:9:149:ASP:HB3	1.72	0.55
1:9:44:VAL:HA	1:9:47:MET:HE3	1.88	0.55
5:G:299:MET:HE2	5:G:331:ALA:HB2	1.88	0.55
5:N:365:ALA:HB3	5:N:369:ILE:HB	1.88	0.55
5:S:299:MET:HE2	5:S:331:ALA:HB2	1.88	0.55
5:P:299:MET:HE2	5:P:331:ALA:HB2	1.87	0.55
2:1:207:LYS:O	2:1:210:TRP:HB3	2.07	0.55
5:G:365:ALA:HB3	5:G:369:ILE:HB	1.88	0.55
2:Y:207:LYS:HZ2	2:Y:208:GLU:HA	1.72	0.55
2:4:243:GLN:HE21	1:6:149:ASP:HB3	1.72	0.55
5:E:365:ALA:HB3	5:E:369:ILE:HB	1.88	0.55
5:I:299:MET:HE2	5:I:331:ALA:HB2	1.88	0.55
5:Q:365:ALA:HB3	5:Q:369:ILE:HB	1.88	0.55
1:6:143:ASN:ND2	1:6:145:ASP:OD1	2.39	0.55
2:7:207:LYS:O	2:7:210:TRP:HB3	2.07	0.55
5:M:299:MET:HE2	5:M:331:ALA:HB2	1.88	0.55
5:O:299:MET:HE2	5:O:331:ALA:HB2	1.88	0.54
2:1:243:GLN:HE21	1:3:149:ASP:HB3	1.72	0.54
1:3:46:ARG:NH1	1:3:51:ASN:HD21	2.05	0.54
5:K:299:MET:HE2	5:K:331:ALA:HB2	1.88	0.54
2:Y:207:LYS:O	2:Y:210:TRP:HB3	2.07	0.54
2:7:187:GLU:C	2:7:189:ARG:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:91:GLU:O	3:8:95:LEU:HG	2.08	0.54
1:9:46:ARG:NH1	1:9:51:ASN:HD21	2.05	0.54
1:0:44:VAL:HA	1:0:47:MET:HE3	1.88	0.54
3:5:91:GLU:O	3:5:95:LEU:HG	2.08	0.54
2:7:202:LEU:H	2:7:202:LEU:HD22	1.73	0.54
3:Z:91:GLU:O	3:Z:95:LEU:HG	2.08	0.54
1:0:149:ASP:HB3	2:Y:243:GLN:HE21	1.72	0.54
2:4:187:GLU:C	2:4:189:ARG:H	2.16	0.54
1:6:46:ARG:NH1	1:6:51:ASN:HD21	2.05	0.54
5:P:23:GLY:HA3	3:Z:100:PHE:HE2	1.73	0.54
2:1:187:GLU:C	2:1:189:ARG:H	2.16	0.54
5:E:288:ASP:CA	5:G:204:ALA:HB2	2.32	0.54
3:2:91:GLU:O	3:2:95:LEU:HG	2.08	0.54
3:5:97:GLN:C	3:5:99:LEU:N	2.65	0.54
5:Q:185:LEU:HD23	5:Q:306:TYR:OH	2.09	0.54
1:0:46:ARG:NH1	1:0:51:ASN:HD21	2.05	0.53
3:8:103:ARG:HA	3:8:103:ARG:HE	1.73	0.53
5:R:185:LEU:HD23	5:R:306:TYR:OH	2.09	0.53
2:Y:187:GLU:C	2:Y:189:ARG:H	2.16	0.53
2:1:202:LEU:H	2:1:202:LEU:HD22	1.73	0.53
3:Z:103:ARG:HA	3:Z:103:ARG:HE	1.74	0.53
5:J:185:LEU:HD23	5:J:306:TYR:OH	2.09	0.53
3:8:97:GLN:C	3:8:99:LEU:N	2.65	0.53
5:H:185:LEU:HD23	5:H:306:TYR:OH	2.09	0.53
3:2:103:ARG:HA	3:2:103:ARG:HE	1.74	0.53
2:Y:207:LYS:HZ1	2:Y:208:GLU:CG	2.17	0.53
5:E:185:LEU:HD23	5:E:306:TYR:OH	2.09	0.53
2:Y:202:LEU:HD22	2:Y:202:LEU:H	1.73	0.53
3:2:100:PHE:HE2	5:R:23:GLY:HA3	1.73	0.53
5:L:185:LEU:HD23	5:L:306:TYR:OH	2.09	0.53
2:7:207:LYS:HZ2	2:7:208:GLU:HA	1.73	0.53
1:0:62:GLU:HG3	5:P:360:GLN:CB	2.22	0.53
1:0:106:LYS:O	1:0:107:ASN:HB3	2.09	0.53
1:9:58:ASP:CB	5:S:360:GLN:NE2	2.62	0.53
1:3:156:MET:HG3	1:3:157:MET:HE2	1.91	0.52
2:4:202:LEU:H	2:4:202:LEU:HD22	1.72	0.52
2:4:207:LYS:HZ2	2:4:208:GLU:HA	1.74	0.52
3:5:103:ARG:HA	3:5:103:ARG:HE	1.73	0.52
5:D:180:LEU:HD22	5:D:267:ILE:HD11	1.91	0.52
5:G:180:LEU:HD22	5:G:267:ILE:HD11	1.92	0.52
5:N:185:LEU:HD23	5:N:306:TYR:OH	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:97:GLN:O	3:5:99:LEU:N	2.43	0.52
1:9:54:LYS:C	5:S:360:GLN:HE22	2.17	0.52
1:9:106:LYS:O	1:9:107:ASN:HB3	2.09	0.52
5:F:180:LEU:HD22	5:F:267:ILE:HD11	1.91	0.52
5:H:180:LEU:HD22	5:H:267:ILE:HD11	1.92	0.52
5:J:180:LEU:HD22	5:J:267:ILE:HD11	1.91	0.52
5:K:180:LEU:HD22	5:K:267:ILE:HD11	1.92	0.52
5:K:185:LEU:HD23	5:K:306:TYR:OH	2.09	0.52
5:S:285:CYS:O	5:S:290:ARG:NH1	2.43	0.52
5:I:180:LEU:HD22	5:I:267:ILE:HD11	1.92	0.52
5:P:285:CYS:O	5:P:290:ARG:NH1	2.43	0.52
5:Q:180:LEU:HD22	5:Q:267:ILE:HD11	1.91	0.52
5:G:185:LEU:HD23	5:G:306:TYR:OH	2.08	0.52
5:K:285:CYS:O	5:K:290:ARG:NH1	2.43	0.52
5:O:180:LEU:HD22	5:O:267:ILE:HD11	1.92	0.52
1:3:106:LYS:O	1:3:107:ASN:HB3	2.09	0.52
2:7:207:LYS:NZ	2:7:208:GLU:HA	2.25	0.52
3:8:97:GLN:O	3:8:99:LEU:N	2.43	0.52
1:9:156:MET:HG3	1:9:157:MET:HE2	1.92	0.52
5:F:185:LEU:HD23	5:F:306:TYR:OH	2.09	0.52
5:G:285:CYS:O	5:G:290:ARG:NH1	2.43	0.52
5:I:185:LEU:HD23	5:I:306:TYR:OH	2.09	0.52
5:L:285:CYS:O	5:L:290:ARG:NH1	2.43	0.52
5:P:180:LEU:HD22	5:P:267:ILE:HD11	1.92	0.52
5:R:285:CYS:O	5:R:290:ARG:NH1	2.43	0.52
2:1:207:LYS:NZ	2:1:208:GLU:HA	2.25	0.52
5:F:285:CYS:O	5:F:290:ARG:NH1	2.43	0.52
5:M:180:LEU:HD22	5:M:267:ILE:HD11	1.92	0.52
5:N:180:LEU:HD22	5:N:267:ILE:HD11	1.92	0.52
2:Y:207:LYS:NZ	2:Y:208:GLU:HA	2.25	0.52
3:5:100:PHE:CB	5:Q:4:GLU:OE2	2.58	0.52
1:6:54:LYS:C	5:Q:360:GLN:HE22	2.17	0.52
1:6:106:LYS:O	1:6:107:ASN:HB3	2.09	0.52
5:E:180:LEU:HD22	5:E:267:ILE:HD11	1.92	0.52
5:M:185:LEU:HD23	5:M:306:TYR:OH	2.09	0.52
5:M:285:CYS:O	5:M:290:ARG:NH1	2.43	0.52
5:O:285:CYS:O	5:O:290:ARG:NH1	2.43	0.52
5:S:180:LEU:HD22	5:S:267:ILE:HD11	1.92	0.52
1:0:156:MET:HG3	1:0:157:MET:HE2	1.92	0.52
2:4:207:LYS:NZ	2:4:208:GLU:HA	2.25	0.52
1:6:156:MET:HG3	1:6:157:MET:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:285:CYS:O	5:H: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
3:Z:97:GLN:O	3:Z:99:LEU:N	2.43	0.52
5:J:285:CYS:O	5:J:290:ARG:NH1	2.43	0.52
5:P:185:LEU:HD23	5:P:306:TYR:OH	2.08	0.52
3:2:97:GLN:O	3:2:99:LEU:N	2.43	0.52
5:D:185:LEU:HD23	5:D:306:TYR:OH	2.09	0.52
5:L:180:LEU:HD22	5:L:267:ILE:HD11	1.92	0.52
5:L:287:ILE:HG22	5:N:204:ALA:HB3	1.92	0.52
5:O:288:ASP:CA	5:S:204:ALA:HB2	2.32	0.52
3:Z:97:GLN:C	3:Z:99:LEU:N	2.65	0.52
1:3:103:ILE:HG22	1:3:104:PHE:CD1	2.46	0.51
1:6:58:ASP:CB	5:Q:360:GLN:HG2	2.38	0.51
5:D:285:CYS:O	5:D:290:ARG:NH1	2.43	0.51
5:N:285:CYS:O	5:N:290:ARG:NH1	2.43	0.51
5:N:287:ILE:HG22	5:R:204:ALA:HB3	1.92	0.51
5:O:185:LEU:HD23	5:O:306:TYR:OH	2.09	0.51
3:2:23:GLN:O	3:2:26:VAL:HG12	2.10	0.51
1:6:103:ILE:HG22	1:6:104:PHE:CD1	2.46	0.51
5:E:285:CYS:O	5:E:290:ARG:NH1	2.43	0.51
5:S:185:LEU:HD23	5:S:306:TYR:OH	2.09	0.51
1:0:100:CYS:SG	3:Z:25:ALA:HB1	2.50	0.51
3:Z:23:GLN:O	3:Z:26:VAL:HG12	2.10	0.51
1:0:149:ASP:HB3	2:Y:243:GLN:NE2	2.26	0.51
3:2:25:ALA:HB1	1:3:100:CYS:SG	2.50	0.51
3:8:23:GLN:O	3:8:26:VAL:HG12	2.10	0.51
5:E:204:ALA:HB2	5:Q:288:ASP:CA	2.32	0.51
5:E:204:ALA:HB3	5:Q:287:ILE:HG22	1.92	0.51
5:O:287:ILE:HG22	5:S:204:ALA:HB3	1.92	0.51
3:5:23:GLN:O	3:5:26:VAL:HG12	2.10	0.51
3:8:25:ALA:HB1	1:9:100:CYS:SG	2.50	0.51
5:J:287:ILE:HG22	5:L:204:ALA:HB3	1.92	0.51
3:2:93:GLU:HG2	3:2:111:LEU:HD21	1.92	0.51
3:2:109:PRO:O	3:2:112:ARG:HG2	2.11	0.51
3:5:25:ALA:HB1	1:6:100:CYS:SG	2.50	0.51
2:7:234:ILE:O	2:7:235:VAL:C	2.53	0.51
1:9:58:ASP:CB	5:S:360:GLN:HG2	2.39	0.51
5:D:204:ALA:HB3	5:P:287:ILE:HG22	1.92	0.51
5:M:287:ILE:HG22	5:O:204:ALA:HB3	1.92	0.51
5:K:287:ILE:HG22	5:M:204:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:234:ILE:O	2:Y:235:VAL:C	2.53	0.51
2:4:243:GLN:NE2	1:6:149:ASP:HB3	2.26	0.51
1:0:103:ILE:HG22	1:0:104:PHE:CD1	2.45	0.51
3:5:93:GLU:HG2	3:5:111:LEU:HD21	1.92	0.51
2:7:243:GLN:NE2	1:9:149:ASP:HB3	2.26	0.51
3:8:100:PHE:CB	5:S:4:GLU:OE2	2.58	0.51
5:E:287:ILE:HG22	5:G:204:ALA:HB3	1.92	0.51
5:H:287:ILE:HG22	5:J:204:ALA:HB3	1.92	0.51
3:5:56:SER:N	3:5:59:GLU:OE1	2.39	0.51
2:1:243:GLN:NE2	1:3:149:ASP:HB3	2.26	0.50
5:I:285:CYS:O	5:I:290:ARG:NH1	2.43	0.50
3:5:109:PRO:O	3:5:112:ARG:HG2	2.11	0.50
5:D:287:ILE:HG22	5:F:204:ALA:HB3	1.92	0.50
3:2:97:GLN:C	3:2:99:LEU:N	2.65	0.50
1:6:46:ARG:NH1	1:6:51:ASN:ND2	2.59	0.50
3:8:93:GLU:HG2	3:8:111:LEU:HD21	1.92	0.50
1:9:103:ILE:HG22	1:9:104:PHE:CD1	2.46	0.50
5:G:287:ILE:HG22	5:I:204:ALA:HB3	1.92	0.50
5:I:287:ILE:HG22	5:K:204:ALA:HB3	1.92	0.50
5:F:287:ILE:HG22	5:H:204:ALA:HB3	1.92	0.50
3:Z:93:GLU:HG2	3:Z:111:LEU:HD21	1.92	0.50
3:Z:109:PRO:O	3:Z:112:ARG:HG2	2.11	0.50
2:1:188:ARG:NH1	3:2:75:ASP:OD2	2.45	0.50
2:4:188:ARG:NH1	3:5:75:ASP:OD2	2.45	0.50
2:Y:246:LYS:C	2:Y:248:SER:H	2.20	0.50
1:6:59:ALA:N	5:Q:360:GLN:HG3	2.27	0.50
2:7:188:ARG:NH1	3:8:75:ASP:OD2	2.45	0.50
3:8:109:PRO:O	3:8:112:ARG:HG2	2.11	0.50
5:I:70:PRO:HG3	5:I:81:ASP:HB3	1.93	0.50
5:Q:253:GLU:HA	5:Q:256:ARG:CG	2.42	0.50
1:3:46:ARG:NH1	1:3:51:ASN:ND2	2.59	0.50
5:M:288:ASP:CA	5:O:204:ALA:HB2	2.32	0.50
2:Y:188:ARG:NH1	3:Z:75:ASP:OD2	2.45	0.50
5:F:70:PRO:HG3	5:F:81:ASP:HB3	1.94	0.50
5:H:318:THR:HA	5:H:327:ILE:HG12	1.94	0.50
1:0:46:ARG:NH1	1:0:51:ASN:ND2	2.59	0.49
1:3:22:LYS:HA	1:3:74:PHE:CE1	2.47	0.49
5:G:70:PRO:HG3	5:G:81:ASP:HB3	1.94	0.49
2:1:207:LYS:HZ2	2:1:208:GLU:HA	1.76	0.49
1:6:107:ASN:HD21	1:6:109:ASP:CG	2.20	0.49
1:6:149:ASP:OD2	1:6:152:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:22:LYS:HA	1:9:74:PHE:CE1	2.47	0.49
5:E:70:PRO:HG3	5:E:81:ASP:HB3	1.94	0.49
5:F:318:THR:HA	5:F:327:ILE:HG12	1.94	0.49
5:J:70:PRO:HG3	5:J:81:ASP:HB3	1.94	0.49
5:K:318:THR:HA	5:K:327:ILE:HG12	1.94	0.49
5:N:318:THR:HA	5:N:327:ILE:HG12	1.94	0.49
5:Q:318:THR:HA	5:Q:327:ILE:HG12	1.94	0.49
1:3:107:ASN:HD21	1:3:109:ASP:CG	2.20	0.49
3:5:53:LEU:H	3:5:53:LEU:CD1	2.10	0.49
1:6:36:ILE:HD12	1:6:72:ILE:HB	1.95	0.49
3:8:26:VAL:HG13	3:8:27:THR:N	2.28	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:H:70:PRO:HG3	5:H:81:ASP:HB3	1.94	0.49
5:L:70:PRO:HG3	5:L:81:ASP:HB3	1.93	0.49
5:L:318:THR:HA	5:L:327:ILE:HG12	1.94	0.49
5:O:318:THR:HA	5:O:327:ILE:HG12	1.94	0.49
5:P:318:THR:HA	5:P:327:ILE:HG12	1.94	0.49
5:S:318:THR:HA	5:S:327:ILE:HG12	1.94	0.49
1:3:149:ASP:OD2	1:3:152:GLU:HG3	2.13	0.49
5:I:318:THR:HA	5:I:327:ILE:HG12	1.95	0.49
5:K:70:PRO:HG3	5:K:81:ASP:HB3	1.94	0.49
5:M:318:THR:HA	5:M:327:ILE:HG12	1.94	0.49
5:R:318:THR:HA	5:R:327:ILE:HG12	1.94	0.49
2:1:234:ILE:O	2:1:235:VAL:C	2.53	0.49
2:1:246:LYS:C	2:1:248:SER:H	2.20	0.49
3:2:26:VAL:HG13	3:2:27:THR:N	2.28	0.49
1:6:22:LYS:HA	1:6:74:PHE:CE1	2.47	0.49
5:D:318:THR:HA	5:D:327:ILE:HG12	1.95	0.49
5:O:124:PHE:CZ	5:O:132:MET:HG3	2.48	0.49
3:Z:26:VAL:HG13	3:Z:27:THR:N	2.28	0.49
3:2:111:LEU:HD22	3:2:111:LEU:N	2.28	0.49
1:3:36:ILE:HD12	1:3:72:ILE:HB	1.95	0.49
1:3:118:GLY:HA2	1:3:133:ILE:HD13	1.95	0.49
1:9:59:ALA:N	5:S:360:GLN:HG3	2.27	0.49
5:D:70:PRO:HG3	5:D:81:ASP:HB3	1.94	0.49
5:J:318:THR:HA	5:J:327:ILE:HG12	1.95	0.49
5:M:124:PHE:CZ	5:M:132:MET:HG3	2.48	0.49
5:Q:124:PHE:CZ	5:Q:132:MET:HG3	2.48	0.49
5:S:70:PRO:HG3	5:S:81:ASP:HB3	1.94	0.49
3:2:56:SER:N	3:2:59:GLU:OE1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:26:VAL:HG13	3:5:27:THR:N	2.28	0.49
1:9:103:ILE:HG22	1:9:104:PHE:HD1	1.78	0.49
5:Q:70:PRO:HG3	5:Q:81:ASP:HB3	1.94	0.49
1:0:107:ASN:HD21	1:0:109:ASP:CG	2.20	0.49
2:7:246:LYS:C	2:7:248:SER:H	2.20	0.49
5:G:124:PHE:CZ	5:G:132:MET:HG3	2.48	0.49
5:G:318:THR:HA	5:G:327:ILE:HG12	1.95	0.49
5:J:198:TYR:CZ	5:J:248:ILE:HG13	2.48	0.49
5:J:288:ASP:CA	5:L:204:ALA:HB2	2.32	0.49
5:L:124:PHE:CZ	5:L:132:MET:HG3	2.48	0.49
5:N:124:PHE:CZ	5:N:132:MET:HG3	2.48	0.49
5:N:288:ASP:CA	5:R:204:ALA:HB2	2.32	0.49
5:O:198:TYR:CZ	5:O:248:ILE:HG13	2.48	0.49
5:P:70:PRO:HG3	5:P:81:ASP:HB3	1.94	0.49
5:R:70:PRO:HG3	5:R:81:ASP:HB3	1.94	0.49
5:S:124:PHE:CZ	5:S:132:MET:HG3	2.48	0.49
5:S:198:TYR:CZ	5:S:248:ILE:HG13	2.48	0.49
5:S:213:LYS:O	5:S:217:CYS:HB2	2.13	0.49
1:0:103:ILE:HG22	1:0:104:PHE:HD1	1.78	0.49
1:3:103:ILE:HG22	1:3:104:PHE:HD1	1.78	0.49
3:5:111:LEU:HD22	3:5:111:LEU:N	2.28	0.49
2:7:165:ALA:O	2:7:169:GLN:HG2	2.13	0.49
3:8:133:ASN:N	3:8:133:ASN:ND2	2.61	0.49
5:D:198:TYR:CZ	5:D:248:ILE:HG13	2.48	0.49
5:H:198:TYR:CZ	5:H:248:ILE:HG13	2.48	0.49
5:I:124:PHE:CZ	5:I:132:MET:HG3	2.48	0.49
5:I:253:GLU:HA	5:I:256:ARG:CG	2.42	0.49
5:L:253:GLU:HA	5:L:256:ARG:CG	2.42	0.49
5:L:288:ASP:CA	5:N:204:ALA:HB2	2.32	0.49
1:6:38:THR:HA	1:6:61:ILE:HD11	1.95	0.49
3:8:56:SER:N	3:8:59:GLU:OE1	2.39	0.49
5:D:213:LYS:O	5:D:217:CYS:HB2	2.13	0.49
5:E:124:PHE:CZ	5:E:132:MET:HG3	2.48	0.49
5:H:124:PHE:CZ	5:H:132:MET:HG3	2.48	0.49
5:J:124:PHE:CZ	5:J:132:MET:HG3	2.48	0.49
5:J:213:LYS:O	5:J:217:CYS:HB2	2.13	0.49
5:L:198:TYR:CZ	5:L:248:ILE:HG13	2.48	0.49
5:M:198:TYR:CZ	5:M:248:ILE:HG13	2.48	0.49
5:N:70:PRO:HG3	5:N:81:ASP:HB3	1.94	0.49
5:O:70:PRO:HG3	5:O:81:ASP:HB3	1.94	0.49
5:P:213:LYS:O	5:P:217:CYS:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:149:ASP:OD2	1:0:152:GLU:HG3	2.13	0.48
2:4:246:LYS:C	2:4:248:SER:H	2.20	0.48
1:6:118:GLY:HA2	1:6:133:ILE:HD13	1.95	0.48
2:7:227:ILE:CD1	2:7:231:LYS:HD3	2.43	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:H:288:ASP:CA	5:J:204:ALA:HB2	2.32	0.48
5:I:213:LYS:O	5:I:217:CYS:HB2	2.13	0.48
5:K:124:PHE:CZ	5:K:132:MET:HG3	2.48	0.48
5:P:198:TYR:CZ	5:P:248:ILE:HG13	2.48	0.48
5:Q:213:LYS:O	5:Q:217:CYS:HB2	2.13	0.48
5:R:124:PHE:CZ	5:R:132:MET:HG3	2.48	0.48
2:Y:165:ALA:O	2:Y:169:GLN:HG2	2.13	0.48
3:Z:111:LEU:HD22	3:Z:111:LEU:N	2.28	0.48
3:2:29:ILE:HG22	3:2:30:GLU:N	2.28	0.48
3:8:111:LEU:HD22	3:8:111:LEU:N	2.28	0.48
5:G:213:LYS:O	5:G:217:CYS:HB2	2.13	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
3:5:29:ILE:HG22	3:5:30:GLU:N	2.28	0.48
1:6:111:PHE:HB3	1:6:147:ARG:HB3	1.95	0.48
3:8:97:GLN:CD	5:S:4:GLU:CD	2.78	0.48
1:9:118:GLY:HA2	1:9:133:ILE:HD13	1.95	0.48
5:E:325:MET:HE2	5:G:244:ASP:HB3	1.96	0.48
5:H:120:THR:HG21	5:H:370:VAL:HG11	1.95	0.48
5:I:120:THR:HG21	5:I:370:VAL:HG11	1.95	0.48
5:K:198:TYR:CZ	5:K:248:ILE:HG13	2.48	0.48
5:K:213:LYS:O	5:K:217:CYS:HB2	2.13	0.48
2:1:194:ILE:HG21	2:1:201:LYS:CE	2.43	0.48
1:3:38:THR:HA	1:3:61:ILE:HD11	1.95	0.48
1:3:111:PHE:HB3	1:3:147:ARG:HB3	1.95	0.48
2:4:194:ILE:HG21	2:4:201:LYS:CE	2.43	0.48
1:9:107:ASN:HD21	1:9:109:ASP:CG	2.20	0.48
5:D:124:PHE:CZ	5:D:132:MET:HG3	2.48	0.48
5:E:213:LYS:O	5:E:217:CYS:HB2	2.13	0.48
5:G:120:THR:HG21	5:G:370:VAL:HG11	1.95	0.48
5:I:325:MET:HE2	5:K:244:ASP:HB3	1.96	0.48
5:N:198:TYR:CZ	5:N:248:ILE:HG13	2.48	0.48
5:O:213:LYS:O	5:O:217:CYS:HB2	2.13	0.48
3:Z:56:SER:N	3:Z:59:GLU:OE1	2.39	0.48
2:1:165:ALA:O	2:1:169:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:250:ILE:HG23	5:E:253:GLU:HG2	1.96	0.48
5:M:213:LYS:O	5:M:217:CYS:HB2	2.13	0.48
5:R:198:TYR:CZ	5:R:248:ILE:HG13	2.48	0.48
2:Y:227:ILE:CD1	2:Y:231:LYS:HD3	2.43	0.48
1:O:22:LYS:HA	1:O:74:PHE:CE1	2.47	0.48
1:O:118:GLY:HA2	1:O:133:ILE:HD13	1.95	0.48
3:2:53:LEU:H	3:2:53:LEU:CD1	2.10	0.48
2:4:227:ILE:CD1	2:4:231:LYS:HD3	2.43	0.48
1:6:55:GLU:CA	5:Q:360:GLN:CD	2.77	0.48
1:9:36:ILE:HD12	1:9:72:ILE:HB	1.94	0.48
1:9:55:GLU:CA	5:S:360:GLN:CD	2.77	0.48
1:9:111:PHE:HB3	1:9:147:ARG:HB3	1.96	0.48
1:9:149:ASP:OD2	1:9:152:GLU:HG3	2.13	0.48
5:F:120:THR:HG21	5:F:370:VAL:HG11	1.95	0.48
5:J:250:ILE:HG23	5:J:253:GLU:HG2	1.96	0.48
5:L:120:THR:HG21	5:L:370:VAL:HG11	1.95	0.48
5:M:325:MET:HE2	5:O:244:ASP:HB3	1.96	0.48
5:P:124:PHE:CZ	5:P:132:MET:HG3	2.48	0.48
5:R:213:LYS:O	5:R:217:CYS:HB2	2.13	0.48
3:2:133:ASN:N	3:2:133:ASN:ND2	2.61	0.48
5:F:288:ASP:CA	5:H:204:ALA:HB2	2.32	0.48
5:H:213:LYS:O	5:H:217:CYS:HB2	2.13	0.48
5:H:250:ILE:HG23	5:H:253:GLU:HG2	1.96	0.48
5:L:213:LYS:O	5:L:217:CYS:HB2	2.13	0.48
3:Z:133:ASN:N	3:Z:133:ASN:ND2	2.61	0.48
1:O:38:THR:HA	1:O:61:ILE:HD11	1.95	0.48
3:5:102:LEU:HD23	3:5:102:LEU:O	2.14	0.48
3:8:29:ILE:HG22	3:8:30:GLU:N	2.28	0.48
3:8:102:LEU:O	3:8:102:LEU:HD23	2.14	0.48
5:D:250:ILE:HG23	5:D:253:GLU:HG2	1.96	0.48
5:E:244:ASP:HB3	5:Q:325:MET:HE2	1.96	0.48
5:F:250:ILE:HG23	5:F:253:GLU:HG2	1.96	0.48
5:I:250:ILE:HG23	5:I:253:GLU:HG2	1.96	0.48
5:K:325:MET:HE2	5:M:244:ASP:HB3	1.96	0.48
5:N:120:THR:HG21	5:N:370:VAL:HG11	1.95	0.48
5:N:250:ILE:HG23	5:N:253:GLU:HG2	1.96	0.48
5:O:253:GLU:HA	5:O:256:ARG:CG	2.42	0.48
5:Q:198:TYR:CZ	5:Q:248:ILE:HG13	2.48	0.48
5:Q:250:ILE:HG23	5:Q:253:GLU:HG2	1.96	0.48
3:Z:29:ILE:HG22	3:Z:30:GLU:N	2.28	0.48
2:4:165:ALA:O	2:4:169:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:103:ILE:HG22	1:6:104:PHE:HD1	1.78	0.48
5:L:250:ILE:HG23	5:L:253:GLU:HG2	1.96	0.48
5:N:213:LYS:O	5:N:217:CYS:HB2	2.13	0.48
2:Y:194:ILE:HG21	2:Y:201:LYS:CE	2.43	0.48
1:0:111:PHE:HB3	1:0:147:ARG:HB3	1.95	0.48
3:2:102:LEU:HD23	3:2:102:LEU:O	2.14	0.48
2:4:234:ILE:O	2:4:235:VAL:C	2.53	0.48
3:5:29:ILE:HA	1:6:103:ILE:HD11	1.95	0.48
5:D:120:THR:HG21	5:D:370:VAL:HG11	1.95	0.48
5:D:244:ASP:HB3	5:P:325:MET:HE2	1.96	0.48
5:G:250:ILE:HG23	5:G:253:GLU:HG2	1.96	0.48
5:G:288:ASP:CA	5:I:204:ALA:HB2	2.32	0.48
5:G:325:MET:HE2	5:I:244:ASP:HB3	1.96	0.48
5:K:120:THR:HG21	5:K:370:VAL:HG11	1.95	0.48
5:K:288:ASP:CA	5:M:204:ALA:HB2	2.32	0.48
5:Q:120:THR:HG21	5:Q:370:VAL:HG11	1.95	0.48
5:R:217:CYS:C	5:R:218:TYR:HD1	2.22	0.48
3:Z:102:LEU:HD23	3:Z:102:LEU:O	2.14	0.48
1:3:10:ARG:HH21	1:3:75:GLU:CD	2.22	0.47
1:9:38:THR:HA	1:9:61:ILE:HD11	1.95	0.47
5:E:120:THR:HG21	5:E:370:VAL:HG11	1.95	0.47
5:E:198:TYR:CZ	5:E:248:ILE:HG13	2.48	0.47
5:F:213:LYS:O	5:F:217:CYS:HB2	2.13	0.47
5:I:198:TYR:CZ	5:I:248:ILE:HG13	2.48	0.47
5:O:325:MET:HE2	5:S:244:ASP:HB3	1.96	0.47
5:R:250:ILE:HG23	5:R:253:GLU:HG2	1.96	0.47
5:S:250:ILE:HG23	5:S:253:GLU:HG2	1.96	0.47
5:K:250:ILE:HG23	5:K:253:GLU:HG2	1.96	0.47
5:M:120:THR:HG21	5:M:370:VAL:HG11	1.95	0.47
5:N:217:CYS:C	5:N:218:TYR:HD1	2.22	0.47
5:N:325:MET:HE2	5:R:244:ASP:HB3	1.96	0.47
5:P:253:GLU:HA	5:P:256:ARG:CG	2.42	0.47
5:S:217:CYS:C	5:S:218:TYR:HD1	2.22	0.47
1:0:103:ILE:HD11	3:Z:29:ILE:HA	1.95	0.47
2:1:212:TRP:CE3	2:1:212:TRP:HA	2.50	0.47
2:4:212:TRP:CE3	2:4:212:TRP:HA	2.50	0.47
3:5:133:ASN:N	3:5:133:ASN:ND2	2.61	0.47
3:8:29:ILE:CG2	3:8:30:GLU:N	2.77	0.47
5:D:288:ASP:CA	5:F:204:ALA:HB2	2.32	0.47
5:D:325:MET:HE2	5:F:244:ASP:HB3	1.96	0.47
5:G:198:TYR:CZ	5:G:248:ILE:HG13	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:120:THR:HG21	5:S:370:VAL:HG11	1.95	0.47
1:0:160:VAL:O	1:0:161:GLN:OXT	2.33	0.47
3:5:123:ARG:HG3	3:5:123:ARG:NH1	2.29	0.47
1:6:13:LEU:HB2	1:6:18:ILE:CD1	2.45	0.47
2:7:194:ILE:HG21	2:7:201:LYS:CE	2.43	0.47
2:7:212:TRP:HA	2:7:212:TRP:CE3	2.50	0.47
1:9:160:VAL:O	1:9:161:GLN:OXT	2.33	0.47
5:L:217:CYS:C	5:L:218:TYR:HD1	2.22	0.47
5:M:162:ASN:OD1	5:M:277:THR:HG22	2.15	0.47
5:O:217:CYS:C	5:O:218:TYR:HD1	2.22	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:29:ILE:CG2	3:Z:30:GLU:N	2.77	0.47
2:1:227:ILE:CD1	2:1:231:LYS:HD3	2.43	0.47
1:6:10:ARG:HH21	1:6:75:GLU:CD	2.22	0.47
1:6:160:VAL:O	1:6:161:GLN:OXT	2.33	0.47
5:D:204:ALA:HB2	5:P:288:ASP:CA	2.32	0.47
5:E:162:ASN:OD1	5:E:277:THR:HG22	2.15	0.47
5:F:217:CYS:C	5:F:218:TYR:HD1	2.22	0.47
5:F:253:GLU:HA	5:F:256:ARG:CG	2.42	0.47
5:H:162:ASN:OD1	5:H:277:THR:HG22	2.15	0.47
5:J:217:CYS:C	5:J:218:TYR:HD1	2.22	0.47
5:J:253:GLU:HA	5:J:256:ARG:CG	2.42	0.47
5:L:325:MET:HE2	5:N:244:ASP:HB3	1.96	0.47
5:M:250:ILE:HG23	5:M:253:GLU:HG2	1.96	0.47
5:P:120:THR:HG21	5:P:370:VAL:HG11	1.95	0.47
1:0:36:ILE:HD12	1:0:72:ILE:HB	1.95	0.47
3:2:123:ARG:HG3	3:2:123:ARG:NH1	2.29	0.47
1:3:160:VAL:O	1:3:161:GLN:OXT	2.33	0.47
3:5:100:PHE:HB3	5:Q:4:GLU:OE2	2.14	0.47
1:6:73:ASP:OD1	1:6:75:GLU:HB2	2.15	0.47
5:G:162:ASN:OD1	5:G:277:THR:HG22	2.15	0.47
5:G:253:GLU:HA	5:G:256:ARG:CG	2.42	0.47
5:H:217:CYS:C	5:H:218:TYR:HD1	2.22	0.47
5:I:162:ASN:OD1	5:I:277:THR:HG22	2.15	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
1:0:13:LEU:HB2	1:0:18:ILE:CD1	2.45	0.47
1:0:73:ASP:OD1	1:0:75:GLU:HB2	2.15	0.47
3:2:29:ILE:HA	1:3:103:ILE:HD11	1.95	0.47
3:2:29:ILE:CG2	3:2:30:GLU:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:124:THR:HG23	1:3:126:GLU:N	2.30	0.47
3:5:11:THR:HA	3:5:14:ARG:HH21	1.80	0.47
1:6:124:THR:HG23	1:6:126:GLU:N	2.30	0.47
3:8:29:ILE:HA	1:9:103:ILE:HD11	1.95	0.47
5:D:162:ASN:OD1	5:D:277:THR:HG22	2.15	0.47
5:D:217:CYS:C	5:D:218:TYR:HD1	2.22	0.47
5:E:217:CYS:C	5:E:218:TYR:HD1	2.22	0.47
5:I:288:ASP:CA	5:K:204:ALA:HB2	2.32	0.47
5:J:325:MET:HE2	5:L:244:ASP:HB3	1.96	0.47
5:L:162:ASN:OD1	5:L:277:THR:HG22	2.15	0.47
5:M:217:CYS:C	5:M:218:TYR:HD1	2.22	0.47
5:O:120:THR:HG21	5:O:370:VAL:HG11	1.95	0.47
5:O:250:ILE:HG23	5:O:253:GLU:HG2	1.96	0.47
5:Q:162:ASN:OD1	5:Q:277:THR:HG22	2.15	0.47
5:Q:217:CYS:C	5:Q:218:TYR:HD1	2.22	0.47
5:R:162:ASN:OD1	5:R:277:THR:HG22	2.15	0.47
5:S:162:ASN:OD1	5:S:277:THR:HG22	2.15	0.47
2:1:223:PHE:O	2:1:227:ILE:HG23	2.15	0.47
3:2:92:LEU:HD12	3:2:93:GLU:N	2.30	0.47
2:4:223:PHE:O	2:4:227:ILE:HG23	2.15	0.47
3:5:100:PHE:O	3:5:104:GLY:N	2.48	0.47
3:8:92:LEU:HD12	3:8:93:GLU:N	2.30	0.47
1:9:13:LEU:HB2	1:9:18:ILE:CD1	2.45	0.47
5:G:217:CYS:C	5:G:218:TYR:HD1	2.22	0.47
5:I:217:CYS:C	5:I:218:TYR:HD1	2.22	0.47
5:J:162:ASN:OD1	5:J:277:THR:HG22	2.15	0.47
5:K:217:CYS:C	5:K:218:TYR:HD1	2.22	0.47
5:K:253:GLU:HA	5:K:256:ARG:CG	2.42	0.47
5:M:290:ARG:HH22	5:O:202:THR:CG2	2.18	0.47
5:N:47:MET:HE2	5:N:47:MET:HB2	1.79	0.47
5:P:217:CYS:C	5:P:218:TYR:HD1	2.22	0.47
2:Y:226:GLN:O	2:Y:227:ILE:C	2.56	0.47
3:2:100:PHE:O	3:2:104:GLY:N	2.48	0.47
2:7:221:TYR:CE2	3:8:40:LYS:HG3	2.50	0.47
5:F:325:MET:HE2	5:H:244:ASP:HB3	1.96	0.47
1:3:73:ASP:OD1	1:3:75:GLU:HB2	2.15	0.47
3:5:92:LEU:HD12	3:5:93:GLU:N	2.30	0.47
3:8:100:PHE:HB3	5:S:4:GLU:OE2	2.14	0.47
5:H:325:MET:HE2	5:J:244:ASP:HB3	1.96	0.47
5:O:162:ASN:OD1	5:O:277:THR:HG22	2.15	0.47
1:0:10:ARG:HH21	1:0:75:GLU:CD	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:17:MET:HE1	3:Z:134:MET:SD	2.56	0.46
1:3:13:LEU:HB2	1:3:18:ILE:CD1	2.45	0.46
3:5:29:ILE:CG2	3:5:30:GLU:N	2.77	0.46
3:5:134:MET:SD	1:6:17:MET:HE1	2.55	0.46
3:8:134:MET:SD	1:9:17:MET:HE1	2.55	0.46
1:9:10:ARG:HH21	1:9:75:GLU:CD	2.22	0.46
5:D:287:ILE:HA	5:F:202:THR:HG21	1.57	0.46
3:8:100:PHE:O	3:8:104:GLY:N	2.48	0.46
1:9:73:ASP:OD1	1:9:75:GLU:HB2	2.15	0.46
5:S:253:GLU:HA	5:S:256:ARG:CG	2.42	0.46
2:Y:221:TYR:CE2	3:Z:40:LYS:HG3	2.50	0.46
3:2:134:MET:SD	1:3:17:MET:HE1	2.56	0.46
2:7:223:PHE:O	2:7:227:ILE:HG23	2.15	0.46
5:N:6:THR:HG22	5:N:101:HIS:HA	1.97	0.46
5:P:162:ASN:OD1	5:P:277:THR:HG22	2.15	0.46
3:Z:92:LEU:HD12	3:Z:93:GLU:N	2.30	0.46
1:0:124:THR:HG23	1:0:126:GLU:N	2.30	0.46
2:1:226:GLN:O	2:1:227:ILE:C	2.55	0.46
3:2:11:THR:HA	3:2:14:ARG:HH21	1.80	0.46
5:L:6:THR:HG22	5:L:101:HIS:HA	1.97	0.46
5:R:6:THR:HG22	5:R:101:HIS:HA	1.98	0.46
2:Y:223:PHE:O	2:Y:227:ILE:HG23	2.15	0.46
2:7:226:GLN:O	2:7:227:ILE:C	2.56	0.46
5:E:288:ASP:CG	5:G:203:THR:C	2.84	0.46
1:0:105:ASP:OD1	1:0:107:ASN:OD1	2.33	0.46
1:3:131:GLU:OE1	1:3:131:GLU:N	2.49	0.46
3:8:123:ARG:HG3	3:8:123:ARG:NH1	2.29	0.46
5:G:290:ARG:HH22	5:I:202:THR:CG2	2.18	0.46
5:N:288:ASP:CG	5:R:203:THR:C	2.84	0.46
5:Q:6:THR:HG22	5:Q:101:HIS:HA	1.98	0.46
3:Z:100:PHE:O	3:Z:104:GLY:N	2.48	0.46
5:E:203:THR:C	5:Q:288:ASP:CG	2.84	0.46
5:E:366:GLY:O	5:E:369:ILE:HG22	2.16	0.46
5:F:6:THR:HG22	5:F:101:HIS:HA	1.97	0.46
5:H:190:MET:O	5:H:194:THR:HG23	2.16	0.46
5:L:288:ASP:CG	5:N:203:THR:C	2.84	0.46
5:M:253:GLU:HA	5:M:256:ARG:CG	2.42	0.46
5:R:190:MET:O	5:R:194:THR:HG23	2.16	0.46
2:Y:212:TRP:HA	2:Y:212:TRP:CE3	2.50	0.46
1:6:5:GLN:C	1:6:7:ALA:N	2.74	0.46
3:8:11:THR:HA	3:8:14:ARG:HH21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:59:ALA:H	5:S:360:GLN:HG3	1.81	0.46
5:E:6:THR:HG22	5:E:101:HIS:HA	1.97	0.46
5:F:47:MET:HE2	5:F:47:MET:HB2	1.79	0.46
5:H:6:THR:HG22	5:H:101:HIS:HA	1.98	0.46
5:J:6:THR:HG22	5:J:101:HIS:HA	1.98	0.46
5:N:366:GLY:O	5:N:369:ILE:HG22	2.16	0.46
2:4:202:LEU:H	2:4:202:LEU:CD2	2.29	0.46
1:6:131:GLU:OE1	1:6:131:GLU:N	2.49	0.46
1:9:124:THR:HG23	1:9:126:GLU:N	2.30	0.46
5:F:162:ASN:OD1	5:F:277:THR:HG22	2.15	0.46
5:I:223:PHE:CD2	5:I:259:GLU:HG3	2.51	0.46
5:J:366:GLY:O	5:J:369:ILE:HG22	2.16	0.46
5:R:47:MET:HE2	5:R:47:MET:HB2	1.79	0.46
5:R:223:PHE:CD2	5:R:259:GLU:HG3	2.51	0.46
3:2:140:LEU:HD12	3:2:140:LEU:HA	1.72	0.46
1:3:105:ASP:OD1	1:3:107:ASN:OD1	2.33	0.46
1:9:105:ASP:OD1	1:9:107:ASN:OD1	2.33	0.46
1:9:131:GLU:OE1	1:9:131:GLU:N	2.49	0.46
5:F:190:MET:O	5:F:194:THR:HG23	2.16	0.46
5:G:190:MET:O	5:G:194:THR:HG23	2.16	0.46
5:K:288:ASP:CG	5:M:203:THR:C	2.84	0.46
5:L:223:PHE:CD2	5:L:259:GLU:HG3	2.51	0.46
5:N:223:PHE:CD2	5:N:259:GLU:HG3	2.51	0.46
5:Q:47:MET:HE2	5:Q:47:MET:HB2	1.79	0.46
5:Q:366:GLY:O	5:Q:369:ILE:HG22	2.16	0.46
5:R:366:GLY:O	5:R:369:ILE:HG22	2.16	0.46
3:2:87:LYS:O	3:2:90:LYS:HB3	2.16	0.45
5:F:366:GLY:O	5:F:369:ILE:HG22	2.16	0.45
5:H:288:ASP:CG	5:J:203:THR:C	2.84	0.45
5:I:190:MET:O	5:I:194:THR:HG23	2.16	0.45
5:I:288:ASP:CG	5:K:203:THR:C	2.84	0.45
5:J:190:MET:O	5:J:194:THR:HG23	2.16	0.45
3:Z:11:THR:HA	3:Z:14:ARG:HH21	1.80	0.45
2:1:221:TYR:CE2	3:2:40:LYS:HG3	2.50	0.45
2:1:245:GLN:O	2:1:246:LYS:C	2.59	0.45
3:8:53:LEU:H	3:8:53:LEU:CD1	2.10	0.45
5:D:366:GLY:O	5:D:369:ILE:HG22	2.16	0.45
5:G:288:ASP:CG	5:I:203:THR:C	2.84	0.45
5:K:223:PHE:CD2	5:K:259:GLU:HG3	2.52	0.45
5:L:324:THR:N	5:N:245:GLY:CA	2.71	0.45
1:0:82:VAL:O	1:0:83:ARG:C	2.58	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
2:4:221:TYR:CE2	3:5:40:LYS:HG3	2.50	0.45
1:6:105:ASP:OD1	1:6:107:ASN:OD1	2.33	0.45
1:9:82:VAL:O	1:9:83:ARG:C	2.59	0.45
5:D:32:PRO:HB2	5:D:34:ILE:HD11	1.98	0.45
5:E:190:MET:O	5:E:194:THR:HG23	2.16	0.45
5:E:223:PHE:CD2	5:E:259:GLU:HG3	2.51	0.45
5:G:6:THR:HG22	5:G:101:HIS:HA	1.97	0.45
5:G:223:PHE:CD2	5:G:259:GLU:HG3	2.52	0.45
5:H:253:GLU:HA	5:H:256:ARG:CG	2.42	0.45
5:N:32:PRO:HB2	5:N:34:ILE:HD11	1.98	0.45
5:N:190:MET:O	5:N:194:THR:HG23	2.16	0.45
5:O:223:PHE:CD2	5:O:259:GLU:HG3	2.52	0.45
1:0:112:ILE:HA	1:0:116:GLU:OE2	2.17	0.45
3:2:49:PRO:O	3:2:50:PRO:C	2.60	0.45
3:5:87:LYS:O	3:5:90:LYS:HB3	2.16	0.45
2:7:202:LEU:H	2:7:202:LEU:CD2	2.29	0.45
5:F:288:ASP:CG	5:H:203:THR:C	2.84	0.45
5:I:366:GLY:O	5:I:369:ILE:HG22	2.16	0.45
5:K:190:MET:O	5:K:194:THR:HG23	2.16	0.45
5:L:366:GLY:O	5:L:369:ILE:HG22	2.16	0.45
5:M:223:PHE:CD2	5:M:259:GLU:HG3	2.52	0.45
5:S:32:PRO:HB2	5:S:34:ILE:HD11	1.98	0.45
3:Z:123:ARG:HG3	3:Z:123:ARG:NH1	2.28	0.45
1:0:105:ASP:O	1:0:106:LYS:O	2.35	0.45
1:0:131:GLU:N	1:0:131:GLU:OE1	2.49	0.45
2:4:245:GLN:O	2:4:246:LYS:C	2.59	0.45
3:5:49:PRO:O	3:5:50:PRO:C	2.60	0.45
3:8:11:THR:HG22	3:8:14:ARG:HH21	1.82	0.45
5:D:6:THR:HG22	5:D:101:HIS:HA	1.98	0.45
5:D:190:MET:O	5:D:194:THR:HG23	2.16	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:366:GLY:O	5:G:369:ILE:HG22	2.16	0.45
5:H:366:GLY:O	5:H:369:ILE:HG22	2.16	0.45
5:O:190:MET:O	5:O:194:THR:HG23	2.16	0.45
5:O:366:GLY:O	5:O:369:ILE:HG22	2.16	0.45
5:P:223:PHE:CD2	5:P:259:GLU:HG3	2.52	0.45
5:R:253:GLU:HA	5:R:256:ARG:CG	2.42	0.45
5:S:6:THR:HG22	5:S:101:HIS:HA	1.97	0.45
5:S:190:MET:O	5:S:194:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:202:LEU:H	2:Y:202:LEU:CD2	2.29	0.45
2:1:227:ILE:HD12	2:1:228:LYS:N	2.32	0.45
3:5:140:LEU:HA	3:5:140:LEU:HD12	1.73	0.45
1:9:112:ILE:HA	1:9:116:GLU:OE2	2.17	0.45
5:H:223:PHE:CD2	5:H:259:GLU:HG3	2.52	0.45
5:M:32:PRO:HB2	5:M:34:ILE:HD11	1.98	0.45
5:M:190:MET:O	5:M:194:THR:HG23	2.16	0.45
5:M:288:ASP:CG	5:O:203:THR:C	2.84	0.45
5:O:32:PRO:HB2	5:O:34:ILE:HD11	1.98	0.45
5:P:32:PRO:HB2	5:P:34:ILE:HD11	1.98	0.45
5:S:223:PHE:CD2	5:S:259:GLU:HG3	2.52	0.45
2:Y:207:LYS:HD2	2:Y:207:LYS:C	2.42	0.45
2:Y:245:GLN:O	2:Y:246:LYS:C	2.59	0.45
3:2:24:LEU:O	3:2:24:LEU:HD23	2.17	0.45
5:D:290:ARG:HH22	5:F:202:THR:CG2	2.18	0.45
5:F:223:PHE:CD2	5:F:259:GLU:HG3	2.52	0.45
5:N:253:GLU:HA	5:N:256:ARG:CG	2.42	0.45
5:P:366:GLY:O	5:P:369:ILE:HG22	2.16	0.45
5:R:32:PRO:HB2	5:R:34:ILE:HD11	1.98	0.45
3:Z:87:LYS:O	3:Z:90:LYS:HB3	2.16	0.45
3:2:141:LYS:CD	3:2:141:LYS:N	2.70	0.45
3:5:11:THR:HG22	3:5:14:ARG:HH21	1.82	0.45
2:7:245:GLN:O	2:7:246:LYS:C	2.59	0.45
5:H:47:MET:HE2	5:H:47:MET:HB2	1.79	0.45
5:I:253:GLU:H	5:I:253:GLU:CD	2.25	0.45
5:J:223:PHE:CD2	5:J:259:GLU:HG3	2.52	0.45
5:J:288:ASP:CG	5:L:203:THR:C	2.84	0.45
5:Q:32:PRO:HB2	5:Q:34:ILE:HD11	1.98	0.45
5:S:366:GLY:O	5:S:369:ILE:HG22	2.16	0.45
3:Z:24:LEU:O	3:Z:24:LEU:HD23	2.17	0.45
3:5:24:LEU:O	3:5:24:LEU:HD23	2.17	0.45
3:8:24:LEU:O	3:8:24:LEU:HD23	2.17	0.45
1:9:105:ASP:O	1:9:106:LYS:O	2.35	0.45
5:D:203:THR:C	5:P:288:ASP:CG	2.84	0.45
5:D:288:ASP:CG	5:F:203:THR:C	2.84	0.45
5:E:32:PRO:HB2	5:E:34:ILE:HD11	1.98	0.45
5:E:253:GLU:HA	5:E:256:ARG:CG	2.42	0.45
5:P:190:MET:O	5:P:194:THR:HG23	2.16	0.45
5:Q:223:PHE:CD2	5:Q:259:GLU:HG3	2.52	0.45
1:3:5:GLN:C	1:3:7:ALA:N	2.74	0.45
2:4:226:GLN:O	2:4:227:ILE:C	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:129:LYS:NZ	3:5:129:LYS:HA	2.32	0.45
3:5:142:GLN:HG2	3:5:143:VAL:N	2.32	0.45
2:7:207:LYS:HD2	2:7:207:LYS:C	2.42	0.45
5:G:253:GLU:H	5:G:253:GLU:CD	2.25	0.45
5:H:32:PRO:HB2	5:H:34:ILE:HD11	1.98	0.45
5:K:32:PRO:HB2	5:K:34:ILE:HD11	1.98	0.45
5:K:253:GLU:CD	5:K:253:GLU:H	2.25	0.45
5:K:324:THR:N	5:M: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
5:M:366:GLY:O	5:M:369:ILE:HG22	2.16	0.45
5:O:288:ASP:CG	5:S:203:THR:C	2.84	0.45
5:P:6:THR:HG22	5:P:101:HIS:HA	1.98	0.45
3:8:87:LYS:O	3:8:90:LYS:HB3	2.16	0.44
5:D:253:GLU:HA	5:D:256:ARG:CG	2.42	0.44
5:O:6:THR:HG22	5:O:101:HIS:HA	1.97	0.44
5:O:324:THR:N	5:S:245:GLY:CA	2.71	0.44
5:Q:190:MET:O	5:Q:194:THR:HG23	2.16	0.44
3:Z:11:THR:HG22	3:Z:14:ARG:HH21	1.82	0.44
3:2:11:THR:HG22	3:2:14:ARG:HH21	1.82	0.44
3:2:129:LYS:HA	3:2:129:LYS:NZ	2.32	0.44
2:4:207:LYS:HD2	2:4:207:LYS:C	2.42	0.44
3:5:97:GLN:NE2	5:Q:4:GLU:OE1	2.46	0.44
1:6:105:ASP:O	1:6:106:LYS:O	2.35	0.44
5:I:6:THR:HG22	5:I:101:HIS:HA	1.98	0.44
5:L:47:MET:HE2	5:L:47:MET:HB2	1.79	0.44
5:L:190:MET:O	5:L:194:THR:HG23	2.16	0.44
1:0:103:ILE:HD13	3:Z:28:GLU:HB3	2.00	0.44
2:4:227:ILE:HD12	2:4:228:LYS:N	2.32	0.44
1:6:59:ALA:H	5:Q:360:GLN:HG3	1.81	0.44
5:J:47:MET:HE2	5:J:47:MET:HB2	1.79	0.44
5:J:223:PHE:HB3	5:J:259:GLU:OE2	2.17	0.44
2:1:207:LYS:HD2	2:1:207:LYS:C	2.42	0.44
1:6:61:ILE:C	1:6:63:GLU:H	2.25	0.44
2:7:227:ILE:HG22	3:8:85:LEU:HG	2.00	0.44
3:8:51:LEU:C	3:8:51:LEU:HD23	2.43	0.44
3:8:114:VAL:HG22	3:8:115:ARG:O	2.17	0.44
5:D:202:THR:HG21	5:P:287:ILE:HA	1.58	0.44
5:E:47:MET:HE2	5:E:47:MET:HB2	1.79	0.44
5:H:223:PHE:HB3	5:H:259:GLU:OE2	2.18	0.44
5:L:223:PHE:HB3	5:L:259:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:223:PHE:HB3	5:N:259:GLU:OE2	2.18	0.44
2:Y:227:ILE:HG22	3:Z:85:LEU:HG	2.00	0.44
3:2:142:GLN:HG2	3:2:143:VAL:N	2.32	0.44
1:3:82:VAL:O	1:3:83:ARG:C	2.59	0.44
3:5:121:MET:HE1	1:6:81:MET:HE1	2.00	0.44
5:E:223:PHE:HB3	5:E:259:GLU:OE2	2.18	0.44
5:F:223:PHE:HB3	5:F:259:GLU:OE2	2.18	0.44
3:Z:18:LYS:O	3:Z:21:MET:HB2	2.18	0.44
3:Z:114:VAL:HG22	3:Z:115:ARG:O	2.18	0.44
2:1:190:LYS:HA	2:1:191:PRO:HD2	1.80	0.44
2:1:221:TYR:CD2	3:2:40:LYS:HG3	2.53	0.44
3:2:18:LYS:O	3:2:21:MET:HB2	2.17	0.44
3:2:85:LEU:CD2	3:2:89:ILE:HG13	2.48	0.44
1:3:105:ASP:O	1:3:106:LYS:O	2.35	0.44
2:4:190:LYS:HA	2:4:191:PRO:HD2	1.80	0.44
1:6:112:ILE:HA	1:6:116:GLU:OE2	2.17	0.44
3:8:28:GLU:HB3	1:9:103:ILE:HD13	2.00	0.44
3:8:49:PRO:O	3:8:50:PRO:C	2.60	0.44
5:D:253:GLU:H	5:D:253:GLU:CD	2.25	0.44
5:E:253:GLU:CD	5:E:253:GLU:H	2.26	0.44
5:G:32:PRO:HB2	5:G:34:ILE:HD11	1.98	0.44
5:H:171:LEU:HA	5:H:172:PRO:HD2	1.84	0.44
5:I:32:PRO:HB2	5:I:34:ILE:HD11	1.98	0.44
5:J:32:PRO:HB2	5:J:34:ILE:HD11	1.98	0.44
5:K:6:THR:HG22	5:K:101:HIS:HA	1.97	0.44
5:L:290:ARG:HH22	5:N:202:THR:CG2	2.18	0.44
5:M:6:THR:HG22	5:M:101:HIS:HA	1.98	0.44
5:M:253:GLU:CD	5:M:253:GLU:H	2.26	0.44
5:N:253:GLU:CD	5:N:253:GLU:H	2.25	0.44
5:N:287:ILE:N	5:R:202:THR:CG2	2.77	0.44
5:Q:315:LYS:HD2	5:Q:315:LYS:HA	1.92	0.44
3:Z:136:LEU:C	3:Z:136:LEU:HD13	2.43	0.44
1:3:112:ILE:HA	1:3:116:GLU:OE2	2.17	0.44
2:4:215:GLN:O	2:4:219:GLU:HG3	2.18	0.44
2:4:227:ILE:HG22	3:5:85:LEU:HG	2.00	0.44
2:7:221:TYR:CD2	3:8:40: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
3:8:121:MET:HE1	1:9:81:MET:HE1	2.00	0.44
3:8:142:GLN:HG2	3:8:143:VAL:N	2.32	0.44
1:9:5:GLN:C	1:9:7:ALA:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:223:PHE:HB3	5:D:259:GLU:OE2	2.18	0.44
5:F:253:GLU:CD	5:F:253:GLU:H	2.26	0.44
5:H:193:LEU:O	5:H:198:TYR:HD2	2.01	0.44
5:J:253:GLU:H	5:J:253:GLU:CD	2.25	0.44
5:L:253:GLU:H	5:L:253:GLU:CD	2.26	0.44
5:M:193:LEU:O	5:M:198:TYR:HD2	2.01	0.44
5:M:220:ALA:HB3	5:M:223:PHE:CD1	2.53	0.44
5:P:223:PHE:HB3	5:P:259:GLU:OE2	2.18	0.44
5:R:223:PHE:HB3	5:R:259:GLU:OE2	2.18	0.44
5:S:223:PHE:HB3	5:S:259:GLU:OE2	2.18	0.44
2:Y:221:TYR:CD2	3:Z:40:LYS:HG3	2.53	0.44
3:5:114:VAL:HG22	3:5:115:ARG:O	2.17	0.44
3:5:140:LEU:O	3:5:141:LYS:C	2.61	0.44
2:7:215:GLN:O	2:7:219:GLU:HG3	2.18	0.44
3:8:18:LYS:O	3:8:21:MET:HB2	2.18	0.44
3:8:140:LEU:O	3:8:141:LYS:C	2.61	0.44
1:9:61:ILE:C	1:9:63:GLU:H	2.25	0.44
5:F:193:LEU:O	5:F:198:TYR:HD2	2.01	0.44
5:F:324:THR:N	5:H:245:GLY:CA	2.71	0.44
5:G:223:PHE:HB3	5:G:259:GLU:OE2	2.18	0.44
5:H:253:GLU:CD	5:H:253:GLU:H	2.25	0.44
5:I:193:LEU:O	5:I:198:TYR:HD2	2.01	0.44
5:K:193:LEU:O	5:K:198:TYR:HD2	2.01	0.44
5:M:299:MET:HE2	5:M:299:MET:HB2	1.82	0.44
5:O:220:ALA:HB3	5:O:223:PHE:CD1	2.53	0.44
5:Q:223:PHE:HB3	5:Q:259:GLU:OE2	2.18	0.44
2:Y:227:ILE:HD12	2:Y:228:LYS:N	2.32	0.44
3:Z:49:PRO:O	3:Z:50:PRO:C	2.60	0.44
3:2:22:LEU:O	3:2:23:GLN:C	2.61	0.44
3:2:28:GLU:HB3	1:3:103:ILE:HD13	2.00	0.44
1:3:61:ILE:C	1:3:63:GLU:H	2.25	0.44
2:4:207:LYS:NZ	2:4:208:GLU:HG2	2.27	0.44
3:5:22:LEU:O	3:5:23:GLN:C	2.61	0.44
3:5:95:LEU:C	3:5:97:GLN:H	2.26	0.44
1:9:5:GLN:C	1:9:7:ALA:H	2.25	0.44
5:I:223:PHE:HB3	5:I:259:GLU:OE2	2.18	0.44
5:K:223:PHE:HB3	5:K:259:GLU:OE2	2.17	0.44
5:O:223:PHE:HB3	5:O:259:GLU:OE2	2.18	0.44
5:Q:205:GLU:O	5:Q:208:ILE:HG22	2.18	0.44
5:S:220:ALA:HB3	5:S:223:PHE:CD1	2.53	0.44
3:Z:51:LEU:HD23	3:Z:51:LEU:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:53:LEU:H	3:Z:53:LEU:CD1	2.10	0.44
1:0:5:GLN:C	1:0:7:ALA:H	2.25	0.43
2:1:227:ILE:HG22	3:2:85:LEU:HG	2.00	0.43
3:2:114:VAL:HG22	3:2:115:ARG:O	2.18	0.43
5:E:287:ILE:CB	5:G:204:ALA:H	2.15	0.43
5:L:205:GLU:O	5:L:208:ILE:HG22	2.18	0.43
5:O:253:GLU:H	5:O:253:GLU:CD	2.25	0.43
5:Q:193:LEU:O	5:Q:198:TYR:HD2	2.01	0.43
5:R:193:LEU:O	5:R:198:TYR:HD2	2.01	0.43
3:5:13:ARG:O	3:5:14:ARG:C	2.61	0.43
3:5:51:LEU:HD23	3:5:51:LEU:C	2.43	0.43
3:5:58:GLN:O	3:5:62:GLU:HB2	2.19	0.43
3:5:85:LEU:CD2	3:5:89:ILE:HG13	2.48	0.43
5:D:220:ALA:HB3	5:D:223:PHE:CD1	2.53	0.43
5:H:149:THR:HA	5:H:165:ILE:O	2.19	0.43
5:K:220:ALA:HB3	5:K:223:PHE:CD1	2.53	0.43
5:M:223:PHE:HB3	5:M:259:GLU:OE2	2.18	0.43
5:P:220:ALA:HB3	5:P:223:PHE:CD1	2.53	0.43
5:P:253:GLU:CD	5:P:253:GLU:H	2.25	0.43
3:Z:63:LEU:O	3:Z:66:LYS:HB3	2.18	0.43
3:Z:142:GLN:HG2	3:Z:143:VAL:N	2.32	0.43
1:0:61:ILE:C	1:0:63:GLU:H	2.25	0.43
3:2:51:LEU:HD23	3:2:51:LEU:C	2.43	0.43
3:2:95:LEU:C	3:2:97:GLN:H	2.26	0.43
1:3:118:GLY:O	1:3:119:GLU:C	2.62	0.43
2:4:221:TYR:O	2:4:224:ALA:HB3	2.19	0.43
3:5:18:LYS:O	3:5:21:MET:HB2	2.18	0.43
1:6:118:GLY:O	1:6:119:GLU:C	2.62	0.43
2:7:230:LYS:NZ	3:8:89:ILE:HG12	2.34	0.43
3:8:95:LEU:C	3:8:97:GLN:H	2.26	0.43
5:E:315:LYS:HD2	5:E:315:LYS:HA	1.92	0.43
5:H:205:GLU:O	5:H:208:ILE:HG22	2.18	0.43
5:I:220:ALA:HB3	5:I:223:PHE:CD1	2.53	0.43
5:L:149:THR:HA	5:L:165:ILE:O	2.18	0.43
5:N:205:GLU:O	5:N:208:ILE:HG22	2.18	0.43
5:O:47:MET:HB2	5:O:47:MET:HE2	1.79	0.43
5:O:287:ILE:HA	5:S:202:THR:HG21	1.57	0.43
2:Y:187:GLU:O	2:Y:189:ARG:N	2.51	0.43
2:Y:215:GLN:O	2:Y:219:GLU:HG3	2.18	0.43
3:Z:68:HIS:HA	3:Z:71:ILE:HD12	2.00	0.43
2:1:221:TYR:O	2:1:224:ALA:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:140:LEU:O	3:2:141:LYS:C	2.61	0.43
1:6:5:GLN:C	1:6:7:ALA:H	2.25	0.43
3:8:85:LEU:CD2	3:8:89:ILE:HG13	2.48	0.43
3:8:129:LYS:HA	3:8:129:LYS:NZ	2.32	0.43
5:F:149:THR:HA	5:F:165:ILE:O	2.19	0.43
5:L:287:ILE:HD11	5:N:202:THR:HA	1.64	0.43
5:Q:253:GLU:H	5:Q:253:GLU:CD	2.25	0.43
5:R:253:GLU:H	5:R:253:GLU:CD	2.26	0.43
3:Z:129:LYS:HA	3:Z:129:LYS:NZ	2.32	0.43
3:Z:140:LEU:O	3:Z:141:LYS:C	2.61	0.43
1:0:5:GLN:C	1:0:7:ALA:N	2.74	0.43
3:2:63:LEU:O	3:2:66:LYS:HB3	2.18	0.43
3:2:121:MET:HE1	1:3:81:MET:HE1	2.00	0.43
1:6:82:VAL:O	1:6:83:ARG:C	2.59	0.43
2:7:198:ASN:HD22	2:7:201:LYS:HB2	1.84	0.43
3:8:63:LEU:O	3:8:66:LYS:HB3	2.18	0.43
3:8:136:LEU:HD13	3:8:136:LEU:C	2.43	0.43
5:D:149:THR:HA	5:D:165:ILE:O	2.19	0.43
5:D:193:LEU:O	5:D:198:TYR:HD2	2.01	0.43
5:G:287:ILE:N	5:I:202:THR:CG2	2.77	0.43
5:J:193:LEU:O	5:J:198:TYR:HD2	2.01	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:149:THR:HA	5:Q:165:ILE:O	2.19	0.43
3:Z:58:GLN:O	3:Z:62:GLU:HB2	2.19	0.43
1:0:136:LEU:HG	3:Z:14:ARG:HG2	2.01	0.43
2:1:198:ASN:HD22	2:1:201:LYS:HB2	1.84	0.43
3:2:58:GLN:O	3:2:62:GLU:HB2	2.19	0.43
1:3:5:GLN:C	1:3:7:ALA:H	2.26	0.43
3:8:58:GLN:O	3:8:62:GLU:HB2	2.19	0.43
5:F:220:ALA:HB3	5:F:223:PHE:CD1	2.53	0.43
5:O:193:LEU:O	5:O:198:TYR:HD2	2.01	0.43
5:R:205:GLU:O	5:R:208:ILE:HG22	2.18	0.43
5:S:193:LEU:O	5:S:198:TYR:HD2	2.01	0.43
5:S:253:GLU:CD	5:S:253:GLU:H	2.25	0.43
2:Y:227:ILE:HD12	2:Y:231:LYS:HD3	2.00	0.43
3:Z:95:LEU:C	3:Z:97:GLN:H	2.26	0.43
2:1:215:GLN:O	2:1:219:GLU:HG3	2.18	0.43
2:1:230:LYS:NZ	3:2:89:ILE:HG12	2.34	0.43
1:3:53:THR:HG1	1:3:56:GLU:HG3	1.79	0.43
3:5:53:LEU:HA	3:5:54:PRO:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:63:LEU:O	3:5:66:LYS:HB3	2.18	0.43
1:6:53:THR:O	1:6:54:LYS:C	2.62	0.43
3:8:121:MET:HE1	1:9:81:MET:SD	2.59	0.43
5:F:205:GLU:O	5:F:208:ILE:HG22	2.18	0.43
5:J:205:GLU:O	5:J:208:ILE:HG22	2.18	0.43
5:N:193:LEU:O	5:N:198:TYR:HD2	2.01	0.43
5:P:149:THR:HA	5:P:165:ILE:O	2.19	0.43
5:S:315:LYS:HD2	5:S:315:LYS:HA	1.92	0.43
1:0:81:MET:HE1	3:Z:121:MET:HE1	2.00	0.43
2:1:187:GLU:O	2:1:189:ARG:N	2.51	0.43
1:3:53:THR:O	1:3:54:LYS:C	2.62	0.43
3:5:97:GLN:CD	5:Q:4:GLU:CD	2.77	0.43
3:5:121:MET:HE1	1:6:81:MET:SD	2.59	0.43
3:5:136:LEU:HD13	3:5:136:LEU:C	2.43	0.43
3:8:13:ARG:O	3:8:14:ARG:C	2.61	0.43
3:8:14:ARG:HG2	1:9:136:LEU:HG	2.01	0.43
5:G:205:GLU:O	5:G:208:ILE:HG22	2.18	0.43
5:G:220:ALA:HB3	5:G:223:PHE:CD1	2.53	0.43
5:I:149:THR:HA	5:I:165:ILE:O	2.19	0.43
5:M:315:LYS:HD2	5:M:315:LYS:HA	1.92	0.43
5:O:149:THR:HA	5:O:165:ILE:O	2.19	0.43
5:R:149:THR:HA	5:R:165:ILE:O	2.18	0.43
5:S:149:THR:HA	5:S:165:ILE:O	2.19	0.43
2:Y:198:ASN:HD22	2:Y:201:LYS:HB2	1.84	0.43
2:Y:221:TYR:O	2:Y:224:ALA:HB3	2.19	0.43
2:1:227:ILE:HD12	2:1:231:LYS:HD3	2.00	0.43
3:2:136:LEU:HD13	3:2:136:LEU:C	2.43	0.43
2:4:221:TYR:CD2	3:5:40:LYS:HG3	2.53	0.43
3:5:28:GLU:HB3	1:6:103:ILE:HD13	2.00	0.43
3:5:68:HIS:HA	3:5:71:ILE:HD12	2.01	0.43
5:D:171:LEU:HA	5:D:172:PRO:HD2	1.84	0.43
5:E:193:LEU:O	5:E:198:TYR:HD2	2.01	0.43
5:G:193:LEU:O	5:G:198:TYR:HD2	2.01	0.43
5:H:220:ALA:HB3	5:H:223:PHE:CD1	2.53	0.43
5:J:220:ALA:HB3	5:J:223:PHE:CD1	2.53	0.43
5:N:149:THR:HA	5:N:165:ILE:O	2.19	0.43
5:R:220:ALA:HB3	5:R:223:PHE:CD1	2.53	0.43
3:Z:85:LEU:CD2	3:Z:89:ILE:HG13	2.48	0.43
3:2:85:LEU:O	3:2:86:GLN:C	2.62	0.43
3:8:140:LEU:HA	3:8:140:LEU:HD12	1.73	0.43
5:J:149:THR:HA	5:J:165:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:287:ILE:HA	5:L:202:THR:HG21	1.58	0.43
5:K:149:THR:HA	5:K:165:ILE:O	2.19	0.43
5:P:222:ASP:OD1	5:P:224:GLU:HB3	2.19	0.43
2:Y:230:LYS:NZ	3:Z:89:ILE:HG12	2.34	0.43
3:2:121:MET:HE1	1:3:81:MET:SD	2.59	0.42
1:6:58:ASP:CB	5:Q:360:GLN:HE21	2.26	0.42
2:7:187:GLU:O	2:7:189:ARG:N	2.51	0.42
2:7:221:TYR:O	2:7:224:ALA:HB3	2.19	0.42
5:E:149:THR:HA	5:E:165:ILE:O	2.19	0.42
5:G:47:MET:HE2	5:G:47:MET:HB2	1.79	0.42
5:G:149:THR:HA	5:G:165:ILE:O	2.19	0.42
5:I:180:LEU:HD11	5:I:261:LEU:HD23	2.01	0.42
5:J:206:ARG:O	5:J:209:VAL:HG12	2.19	0.42
5:L:180:LEU:HD11	5:L:261:LEU:HD23	2.01	0.42
5:L:193:LEU:O	5:L:198:TYR:HD2	2.01	0.42
5:M:149:THR:HA	5:M:165:ILE:O	2.19	0.42
5:M:287:ILE:HA	5:O:202:THR:HG21	1.57	0.42
5:N:180:LEU:HD11	5:N:261:LEU:HD23	2.01	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
5:S:222:ASP:OD1	5:S:224:GLU:HB3	2.19	0.42
3:Z:130:HIS:HE1	3:Z:134:MET:CE	2.32	0.42
2:4:198:ASN:HD22	2:4:201:LYS:HB2	1.84	0.42
2:4:230:LYS:NZ	3:5:89:ILE:HG12	2.34	0.42
3:5:14:ARG:HG2	1:6:136:LEU:HG	2.01	0.42
5:D:245:GLY:CA	5:P:324:THR:N	2.71	0.42
5:E:180:LEU:HD11	5:E:261:LEU:HD23	2.01	0.42
5:E:205:GLU:O	5:E:208:ILE:HG22	2.18	0.42
5:G:324:THR:N	5:I:245:GLY:CA	2.71	0.42
5:I:222:ASP:OD1	5:I:224:GLU:HB3	2.19	0.42
5:I:315:LYS:HD2	5:I:315:LYS:HA	1.91	0.42
5:P:193:LEU:O	5:P:198:TYR:HD2	2.01	0.42
5:S:206:ARG:O	5:S:209:VAL:HG12	2.20	0.42
3:Z:88:THR:O	3:Z:89:ILE:C	2.62	0.42
3:2:14:ARG:HG2	1:3:136:LEU:HG	2.01	0.42
1:3:8:GLU:HA	1:3:11:ALA:HB3	2.01	0.42
3:5:32:GLU:O	3:5:36:LYS:HB2	2.19	0.42
3:5:132:VAL:O	3:5:134:MET:N	2.47	0.42
2:7:190:LYS:HA	2:7:191:PRO:HD2	1.80	0.42
5:D:205:GLU:O	5:D:208:ILE:HG22	2.19	0.42
5:G:315:LYS:HD2	5:G:315:LYS:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:287:ILE:HA	5:K:202:THR:HG21	1.58	0.42
5:I:324:THR:O	5:K:244:ASP:HA	2.09	0.42
5:J:180:LEU:HD11	5:J:261:LEU:HD23	2.02	0.42
5:K:180:LEU:HD11	5:K:261:LEU:HD23	2.01	0.42
5:K:287:ILE:HA	5:M:202:THR:HG21	1.57	0.42
5:K:315:LYS:HD2	5:K:315:LYS:HA	1.92	0.42
5:M:180:LEU:HD11	5:M:261:LEU:HD23	2.01	0.42
5:P:205:GLU:O	5:P:208:ILE:HG22	2.18	0.42
5:S:205:GLU:O	5:S:208:ILE:HG22	2.18	0.42
3:2:68:HIS:HA	3:2:71:ILE:HD12	2.00	0.42
2:4:227:ILE:HD12	2:4:231:LYS:HD3	2.00	0.42
5:D:222:ASP:OD1	5:D:224:GLU:HB3	2.20	0.42
5:E:202:THR:CG2	5:Q:287:ILE:N	2.76	0.42
5:E:287:ILE:N	5:G:202:THR:CG2	2.76	0.42
5:G:180:LEU:HD11	5:G:261:LEU:HD23	2.01	0.42
5:G:206:ARG:O	5:G:209:VAL:HG12	2.20	0.42
5:H:180:LEU:HD11	5:H:261:LEU:HD23	2.02	0.42
5:I:205:GLU:O	5:I:208:ILE:HG22	2.18	0.42
5:K:222:ASP:OD1	5:K:224:GLU:HB3	2.19	0.42
5:M:47:MET:HB2	5:M:47:MET:HE2	1.79	0.42
5:M:206:ARG:O	5:M:209:VAL:HG12	2.20	0.42
3:Z:13:ARG:O	3:Z:14:ARG:C	2.61	0.42
3:Z:22:LEU:O	3:Z:23:GLN:C	2.61	0.42
1:0:81:MET:SD	3:Z:121:MET:HE1	2.59	0.42
3:2:13:ARG:O	3:2:14:ARG:C	2.61	0.42
3:2:88:THR:O	3:2:89:ILE:C	2.62	0.42
2:4:187:GLU:O	2:4:189:ARG:N	2.51	0.42
1:6:8:GLU:HA	1:6:11:ALA:HB3	2.01	0.42
5:D:287:ILE:N	5:F:202:THR:CG2	2.76	0.42
5:E:220:ALA:HB3	5:E:223:PHE:CD1	2.53	0.42
5:E:244:ASP:CG	5:Q:322:PRO:CB	2.73	0.42
5:F:180:LEU:HD11	5:F:261:LEU:HD23	2.02	0.42
5:F:196:ARG:HH21	5:F:249:THR:HG23	1.85	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:K:206:ARG:O	5:K:209:VAL:HG12	2.20	0.42
5:M:205:GLU:O	5:M:208:ILE:HG22	2.18	0.42
5:N:324:THR:N	5:R:245:GLY:CA	2.71	0.42
5:O:205:GLU:O	5:O:208:ILE:HG22	2.18	0.42
5:S:180:LEU:HD11	5:S:261:LEU:HD23	2.01	0.42
1:3:13:LEU:HB2	1:3:18:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:92:LEU:HD12	3:8:92:LEU:C	2.45	0.42
3:8:105:LYS:HG3	5:S:1:ASP:OD1	2.20	0.42
1:9:118:GLY:O	1:9:119:GLU:C	2.62	0.42
5:D:180:LEU:HD11	5:D:261:LEU:HD23	2.02	0.42
5:E:206:ARG:O	5:E:209:VAL:HG12	2.20	0.42
5:H:206:ARG:O	5:H:209:VAL:HG12	2.20	0.42
5:J:171:LEU:HA	5:J:172:PRO:HD2	1.84	0.42
5:K:287:ILE:HD11	5:M:202:THR:HA	1.64	0.42
5:O:180:LEU:HD11	5:O:261:LEU:HD23	2.01	0.42
5:O:196:ARG:HH21	5:O:249:THR:HG23	1.85	0.42
5:O:222:ASP:OD1	5:O:224:GLU:HB3	2.20	0.42
5:P:180:LEU:HD11	5:P:261:LEU:HD23	2.02	0.42
5:P:315:LYS:HD2	5:P:315:LYS:HA	1.92	0.42
2:Y:202:LEU:HD22	2:Y:202:LEU:N	2.35	0.42
2:Y:207:LYS:HG3	2:Y:208:GLU:N	2.35	0.42
3:Z:32:GLU:O	3:Z:36:LYS:HB2	2.19	0.42
1:0:53:THR:O	1:0:54:LYS:C	2.62	0.42
1:0:74:PHE:O	1:0:78:LEU:HG	2.19	0.42
1:0:118:GLY:O	1:0:119:GLU:C	2.62	0.42
3:2:46:GLU:HA	3:2:49:PRO:HG3	2.02	0.42
3:2:132:VAL:C	3:2:134:MET:H	2.28	0.42
3:8:68:HIS:HA	3:8:71:ILE:HD12	2.01	0.42
3:8:82:GLU:O	3:8:86:GLN:HG3	2.20	0.42
1:9:74:PHE:O	1:9:78:LEU:HG	2.19	0.42
5:G:222:ASP:OD1	5:G:224:GLU:HB3	2.19	0.42
5:L:206:ARG:O	5:L:209:VAL:HG12	2.20	0.42
5:M:196:ARG:HH21	5:M:249:THR:HG23	1.85	0.42
5:O:287:ILE:N	5:S:202:THR:CG2	2.76	0.42
5:P:206:ARG:O	5:P:209:VAL:HG12	2.20	0.42
5:Q:193:LEU:HD11	5:Q:250:ILE:HG13	2.02	0.42
5:Q:196:ARG:HH21	5:Q:249:THR:HG23	1.85	0.42
3:Z:122:LEU:HD23	3:Z:134:MET:HE1	2.02	0.42
2:4:207:LYS:HG3	2:4:208:GLU:N	2.35	0.42
3:8:7:ARG:O	3:8:7:ARG:HG2	2.20	0.42
5:F:193:LEU:HD11	5:F:250:ILE:HG13	2.02	0.42
5:J:222:ASP:OD1	5:J:224:GLU:HB3	2.19	0.42
5:N:222:ASP:OD1	5:N:224:GLU:HB3	2.19	0.42
5:O:193:LEU:HD11	5:O:250:ILE:HG13	2.02	0.42
5:O:206:ARG:O	5:O:209:VAL:HG12	2.20	0.42
3:Z:35:ALA:O	3:Z:36:LYS:C	2.63	0.42
3:Z:82:GLU:O	3:Z:86:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:132:VAL:C	3:5:134:MET:H	2.28	0.42
3:8:32:GLU:O	3:8:36:LYS:HB2	2.19	0.42
3:8:88:THR:O	3:8:89:ILE:C	2.62	0.42
5:D:193:LEU:HD11	5:D:250:ILE:HG13	2.02	0.42
5:E:193:LEU:HD11	5:E:250:ILE:HG13	2.02	0.42
5:F:206:ARG:O	5:F:209:VAL:HG12	2.20	0.42
5:G:193:LEU:HD11	5:G:250:ILE:HG13	2.02	0.42
5:G:196:ARG:HH21	5:G:249:THR:HG23	1.85	0.42
5:I:47:MET:HE2	5:I:47:MET:HB2	1.79	0.42
5:L:299:MET:HE2	5:L:299:MET:HB2	1.82	0.42
5:O:299:MET:HE2	5:O:299:MET:HB2	1.82	0.42
5:P:196:ARG:HH21	5:P:249:THR:HG23	1.85	0.42
5:R:206:ARG:O	5:R:209:VAL:HG12	2.20	0.42
3:Z:53:LEU:HA	3:Z:54:PRO:HD3	1.83	0.42
3:Z:140:LEU:HA	3:Z:140:LEU:HD12	1.73	0.42
3:5:85:LEU:O	3:5:86:GLN:C	2.62	0.42
3:5:92:LEU:HD12	3:5:92:LEU:C	2.45	0.42
2:7:207:LYS:HG3	2:7:208:GLU:N	2.35	0.42
3:8:46:GLU:HA	3:8:49:PRO:HG3	2.02	0.42
3:8:122:LEU:HD23	3:8:134:MET:HE1	2.02	0.42
1:9:150:PHE:O	1:9:154:LEU:HD22	2.20	0.42
5:E:202:THR:HG21	5:Q:287:ILE:HA	1.58	0.42
5:E:287:ILE:HA	5:G:202:THR:HG21	1.58	0.42
5:E:369:ILE:HG23	5:E:370:VAL:N	2.35	0.42
5:I:193:LEU:HD11	5:I:250:ILE:HG13	2.02	0.42
5:L:222:ASP:OD1	5:L:224:GLU:HB3	2.20	0.42
5:M:193:LEU:HD11	5:M:250:ILE:HG13	2.02	0.42
5:N:193:LEU:HD11	5:N:250:ILE:HG13	2.02	0.42
5:R:193:LEU:HD11	5:R:250:ILE:HG13	2.02	0.42
5:S:299:MET:HE2	5:S:299:MET:HB2	1.82	0.42
3:Z:92:LEU:HD12	3:Z:92:LEU:C	2.45	0.42
1:0:80:MET:HG2	1:0:81:MET:HE2	2.02	0.41
1:0:150:PHE:O	1:0:154:LEU:HD22	2.20	0.41
3:2:7:ARG:O	3:2:7:ARG:HG2	2.20	0.41
1:6:13:LEU:HB2	1:6:18:ILE:HD11	2.01	0.41
3:8:22:LEU:O	3:8:23:GLN:C	2.61	0.41
1:9:8:GLU:HA	1:9:11:ALA:HB3	2.01	0.41
1:9:13:LEU:HB2	1:9:18:ILE:HD11	2.01	0.41
5:E:196:ARG:HH21	5:E:249:THR:HG23	1.85	0.41
5:H:222:ASP:OD1	5:H:224:GLU:HB3	2.19	0.41
5:I:226:GLU:HG3	5:I:255:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:196:ARG:HH21	5:J:249:THR:HG23	1.85	0.41
5:K:226:GLU:HG3	5:K:255:PHE:CE2	2.55	0.41
5:P:193:LEU:HD11	5:P:250:ILE:HG13	2.02	0.41
5:Q:220:ALA:HB3	5:Q:223:PHE:CD1	2.53	0.41
1:0:13:LEU:HB2	1:0:18:ILE:HD11	2.01	0.41
3:2:32:GLU:O	3:2:36:LYS:HB2	2.19	0.41
1:9:53:THR:O	1:9:54:LYS:C	2.62	0.41
5:H:193:LEU:HD11	5:H:250:ILE:HG13	2.02	0.41
5:J:287:ILE:N	5:L:202:THR:CG2	2.76	0.41
5:K:193:LEU:HD11	5:K:250:ILE:HG13	2.02	0.41
5:L:193:LEU:HD11	5:L:250:ILE:HG13	2.02	0.41
5:Q:206:ARG:O	5:Q:209:VAL:HG12	2.20	0.41
5:R:227:MET:O	5:R:230:ALA:HB3	2.21	0.41
3:Z:46:GLU:HA	3:Z:49:PRO:HG3	2.02	0.41
2:1:207:LYS:HG3	2:1:208:GLU:N	2.35	0.41
3:2:105:LYS:CB	5:R:5:THR:CG2	2.74	0.41
3:5:130:HIS:CE1	3:5:134:MET:HE3	2.53	0.41
5:D:196:ARG:HH21	5:D:249:THR:HG23	1.85	0.41
5:F:222:ASP:OD1	5:F:224:GLU:HB3	2.20	0.41
5:F:369:ILE:HG23	5:F:370:VAL:N	2.35	0.41
5:G:287:ILE:HA	5:I:202:THR:HG21	1.58	0.41
5:I:206:ARG:O	5:I:209:VAL:HG12	2.20	0.41
5:J:193:LEU:HD11	5:J:250:ILE:HG13	2.02	0.41
5:K:369:ILE:HG23	5:K:370:VAL:N	2.35	0.41
5:N:196:ARG:HH21	5:N:249:THR:HG23	1.85	0.41
5:N:287:ILE:CB	5:R:204:ALA:H	2.15	0.41
5:O:369:ILE:HG23	5:O:370:VAL:N	2.35	0.41
5:Q:222:ASP:OD1	5:Q:224:GLU:HB3	2.20	0.41
5:Q:226:GLU:HG3	5:Q:255:PHE:CE2	2.55	0.41
5:R:196:ARG:HH21	5:R:249:THR:HG23	1.85	0.41
5:R:222:ASP:OD1	5:R:224:GLU:HB3	2.20	0.41
5:S:193:LEU:HD11	5:S:250:ILE:HG13	2.02	0.41
2:4:234:ILE:HG12	3:5:92:LEU:HB3	2.02	0.41
3:5:46:GLU:HA	3:5:49:PRO:HG3	2.02	0.41
3:5:122:LEU:HD23	3:5:134:MET:HE1	2.02	0.41
3:8:130:HIS:HE1	3:8:134:MET:CE	2.32	0.41
1:9:80:MET:HG2	1:9:81:MET:HE2	2.02	0.41
5:I:171:LEU:HA	5:I:172:PRO:HD2	1.84	0.41
5:I:369:ILE:HG23	5:I:370:VAL:N	2.35	0.41
5:K:47:MET:HB2	5:K:47:MET:HE2	1.79	0.41
5:K:144:ALA:HB2	5:K:342:GLY:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:206:ARG:O	5:N:209:VAL:HG12	2.20	0.41
5:S:226:GLU:HG3	5:S:255:PHE:CE2	2.55	0.41
5:S:369:ILE:HG23	5:S:370:VAL:N	2.35	0.41
3:Z:7:ARG:O	3:Z:7:ARG:HG2	2.20	0.41
3:Z:132:VAL:C	3:Z:134:MET:H	2.28	0.41
1:O:8:GLU:HA	1:O:11:ALA:HB3	2.01	0.41
2:1:202:LEU:HD22	2:1:202:LEU:N	2.35	0.41
3:2:92:LEU:HD12	3:2:92:LEU:C	2.45	0.41
2:4:202:LEU:HD22	2:4:202:LEU:N	2.35	0.41
1:6:74:PHE:O	1:6:78:LEU:HG	2.19	0.41
5:E:227:MET:O	5:E:230:ALA:HB3	2.21	0.41
5:G:227:MET:O	5:G:230:ALA:HB3	2.21	0.41
5:I:144:ALA:HB2	5:I:342:GLY:CA	2.51	0.41
5:M:226:GLU:HG3	5:M:255:PHE:CE2	2.55	0.41
5:N:287:ILE:HA	5:R:202:THR:HG21	1.58	0.41
5:P:226:GLU:HG3	5:P:255:PHE:CE2	2.55	0.41
5:P:369:ILE:HG23	5:P:370:VAL:N	2.35	0.41
5:Q:32:PRO:HB2	5:Q:34:ILE:CD1	2.51	0.41
2:1:234:ILE:HG12	3:2:92:LEU:HB3	2.02	0.41
3:2:34:ALA:O	3:2:35:ALA:C	2.64	0.41
2:4:212:TRP:HA	2:4:212:TRP:HE3	1.86	0.41
3:5:88:THR:O	3:5:89:ILE:C	2.62	0.41
2:7:235:VAL:HG23	2:7:235:VAL:H	1.65	0.41
3:8:66:LYS:HB2	3:8:66:LYS:HE2	1.90	0.41
3:8:132:VAL:C	3:8:134:MET:H	2.28	0.41
1:9:144:ASN:ND2	1:9:144:ASN:O	2.54	0.41
5:D:206:ARG:O	5:D:209:VAL:HG12	2.20	0.41
5:D:324:THR:N	5:F:245:GLY:CA	2.71	0.41
5:D:369:ILE:HG23	5:D:370:VAL:N	2.35	0.41
5:E:32:PRO:HB2	5:E:34:ILE:CD1	2.51	0.41
5:E:222:ASP:OD1	5:E:224:GLU:HB3	2.19	0.41
5:F:32:PRO:HB2	5:F:34:ILE:CD1	2.51	0.41
5:F:171:LEU:HA	5:F:172:PRO:HD2	1.84	0.41
5:H:32:PRO:HB2	5:H:34:ILE:CD1	2.51	0.41
5:J:221:LEU:HA	5:J:312:ARG:HG2	2.02	0.41
5:J:290:ARG:HH22	5:L:202:THR:CG2	2.18	0.41
5:K:196:ARG:HH21	5:K:249:THR:HG23	1.85	0.41
5:L:221:LEU:HA	5:L:312:ARG:HG2	2.02	0.41
5:M:369:ILE:HG23	5:M:370:VAL:N	2.35	0.41
2:1:212:TRP:HA	2:1:212:TRP:HE3	1.85	0.41
3:2:66:LYS:HE2	3:2:66:LYS:HB2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:82:GLU:O	3:2:86:GLN:HG3	2.20	0.41
3:2:132:VAL:O	3:2:134:MET:N	2.47	0.41
1:3:74:PHE:O	1:3:78:LEU:HG	2.19	0.41
3:8:97:GLN:HE21	5:S:4:GLU:CD	2.12	0.41
5:E:226:GLU:HG3	5:E:255:PHE:CE2	2.56	0.41
5:G:32:PRO:HB2	5:G:34:ILE:CD1	2.51	0.41
5:G:144:ALA:HB2	5:G:342:GLY:CA	2.51	0.41
5:G:288:ASP:OD1	5:I:204:ALA:HA	2.21	0.41
5:J:32:PRO:HB2	5:J:34:ILE:CD1	2.51	0.41
5:M:222:ASP:OD1	5:M:224:GLU:HB3	2.20	0.41
5:N:32:PRO:HB2	5:N:34:ILE:CD1	2.51	0.41
5:N:221:LEU:HA	5:N:312:ARG:HG2	2.02	0.41
5:O:144:ALA:HB2	5:O:342:GLY:CA	2.51	0.41
5:O:315:LYS:HD2	5:O:315:LYS:HA	1.92	0.41
5:P:227:MET:O	5:P:230:ALA:HB3	2.21	0.41
2:Y:234:ILE:HG12	3:Z:92:LEU:HB3	2.02	0.41
3:2:122:LEU:HD23	3:2:134:MET:HE1	2.02	0.41
3:5:130:HIS:HE1	3:5:134:MET:CE	2.32	0.41
1:6:150:PHE:O	1:6:154:LEU:HD22	2.20	0.41
1:9:58:ASP:CB	5:S:360:GLN:HE21	2.26	0.41
5:E:144:ALA:HB2	5:E:342:GLY:CA	2.51	0.41
5:E:288:ASP:OD1	5:G:204:ALA:HA	2.21	0.41
5:E:299:MET:HE2	5:E:299:MET:HB2	1.82	0.41
5:G:369:ILE:HG23	5:G:370:VAL:N	2.35	0.41
5:J:144:ALA:HB2	5:J:342:GLY:CA	2.51	0.41
5:J:369:ILE:HG23	5:J:370:VAL:N	2.35	0.41
5:M:144:ALA:HB2	5:M:342:GLY:CA	2.51	0.41
5:M:227:MET:O	5:M:230:ALA:HB3	2.21	0.41
5:N:144:ALA:HB2	5:N:342:GLY:CA	2.51	0.41
5:O:226:GLU:HG3	5:O:255:PHE:CE2	2.55	0.41
5:R:144:ALA:HB2	5:R:342:GLY:CA	2.51	0.41
5:S:196:ARG:HH21	5:S:249:THR:HG23	1.85	0.41
1:3:79:VAL:HG12	1:3:83:ARG:NE	2.36	0.41
1:3:121:LEU:HA	1:3:121:LEU:HD12	1.89	0.41
1:3:144:ASN:O	1:3:144:ASN:ND2	2.54	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
3:5:66:LYS:HE2	3:5:66:LYS:HB2	1.90	0.41
3:5:105:LYS:HG3	5:Q:1:ASP:OD1	2.20	0.41
1:6:22:LYS:O	1:6:23:ALA:C	2.64	0.41
1:6:79:VAL:HG12	1:6:83:ARG:NE	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:191:PRO:C	2:7:193:ASN:H	2.29	0.41
2:7:230:LYS:HA	2:7:233:GLU:HG3	2.02	0.41
2:7:234:ILE:HG12	3:8:92:LEU:HB3	2.02	0.41
3:8:132:VAL:O	3:8:134:MET:N	2.47	0.41
5:D:32:PRO:HB2	5:D:34:ILE:CD1	2.51	0.41
5:E:219:VAL:HG22	5:E:258:PRO:CB	2.51	0.41
5:E:290:ARG:HH22	5:G:202:THR:CG2	2.18	0.41
5:F:221:LEU:HA	5:F:312:ARG:HG2	2.02	0.41
5:F:227:MET:O	5:F:230:ALA:HB3	2.21	0.41
5:F:287:ILE:N	5:H:202:THR:CG2	2.76	0.41
5:G:171:LEU:HA	5:G:172:PRO:HD2	1.84	0.41
5:H:221:LEU:HA	5:H:312:ARG:HG2	2.02	0.41
5:H:226:GLU:HG3	5:H:255:PHE:CE2	2.55	0.41
5:H:369:ILE:HG23	5:H:370:VAL:N	2.35	0.41
5:J:226:GLU:HG3	5:J:255:PHE:CE2	2.55	0.41
5:K:171:LEU:HA	5:K:172:PRO:HD2	1.84	0.41
5:L:32:PRO:HB2	5:L:34:ILE:CD1	2.51	0.41
5:L:144:ALA:HB2	5:L:342:GLY:CA	2.51	0.41
5:L:196:ARG:HH21	5:L:249:THR:HG23	1.85	0.41
5:L:226:GLU:HG3	5:L:255:PHE:CE2	2.55	0.41
5:N:227:MET:O	5:N:230:ALA:HB3	2.21	0.41
5:N:369:ILE:HG23	5:N:370:VAL:N	2.35	0.41
5:O:227:MET:O	5:O:230:ALA:HB3	2.21	0.41
5:P:144:ALA:HB2	5:P:342:GLY:CA	2.51	0.41
5:P:299:MET:HE2	5:P:299:MET:HB2	1.82	0.41
5:R:32:PRO:HB2	5:R:34:ILE:CD1	2.51	0.41
5:S:227:MET:O	5:S:230:ALA:HB3	2.21	0.41
1:0:22:LYS:O	1:0:23:ALA:C	2.64	0.41
3:8:4:GLU:OE2	3:8:7:ARG:CZ	2.69	0.41
1:9:79:VAL:HG12	1:9:83:ARG:NE	2.36	0.41
5:D:221:LEU:HA	5:D:312:ARG:HG2	2.02	0.41
5:D:299:MET:HE2	5:D:299:MET:HB2	1.82	0.41
5:E:75:ILE:HD12	5:E:75:ILE:HG23	1.92	0.41
5:F:226:GLU:HG3	5:F:255:PHE:CE2	2.55	0.41
5:H:227:MET:O	5:H:230:ALA:HB3	2.21	0.41
5:I:219:VAL:HG22	5:I:258:PRO:CB	2.51	0.41
5:K:288:ASP:OD1	5:M:204:ALA:HA	2.21	0.41
5:L:171:LEU:HA	5:L:172:PRO:HD2	1.84	0.41
5:M:219:VAL:HG22	5:M:258:PRO:CB	2.51	0.41
5:N:226:GLU:HG3	5:N:255:PHE:CE2	2.55	0.41
5:P:219:VAL:HG22	5:P:258:PRO:CB	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:144:ALA:HB2	5:Q:342:GLY:CA	2.51	0.41
5:Q:221:LEU:HA	5:Q:312:ARG:HG2	2.02	0.41
5:S:144:ALA:HB2	5:S:342:GLY:CA	2.51	0.41
2:Y:230:LYS:HA	2:Y:233:GLU:HG3	2.02	0.41
3:Z:85:LEU:O	3:Z:86:GLN:C	2.62	0.41
3:2:35:ALA:O	3:2:36:LYS:C	2.63	0.40
1:3:80:MET:HG2	1:3:81:MET:HE2	2.02	0.40
3:5:7:ARG:O	3:5:7:ARG:HG2	2.20	0.40
5:D:288:ASP:OD1	5:F:204:ALA:HA	2.21	0.40
5:E:204:ALA:HA	5:Q:288:ASP:OD1	2.21	0.40
5:G:226:GLU:HG3	5:G:255:PHE:CE2	2.56	0.40
5:G:287:ILE:CB	5:I:204:ALA:H	2.14	0.40
5:H:196:ARG:HH21	5:H:249:THR:HG23	1.85	0.40
5:I:288:ASP:OD1	5:K:204:ALA:HA	2.21	0.40
5:L:369:ILE:HG23	5:L:370:VAL:N	2.35	0.40
5:M:287:ILE:N	5:O:202:THR:CG2	2.76	0.40
5:Q:369:ILE:HG23	5:Q:370:VAL:N	2.35	0.40
5:R:221:LEU:HA	5:R:312:ARG:HG2	2.02	0.40
5:S:32:PRO:HB2	5:S:34:ILE:CD1	2.51	0.40
5:S:221:LEU:HA	5:S:312:ARG:HG2	2.02	0.40
3:2:137:ARG:H	3:2:137:ARG:HG2	1.49	0.40
1:6:144:ASN:ND2	1:6:144:ASN:O	2.54	0.40
3:8:34:ALA:O	3:8:35:ALA:C	2.64	0.40
5:D:120:THR:HG21	5:D:370:VAL:CG1	2.52	0.40
5:H:287:ILE:N	5:J:202:THR:CG2	2.77	0.40
5:K:227:MET:O	5:K:230:ALA:HB3	2.21	0.40
5:K:290:ARG:HH22	5:M:202:THR:CG2	2.18	0.40
5:M:250:ILE:HG22	5:M:254:ARG:HB2	2.04	0.40
5:P:221:LEU:HA	5:P:312:ARG:HG2	2.02	0.40
5:R:369:ILE:HG23	5:R:370:VAL:N	2.35	0.40
2:Y:191:PRO:C	2:Y:193:ASN:H	2.29	0.40
1:0:144:ASN:O	1:0:144:ASN:ND2	2.54	0.40
2:1:189:ARG:NE	3:2:72:ASP:OD1	2.47	0.40
2:1:199:GLU:OE2	3:2:56:SER:O	2.39	0.40
3:2:130:HIS:HE1	3:2:134:MET:CE	2.32	0.40
2:4:191:PRO:C	2:4:193:ASN:H	2.29	0.40
2:4:223:PHE:HB3	3:5:81:THR:HG22	2.03	0.40
3:5:82:GLU:O	3:5:86:GLN:HG3	2.20	0.40
3:8:141:LYS:CD	3:8:141:LYS:N	2.70	0.40
5:D:227:MET:O	5:D:230:ALA:HB3	2.21	0.40
5:D:250:ILE:HG22	5:D:254:ARG:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:171:LEU:HA	5:E:172:PRO:HD2	1.84	0.40
5:F:288:ASP:OD1	5:H:204:ALA:HA	2.21	0.40
5:G:219:VAL:HG22	5:G:258:PRO:CB	2.51	0.40
5:H:120:THR:HG21	5:H:370:VAL:CG1	2.52	0.40
5:H:144:ALA:HB2	5:H:342:GLY:CA	2.51	0.40
5:I:32:PRO:HB2	5:I:34:ILE:CD1	2.51	0.40
5:I:256:ARG:HH11	5:I:256:ARG:HD2	1.79	0.40
5:L:120:THR:HG21	5:L:370:VAL:CG1	2.52	0.40
5:O:120:THR:HG21	5:O:370:VAL:CG1	2.52	0.40
5:Q:120:THR:HG21	5:Q:370:VAL:CG1	2.52	0.40
5:S:256:ARG:HH11	5:S:256:ARG:HD2	1.78	0.40
1:3:118:GLY:CA	1:3:133:ILE:HD13	2.52	0.40
1:6:51:ASN:HD22	1:6:51:ASN:HA	1.67	0.40
1:6:80:MET:HG2	1:6:81:MET:HE2	2.03	0.40
2:7:201:LYS:O	2:7:202:LEU:C	2.64	0.40
5:D:144:ALA:HB2	5:D:342:GLY:CA	2.51	0.40
5:D:226:GLU:HG3	5:D:255:PHE:CE2	2.55	0.40
5:E:221:LEU:HA	5:E:312:ARG:HG2	2.02	0.40
5:J:227:MET:O	5:J:230:ALA:HB3	2.21	0.40
5:K:219:VAL:HG22	5:K:258:PRO:CB	2.52	0.40
5:L:227:MET:O	5:L:230:ALA:HB3	2.21	0.40
5:M:288:ASP:OD1	5:O:204:ALA:HA	2.21	0.40
5:N:120:THR:HG21	5:N:370:VAL:CG1	2.51	0.40
5:O:219:VAL:HG22	5:O:258:PRO:CB	2.52	0.40
5:O:221:LEU:HA	5:O:312:ARG:HG2	2.02	0.40
5:Q:219:VAL:HG22	5:Q:258:PRO:CB	2.52	0.40
5:Q:227:MET:O	5:Q:230:ALA:HB3	2.21	0.40
5:S:219:VAL:HG22	5:S:258:PRO:CB	2.51	0.40
2:Y:198:ASN:CB	2:Y:201:LYS:HB2	2.39	0.40
3:Z:4:GLU:OE2	3:Z:7:ARG:CZ	2.70	0.40
1:0:79:VAL:HG12	1:0:83:ARG:NE	2.36	0.40
5:D:204:ALA:HA	5:P:288:ASP:OD1	2.21	0.40
5:E:250:ILE:HG22	5:E:254:ARG:HB2	2.04	0.40
5:H:288:ASP:OD1	5:J:204:ALA:HA	2.21	0.40
5:I:120:THR:HG21	5:I:370:VAL:CG1	2.52	0.40
5:I:227:MET:O	5:I:230:ALA:HB3	2.21	0.40
5:I:250:ILE:HG22	5:I:254:ARG:HB2	2.04	0.40
5:J:120:THR:HG21	5:J:370:VAL:CG1	2.51	0.40
5:J:250:ILE:HG22	5:J:254:ARG:HB2	2.04	0.40
5:K:32:PRO:HB2	5:K:34:ILE:CD1	2.51	0.40
5:P:32:PRO:HB2	5:P:34:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:219:VAL:HG22	5:R:258:PRO:CB	2.51	0.40
5:R:250:ILE:HG22	5:R:254:ARG:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	157/159 (99%)	130 (83%)	20 (13%)	7 (4%)	2	17
1	3	157/159 (99%)	130 (83%)	20 (13%)	7 (4%)	2	17
1	6	157/159 (99%)	130 (83%)	20 (13%)	7 (4%)	2	17
1	9	157/159 (99%)	130 (83%)	20 (13%)	7 (4%)	2	17
2	1	88/90 (98%)	66 (75%)	18 (20%)	4 (4%)	2	17
2	4	88/90 (98%)	65 (74%)	19 (22%)	4 (4%)	2	17
2	7	88/90 (98%)	65 (74%)	19 (22%)	4 (4%)	2	17
2	Y	88/90 (98%)	66 (75%)	18 (20%)	4 (4%)	2	17
3	2	139/141 (99%)	107 (77%)	19 (14%)	13 (9%)	0	8
3	5	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	0	8
3	8	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	0	8
3	Z	139/141 (99%)	107 (77%)	19 (14%)	13 (9%)	0	8
4	A	258/277 (93%)	249 (96%)	7 (3%)	2 (1%)	16	54
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%)	18	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	7	38
5	E	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	7	38
5	F	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	7	38
5	G	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	7	38
5	H	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	7	38
5	I	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	7	38
5	J	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	7	38
5	K	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	7	38
5	L	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	7	38
5	M	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	7	38
5	N	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	7	38
5	O	370/372 (100%)	333 (90%)	31 (8%)	6 (2%)	7	38
5	P	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	7	38
5	Q	370/372 (100%)	334 (90%)	30 (8%)	6 (2%)	7	38
5	R	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	7	38
5	S	370/372 (100%)	335 (90%)	29 (8%)	6 (2%)	7	38
All	All	8687/9728 (89%)	7744 (89%)	747 (9%)	196 (2%)	7	28

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
5	H	2	GLU
5	H	253	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	R	253	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	J	253	GLU
5	K	253	GLU
5	N	253	GLU
5	P	253	GLU
5	Q	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

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Mol	Chain	Res	Type
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%)	117 (87%)	17 (13%)	4	16
1	3	134/134 (100%)	117 (87%)	17 (13%)	4	16
1	6	134/134 (100%)	117 (87%)	17 (13%)	4	16
1	9	134/134 (100%)	117 (87%)	17 (13%)	4	16
2	1	82/82 (100%)	72 (88%)	10 (12%)	5	17
2	4	82/82 (100%)	72 (88%)	10 (12%)	5	17
2	7	82/82 (100%)	72 (88%)	10 (12%)	5	17
2	Y	82/82 (100%)	72 (88%)	10 (12%)	5	17
3	2	124/124 (100%)	108 (87%)	16 (13%)	4	15
3	5	124/124 (100%)	108 (87%)	16 (13%)	4	15
3	8	124/124 (100%)	108 (87%)	16 (13%)	4	15
3	Z	124/124 (100%)	108 (87%)	16 (13%)	4	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	224/239 (94%)	195 (87%)	29 (13%)	4	15
4	B	239/239 (100%)	203 (85%)	36 (15%)	3	12
4	C	36/239 (15%)	30 (83%)	6 (17%)	2	10
4	T	36/239 (15%)	27 (75%)	9 (25%)	0	4
4	U	239/239 (100%)	203 (85%)	36 (15%)	3	12
4	V	239/239 (100%)	210 (88%)	29 (12%)	5	17
4	W	36/239 (15%)	27 (75%)	9 (25%)	0	4
4	X	36/239 (15%)	30 (83%)	6 (17%)	2	10
5	D	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	E	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	F	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	G	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	H	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	I	315/315 (100%)	265 (84%)	50 (16%)	2	11
5	J	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	K	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	L	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	M	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	N	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	O	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	P	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	Q	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	R	315/315 (100%)	264 (84%)	51 (16%)	2	11
5	S	315/315 (100%)	264 (84%)	51 (16%)	2	11
All	All	7485/8312 (90%)	6338 (85%)	1147 (15%)	5	12

All (1147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	17	MET
1	0	22	LYS
1	0	45	MET
1	0	46	ARG
1	0	62	GLU

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Mol	Chain	Res	Type
1	0	64	VAL
1	0	95	GLU
1	0	103	ILE
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
2	1	185	LEU
2	1	190	LYS
2	1	192	LEU
2	1	207	LYS
2	1	215	GLN
2	1	218	THR
2	1	227	ILE
2	1	231	LYS
2	1	243	GLN
2	1	248	SER
3	2	3	GLU
3	2	4	GLU
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	121	MET
3	2	122	LEU
3	2	129	LYS
3	2	131	LYS
3	2	133	ASN
3	2	137	ARG
1	3	17	MET
1	3	22	LYS
1	3	45	MET
1	3	46	ARG

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Mol	Chain	Res	Type
1	3	62	GLU
1	3	64	VAL
1	3	95	GLU
1	3	103	ILE
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
2	4	185	LEU
2	4	190	LYS
2	4	192	LEU
2	4	207	LYS
2	4	215	GLN
2	4	218	THR
2	4	227	ILE
2	4	231	LYS
2	4	243	GLN
2	4	248	SER
3	5	3	GLU
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	121	MET
3	5	122	LEU
3	5	129	LYS
3	5	131	LYS
3	5	133	ASN
3	5	137	ARG
1	6	17	MET
1	6	22	LYS
1	6	45	MET

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Mol	Chain	Res	Type
1	6	46	ARG
1	6	62	GLU
1	6	64	VAL
1	6	95	GLU
1	6	103	ILE
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
2	7	185	LEU
2	7	190	LYS
2	7	192	LEU
2	7	207	LYS
2	7	215	GLN
2	7	218	THR
2	7	227	ILE
2	7	231	LYS
2	7	243	GLN
2	7	248	SER
3	8	3	GLU
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	121	MET
3	8	122	LEU
3	8	129	LYS
3	8	131	LYS
3	8	133	ASN
3	8	137	ARG
1	9	17	MET
1	9	22	LYS

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Mol	Chain	Res	Type
1	9	45	MET
1	9	46	ARG
1	9	62	GLU
1	9	64	VAL
1	9	95	GLU
1	9	103	ILE
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
1	9	155	LYS
4	A	29	SER
4	A	37	VAL
4	A	53	TYR
4	A	57	LEU
4	A	89	GLU
4	A	99	LEU
4	A	106	LEU
4	A	122	VAL
4	A	125	SER
4	A	131	GLU
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	206	LYS
4	A	207	TYR
4	A	214	TYR
4	A	220	VAL
4	A	222	SER
4	A	234	PHE
4	A	241	LYS
4	A	251	ASP
4	A	254	TYR
4	A	263	ILE

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Mol	Chain	Res	Type
4	A	269	HIS
4	A	277	ILE
4	B	29	SER
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	89	GLU
4	B	99	LEU
4	B	106	LEU
4	B	122	VAL
4	B	131	GLU
4	B	146	HIS
4	B	158	VAL
4	B	162	LEU
4	B	163	VAL
4	B	164	ILE
4	B	165	ILE
4	B	188	GLU
4	B	193	VAL
4	B	206	LYS
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	252	GLU
4	B	253	LEU
4	B	254	TYR
4	B	263	ILE
4	B	264	SER
4	B	269	HIS
4	B	276	SER
4	C	241	LYS
4	C	251	ASP
4	C	254	TYR
4	C	263	ILE

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Mol	Chain	Res	Type
4	C	269	HIS
4	C	277	ILE
5	D	16	LEU
5	D	33	SER
5	D	34	ILE
5	D	37	ARG
5	D	65	LEU
5	D	66	THR
5	D	67	LEU
5	D	72	GLU
5	D	80	ASP
5	D	99	GLU
5	D	100	GLU
5	D	109	PRO
5	D	145	SER
5	D	153	LEU
5	D	159	VAL
5	D	180	LEU
5	D	196	ARG
5	D	199	SER
5	D	201	VAL
5	D	206	ARG
5	D	221	LEU
5	D	223	PHE
5	D	229	THR
5	D	238	LYS
5	D	239	SER
5	D	242	LEU
5	D	246	GLN
5	D	253	GLU
5	D	263	GLN
5	D	274	ILE
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	305	MET
5	D	312	ARG
5	D	315	LYS

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Mol	Chain	Res	Type
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	353	GLN
5	D	354	GLN
5	D	361	GLU
5	D	368	SER
5	E	16	LEU
5	E	33	SER
5	E	34	ILE
5	E	37	ARG
5	E	65	LEU
5	E	66	THR
5	E	67	LEU
5	E	72	GLU
5	E	80	ASP
5	E	99	GLU
5	E	100	GLU
5	E	109	PRO
5	E	145	SER
5	E	153	LEU
5	E	159	VAL
5	E	180	LEU
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	238	LYS
5	E	239	SER
5	E	242	LEU
5	E	246	GLN
5	E	253	GLU
5	E	263	GLN
5	E	274	ILE
5	E	281	SER

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Mol	Chain	Res	Type
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	305	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	353	GLN
5	E	354	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	65	LEU
5	F	66	THR
5	F	67	LEU
5	F	72	GLU
5	F	80	ASP
5	F	99	GLU
5	F	100	GLU
5	F	109	PRO
5	F	145	SER
5	F	153	LEU
5	F	159	VAL
5	F	180	LEU
5	F	196	ARG
5	F	199	SER
5	F	201	VAL
5	F	206	ARG
5	F	221	LEU
5	F	223	PHE

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Mol	Chain	Res	Type
5	F	229	THR
5	F	238	LYS
5	F	239	SER
5	F	242	LEU
5	F	246	GLN
5	F	253	GLU
5	F	263	GLN
5	F	274	ILE
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	305	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	353	GLN
5	F	354	GLN
5	F	361	GLU
5	F	368	SER
5	G	16	LEU
5	G	33	SER
5	G	34	ILE
5	G	37	ARG
5	G	65	LEU
5	G	66	THR
5	G	67	LEU
5	G	72	GLU
5	G	80	ASP
5	G	99	GLU
5	G	100	GLU
5	G	109	PRO
5	G	145	SER

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Mol	Chain	Res	Type
5	G	153	LEU
5	G	159	VAL
5	G	180	LEU
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	238	LYS
5	G	239	SER
5	G	242	LEU
5	G	246	GLN
5	G	253	GLU
5	G	263	GLN
5	G	274	ILE
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	305	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	353	GLN
5	G	354	GLN
5	G	361	GLU
5	G	368	SER
5	H	16	LEU
5	H	33	SER
5	H	34	ILE
5	H	37	ARG

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Mol	Chain	Res	Type
5	H	65	LEU
5	H	66	THR
5	H	67	LEU
5	H	72	GLU
5	H	80	ASP
5	H	99	GLU
5	H	100	GLU
5	H	109	PRO
5	H	145	SER
5	H	153	LEU
5	H	159	VAL
5	H	180	LEU
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	238	LYS
5	H	239	SER
5	H	242	LEU
5	H	246	GLN
5	H	253	GLU
5	H	263	GLN
5	H	274	ILE
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	305	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

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Mol	Chain	Res	Type
5	H	351	THR
5	H	353	GLN
5	H	354	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	67	LEU
5	I	72	GLU
5	I	80	ASP
5	I	99	GLU
5	I	100	GLU
5	I	109	PRO
5	I	145	SER
5	I	153	LEU
5	I	159	VAL
5	I	180	LEU
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	238	LYS
5	I	239	SER
5	I	242	LEU
5	I	246	GLN
5	I	253	GLU
5	I	263	GLN
5	I	274	ILE
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	305	MET

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Mol	Chain	Res	Type
5	I	312	ARG
5	I	315	LYS
5	I	318	THR
5	I	320	LEU
5	I	327	ILE
5	I	334	GLU
5	I	349	LEU
5	I	350	SER
5	I	351	THR
5	I	353	GLN
5	I	354	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	65	LEU
5	J	66	THR
5	J	67	LEU
5	J	72	GLU
5	J	80	ASP
5	J	99	GLU
5	J	100	GLU
5	J	109	PRO
5	J	145	SER
5	J	153	LEU
5	J	159	VAL
5	J	180	LEU
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	238	LYS
5	J	239	SER
5	J	242	LEU
5	J	246	GLN
5	J	253	GLU
5	J	263	GLN

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Mol	Chain	Res	Type
5	J	274	ILE
5	J	281	SER
5	J	283	MET
5	J	287	ILE
5	J	291	LYS
5	J	293	LEU
5	J	297	ASN
5	J	299	MET
5	J	305	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	353	GLN
5	J	354	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	65	LEU
5	K	66	THR
5	K	67	LEU
5	K	72	GLU
5	K	80	ASP
5	K	99	GLU
5	K	100	GLU
5	K	109	PRO
5	K	145	SER
5	K	153	LEU
5	K	159	VAL
5	K	180	LEU
5	K	196	ARG
5	K	199	SER
5	K	201	VAL
5	K	206	ARG

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Mol	Chain	Res	Type
5	K	221	LEU
5	K	223	PHE
5	K	229	THR
5	K	238	LYS
5	K	239	SER
5	K	242	LEU
5	K	246	GLN
5	K	253	GLU
5	K	263	GLN
5	K	274	ILE
5	K	281	SER
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	305	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	353	GLN
5	K	354	GLN
5	K	361	GLU
5	K	368	SER
5	L	16	LEU
5	L	33	SER
5	L	34	ILE
5	L	37	ARG
5	L	65	LEU
5	L	66	THR
5	L	67	LEU
5	L	72	GLU
5	L	80	ASP
5	L	99	GLU
5	L	100	GLU

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Mol	Chain	Res	Type
5	L	109	PRO
5	L	145	SER
5	L	153	LEU
5	L	159	VAL
5	L	180	LEU
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	238	LYS
5	L	239	SER
5	L	242	LEU
5	L	246	GLN
5	L	253	GLU
5	L	263	GLN
5	L	274	ILE
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	305	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	353	GLN
5	L	354	GLN
5	L	361	GLU
5	L	368	SER
5	M	16	LEU
5	M	33	SER

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Mol	Chain	Res	Type
5	M	34	ILE
5	M	37	ARG
5	M	65	LEU
5	M	66	THR
5	M	67	LEU
5	M	72	GLU
5	M	80	ASP
5	M	99	GLU
5	M	100	GLU
5	M	109	PRO
5	M	145	SER
5	M	153	LEU
5	M	159	VAL
5	M	180	LEU
5	M	196	ARG
5	M	199	SER
5	M	201	VAL
5	M	206	ARG
5	M	221	LEU
5	M	223	PHE
5	M	229	THR
5	M	238	LYS
5	M	239	SER
5	M	242	LEU
5	M	246	GLN
5	M	253	GLU
5	M	263	GLN
5	M	274	ILE
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	305	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

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Mol	Chain	Res	Type
5	M	349	LEU
5	M	350	SER
5	M	351	THR
5	M	353	GLN
5	M	354	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	65	LEU
5	N	66	THR
5	N	67	LEU
5	N	72	GLU
5	N	80	ASP
5	N	99	GLU
5	N	100	GLU
5	N	109	PRO
5	N	145	SER
5	N	153	LEU
5	N	159	VAL
5	N	180	LEU
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	238	LYS
5	N	239	SER
5	N	242	LEU
5	N	246	GLN
5	N	253	GLU
5	N	263	GLN
5	N	274	ILE
5	N	281	SER
5	N	283	MET
5	N	287	ILE
5	N	291	LYS
5	N	293	LEU

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Mol	Chain	Res	Type
5	N	297	ASN
5	N	299	MET
5	N	305	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	353	GLN
5	N	354	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	65	LEU
5	O	66	THR
5	O	67	LEU
5	O	72	GLU
5	O	80	ASP
5	O	99	GLU
5	O	100	GLU
5	O	109	PRO
5	O	145	SER
5	O	153	LEU
5	O	159	VAL
5	O	180	LEU
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	238	LYS
5	O	239	SER
5	O	242	LEU

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Mol	Chain	Res	Type
5	O	246	GLN
5	O	253	GLU
5	O	263	GLN
5	O	274	ILE
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	305	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	353	GLN
5	O	354	GLN
5	O	361	GLU
5	O	368	SER
5	P	16	LEU
5	P	33	SER
5	P	34	ILE
5	P	37	ARG
5	P	65	LEU
5	P	66	THR
5	P	67	LEU
5	P	72	GLU
5	P	80	ASP
5	P	99	GLU
5	P	100	GLU
5	P	109	PRO
5	P	145	SER
5	P	153	LEU
5	P	159	VAL
5	P	180	LEU
5	P	196	ARG

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Mol	Chain	Res	Type
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	238	LYS
5	P	239	SER
5	P	242	LEU
5	P	246	GLN
5	P	253	GLU
5	P	263	GLN
5	P	274	ILE
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	305	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	353	GLN
5	P	354	GLN
5	P	361	GLU
5	P	368	SER
5	Q	16	LEU
5	Q	33	SER
5	Q	34	ILE
5	Q	37	ARG
5	Q	65	LEU
5	Q	66	THR
5	Q	67	LEU
5	Q	72	GLU

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Mol	Chain	Res	Type
5	Q	80	ASP
5	Q	99	GLU
5	Q	100	GLU
5	Q	109	PRO
5	Q	145	SER
5	Q	153	LEU
5	Q	159	VAL
5	Q	180	LEU
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	238	LYS
5	Q	239	SER
5	Q	242	LEU
5	Q	246	GLN
5	Q	253	GLU
5	Q	263	GLN
5	Q	274	ILE
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	305	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
5	Q	353	GLN
5	Q	354	GLN
5	Q	361	GLU

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Mol	Chain	Res	Type
5	Q	368	SER
5	R	16	LEU
5	R	33	SER
5	R	34	ILE
5	R	37	ARG
5	R	65	LEU
5	R	66	THR
5	R	67	LEU
5	R	72	GLU
5	R	80	ASP
5	R	99	GLU
5	R	100	GLU
5	R	109	PRO
5	R	145	SER
5	R	153	LEU
5	R	159	VAL
5	R	180	LEU
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	238	LYS
5	R	239	SER
5	R	242	LEU
5	R	246	GLN
5	R	253	GLU
5	R	263	GLN
5	R	274	ILE
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	305	MET
5	R	312	ARG
5	R	315	LYS
5	R	318	THR

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Mol	Chain	Res	Type
5	R	320	LEU
5	R	327	ILE
5	R	334	GLU
5	R	349	LEU
5	R	350	SER
5	R	351	THR
5	R	353	GLN
5	R	354	GLN
5	R	361	GLU
5	R	368	SER
5	S	16	LEU
5	S	33	SER
5	S	34	ILE
5	S	37	ARG
5	S	65	LEU
5	S	66	THR
5	S	67	LEU
5	S	72	GLU
5	S	80	ASP
5	S	99	GLU
5	S	100	GLU
5	S	109	PRO
5	S	145	SER
5	S	153	LEU
5	S	159	VAL
5	S	180	LEU
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	238	LYS
5	S	239	SER
5	S	242	LEU
5	S	246	GLN
5	S	253	GLU
5	S	263	GLN
5	S	274	ILE
5	S	281	SER
5	S	283	MET

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Mol	Chain	Res	Type
5	S	287	ILE
5	S	291	LYS
5	S	293	LEU
5	S	297	ASN
5	S	299	MET
5	S	305	MET
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	353	GLN
5	S	354	GLN
5	S	361	GLU
5	S	368	SER
4	T	241	LYS
4	T	251	ASP
4	T	252	GLU
4	T	253	LEU
4	T	254	TYR
4	T	263	ILE
4	T	264	SER
4	T	269	HIS
4	T	276	SER
4	U	29	SER
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	89	GLU
4	U	99	LEU
4	U	106	LEU
4	U	122	VAL
4	U	131	GLU
4	U	146	HIS

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Mol	Chain	Res	Type
4	U	158	VAL
4	U	162	LEU
4	U	163	VAL
4	U	164	ILE
4	U	165	ILE
4	U	188	GLU
4	U	193	VAL
4	U	206	LYS
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	252	GLU
4	U	253	LEU
4	U	254	TYR
4	U	263	ILE
4	U	264	SER
4	U	269	HIS
4	U	276	SER
4	V	29	SER
4	V	37	VAL
4	V	53	TYR
4	V	57	LEU
4	V	89	GLU
4	V	99	LEU
4	V	106	LEU
4	V	122	VAL
4	V	125	SER
4	V	131	GLU
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	206	LYS
4	V	207	TYR
4	V	214	TYR

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Mol	Chain	Res	Type
4	V	220	VAL
4	V	222	SER
4	V	234	PHE
4	V	241	LYS
4	V	251	ASP
4	V	254	TYR
4	V	263	ILE
4	V	269	HIS
4	V	277	ILE
4	W	241	LYS
4	W	251	ASP
4	W	252	GLU
4	W	253	LEU
4	W	254	TYR
4	W	263	ILE
4	W	264	SER
4	W	269	HIS
4	W	276	SER
4	X	241	LYS
4	X	251	ASP
4	X	254	TYR
4	X	263	ILE
4	X	269	HIS
4	X	277	ILE
2	Y	185	LEU
2	Y	190	LYS
2	Y	192	LEU
2	Y	207	LYS
2	Y	215	GLN
2	Y	218	THR
2	Y	227	ILE
2	Y	231	LYS
2	Y	243	GLN
2	Y	248	SER
3	Z	3	GLU
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

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Mol	Chain	Res	Type
3	Z	59	GLU
3	Z	103	ARG
3	Z	121	MET
3	Z	122	LEU
3	Z	129	LYS
3	Z	131	LYS
3	Z	133	ASN
3	Z	137	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (174) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	50	GLN
1	0	51	ASN
1	0	144	ASN
2	1	175	GLN
2	1	198	ASN
2	1	226	GLN
2	1	243	GLN
2	1	245	GLN
3	2	42	ASN
3	2	47	HIS
3	2	58	GLN
3	2	86	GLN
3	2	97	GLN
3	2	133	ASN
3	2	142	GLN
1	3	50	GLN
1	3	51	ASN
1	3	144	ASN
2	4	175	GLN
2	4	198	ASN
2	4	226	GLN
2	4	243	GLN
2	4	245	GLN
3	5	42	ASN
3	5	47	HIS
3	5	58	GLN
3	5	86	GLN
3	5	97	GLN
3	5	133	ASN
3	5	142	GLN

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Mol	Chain	Res	Type
1	6	50	GLN
1	6	51	ASN
1	6	144	ASN
2	7	175	GLN
2	7	198	ASN
2	7	226	GLN
2	7	243	GLN
2	7	245	GLN
3	8	42	ASN
3	8	47	HIS
3	8	58	GLN
3	8	86	GLN
3	8	97	GLN
3	8	133	ASN
3	8	142	GLN
1	9	6	GLN
1	9	50	GLN
1	9	51	ASN
1	9	144	ASN
5	D	40	HIS
5	D	41	GLN
5	D	78	ASN
5	D	137	GLN
5	D	252	ASN
5	D	263	GLN
5	D	354	GLN
5	D	360	GLN
5	E	40	HIS
5	E	41	GLN
5	E	78	ASN
5	E	137	GLN
5	E	252	ASN
5	E	263	GLN
5	E	354	GLN
5	E	360	GLN
5	F	40	HIS
5	F	41	GLN
5	F	78	ASN
5	F	252	ASN
5	F	263	GLN
5	F	354	GLN
5	G	40	HIS

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Mol	Chain	Res	Type
5	G	41	GLN
5	G	78	ASN
5	G	137	GLN
5	G	252	ASN
5	G	263	GLN
5	G	354	GLN
5	H	40	HIS
5	H	41	GLN
5	H	78	ASN
5	H	252	ASN
5	H	263	GLN
5	H	354	GLN
5	I	40	HIS
5	I	41	GLN
5	I	78	ASN
5	I	137	GLN
5	I	252	ASN
5	I	263	GLN
5	I	354	GLN
5	J	40	HIS
5	J	41	GLN
5	J	78	ASN
5	J	137	GLN
5	J	252	ASN
5	J	263	GLN
5	J	354	GLN
5	K	40	HIS
5	K	41	GLN
5	K	78	ASN
5	K	137	GLN
5	K	252	ASN
5	K	263	GLN
5	K	354	GLN
5	L	40	HIS
5	L	41	GLN
5	L	78	ASN
5	L	252	ASN
5	L	263	GLN
5	L	354	GLN
5	M	40	HIS
5	M	41	GLN
5	M	78	ASN

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Mol	Chain	Res	Type
5	M	137	GLN
5	M	252	ASN
5	M	263	GLN
5	M	354	GLN
5	N	40	HIS
5	N	41	GLN
5	N	78	ASN
5	N	137	GLN
5	N	252	ASN
5	N	263	GLN
5	N	354	GLN
5	N	360	GLN
5	O	40	HIS
5	O	41	GLN
5	O	78	ASN
5	O	137	GLN
5	O	263	GLN
5	O	354	GLN
5	O	360	GLN
5	P	40	HIS
5	P	41	GLN
5	P	78	ASN
5	P	137	GLN
5	P	252	ASN
5	P	263	GLN
5	P	280	ASN
5	P	354	GLN
5	Q	40	HIS
5	Q	41	GLN
5	Q	78	ASN
5	Q	252	ASN
5	Q	263	GLN
5	Q	354	GLN
5	Q	360	GLN
5	R	40	HIS
5	R	41	GLN
5	R	78	ASN
5	R	137	GLN
5	R	252	ASN
5	R	263	GLN
5	R	354	GLN
5	S	40	HIS

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Mol	Chain	Res	Type
5	S	41	GLN
5	S	78	ASN
5	S	111	ASN
5	S	252	ASN
5	S	263	GLN
5	S	354	GLN
5	S	360	GLN
2	Y	175	GLN
2	Y	198	ASN
2	Y	226	GLN
2	Y	243	GLN
2	Y	245	GLN
3	Z	42	ASN
3	Z	58	GLN
3	Z	86	GLN
3	Z	97	GLN
3	Z	133	ASN
3	Z	142	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1584. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.