



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 06:30 PM UTC

PDB ID : 7KON / pdb_00007kon
EMDB ID : EMD-22978
Title : Structure of upper Tn Ca²⁺ free (rotated) and lower Tn Ca²⁺ bound cardiac native thin filament at pCa=5.8
Authors : Galkin, V.E.; Risi, C.M.
Deposited on : 2020-11-09
Resolution : 8.10 Å (reported)
Based on initial models : 6KN7, 6KN8

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 : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

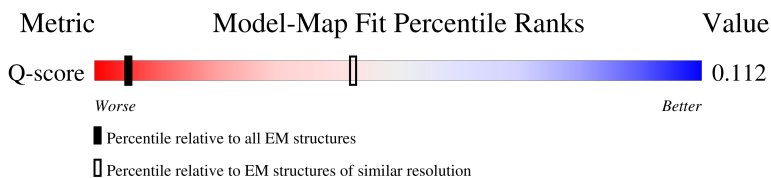
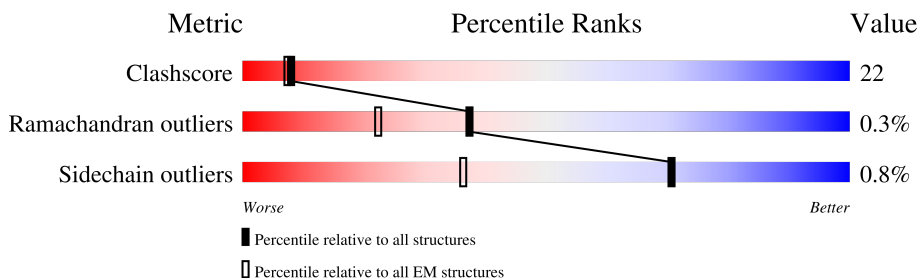
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

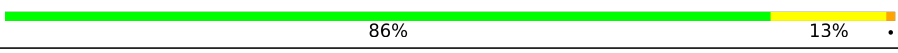
The reported resolution of this entry is 8.10 Å.

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.



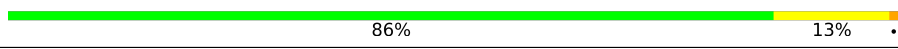
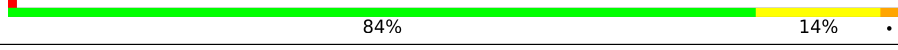
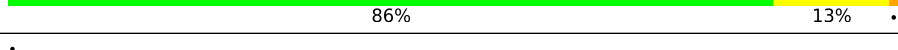
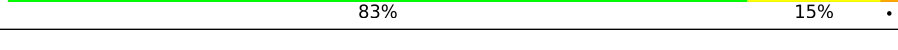
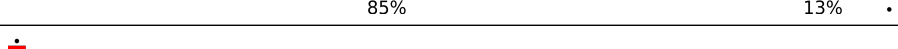
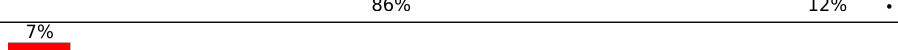
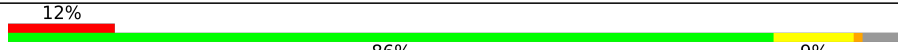
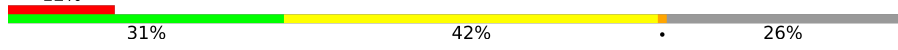
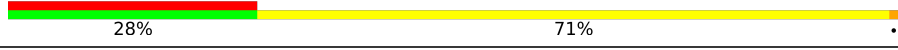
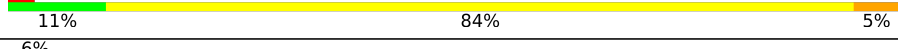
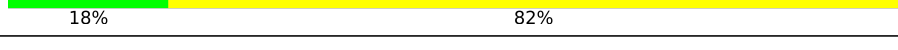
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	342 (7.60 - 8.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	375	
1	B	375	
1	C	375	
1	D	375	

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Mol	Chain	Length	Quality of chain
1	E	375	
1	F	375	
1	G	375	
1	H	375	
1	I	375	
1	J	375	
1	K	375	
1	L	375	
1	M	375	
1	N	375	
1	O	375	
2	P	286	
2	Q	286	
2	R	286	
2	S	286	
2	W	286	
2	X	286	
2	Y	286	
2	Z	286	
3	T	186	
3	a	186	
4	U	170	
4	b	170	
5	V	160	
5	c	160	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 60987 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	B	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	C	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	F	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	G	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	H	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	I	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	J	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	K	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	L	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	M	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	N	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	O	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		

- Molecule 2 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	Q	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	R	29	Total	C	N	O	S	0	0
			231	141	41	46	3		
2	S	29	Total	C	N	O	S	0	0
			231	141	41	46	3		
2	W	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	X	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	Y	29	Total	C	N	O	S	0	0
			231	141	41	46	3		
2	Z	29	Total	C	N	O	S	0	0
			231	141	41	46	3		

- Molecule 3 is a protein called Troponin T, cardiac muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	126	Total	C	N	O		0	0
			1101	673	219	209			
3	a	138	Total	C	N	O	S	0	0
			1211	740	241	229	1		

- Molecule 4 is a protein called Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	170	Total	C	N	O	S	0	0
			1374	848	263	258	5		
4	b	126	Total	C	N	O	S	0	0
			1008	624	193	187	4		

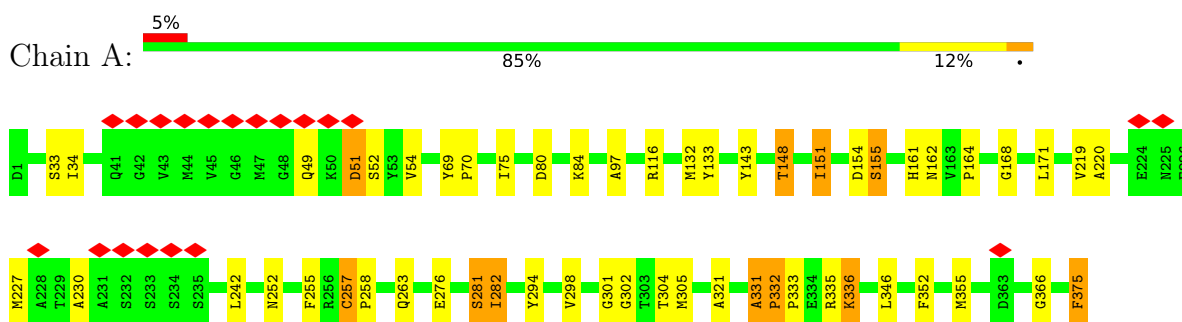
- Molecule 5 is a protein called Troponin C.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	160	Total	C	N	O	S	0	0
			1273	788	195	278	12		
5	c	160	Total	C	N	O	S	0	0
			1273	788	195	278	12		

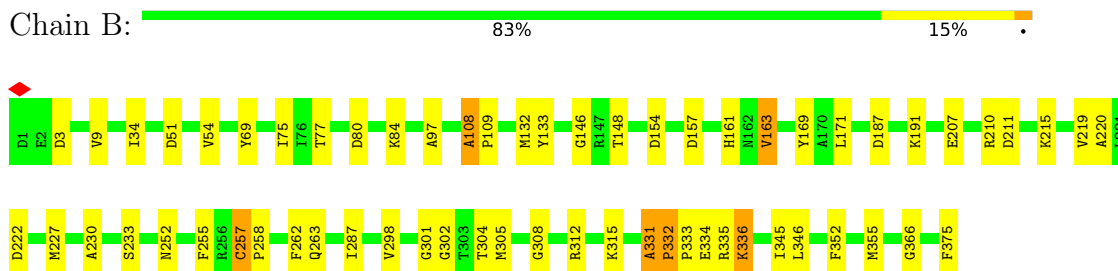
3 Residue-property plots

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

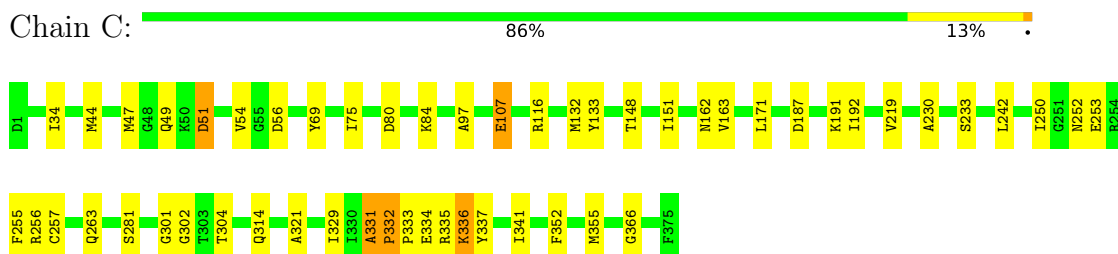
- Molecule 1: Actin, alpha skeletal muscle



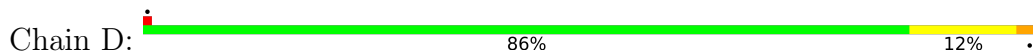
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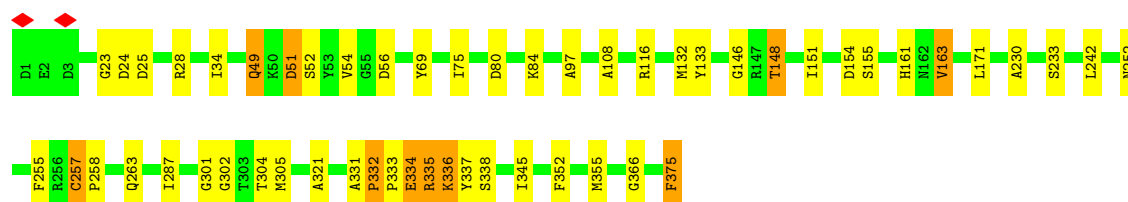


- Molecule 1: Actin, alpha skeletal muscle

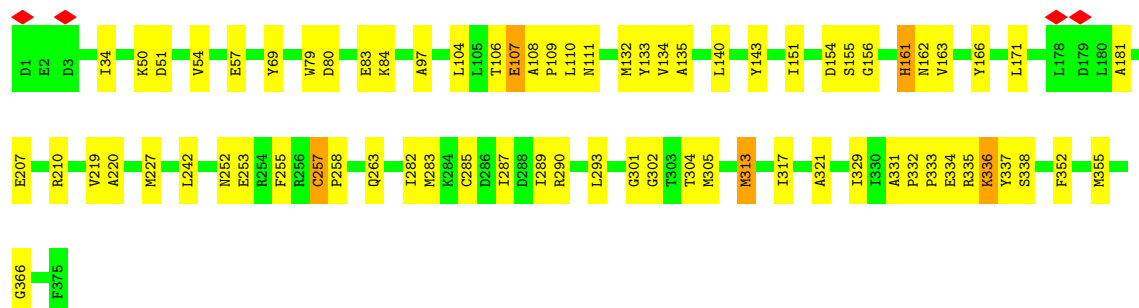
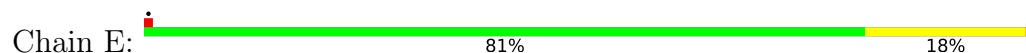


- Molecule 1: Actin, alpha skeletal muscle

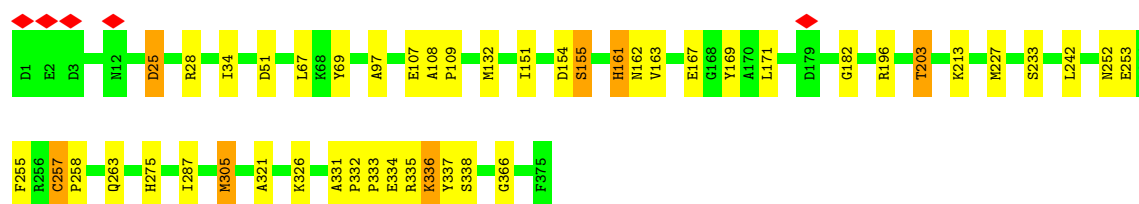
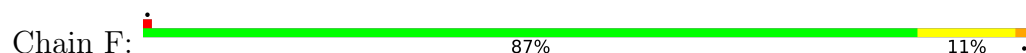




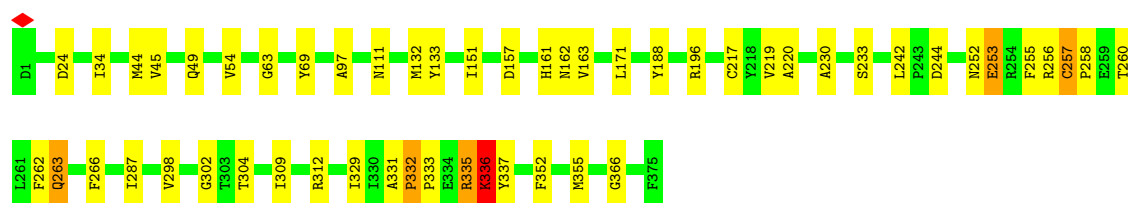
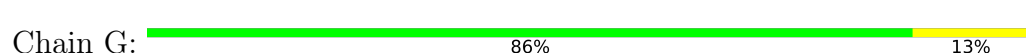
- Molecule 1: Actin, alpha skeletal muscle



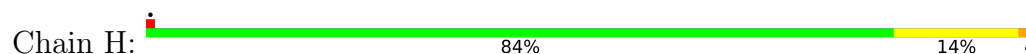
- Molecule 1: Actin, alpha skeletal muscle

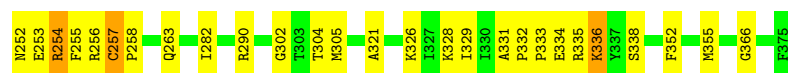


- Molecule 1: Actin, alpha skeletal muscle

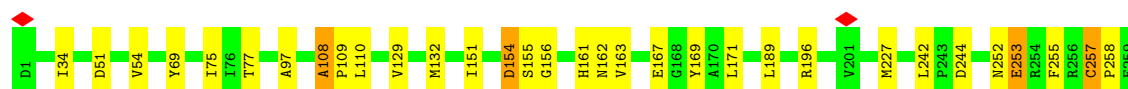
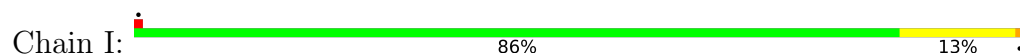


- Molecule 1: Actin, alpha skeletal muscle

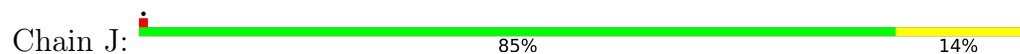




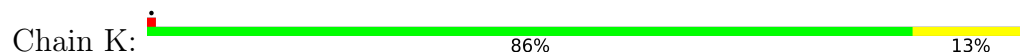
- Molecule 1: Actin, alpha skeletal muscle



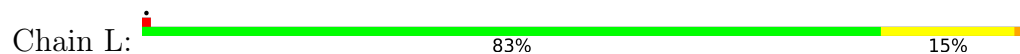
- Molecule 1: Actin, alpha skeletal muscle



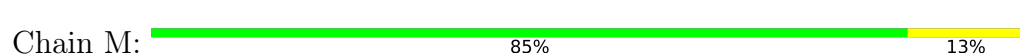
- Molecule 1: Actin, alpha skeletal muscle

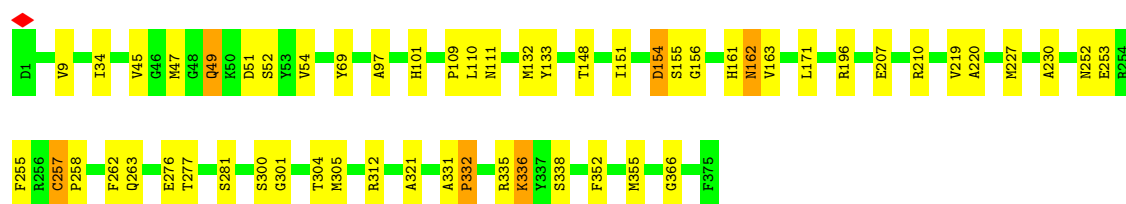


- Molecule 1: Actin, alpha skeletal muscle

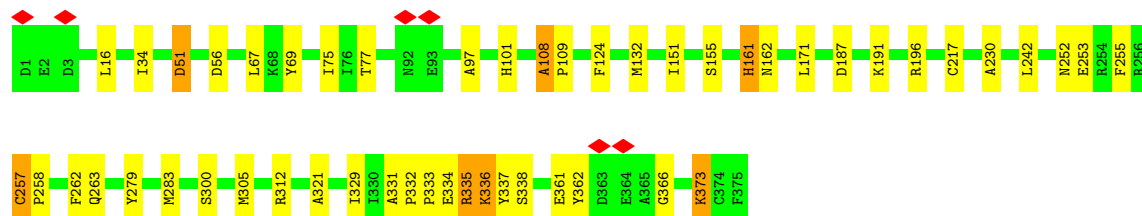
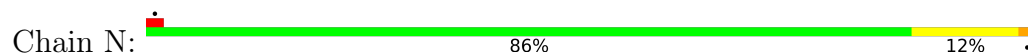


- Molecule 1: Actin, alpha skeletal muscle

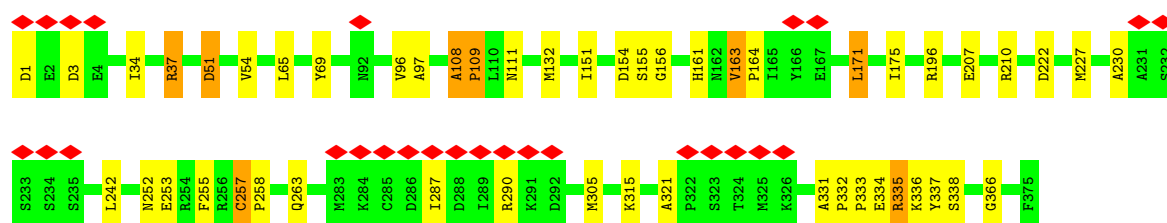
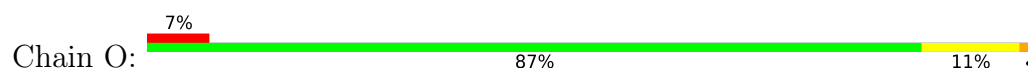




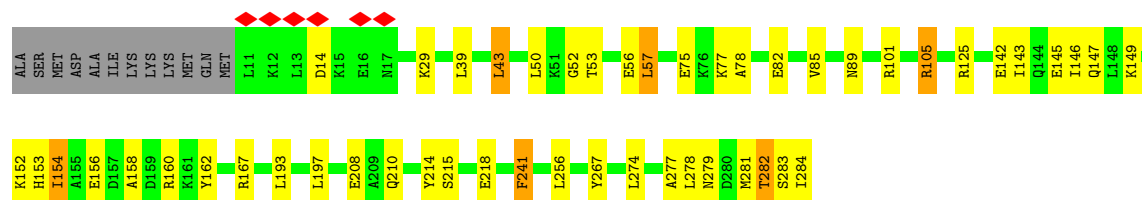
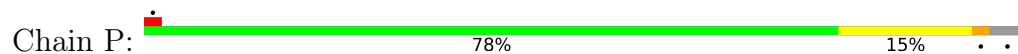
- Molecule 1: Actin, alpha skeletal muscle



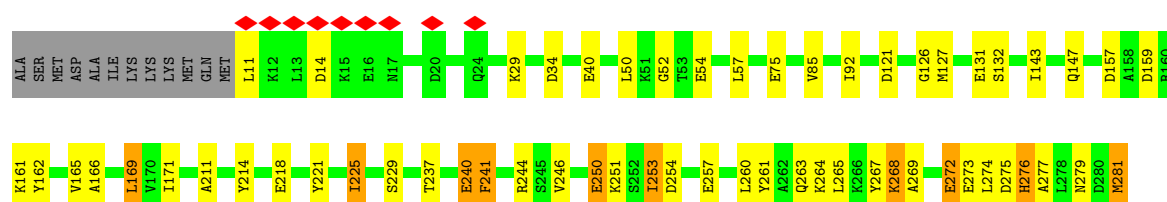
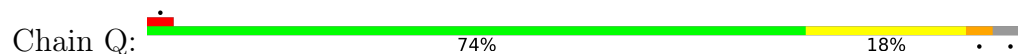
- Molecule 1: Actin, alpha skeletal muscle

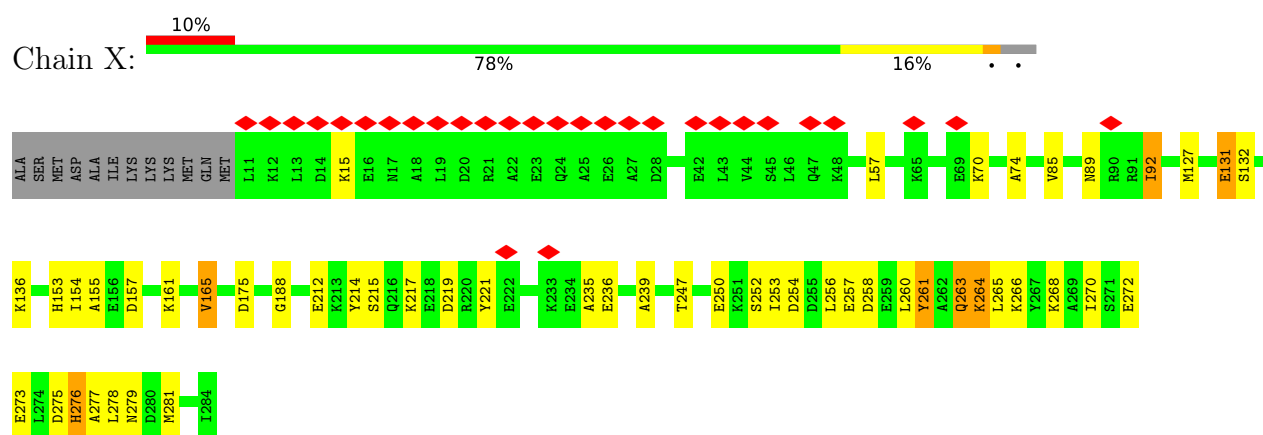


- Molecule 2: Tropomyosin alpha-1 chain

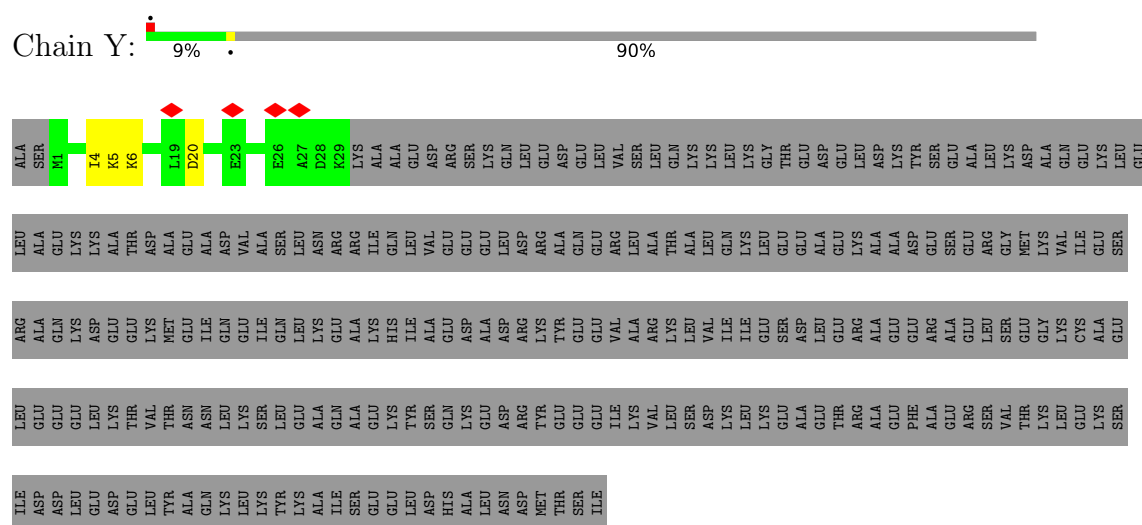


- Molecule 2: Tropomyosin alpha-1 chain

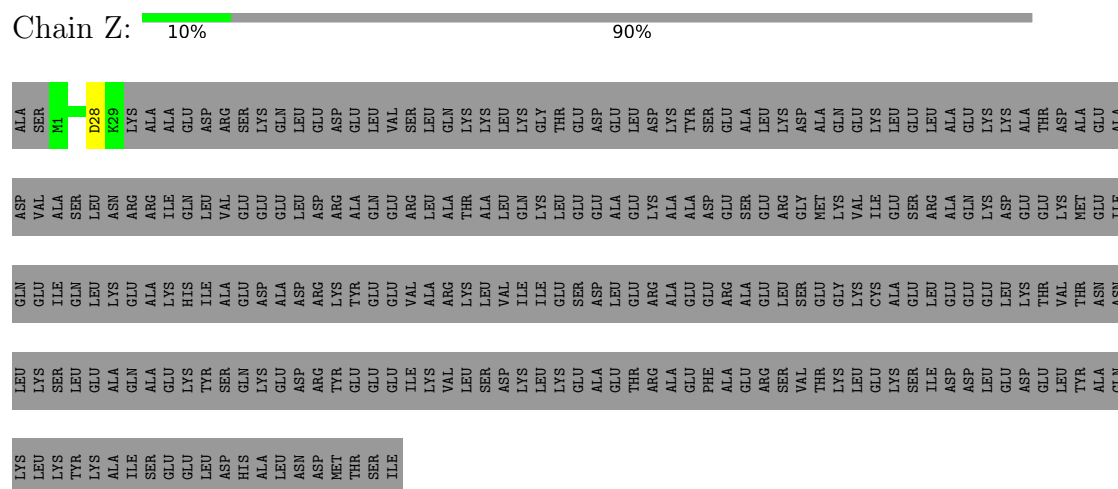




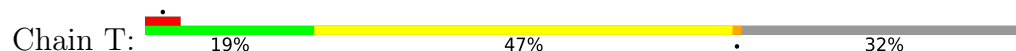
- Molecule 2: Tropomyosin alpha-1 chain



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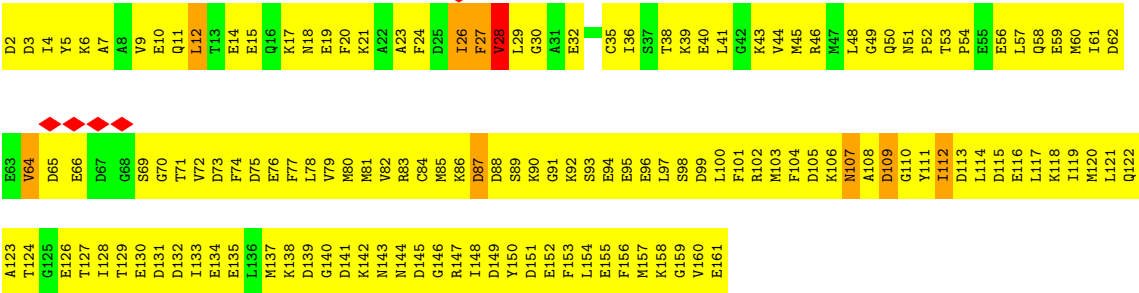


- Molecule 3: Troponin T, cardiac muscle



S166	LEU	ASP	LEU	ARG	ALA	HIS	LEU	LYS	GLN	VAL	LYS	LYS	GLU	ASP	THR	LYS	GLU	ASN	ARG	GLU	VAL	GLY	ASP	TRP	ARG	LYS	ASN	ILE	ASP	ALA	LEU	SER	GLY	MET	GLU	GLY	ARG	LYS	LYS	PHE	GLU	SER
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• Molecule 5: Troponin C



• Molecule 5: Troponin C



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10593	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.031	Depositor
Map size ($\text{\AA}$)	439.344, 439.344, 439.344	wwPDB
Map dimensions	162, 162, 162	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.712, 2.712, 2.712	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	A	0.92	1/2996 (0.0%)	1.30	31/4058 (0.8%)
1	B	0.92	0/2996	1.33	33/4058 (0.8%)
1	C	0.93	0/2996	1.32	37/4058 (0.9%)
1	D	0.92	1/2996 (0.0%)	1.33	36/4058 (0.9%)
1	E	0.93	0/2996	1.33	36/4058 (0.9%)
1	F	0.89	0/2996	1.32	35/4058 (0.9%)
1	G	0.94	2/2996 (0.1%)	1.33	36/4058 (0.9%)
1	H	0.91	1/2996 (0.0%)	1.33	34/4058 (0.8%)
1	I	0.91	0/2996	1.31	33/4058 (0.8%)
1	J	0.90	0/2996	1.33	31/4058 (0.8%)
1	K	0.91	1/2996 (0.0%)	1.31	36/4058 (0.9%)
1	L	0.88	0/2996	1.31	35/4058 (0.9%)
1	M	0.90	0/2996	1.31	35/4058 (0.9%)
1	N	0.92	1/2996 (0.0%)	1.33	36/4058 (0.9%)
1	O	0.90	0/2996	1.31	32/4058 (0.8%)
2	P	1.37	0/2215	1.34	17/2954 (0.6%)
2	Q	1.37	2/2215 (0.1%)	1.39	22/2954 (0.7%)
2	R	1.39	1/230 (0.4%)	1.28	2/301 (0.7%)
2	S	1.35	1/230 (0.4%)	1.22	0/301
2	W	1.30	1/2215 (0.0%)	1.27	7/2954 (0.2%)
2	X	1.32	2/2215 (0.1%)	1.30	9/2954 (0.3%)
2	Y	1.23	0/230	1.09	0/301
2	Z	1.16	0/230	1.14	1/301 (0.3%)
3	T	0.79	0/1108	0.97	2/1466 (0.1%)
3	a	0.83	1/1220 (0.1%)	0.94	4/1613 (0.2%)
4	U	0.28	0/1384	0.65	1/1840 (0.1%)
4	b	0.31	0/1014	0.57	0/1352
5	V	0.46	0/1286	0.96	8/1719 (0.5%)
5	c	0.28	0/1286	0.55	0/1719
All	All	0.96	15/62018 (0.0%)	1.27	589/83599 (0.7%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	8	MET	SD-CE	-6.28	1.63	1.79
1	H	161	HIS	CB-CG	-6.01	1.41	1.50
2	R	4	ILE	CA-CB	-6.01	1.47	1.54
2	W	256	LEU	CB-CG	-5.90	1.41	1.53
1	K	161	HIS	CB-CG	-5.83	1.42	1.50
2	X	57	LEU	CG-CD2	-5.76	1.33	1.52
2	Q	241	PHE	CA-C	-5.65	1.45	1.52
1	D	161	HIS	CB-CG	-5.61	1.42	1.50
2	X	276	HIS	CB-CG	-5.52	1.42	1.50
1	G	161	HIS	CG-CD2	-5.42	1.29	1.35
1	N	67	LEU	CB-CG	5.27	1.64	1.53
3	a	109	HIS	CB-CG	-5.17	1.43	1.50
1	G	256	ARG	NE-CZ	5.15	1.38	1.33
2	Q	281	MET	CA-C	-5.14	1.46	1.52
1	A	161	HIS	CB-CG	-5.04	1.43	1.50

All (589) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	26	ILE	N-CA-C	14.57	123.70	111.90
2	P	282	THR	N-CA-C	-14.16	95.54	110.97
5	V	26	ILE	CB-CA-C	-12.78	99.03	111.30
3	a	125	ASP	N-CA-C	-9.23	101.30	111.36
1	J	163	VAL	N-CA-C	9.15	116.61	107.55
1	K	163	VAL	N-CA-C	8.96	117.95	107.73
2	Q	268	LYS	N-CA-C	-8.74	100.73	111.40
1	O	163	VAL	N-CA-C	8.66	117.07	109.02
1	C	163	VAL	N-CA-C	8.57	117.50	107.73
1	N	263	GLN	CA-C-N	8.52	128.16	119.82
1	N	263	GLN	C-N-CA	8.52	128.16	119.82
1	D	163	VAL	N-CA-C	8.48	117.40	107.73
2	Q	272	GLU	N-CA-C	-8.43	102.04	111.14
1	O	263	GLN	CA-C-N	8.36	128.00	119.56
1	O	263	GLN	C-N-CA	8.36	128.00	119.56
1	F	69	TYR	CA-C-N	8.32	128.04	119.56
1	F	69	TYR	C-N-CA	8.32	128.04	119.56
1	K	111	ASN	CA-CB-CG	8.25	120.85	112.60
2	Q	250	GLU	N-CA-C	-8.25	102.37	111.36
1	B	69	TYR	CA-C-N	8.21	127.85	119.56
1	B	69	TYR	C-N-CA	8.21	127.85	119.56
1	E	163	VAL	N-CA-C	8.19	116.82	107.89
1	K	263	GLN	CA-C-N	8.18	127.90	119.56
1	K	263	GLN	C-N-CA	8.18	127.90	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	263	GLN	CA-C-N	8.17	127.90	119.56
1	H	263	GLN	C-N-CA	8.17	127.90	119.56
1	G	163	VAL	N-CA-C	8.11	117.26	107.61
1	O	69	TYR	CA-C-N	8.09	127.81	119.56
1	O	69	TYR	C-N-CA	8.09	127.81	119.56
1	A	263	GLN	CA-C-N	8.07	127.71	119.56
1	A	263	GLN	C-N-CA	8.07	127.71	119.56
1	L	163	VAL	N-CA-C	8.02	116.63	107.89
1	E	69	TYR	CA-C-N	8.01	127.73	119.56
1	E	69	TYR	C-N-CA	8.01	127.73	119.56
1	K	366	GLY	CA-C-N	7.94	127.66	119.56
1	K	366	GLY	C-N-CA	7.94	127.66	119.56
1	B	366	GLY	CA-C-N	7.93	127.65	119.56
1	B	366	GLY	C-N-CA	7.93	127.65	119.56
1	N	69	TYR	CA-C-N	7.92	128.11	119.87
1	N	69	TYR	C-N-CA	7.92	128.11	119.87
1	N	34	ILE	N-CA-C	7.91	120.24	108.46
1	J	366	GLY	CA-C-N	7.90	127.62	119.56
1	J	366	GLY	C-N-CA	7.90	127.62	119.56
1	F	263	GLN	CA-C-N	7.88	127.59	119.56
1	F	263	GLN	C-N-CA	7.88	127.59	119.56
1	H	366	GLY	CA-C-N	7.88	127.54	119.82
1	H	366	GLY	C-N-CA	7.88	127.54	119.82
1	J	219	VAL	N-CA-C	7.85	118.65	110.72
1	E	263	GLN	CA-C-N	7.84	127.55	119.56
1	E	263	GLN	C-N-CA	7.84	127.55	119.56
1	E	111	ASN	CA-CB-CG	7.77	120.37	112.60
1	K	69	TYR	CA-C-N	7.75	127.47	119.56
1	K	69	TYR	C-N-CA	7.75	127.47	119.56
1	D	263	GLN	CA-C-N	7.75	127.39	119.56
1	D	263	GLN	C-N-CA	7.75	127.39	119.56
1	G	69	TYR	CA-C-N	7.72	127.43	119.56
1	G	69	TYR	C-N-CA	7.72	127.43	119.56
1	G	366	GLY	CA-C-N	7.69	127.40	119.56
1	G	366	GLY	C-N-CA	7.69	127.40	119.56
1	J	263	GLN	CA-C-N	7.68	127.40	119.56
1	J	263	GLN	C-N-CA	7.68	127.40	119.56
1	M	69	TYR	CA-C-N	7.68	127.39	119.56
1	M	69	TYR	C-N-CA	7.68	127.39	119.56
1	L	69	TYR	CA-C-N	7.66	127.38	119.56
1	L	69	TYR	C-N-CA	7.66	127.38	119.56
1	L	366	GLY	CA-C-N	7.66	127.38	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	366	GLY	C-N-CA	7.66	127.38	119.56
2	P	241	PHE	CA-CB-CG	-7.66	106.14	113.80
1	H	69	TYR	CA-C-N	7.65	127.36	119.56
1	H	69	TYR	C-N-CA	7.65	127.36	119.56
1	A	69	TYR	CA-C-N	7.62	127.80	119.87
1	A	69	TYR	C-N-CA	7.62	127.80	119.87
1	E	366	GLY	CA-C-N	7.60	127.31	119.56
1	E	366	GLY	C-N-CA	7.60	127.31	119.56
1	J	69	TYR	CA-C-N	7.59	128.23	120.04
1	J	69	TYR	C-N-CA	7.59	128.23	120.04
1	C	69	TYR	CA-C-N	7.55	127.26	119.56
1	C	69	TYR	C-N-CA	7.55	127.26	119.56
1	D	366	GLY	CA-C-N	7.50	127.21	119.56
1	D	366	GLY	C-N-CA	7.50	127.21	119.56
1	M	366	GLY	CA-C-N	7.48	127.19	119.56
1	M	366	GLY	C-N-CA	7.48	127.19	119.56
1	G	263	GLN	CA-C-N	7.48	127.11	119.56
1	G	263	GLN	C-N-CA	7.48	127.11	119.56
2	P	43	LEU	N-CA-C	-7.48	102.81	112.23
1	F	366	GLY	CA-C-N	7.45	128.11	119.47
1	F	366	GLY	C-N-CA	7.45	128.11	119.47
1	B	263	GLN	CA-C-N	7.39	127.02	119.56
1	B	263	GLN	C-N-CA	7.39	127.02	119.56
1	H	97	ALA	CA-C-N	7.36	127.07	119.56
1	H	97	ALA	C-N-CA	7.36	127.07	119.56
1	F	331	ALA	CA-C-N	7.34	127.94	120.38
1	F	331	ALA	C-N-CA	7.34	127.94	120.38
1	L	332	PRO	CA-C-N	7.32	127.03	119.56
1	L	332	PRO	C-N-CA	7.32	127.03	119.56
1	C	263	GLN	CA-C-N	7.32	127.03	119.56
1	C	263	GLN	C-N-CA	7.32	127.03	119.56
1	M	263	GLN	CA-C-N	7.30	126.94	119.56
1	M	263	GLN	C-N-CA	7.30	126.94	119.56
1	B	148	THR	N-CA-C	-7.29	104.91	114.31
1	D	34	ILE	N-CA-C	7.28	119.31	108.46
1	L	263	GLN	CA-C-N	7.23	126.87	119.56
1	L	263	GLN	C-N-CA	7.23	126.87	119.56
1	J	97	ALA	CA-C-N	7.23	126.93	119.56
1	J	97	ALA	C-N-CA	7.23	126.93	119.56
1	D	69	TYR	CA-C-N	7.22	127.84	120.04
1	D	69	TYR	C-N-CA	7.22	127.84	120.04
1	E	34	ILE	N-CA-C	7.21	119.20	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	171	LEU	CA-C-N	7.18	126.89	119.56
1	L	171	LEU	C-N-CA	7.18	126.89	119.56
1	N	329	ILE	N-CA-C	7.18	118.22	108.17
1	C	366	GLY	CA-C-N	7.15	126.86	119.56
1	C	366	GLY	C-N-CA	7.15	126.86	119.56
1	L	34	ILE	N-CA-C	7.14	118.11	108.11
1	I	263	GLN	CA-C-N	7.13	126.76	119.56
1	I	263	GLN	C-N-CA	7.13	126.76	119.56
1	F	25	ASP	CA-CB-CG	7.12	119.72	112.60
1	O	366	GLY	CA-C-N	7.10	126.80	119.56
1	O	366	GLY	C-N-CA	7.10	126.80	119.56
1	B	331	ALA	CA-C-N	7.09	127.68	120.38
1	B	331	ALA	C-N-CA	7.09	127.68	120.38
1	O	151	ILE	CB-CA-C	-7.09	102.12	110.91
1	O	97	ALA	CA-C-N	7.07	126.77	119.56
1	O	97	ALA	C-N-CA	7.07	126.77	119.56
1	A	366	GLY	CA-C-N	7.06	126.76	119.56
1	A	366	GLY	C-N-CA	7.06	126.76	119.56
1	D	97	ALA	CA-C-N	7.06	126.76	119.56
1	D	97	ALA	C-N-CA	7.06	126.76	119.56
1	O	171	LEU	CA-C-N	7.04	126.74	119.56
1	O	171	LEU	C-N-CA	7.04	126.74	119.56
1	I	171	LEU	CA-C-N	7.03	126.73	119.56
1	I	171	LEU	C-N-CA	7.03	126.73	119.56
1	J	148	THR	N-CA-C	-7.03	105.24	114.31
1	A	171	LEU	CA-C-N	7.02	126.72	119.56
1	A	171	LEU	C-N-CA	7.02	126.72	119.56
1	A	97	ALA	CA-C-N	7.00	126.70	119.56
1	A	97	ALA	C-N-CA	7.00	126.70	119.56
1	H	171	LEU	CA-C-N	6.99	126.69	119.56
1	H	171	LEU	C-N-CA	6.99	126.69	119.56
1	J	321	ALA	CA-C-N	6.99	126.97	119.78
1	J	321	ALA	C-N-CA	6.99	126.97	119.78
1	N	257	CYS	CA-C-N	6.98	127.57	119.47
1	N	257	CYS	C-N-CA	6.98	127.57	119.47
1	I	366	GLY	CA-C-N	6.98	126.68	119.56
1	I	366	GLY	C-N-CA	6.98	126.68	119.56
1	A	75	ILE	N-CA-C	6.96	117.91	108.17
1	I	97	ALA	CA-C-N	6.95	126.65	119.56
1	I	97	ALA	C-N-CA	6.95	126.65	119.56
1	E	161	HIS	N-CA-C	6.94	120.23	111.69
1	E	332	PRO	CA-C-N	6.93	126.63	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	332	PRO	C-N-CA	6.93	126.63	119.56
1	C	171	LEU	CA-C-N	6.92	126.62	119.56
1	C	171	LEU	C-N-CA	6.92	126.62	119.56
2	P	154	ILE	N-CA-C	-6.89	103.76	110.72
2	P	208	GLU	N-CA-C	-6.88	103.87	111.36
2	Q	283	SER	N-CA-C	-6.87	101.66	110.53
1	N	366	GLY	CA-C-N	6.84	126.53	119.56
1	N	366	GLY	C-N-CA	6.84	126.53	119.56
1	M	171	LEU	CA-C-N	6.83	126.53	119.56
1	M	171	LEU	C-N-CA	6.83	126.53	119.56
1	G	171	LEU	CA-C-N	6.82	126.52	119.56
1	G	171	LEU	C-N-CA	6.82	126.52	119.56
1	I	69	TYR	CA-C-N	6.81	126.51	119.56
1	I	69	TYR	C-N-CA	6.81	126.51	119.56
3	T	110	PHE	N-CA-C	6.80	118.35	111.07
2	P	52	GLY	N-CA-C	-6.79	104.62	112.50
1	G	332	PRO	CA-C-N	6.79	126.48	119.56
1	G	332	PRO	C-N-CA	6.79	126.48	119.56
2	W	208	GLU	N-CA-C	-6.78	103.81	111.14
1	B	132	MET	N-CA-C	6.76	119.45	109.24
1	F	257	CYS	CA-C-N	6.75	127.31	119.47
1	F	257	CYS	C-N-CA	6.75	127.31	119.47
1	J	171	LEU	CA-C-N	6.75	126.44	119.56
1	J	171	LEU	C-N-CA	6.75	126.44	119.56
1	A	331	ALA	CA-C-N	6.75	127.33	120.38
1	A	331	ALA	C-N-CA	6.75	127.33	120.38
1	I	151	ILE	CA-C-N	-6.74	114.10	122.93
1	I	151	ILE	C-N-CA	-6.74	114.10	122.93
2	W	126	GLY	N-CA-C	-6.73	104.69	112.50
1	E	257	CYS	CA-C-N	6.71	127.25	119.47
1	E	257	CYS	C-N-CA	6.71	127.25	119.47
1	I	331	ALA	CA-C-N	6.70	127.28	120.38
1	I	331	ALA	C-N-CA	6.70	127.28	120.38
1	L	31	PHE	CA-C-N	6.70	126.66	119.76
1	L	31	PHE	C-N-CA	6.70	126.66	119.76
1	N	151	ILE	CA-C-N	-6.70	114.42	123.12
1	N	151	ILE	C-N-CA	-6.70	114.42	123.12
1	M	111	ASN	CA-CB-CG	6.69	119.29	112.60
2	Q	121	ASP	CA-CB-CG	6.67	119.27	112.60
1	A	257	CYS	CA-C-N	6.67	127.20	119.47
1	A	257	CYS	C-N-CA	6.67	127.20	119.47
1	F	171	LEU	CA-C-N	6.65	126.34	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	171	LEU	C-N-CA	6.65	126.34	119.56
1	N	331	ALA	CA-C-N	6.65	127.23	120.38
1	N	331	ALA	C-N-CA	6.65	127.23	120.38
2	X	263	GLN	N-CA-C	-6.65	103.73	110.97
3	a	109	HIS	CA-CB-CG	6.62	120.42	113.80
1	C	331	ALA	CA-C-N	6.62	127.19	120.38
1	C	331	ALA	C-N-CA	6.62	127.19	120.38
1	C	148	THR	N-CA-C	-6.60	105.79	114.31
1	D	171	LEU	CA-C-N	6.59	126.28	119.56
1	D	171	LEU	C-N-CA	6.59	126.28	119.56
1	K	171	LEU	CA-C-N	6.59	126.28	119.56
1	K	171	LEU	C-N-CA	6.59	126.28	119.56
1	B	171	LEU	CA-C-N	6.58	126.27	119.56
1	B	171	LEU	C-N-CA	6.58	126.27	119.56
1	C	329	ILE	N-CA-C	6.56	117.74	108.36
1	H	108	ALA	CA-C-N	6.55	126.24	119.82
1	H	108	ALA	C-N-CA	6.55	126.24	119.82
1	N	97	ALA	CA-C-N	6.54	127.05	119.47
1	N	97	ALA	C-N-CA	6.54	127.05	119.47
1	C	34	ILE	N-CA-C	6.53	118.18	108.46
1	I	257	CYS	CA-C-N	6.52	127.03	119.47
1	I	257	CYS	C-N-CA	6.52	127.03	119.47
1	O	321	ALA	CA-C-N	6.50	126.46	120.03
1	O	321	ALA	C-N-CA	6.50	126.46	120.03
1	F	151	ILE	CA-C-N	-6.45	114.64	122.90
1	F	151	ILE	C-N-CA	-6.45	114.64	122.90
1	J	298	VAL	N-CA-C	6.43	117.12	108.11
3	a	90	ILE	N-CA-C	-6.43	104.22	110.72
2	Q	126	GLY	N-CA-C	-6.42	105.05	112.50
1	M	257	CYS	CA-C-N	6.41	126.91	119.47
1	M	257	CYS	C-N-CA	6.41	126.91	119.47
1	J	108	ALA	CA-C-N	6.38	126.07	119.56
1	J	108	ALA	C-N-CA	6.38	126.07	119.56
1	N	171	LEU	CA-C-N	6.38	126.00	119.56
1	N	171	LEU	C-N-CA	6.38	126.00	119.56
1	G	329	ILE	N-CA-C	6.38	117.10	108.17
1	K	151	ILE	CA-C-N	-6.38	114.74	122.90
1	K	151	ILE	C-N-CA	-6.38	114.74	122.90
1	M	148	THR	N-CA-C	-6.37	105.26	114.12
1	K	332	PRO	CA-C-N	6.36	126.05	119.56
1	K	332	PRO	C-N-CA	6.36	126.05	119.56
1	I	34	ILE	N-CA-C	6.36	117.94	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	257	CYS	CA-C-N	6.36	126.84	119.47
1	O	257	CYS	C-N-CA	6.36	126.84	119.47
2	R	20	ASP	N-CA-C	-6.36	104.27	111.07
1	G	257	CYS	CA-C-N	6.36	126.84	119.47
1	G	257	CYS	C-N-CA	6.36	126.84	119.47
1	O	34	ILE	N-CA-C	6.35	117.92	108.46
1	O	108	ALA	CA-C-N	6.34	126.55	119.32
1	O	108	ALA	C-N-CA	6.34	126.55	119.32
2	P	125	ARG	N-CA-C	-6.33	104.31	111.14
1	B	34	ILE	N-CA-C	6.31	117.21	108.12
1	L	217	CYS	N-CA-C	6.30	119.80	110.48
1	H	148	THR	N-CA-C	-6.28	106.21	114.31
1	F	132	MET	N-CA-C	6.26	118.93	109.23
1	K	34	ILE	N-CA-C	6.25	116.86	108.11
1	N	75	ILE	N-CA-C	6.25	116.92	108.17
1	C	242	LEU	CA-C-N	6.23	125.92	119.56
1	C	242	LEU	C-N-CA	6.23	125.92	119.56
1	I	163	VAL	N-CA-C	6.23	114.83	107.73
1	D	75	ILE	N-CA-C	6.22	116.88	108.17
1	B	332	PRO	CA-C-N	6.22	126.68	119.47
1	B	332	PRO	C-N-CA	6.22	126.68	119.47
1	A	332	PRO	CA-C-N	6.21	125.89	119.56
1	A	332	PRO	C-N-CA	6.21	125.89	119.56
1	F	332	PRO	CA-C-N	6.20	125.88	119.56
1	F	332	PRO	C-N-CA	6.20	125.88	119.56
1	D	148	THR	N-CA-C	-6.19	106.32	114.31
1	J	332	PRO	CA-C-N	6.18	125.81	119.56
1	J	332	PRO	C-N-CA	6.18	125.81	119.56
1	H	332	PRO	CA-C-N	6.17	125.80	119.56
1	H	332	PRO	C-N-CA	6.17	125.80	119.56
1	H	257	CYS	CA-C-N	6.16	126.61	119.47
1	H	257	CYS	C-N-CA	6.16	126.61	119.47
1	G	217	CYS	N-CA-C	6.14	118.84	110.55
1	M	163	VAL	N-CA-C	6.13	114.91	107.61
1	M	34	ILE	N-CA-C	6.12	116.93	108.12
1	D	257	CYS	CA-C-N	6.12	126.56	119.47
1	D	257	CYS	C-N-CA	6.12	126.56	119.47
1	E	151	ILE	CA-C-N	-6.11	114.92	122.93
1	E	151	ILE	C-N-CA	-6.11	114.92	122.93
1	E	331	ALA	CA-C-N	6.11	126.68	120.38
1	E	331	ALA	C-N-CA	6.11	126.68	120.38
2	R	5	LYS	N-CA-C	-6.11	104.62	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	332	PRO	CA-C-N	6.11	125.79	119.56
1	D	332	PRO	C-N-CA	6.11	125.79	119.56
1	C	332	PRO	CA-C-N	6.09	126.21	119.87
1	C	332	PRO	C-N-CA	6.09	126.21	119.87
1	M	151	ILE	CA-C-N	-6.08	115.12	122.90
1	M	151	ILE	C-N-CA	-6.08	115.12	122.90
1	K	97	ALA	CA-C-N	6.06	127.42	119.84
1	K	97	ALA	C-N-CA	6.06	127.42	119.84
1	H	132	MET	N-CA-C	6.04	118.59	109.23
1	M	162	ASN	CA-C-N	-6.03	118.08	123.33
1	M	162	ASN	C-N-CA	-6.03	118.08	123.33
1	B	75	ILE	N-CA-C	6.01	116.58	108.17
1	G	242	LEU	N-CA-C	-6.00	102.01	110.29
1	J	331	ALA	CA-C-N	6.00	126.56	120.38
1	J	331	ALA	C-N-CA	6.00	126.56	120.38
1	I	154	ASP	N-CA-C	6.00	119.91	112.59
1	F	163	VAL	N-CA-C	5.99	114.74	107.61
2	P	57	LEU	CB-CA-C	-5.99	100.85	110.79
1	A	148	THR	N-CA-C	-5.98	106.59	114.31
2	Z	28	ASP	CA-CB-CG	5.98	118.58	112.60
1	B	257	CYS	CA-C-N	5.98	126.40	119.47
1	B	257	CYS	C-N-CA	5.98	126.40	119.47
2	X	15	LYS	N-CA-C	-5.97	104.89	111.82
1	F	97	ALA	CA-C-N	5.97	126.40	119.47
1	F	97	ALA	C-N-CA	5.97	126.40	119.47
1	A	276	GLU	N-CA-C	-5.96	105.10	112.90
1	D	331	ALA	CA-C-N	5.95	126.51	120.38
1	D	331	ALA	C-N-CA	5.95	126.51	120.38
1	L	54	VAL	N-CA-C	5.94	117.03	108.48
1	H	331	ALA	CA-C-N	5.93	126.49	120.38
1	H	331	ALA	C-N-CA	5.93	126.49	120.38
1	G	309	ILE	N-CA-C	5.93	116.71	110.72
1	K	101	HIS	CA-C-N	5.92	127.24	119.84
1	K	101	HIS	C-N-CA	5.92	127.24	119.84
2	P	14	ASP	N-CA-C	-5.90	105.17	112.90
1	N	217	CYS	N-CA-C	5.90	119.25	110.52
1	O	332	PRO	CA-C-N	5.90	126.31	119.47
1	O	332	PRO	C-N-CA	5.90	126.31	119.47
2	W	154	ILE	N-CA-C	-5.90	104.76	110.42
1	I	75	ILE	N-CA-C	5.89	116.96	108.48
1	K	154	ASP	CA-C-N	5.88	132.77	121.54
1	K	154	ASP	C-N-CA	5.88	132.77	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	PHE	CA-CB-CG	5.87	119.67	113.80
1	A	34	ILE	N-CA-C	5.87	117.21	108.46
1	N	321	ALA	CA-C-N	5.86	125.84	120.21
1	N	321	ALA	C-N-CA	5.86	125.84	120.21
1	K	242	LEU	CA-C-N	5.86	126.27	119.47
1	K	242	LEU	C-N-CA	5.86	126.27	119.47
1	M	154	ASP	CA-C-N	5.86	132.73	121.54
1	M	154	ASP	C-N-CA	5.86	132.73	121.54
1	O	51	ASP	CA-CB-CG	-5.86	106.74	112.60
2	Q	225	ILE	N-CA-C	-5.86	105.02	110.53
1	M	101	HIS	CA-C-N	5.86	125.81	119.78
1	M	101	HIS	C-N-CA	5.86	125.81	119.78
1	O	151	ILE	N-CA-CB	5.86	117.10	110.72
2	Q	52	GLY	N-CA-C	-5.86	105.71	112.50
1	F	161	HIS	N-CA-C	5.84	118.87	111.69
1	D	375	PHE	CA-CB-CG	5.83	119.63	113.80
1	A	298	VAL	N-CA-C	5.83	116.25	107.80
1	K	163	VAL	CA-C-N	5.83	126.28	119.99
1	K	163	VAL	C-N-CA	5.83	126.28	119.99
1	N	332	PRO	CA-C-N	5.82	126.23	119.47
1	N	332	PRO	C-N-CA	5.82	126.23	119.47
1	A	54	VAL	N-CA-C	5.81	116.24	108.11
5	V	27	PHE	CA-C-N	-5.80	111.52	121.97
5	V	27	PHE	C-N-CA	-5.80	111.52	121.97
2	Q	171	ILE	CA-C-N	5.80	128.41	120.46
2	Q	171	ILE	C-N-CA	5.80	128.41	120.46
1	M	9	VAL	N-CA-C	5.78	116.20	108.11
1	N	242	LEU	CA-C-N	5.78	126.17	119.47
1	N	242	LEU	C-N-CA	5.78	126.17	119.47
1	J	34	ILE	N-CA-C	5.78	116.44	108.12
3	a	106	ILE	N-CA-C	-5.78	104.88	110.42
1	N	161	HIS	N-CA-C	5.77	117.65	111.36
1	O	132	MET	N-CA-C	5.76	118.61	109.50
1	H	34	ILE	N-CA-C	5.76	117.04	108.46
1	L	148	THR	N-CA-C	-5.76	106.60	113.97
1	C	321	ALA	CA-C-N	5.75	125.70	119.78
1	C	321	ALA	C-N-CA	5.75	125.70	119.78
1	L	97	ALA	CA-C-N	5.74	126.13	119.47
1	L	97	ALA	C-N-CA	5.74	126.13	119.47
1	G	132	MET	N-CA-C	5.74	118.12	109.23
1	N	162	ASN	N-CA-C	5.74	119.16	111.24
1	L	298	VAL	N-CA-C	5.74	116.12	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	105	ARG	N-CA-C	-5.73	105.11	111.36
1	C	75	ILE	N-CA-C	5.73	116.19	108.17
1	H	329	ILE	N-CA-C	5.73	116.19	108.17
1	E	242	LEU	CA-C-N	5.71	126.10	119.47
1	E	242	LEU	C-N-CA	5.71	126.10	119.47
1	C	54	VAL	N-CA-C	5.70	116.69	108.48
5	V	26	ILE	CA-C-N	-5.70	110.54	121.94
5	V	26	ILE	C-N-CA	-5.70	110.54	121.94
1	B	163	VAL	CA-C-N	5.69	126.17	120.14
1	B	163	VAL	C-N-CA	5.69	126.17	120.14
1	C	107	GLU	N-CA-C	5.68	117.16	108.52
1	E	321	ALA	CA-C-N	5.68	125.63	119.78
1	E	321	ALA	C-N-CA	5.68	125.63	119.78
1	H	233	SER	N-CA-C	5.67	118.73	108.69
2	X	89	ASN	N-CA-C	-5.67	105.18	111.36
2	W	154	ILE	N-CA-CB	5.66	117.18	110.55
1	B	157	ASP	CA-CB-CG	5.66	118.26	112.60
1	I	132	MET	N-CA-C	5.66	118.00	109.23
1	M	331	ALA	CA-C-N	5.66	126.21	120.38
1	M	331	ALA	C-N-CA	5.66	126.21	120.38
1	C	97	ALA	CA-C-N	5.66	126.03	119.47
1	C	97	ALA	C-N-CA	5.66	126.03	119.47
1	K	298	VAL	N-CA-C	5.65	115.99	107.80
1	E	181	ALA	N-CA-C	5.65	116.53	108.74
1	A	242	LEU	CA-C-N	5.64	126.02	119.47
1	A	242	LEU	C-N-CA	5.64	126.02	119.47
1	G	54	VAL	N-CA-C	5.64	116.01	108.11
1	E	97	ALA	CA-C-N	5.64	125.31	119.56
1	E	97	ALA	C-N-CA	5.64	125.31	119.56
1	C	151	ILE	CB-CA-C	-5.63	103.26	110.98
1	J	257	CYS	CA-C-N	5.62	125.30	119.56
1	J	257	CYS	C-N-CA	5.62	125.30	119.56
1	M	132	MET	N-CA-C	5.61	117.93	109.23
1	F	108	ALA	CA-C-N	5.60	125.96	119.47
1	F	108	ALA	C-N-CA	5.60	125.96	119.47
2	P	29	LYS	N-CA-C	-5.60	105.26	111.36
2	Q	132	SER	N-CA-C	-5.60	105.26	111.36
1	B	108	ALA	CA-C-N	5.59	125.95	119.47
1	B	108	ALA	C-N-CA	5.59	125.95	119.47
1	F	162	ASN	CA-C-N	-5.59	118.47	123.33
1	F	162	ASN	C-N-CA	-5.59	118.47	123.33
1	G	331	ALA	CA-C-N	5.59	126.14	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	331	ALA	C-N-CA	5.59	126.14	120.38
1	M	54	VAL	N-CA-C	5.59	116.53	108.48
1	A	132	MET	N-CA-C	5.59	117.89	109.23
1	C	51	ASP	CA-CB-CG	-5.59	107.01	112.60
2	Q	75	GLU	N-CA-C	-5.59	105.27	111.36
1	E	171	LEU	CA-C-N	5.58	125.26	119.56
1	E	171	LEU	C-N-CA	5.58	125.26	119.56
1	M	276	GLU	N-CA-C	-5.58	105.59	112.90
1	B	77	THR	N-CA-C	-5.58	107.02	113.88
2	P	215	SER	N-CA-C	-5.58	105.35	111.82
1	N	108	ALA	CA-C-N	5.56	125.92	119.47
1	N	108	ALA	C-N-CA	5.56	125.92	119.47
5	V	112	ILE	CA-C-N	-5.55	112.23	120.94
5	V	112	ILE	C-N-CA	-5.55	112.23	120.94
1	D	108	ALA	CA-C-N	5.54	125.90	119.47
1	D	108	ALA	C-N-CA	5.54	125.90	119.47
1	D	54	VAL	N-CA-C	5.53	116.45	108.48
1	C	132	MET	N-CA-C	5.53	117.59	109.24
1	D	151	ILE	CA-C-N	-5.53	115.46	122.37
1	D	151	ILE	C-N-CA	-5.53	115.46	122.37
1	G	151	ILE	CA-C-N	-5.53	115.93	123.12
1	G	151	ILE	C-N-CA	-5.53	115.93	123.12
1	K	331	ALA	CA-C-N	5.52	126.07	120.38
1	K	331	ALA	C-N-CA	5.52	126.07	120.38
1	I	108	ALA	CA-C-N	5.51	125.87	119.47
1	I	108	ALA	C-N-CA	5.51	125.87	119.47
1	C	257	CYS	CA-C-N	5.51	125.18	119.56
1	C	257	CYS	C-N-CA	5.51	125.18	119.56
1	G	97	ALA	CA-C-N	5.51	126.72	119.84
1	G	97	ALA	C-N-CA	5.51	126.72	119.84
1	N	132	MET	N-CA-C	5.51	117.76	109.23
1	D	321	ALA	CA-C-N	5.50	125.45	119.78
1	D	321	ALA	C-N-CA	5.50	125.45	119.78
1	J	132	MET	N-CA-C	5.50	117.76	109.23
1	K	132	MET	N-CA-C	5.50	117.75	109.23
1	G	162	ASN	CA-C-N	-5.49	118.55	123.33
1	G	162	ASN	C-N-CA	-5.49	118.55	123.33
1	H	321	ALA	CA-C-N	5.48	125.46	120.03
1	H	321	ALA	C-N-CA	5.48	125.46	120.03
1	N	51	ASP	CA-CB-CG	-5.47	107.13	112.60
1	G	34	ILE	N-CA-C	5.46	116.60	108.46
1	M	97	ALA	CA-C-N	5.46	126.66	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	97	ALA	C-N-CA	5.46	126.66	119.84
1	F	242	LEU	CA-C-N	5.46	125.80	119.47
1	F	242	LEU	C-N-CA	5.46	125.80	119.47
2	P	77	LYS	N-CA-C	-5.46	105.33	111.28
1	K	309	ILE	N-CA-C	5.45	116.22	110.72
1	O	242	LEU	CA-C-N	5.45	125.79	119.47
1	O	242	LEU	C-N-CA	5.45	125.79	119.47
1	L	242	LEU	CA-C-N	5.43	125.77	119.47
1	L	242	LEU	C-N-CA	5.43	125.77	119.47
2	P	282	THR	CB-CA-C	5.43	119.33	110.96
1	L	154	ASP	CA-C-N	5.43	131.91	121.54
1	L	154	ASP	C-N-CA	5.43	131.91	121.54
1	I	77	THR	N-CA-C	-5.42	107.03	113.97
1	H	80	ASP	N-CA-C	-5.41	105.04	111.69
1	G	233	SER	N-CA-C	5.40	117.46	108.99
1	N	373	LYS	N-CA-C	5.38	120.50	113.88
1	G	244	ASP	N-CA-C	-5.37	106.21	114.16
2	X	188	GLY	N-CA-C	-5.37	106.27	112.50
1	O	111	ASN	CA-C-N	5.37	125.37	119.90
1	O	111	ASN	C-N-CA	5.37	125.37	119.90
1	C	314	GLN	N-CA-C	-5.36	105.10	111.69
1	K	321	ALA	CA-C-N	5.35	125.29	119.78
1	K	321	ALA	C-N-CA	5.35	125.29	119.78
1	B	97	ALA	CA-C-N	5.34	125.67	119.47
1	B	97	ALA	C-N-CA	5.34	125.67	119.47
1	I	54	VAL	N-CA-C	5.34	116.17	108.48
1	K	108	ALA	CA-C-N	5.34	125.41	119.32
1	K	108	ALA	C-N-CA	5.34	125.41	119.32
1	F	107	GLU	N-CA-C	5.34	117.30	109.24
1	M	277	THR	N-CA-C	-5.34	105.36	111.07
2	P	75	GLU	N-CA-C	-5.33	105.55	111.36
1	J	222	ASP	CA-CB-CG	5.33	117.93	112.60
2	Q	169	LEU	N-CA-C	-5.33	105.36	111.07
1	I	162	ASN	N-CA-C	5.33	118.59	111.24
2	X	131	GLU	N-CA-C	-5.33	105.55	111.36
1	E	54	VAL	N-CA-C	5.32	116.15	108.48
2	W	113	LEU	N-CA-C	-5.32	105.57	111.36
1	I	275	HIS	CA-CB-CG	-5.31	108.49	113.80
1	C	163	VAL	CA-C-N	5.31	125.72	119.99
1	C	163	VAL	C-N-CA	5.31	125.72	119.99
1	D	242	LEU	N-CA-C	-5.31	102.49	110.24
1	J	54	VAL	N-CA-C	5.30	116.36	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	34	ILE	N-CA-C	5.30	115.75	108.12
2	Q	34	ASP	N-CA-C	-5.30	105.58	111.36
1	K	233	SER	N-CA-C	5.30	117.31	108.99
2	X	175	ASP	CA-CB-CG	5.29	117.89	112.60
1	N	16	LEU	N-CA-C	5.29	118.20	109.85
1	F	321	ALA	CA-C-N	5.28	125.22	119.78
1	F	321	ALA	C-N-CA	5.28	125.22	119.78
1	E	253	GLU	CA-C-N	5.27	127.87	120.28
1	E	253	GLU	C-N-CA	5.27	127.87	120.28
1	D	242	LEU	CA-C-N	5.27	124.94	119.56
1	D	242	LEU	C-N-CA	5.27	124.94	119.56
1	I	242	LEU	CA-C-N	5.26	125.58	119.47
1	I	242	LEU	C-N-CA	5.26	125.58	119.47
2	X	276	HIS	CA-CB-CG	-5.25	108.55	113.80
1	F	233	SER	N-CA-C	5.25	117.99	109.06
1	B	9	VAL	N-CA-C	5.24	115.67	108.12
1	E	151	ILE	CB-CA-C	-5.24	103.80	110.98
2	X	92	ILE	CB-CA-C	-5.24	105.26	111.97
1	B	298	VAL	N-CA-C	5.24	115.40	107.80
1	N	77	THR	N-CA-C	-5.24	107.26	113.97
1	C	151	ILE	CA-C-N	-5.23	116.07	122.93
1	C	151	ILE	C-N-CA	-5.23	116.07	122.93
1	H	242	LEU	CA-C-N	5.23	125.54	119.47
1	H	242	LEU	C-N-CA	5.23	125.54	119.47
1	H	101	HIS	CA-C-N	5.23	125.16	119.78
1	H	101	HIS	C-N-CA	5.23	125.16	119.78
1	B	375	PHE	CA-CB-CG	5.23	119.03	113.80
1	O	331	ALA	CA-C-N	5.22	125.75	120.38
1	O	331	ALA	C-N-CA	5.22	125.75	120.38
1	N	101	HIS	CA-CB-CG	5.22	119.02	113.80
1	E	162	ASN	N-CA-C	5.22	118.44	111.24
2	Q	29	LYS	N-CA-C	-5.21	105.77	111.82
2	Q	276	HIS	N-CA-C	-5.21	105.51	111.14
1	D	233	SER	N-CA-C	5.21	117.17	108.99
1	M	332	PRO	CA-C-N	5.21	125.52	119.47
1	M	332	PRO	C-N-CA	5.21	125.52	119.47
1	H	161	HIS	CA-CB-CG	5.21	119.01	113.80
4	U	141	ARG	N-CA-C	5.21	120.55	113.16
1	F	203	THR	N-CA-C	5.20	117.35	111.11
1	E	51	ASP	CA-CB-CG	-5.20	107.40	112.60
1	J	148	THR	CA-C-O	5.18	124.52	118.77
1	J	75	ILE	N-CA-C	5.16	116.80	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	MET	N-CA-C	5.16	117.23	109.23
1	C	233	SER	N-CA-C	5.15	117.07	108.99
2	P	167	ARG	N-CA-C	-5.14	105.75	111.36
1	L	108	ALA	CA-C-N	5.14	125.43	119.47
1	L	108	ALA	C-N-CA	5.14	125.43	119.47
1	L	151	ILE	CA-C-N	-5.14	115.94	122.37
1	L	151	ILE	C-N-CA	-5.14	115.94	122.37
2	Q	229	SER	N-CA-C	-5.14	105.76	111.36
2	W	29	LYS	N-CA-C	-5.14	105.75	112.23
1	D	163	VAL	CA-C-N	5.14	125.54	119.99
1	D	163	VAL	C-N-CA	5.14	125.54	119.99
1	I	253	GLU	CA-C-N	5.13	127.67	120.28
1	I	253	GLU	C-N-CA	5.13	127.67	120.28
1	A	321	ALA	CA-C-N	5.13	125.11	120.03
1	A	321	ALA	C-N-CA	5.13	125.11	120.03
2	Q	159	ASP	CA-CB-CG	5.12	117.72	112.60
1	L	257	CYS	CA-C-N	5.11	125.40	119.47
1	L	257	CYS	C-N-CA	5.11	125.40	119.47
1	G	253	GLU	CA-C-N	5.11	127.64	120.28
1	G	253	GLU	C-N-CA	5.11	127.64	120.28
1	L	233	SER	N-CA-C	5.11	117.01	108.99
2	Q	253	ILE	N-CA-C	-5.11	105.56	110.72
1	L	321	ALA	CA-C-N	5.10	125.08	120.03
1	L	321	ALA	C-N-CA	5.10	125.08	120.03
1	G	111	ASN	CA-C-N	5.09	125.10	119.90
1	G	111	ASN	C-N-CA	5.09	125.10	119.90
2	Q	85	VAL	CB-CA-C	-5.09	105.45	111.97
1	D	51	ASP	CA-CB-CG	-5.09	107.51	112.60
1	G	157	ASP	N-CA-C	-5.09	106.24	112.90
1	O	54	VAL	N-CA-C	5.08	115.80	108.48
1	F	151	ILE	CB-CA-C	-5.08	104.02	110.98
3	T	102	LEU	N-CA-C	-5.08	105.93	111.82
1	J	51	ASP	CA-CB-CG	-5.07	107.53	112.60
1	L	51	ASP	CA-CB-CG	-5.07	107.53	112.60
1	H	77	THR	N-CA-C	-5.07	107.48	113.97
2	Q	92	ILE	N-CA-C	-5.06	105.61	110.72
1	G	298	VAL	N-CA-C	5.06	115.13	107.80
1	I	129	VAL	CA-C-N	5.06	124.67	119.56
1	I	129	VAL	C-N-CA	5.06	124.67	119.56
1	B	51	ASP	CA-CB-CG	-5.05	107.55	112.60
1	B	54	VAL	N-CA-C	5.05	115.18	108.11
1	O	109	PRO	N-CA-C	5.05	121.27	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	VAL	N-CA-C	5.04	116.50	111.00
1	E	132	MET	N-CA-C	5.04	117.05	109.23
2	X	153	HIS	N-CA-C	-5.04	105.68	111.07
1	L	163	VAL	CB-CA-C	-5.04	104.98	110.37
1	B	148	THR	CA-C-O	5.04	124.36	118.77
1	E	162	ASN	CA-C-N	-5.03	117.89	123.43
1	E	162	ASN	C-N-CA	-5.03	117.89	123.43
1	B	233	SER	N-CA-C	5.03	117.35	108.75
1	A	51	ASP	CA-CB-CG	-5.03	107.57	112.60
1	A	151	ILE	CA-C-N	-5.02	116.35	122.93
1	A	151	ILE	C-N-CA	-5.02	116.35	122.93
2	W	261	TYR	N-CA-C	-5.02	105.89	111.36
1	H	111	ASN	CA-C-N	5.01	126.11	119.84
1	H	111	ASN	C-N-CA	5.01	126.11	119.84
2	Q	240	GLU	N-CA-C	-5.01	105.52	111.69
1	K	151	ILE	CB-CA-C	-5.01	104.12	110.98
1	M	321	ALA	CA-C-N	5.01	124.94	119.78
1	M	321	ALA	C-N-CA	5.01	124.94	119.78
2	P	50	LEU	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2933	0	2894	69	0
1	B	2933	0	2894	78	0
1	C	2933	0	2894	56	0
1	D	2933	0	2894	70	0
1	E	2933	0	2894	80	0
1	F	2933	0	2894	62	0
1	G	2933	0	2894	42	0
1	H	2933	0	2894	92	0
1	I	2933	0	2894	52	0
1	J	2933	0	2894	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2933	0	2894	64	0
1	L	2933	0	2894	84	0
1	M	2933	0	2894	64	0
1	N	2933	0	2894	56	0
1	O	2933	0	2894	43	0
2	P	2207	0	2200	108	0
2	Q	2207	0	2200	215	0
2	R	231	0	245	24	0
2	S	231	0	245	58	0
2	W	2207	0	2200	65	0
2	X	2207	0	2200	150	0
2	Y	231	0	245	8	0
2	Z	231	0	245	0	0
3	T	1101	0	1120	543	0
3	a	1211	0	1226	221	0
4	U	1374	0	1436	522	0
4	b	1008	0	1064	196	0
5	V	1273	0	1201	400	0
5	c	1273	0	1201	231	0
All	All	60987	0	60438	2701	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 22.

All (2701) 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:T:229:LEU:HD13	4:U:93:LEU:CB	1.22	1.63
3:T:208:LYS:HD2	4:U:112:TYR:CE2	1.33	1.58
1:F:25:ASP:HB3	4:U:147:VAL:CG2	1.16	1.57
2:Q:276:HIS:HA	3:T:110:PHE:CE1	1.03	1.55
3:T:208:LYS:CD	4:U:112:TYR:HE2	1.24	1.50
1:D:146:GLY:CA	4:U:173:LEU:HD13	1.43	1.49
2:Q:276:HIS:CA	3:T:110:PHE:CE1	1.97	1.45
1:F:25:ASP:CB	4:U:147:VAL:CG2	1.94	1.44
2:Q:282:THR:CG2	2:R:1:MET:HE1	1.47	1.43
2:Q:269:ALA:HA	3:T:118:GLU:CD	1.41	1.41
4:U:48:GLN:NE2	5:V:3:ASP:CG	1.75	1.41
1:B:146:GLY:HA2	4:U:209:GLU:CG	1.51	1.40
3:T:256:GLN:NE2	4:U:68:ARG:HH12	1.14	1.39
2:Q:273:GLU:HA	3:T:114:LYS:CE	1.50	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:50:LYS:HD3	5:V:156:PHE:CE1	1.55	1.39
1:F:25:ASP:CB	4:U:147:VAL:HG21	1.51	1.38
1:H:163:VAL:HG22	1:H:175:ILE:CG1	1.50	1.37
2:P:284:ILE:HG23	2:S:8:MET:CG	1.53	1.37
3:T:208:LYS:CD	4:U:112:TYR:CE2	2.03	1.37
4:U:48:GLN:HE21	5:V:3:ASP:CG	1.29	1.36
2:Q:272:GLU:O	3:T:114:LYS:HD3	1.18	1.35
2:X:272:GLU:HB3	3:a:113:ARG:NE	1.40	1.34
3:T:229:LEU:CD1	4:U:93:LEU:HB2	1.55	1.34
2:Q:251:LYS:HA	3:T:139:ARG:NH2	1.43	1.34
3:T:241:TYR:CE1	4:U:76:LEU:O	1.81	1.33
2:Q:282:THR:HG22	2:R:1:MET:CE	1.56	1.33
2:Q:253:ILE:CG2	3:T:135:ALA:HB2	1.59	1.32
3:T:261:ILE:CD1	4:U:125:ILE:HG22	1.60	1.31
3:T:261:ILE:HD11	4:U:125:ILE:CG2	1.60	1.31
3:T:226:GLU:HA	4:U:93:LEU:CD1	1.58	1.31
2:X:247:THR:CG2	3:a:142:ASN:HD21	1.43	1.30
3:T:215:ARG:NH1	4:U:112:TYR:HB2	1.46	1.30
4:U:50:LYS:CD	5:V:156:PHE:CE1	2.13	1.30
4:U:204:ARG:NH1	2:W:76:LYS:NZ	1.77	1.30
2:P:281:MET:O	2:S:4:ILE:CG2	1.80	1.29
2:X:265:LEU:CD1	3:a:121:VAL:HG12	1.62	1.28
2:Q:272:GLU:C	3:T:114:LYS:HD3	1.57	1.28
2:Q:269:ALA:HA	3:T:118:GLU:OE1	1.31	1.27
2:Q:264:LYS:CE	3:T:128:GLU:OE2	1.83	1.25
2:X:247:THR:HG21	3:a:142:ASN:ND2	1.52	1.24
1:A:133:TYR:CD2	1:A:352:PHE:HZ	1.55	1.24
1:B:146:GLY:CA	4:U:209:GLU:CG	2.16	1.24
1:J:306:TYR:O	1:J:309:ILE:HG22	1.31	1.23
3:T:257:GLN:OE1	4:U:125:ILE:CG2	1.87	1.23
2:X:272:GLU:HG3	3:a:117:GLU:OE2	1.39	1.23
1:D:146:GLY:HA3	4:U:173:LEU:CD1	1.66	1.23
1:H:133:TYR:CD2	1:H:352:PHE:HZ	1.54	1.23
1:B:252:ASN:HA	1:B:255:PHE:CZ	1.73	1.22
1:D:146:GLY:C	4:U:173:LEU:HD22	1.63	1.22
1:F:252:ASN:HB2	1:F:255:PHE:CZ	1.71	1.22
1:D:252:ASN:HA	1:D:255:PHE:CE2	1.73	1.22
4:U:50:LYS:HD3	5:V:156:PHE:CD1	1.75	1.21
1:E:313:MET:SD	1:E:329:ILE:HD13	1.79	1.21
2:Q:251:LYS:CA	3:T:139:ARG:HH21	1.53	1.21
2:Q:269:ALA:HA	3:T:118:GLU:OE2	1.40	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:265:LEU:CD1	3:a:121:VAL:CG1	2.18	1.21
1:L:305:MET:CE	1:L:335:ARG:HB2	1.69	1.21
1:B:332:PRO:O	1:B:335:ARG:HG3	1.36	1.20
3:T:251:GLN:CG	4:U:114:ILE:HD11	1.72	1.20
1:E:313:MET:SD	1:E:329:ILE:CD1	2.30	1.19
1:L:326:LYS:HD2	2:Y:20:ASP:CG	1.67	1.19
2:Q:273:GLU:CA	3:T:114:LYS:HE2	1.71	1.19
3:T:208:LYS:CG	4:U:112:TYR:CE2	2.23	1.19
2:X:279:ASN:HB2	3:a:109:HIS:CE1	1.74	1.19
1:B:146:GLY:CA	4:U:209:GLU:HG2	1.72	1.19
2:W:88:LEU:HD11	2:X:85:VAL:HG13	1.21	1.19
1:I:305:MET:CE	1:I:335:ARG:HG3	1.72	1.19
1:H:163:VAL:HG22	1:H:175:ILE:CD1	1.73	1.18
2:P:284:ILE:CG2	2:S:8:MET:HG2	1.73	1.18
2:Q:273:GLU:CA	3:T:114:LYS:CE	2.21	1.18
1:A:332:PRO:O	1:A:335:ARG:HG3	1.38	1.18
1:J:252:ASN:HA	1:J:255:PHE:CE2	1.78	1.18
2:P:281:MET:O	2:S:4:ILE:HG22	1.38	1.18
3:T:229:LEU:CD1	4:U:93:LEU:CB	2.18	1.18
2:Q:276:HIS:HA	3:T:110:PHE:CD1	1.78	1.17
1:B:252:ASN:HA	1:B:255:PHE:CE2	1.78	1.17
1:H:133:TYR:CZ	1:H:352:PHE:CE1	2.31	1.17
2:Q:261:TYR:HE1	3:T:126:ARG:NH2	1.42	1.17
1:A:133:TYR:CE2	1:A:352:PHE:CZ	2.32	1.17
3:T:256:GLN:NE2	4:U:68:ARG:NH1	1.91	1.17
2:P:278:LEU:HD11	2:S:1:MET:SD	1.84	1.16
1:D:146:GLY:O	4:U:173:LEU:HD22	1.42	1.16
1:G:252:ASN:HA	1:G:255:PHE:CE2	1.80	1.16
3:T:237:TRP:NE1	4:U:81:GLN:O	1.76	1.16
2:Q:261:TYR:CE1	3:T:126:ARG:NH2	2.14	1.16
2:Q:276:HIS:CD2	3:T:110:PHE:HZ	1.62	1.16
1:H:133:TYR:CZ	1:H:352:PHE:HE1	1.63	1.16
1:K:252:ASN:HA	1:K:255:PHE:CE2	1.80	1.16
3:T:118:GLU:O	3:T:121:VAL:HG12	1.43	1.16
2:Q:268:LYS:CB	3:T:121:VAL:HB	1.75	1.15
1:A:133:TYR:CD2	1:A:352:PHE:CZ	2.34	1.15
3:T:257:GLN:OE1	4:U:125:ILE:HG21	1.00	1.15
1:A:148:THR:HB	1:C:47:MET:HE1	1.20	1.15
2:Q:268:LYS:HB2	3:T:121:VAL:CB	1.77	1.13
3:T:229:LEU:HD13	4:U:93:LEU:HB3	1.24	1.13
1:N:252:ASN:HA	1:N:255:PHE:CE2	1.82	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:100:LEU:HD23	4:U:103:ARG:HE	1.04	1.13
2:Q:276:HIS:CD2	3:T:110:PHE:CZ	2.36	1.13
4:U:56:ILE:CG2	5:V:124:THR:HG22	1.78	1.13
3:T:251:GLN:HG3	4:U:114:ILE:HD11	1.20	1.12
2:X:254:ASP:OD2	3:a:135:ALA:HB2	1.47	1.12
1:H:133:TYR:CE2	1:H:352:PHE:CZ	2.37	1.12
2:X:257:GLU:HB3	3:a:131:ARG:NH1	1.65	1.12
2:X:265:LEU:HD11	3:a:121:VAL:HG11	1.32	1.12
1:D:332:PRO:O	1:D:335:ARG:HG2	1.46	1.11
1:L:257:CYS:HB3	1:L:258:PRO:HD3	1.14	1.11
2:Q:276:HIS:CA	3:T:110:PHE:HE1	1.43	1.11
2:W:84:ASP:OD1	2:W:88:LEU:HG	1.50	1.11
2:X:272:GLU:CB	3:a:113:ARG:HE	1.62	1.11
1:B:146:GLY:HA3	4:U:209:GLU:HB3	1.23	1.11
1:C:252:ASN:HA	1:C:255:PHE:CE2	1.84	1.11
1:M:252:ASN:HA	1:M:255:PHE:CE2	1.86	1.11
2:X:265:LEU:HD13	3:a:121:VAL:CG1	1.75	1.11
1:N:305:MET:SD	1:N:335:ARG:NE	2.24	1.11
1:L:305:MET:HE2	1:L:335:ARG:HB2	1.30	1.10
2:Q:276:HIS:HB2	3:T:114:LYS:HG2	1.13	1.10
1:L:332:PRO:O	1:L:335:ARG:HG2	1.50	1.10
3:T:215:ARG:HH12	4:U:112:TYR:CA	1.64	1.10
2:X:161:LYS:O	2:X:165:VAL:HG12	1.50	1.10
3:T:233:ALA:HB1	4:U:100:LEU:CD1	1.82	1.10
3:T:256:GLN:CD	4:U:68:ARG:HH12	1.59	1.10
1:L:342:GLY:O	1:L:345:ILE:HG22	1.52	1.10
2:X:247:THR:HG21	3:a:142:ASN:HD21	0.94	1.09
1:C:332:PRO:O	1:C:335:ARG:HG3	1.52	1.09
2:Q:272:GLU:CD	3:T:117:GLU:CB	2.25	1.09
1:B:133:TYR:CD2	1:B:352:PHE:HZ	1.70	1.09
1:H:163:VAL:CG2	1:H:175:ILE:HD13	1.81	1.09
3:T:226:GLU:HA	4:U:93:LEU:HD13	1.12	1.09
1:F:252:ASN:HA	1:F:255:PHE:CE2	1.88	1.09
2:Q:272:GLU:CD	3:T:117:GLU:HB3	1.75	1.09
2:Q:257:GLU:OE2	3:T:131:ARG:HB3	1.48	1.09
2:Q:275:ASP:O	3:T:110:PHE:CD1	2.04	1.08
1:H:95:ARG:NH1	3:T:265:ARG:HB2	1.67	1.08
3:T:241:TYR:CD1	4:U:76:LEU:O	2.06	1.08
2:X:273:GLU:HG3	3:a:113:ARG:HH22	1.15	1.08
1:F:305:MET:HE3	1:F:336:LYS:CD	1.83	1.08
3:T:208:LYS:HG3	4:U:112:TYR:CE2	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:54:LEU:HD12	5:V:157:MET:HG2	1.31	1.08
3:T:250:LEU:HD11	4:U:115:GLU:HG3	1.13	1.07
3:T:250:LEU:HD22	4:U:118:VAL:HG11	1.33	1.07
1:B:146:GLY:HA3	4:U:209:GLU:CB	1.84	1.07
1:H:133:TYR:CD2	1:H:352:PHE:CZ	2.42	1.07
3:T:250:LEU:CD1	4:U:115:GLU:HG3	1.83	1.07
1:H:163:VAL:HG22	1:H:175:ILE:HG12	1.08	1.07
1:L:333:PRO:HG2	2:Y:6:LYS:HZ1	1.19	1.07
1:A:148:THR:CB	1:C:47:MET:HE1	1.84	1.07
2:Q:264:LYS:HE3	3:T:128:GLU:OE2	1.54	1.07
2:W:91:ARG:HH21	2:X:92:ILE:HG13	1.07	1.07
2:X:247:THR:CB	3:a:142:ASN:HD21	1.68	1.07
1:C:192:ILE:CD1	1:C:256:ARG:HD3	1.83	1.06
4:U:204:ARG:NH1	2:W:76:LYS:HZ3	1.40	1.06
3:T:226:GLU:CG	4:U:93:LEU:HD11	1.86	1.05
2:Q:273:GLU:N	3:T:114:LYS:HE2	1.70	1.05
1:N:109:PRO:HD2	1:N:161:HIS:NE2	1.70	1.05
2:P:281:MET:HG3	2:R:1:MET:HB3	1.38	1.05
4:U:48:GLN:OE1	5:V:6:LYS:NZ	1.90	1.05
2:Q:269:ALA:CA	3:T:118:GLU:OE2	2.04	1.05
2:Q:272:GLU:C	3:T:114:LYS:CD	2.29	1.05
3:T:208:LYS:NZ	4:U:112:TYR:HD2	1.53	1.05
3:T:240:ILE:HB	4:U:80:CYS:SG	1.97	1.05
4:U:204:ARG:HH11	2:W:76:LYS:NZ	1.40	1.05
1:C:192:ILE:HD12	1:C:256:ARG:CD	1.87	1.04
1:H:95:ARG:HH11	3:T:265:ARG:HD3	1.21	1.04
2:Q:253:ILE:CG2	3:T:135:ALA:CB	2.34	1.04
3:T:215:ARG:NH1	4:U:112:TYR:CB	2.19	1.04
1:A:143:TYR:CZ	1:C:44:MET:HE2	1.91	1.04
1:N:252:ASN:HB2	1:N:255:PHE:CZ	1.93	1.04
1:A:143:TYR:CE2	1:C:44:MET:HE2	1.94	1.03
1:F:305:MET:HE3	1:F:336:LYS:HD2	1.34	1.03
3:T:212:LEU:HD13	4:U:109:GLU:HG3	1.04	1.03
1:H:163:VAL:HG21	1:H:175:ILE:HD13	1.39	1.03
2:P:281:MET:HG3	2:R:1:MET:CB	1.88	1.03
2:Q:264:LYS:C	3:T:121:VAL:HG23	1.82	1.03
3:T:216:ARG:HD3	4:U:105:ASP:OD1	1.59	1.03
3:T:261:ILE:HG13	4:U:124:GLU:OE2	1.59	1.03
3:T:234:LYS:HD3	4:U:85:LEU:HD21	1.06	1.03
1:D:146:GLY:HA2	4:U:173:LEU:HD13	1.41	1.02
2:Q:257:GLU:CB	3:T:132:ALA:HB2	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:282:THR:CG2	2:R:1:MET:CE	2.25	1.02
4:U:100:LEU:HD23	4:U:103:ARG:NE	1.74	1.02
2:X:276:HIS:HE1	3:a:110:PHE:HB2	1.24	1.02
1:H:163:VAL:CG2	1:H:175:ILE:CD1	2.35	1.02
1:I:305:MET:SD	1:I:335:ARG:NE	2.32	1.02
1:E:289:ILE:HD11	1:G:63:GLY:O	1.58	1.02
2:X:273:GLU:HG3	3:a:113:ARG:NH2	1.73	1.02
1:J:252:ASN:HB2	1:J:255:PHE:CZ	1.95	1.01
2:Q:273:GLU:HA	3:T:114:LYS:HE3	1.02	1.01
1:H:252:ASN:HA	1:H:255:PHE:CE2	1.94	1.01
2:P:282:THR:O	2:S:3:ALA:C	2.04	1.01
4:U:56:ILE:HG21	5:V:124:THR:CG2	1.89	1.01
1:A:133:TYR:CG	1:A:352:PHE:HZ	1.78	1.01
2:P:142:GLU:HG2	2:P:145:GLU:OE2	1.61	1.00
4:U:147:VAL:HG22	4:U:148:ARG:H	1.23	1.00
1:A:148:THR:HB	1:C:47:MET:CE	1.91	1.00
1:I:305:MET:HE2	1:I:335:ARG:CG	1.91	1.00
2:Q:253:ILE:HG23	3:T:135:ALA:CB	1.91	1.00
2:W:91:ARG:NH2	2:X:92:ILE:HG13	1.75	1.00
2:W:91:ARG:HE	2:X:92:ILE:CD1	1.74	1.00
2:X:265:LEU:HD11	3:a:121:VAL:CG1	1.87	1.00
1:F:25:ASP:CB	4:U:147:VAL:HG23	1.90	1.00
1:L:333:PRO:HG2	2:Y:6:LYS:NZ	1.75	1.00
2:Q:250:GLU:OE1	3:T:139:ARG:HA	1.59	1.00
2:Q:257:GLU:HB2	3:T:132:ALA:HB2	1.42	1.00
1:K:305:MET:HG3	1:K:335:ARG:HD2	1.44	1.00
1:L:257:CYS:HB3	1:L:258:PRO:CD	1.91	0.99
4:U:50:LYS:HG2	5:V:156:PHE:CZ	1.97	0.99
3:T:226:GLU:HG3	4:U:93:LEU:HD11	1.00	0.99
2:X:268:LYS:O	2:X:272:GLU:HG2	1.62	0.99
1:E:305:MET:HE3	1:E:336:LYS:HD2	1.44	0.99
3:T:236:LEU:HD11	4:U:104:VAL:HG11	1.40	0.99
1:D:146:GLY:CA	4:U:173:LEU:CD1	2.29	0.99
2:S:1:MET:HB3	2:S:4:ILE:HG12	1.42	0.99
1:I:305:MET:HE2	1:I:335:ARG:HG3	1.00	0.99
3:T:271:ASN:HB3	4:U:135:LEU:HD22	1.41	0.99
3:T:233:ALA:HB1	4:U:100:LEU:HD12	1.38	0.98
2:Q:264:LYS:HE2	3:T:128:GLU:OE2	1.63	0.98
4:U:56:ILE:HG21	5:V:124:THR:HG22	1.43	0.98
1:H:163:VAL:HG23	1:H:175:ILE:CG2	1.93	0.98
1:D:305:MET:SD	1:D:335:ARG:HB2	2.02	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:133:TYR:CE1	1:K:352:PHE:HZ	1.81	0.98
1:C:192:ILE:HD12	1:C:256:ARG:HD3	0.98	0.97
2:Q:253:ILE:HG23	3:T:135:ALA:HB2	1.00	0.97
3:T:226:GLU:HG3	4:U:93:LEU:CD1	1.94	0.97
1:K:305:MET:CG	1:K:335:ARG:HD2	1.93	0.97
1:F:25:ASP:HB2	4:U:147:VAL:HB	1.46	0.97
1:I:305:MET:CE	1:I:335:ARG:CG	2.43	0.97
1:L:305:MET:HE1	1:L:335:ARG:HB2	1.47	0.97
5:c:53:THR:H	5:c:56:GLU:HB2	1.26	0.97
5:V:104:PHE:HA	5:V:120:MET:HG3	1.47	0.97
3:T:208:LYS:HZ2	4:U:112:TYR:HD2	0.97	0.97
3:T:226:GLU:CA	4:U:93:LEU:CD1	2.43	0.97
1:L:216:LEU:HG	1:L:238:LYS:HD3	1.46	0.96
5:V:28:VAL:HG23	5:V:32:GLU:H	1.30	0.96
1:E:313:MET:SD	1:E:329:ILE:HD11	2.05	0.96
1:H:163:VAL:CG2	1:H:175:ILE:CG1	2.42	0.96
2:P:284:ILE:HG23	2:S:8:MET:HG2	1.00	0.96
2:Q:269:ALA:CA	3:T:118:GLU:OE1	2.13	0.96
2:Q:269:ALA:CA	3:T:118:GLU:CD	2.37	0.96
4:U:50:LYS:CG	5:V:156:PHE:CE1	2.47	0.96
1:K:252:ASN:HB2	1:K:255:PHE:CZ	2.00	0.96
1:N:305:MET:HE1	1:N:335:ARG:HH21	1.29	0.96
4:U:204:ARG:NH1	2:W:76:LYS:HZ2	1.51	0.96
1:A:252:ASN:HA	1:A:255:PHE:CE2	2.00	0.96
2:X:276:HIS:CE1	3:a:110:PHE:HB2	2.00	0.96
3:T:229:LEU:HD12	4:U:93:LEU:HD12	1.44	0.96
2:W:256:LEU:CD1	2:X:260:LEU:HD13	1.95	0.96
1:B:133:TYR:CD2	1:B:352:PHE:CZ	2.54	0.95
1:C:253:GLU:HA	1:C:256:ARG:HG2	1.48	0.95
4:U:54:LEU:HD11	5:V:97:LEU:HG	1.47	0.95
2:X:272:GLU:CG	3:a:117:GLU:OE2	2.14	0.95
4:U:83:LEU:HD12	4:U:100:LEU:HD21	1.45	0.95
1:C:253:GLU:HA	1:C:256:ARG:CG	1.96	0.95
1:E:109:PRO:HD2	1:E:161:HIS:NE2	1.81	0.95
1:M:300:SER:HA	1:M:336:LYS:HA	1.46	0.95
1:H:163:VAL:HG23	1:H:175:ILE:HG23	1.48	0.95
3:T:237:TRP:O	4:U:80:CYS:SG	2.25	0.95
1:H:133:TYR:CG	1:H:352:PHE:HZ	1.84	0.95
1:L:252:ASN:HA	1:L:255:PHE:CE2	2.01	0.95
4:U:54:LEU:CD1	5:V:157:MET:HG2	1.96	0.95
2:X:257:GLU:CB	3:a:131:ARG:NH1	2.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:247:THR:HG21	3:a:142:ASN:CG	1.92	0.94
1:A:252:ASN:HA	1:A:255:PHE:CZ	2.03	0.94
5:V:94:GLU:O	5:V:97:LEU:HB2	1.66	0.94
1:E:106:THR:HG22	1:E:135:ALA:HB3	1.50	0.94
1:A:133:TYR:CZ	1:A:352:PHE:CE1	2.55	0.94
4:U:53:LEU:HD13	5:V:121:LEU:HG	1.49	0.94
3:T:237:TRP:HA	3:T:240:ILE:HD12	1.50	0.94
3:T:254:PHE:HE1	4:U:121:ASN:HB2	1.31	0.94
1:N:305:MET:CE	1:N:335:ARG:HH21	1.81	0.93
1:H:163:VAL:CG2	1:H:175:ILE:HG12	1.98	0.93
1:H:326:LYS:HE2	2:X:215:SER:HB3	1.47	0.93
2:P:283:SER:HA	2:S:7:LYS:HD2	1.48	0.93
2:P:284:ILE:CG2	2:S:8:MET:CG	2.38	0.93
3:T:201:ARG:O	3:T:205:ARG:N	2.01	0.93
1:B:146:GLY:CA	4:U:209:GLU:CB	2.42	0.93
2:P:282:THR:O	2:S:3:ALA:CB	2.16	0.93
1:B:305:MET:CE	1:B:335:ARG:HB2	1.98	0.93
2:Q:250:GLU:OE2	3:T:142:ASN:ND2	2.02	0.93
1:O:252:ASN:HA	1:O:255:PHE:CE2	2.04	0.92
1:C:133:TYR:CD2	1:C:352:PHE:HZ	1.86	0.92
1:K:352:PHE:CD1	1:K:355:MET:HG3	2.05	0.92
3:T:212:LEU:CD1	4:U:109:GLU:HG3	1.99	0.92
1:H:133:TYR:CE2	1:H:352:PHE:HZ	1.82	0.92
2:Q:257:GLU:CD	3:T:131:ARG:CB	2.42	0.92
3:T:212:LEU:HD22	4:U:109:GLU:HA	1.49	0.92
3:T:271:ASN:HB3	4:U:135:LEU:CD2	1.99	0.92
4:U:50:LYS:HG2	5:V:156:PHE:CE1	2.05	0.92
3:T:230:ARG:HH21	4:U:88:LEU:H	1.17	0.92
4:U:41:ILE:HG13	5:V:135:GLU:HA	1.52	0.92
2:Q:269:ALA:CB	3:T:118:GLU:OE2	2.17	0.92
1:F:326:LYS:HE3	2:W:177:GLU:OE2	1.70	0.91
1:N:109:PRO:HD2	1:N:161:HIS:CD2	2.04	0.91
3:T:212:LEU:HA	3:T:215:ARG:HB2	1.48	0.91
2:P:281:MET:O	2:S:4:ILE:HG23	1.67	0.91
1:D:146:GLY:HA3	4:U:173:LEU:HD13	0.93	0.91
3:T:251:GLN:HG3	4:U:114:ILE:CD1	1.99	0.91
1:N:109:PRO:CD	1:N:161:HIS:NE2	2.34	0.91
1:H:95:ARG:HH22	3:T:269:ASN:ND2	1.68	0.90
1:F:25:ASP:CB	4:U:147:VAL:CB	2.49	0.90
1:B:207:GLU:HA	1:B:210:ARG:HG2	1.50	0.90
1:B:133:TYR:CE2	1:B:352:PHE:CE1	2.60	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:208:LYS:HD2	4:U:112:TYR:CD2	2.05	0.90
1:D:146:GLY:HA2	4:U:173:LEU:HB2	1.53	0.90
1:F:25:ASP:HB3	4:U:147:VAL:HG23	1.44	0.90
2:Q:276:HIS:HD2	3:T:110:PHE:CZ	1.88	0.90
3:T:250:LEU:HD11	4:U:115:GLU:CG	2.02	0.90
5:c:79:VAL:O	5:c:83:ARG:HB2	1.71	0.90
1:F:252:ASN:CB	1:F:255:PHE:CZ	2.55	0.90
2:X:272:GLU:CB	3:a:113:ARG:NE	2.28	0.90
2:Q:264:LYS:O	3:T:121:VAL:CG2	2.19	0.90
3:T:244:GLU:OE1	4:U:79:ARG:HB3	1.72	0.90
3:T:230:ARG:HH21	4:U:88:LEU:N	1.70	0.89
1:B:133:TYR:CZ	1:B:352:PHE:HE1	1.90	0.89
3:T:215:ARG:HH12	4:U:112:TYR:N	1.70	0.89
1:C:133:TYR:CZ	1:C:352:PHE:HE1	1.90	0.89
1:G:24:ASP:OD1	4:b:146:ARG:HG3	1.73	0.89
1:L:326:LYS:HD2	2:Y:20:ASP:OD2	1.71	0.89
1:A:133:TYR:CE2	1:A:352:PHE:HZ	1.79	0.89
1:N:305:MET:CE	1:N:335:ARG:NH2	2.36	0.89
4:U:83:LEU:CD1	4:U:100:LEU:HD21	2.01	0.89
3:a:237:TRP:HA	3:a:240:ILE:HD12	1.53	0.89
1:B:252:ASN:CA	1:B:255:PHE:CZ	2.56	0.89
1:F:109:PRO:HG2	1:F:161:HIS:NE2	1.88	0.88
2:P:142:GLU:HA	2:P:145:GLU:HG2	1.50	0.88
1:A:133:TYR:CZ	1:A:352:PHE:CZ	2.61	0.88
1:E:283:MET:HA	1:E:290:ARG:HD3	1.54	0.88
2:Q:275:ASP:O	3:T:110:PHE:HD1	1.51	0.88
2:Q:282:THR:HG21	2:R:1:MET:SD	2.13	0.88
3:T:257:GLN:CD	4:U:125:ILE:HG21	1.98	0.88
2:Q:161:LYS:O	2:Q:165:VAL:HG22	1.72	0.88
2:Q:264:LYS:O	3:T:121:VAL:HG23	1.72	0.88
2:X:265:LEU:HD13	3:a:121:VAL:HG12	0.90	0.88
3:a:215:ARG:NE	4:b:108:ASP:OD1	2.06	0.88
2:Q:251:LYS:HD2	3:T:139:ARG:HH22	1.38	0.88
3:T:250:LEU:HD22	4:U:118:VAL:CG1	2.03	0.88
1:I:257:CYS:HB2	1:I:258:PRO:HD3	1.54	0.88
4:U:147:VAL:HG22	4:U:148:ARG:N	1.89	0.88
3:T:216:ARG:HB3	4:U:105:ASP:CG	1.97	0.88
2:P:278:LEU:HD11	2:S:1:MET:CG	2.03	0.88
2:X:257:GLU:HB3	3:a:131:ARG:HH12	1.35	0.88
1:H:95:ARG:NH1	3:T:265:ARG:HD3	1.89	0.88
2:P:284:ILE:HG23	2:S:8:MET:HG3	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:215:ARG:NH1	4:U:112:TYR:CA	2.37	0.88
2:X:236:GLU:OE2	3:a:149:GLN:CD	2.17	0.88
1:A:148:THR:CG2	1:C:47:MET:HE1	2.02	0.88
3:T:212:LEU:HD13	4:U:109:GLU:CG	1.99	0.88
3:T:216:ARG:CD	4:U:105:ASP:OD1	2.22	0.88
3:T:251:GLN:CG	4:U:114:ILE:CD1	2.52	0.88
1:D:146:GLY:O	4:U:173:LEU:CD2	2.21	0.87
2:Q:257:GLU:CD	3:T:131:ARG:HB3	1.99	0.87
3:T:243:LEU:HB3	4:U:111:ARG:HD3	1.55	0.87
3:T:254:PHE:CE1	4:U:121:ASN:HB2	2.10	0.87
1:B:109:PRO:HD2	1:B:161:HIS:CD2	2.09	0.87
1:O:1:ASP:HA	1:O:96:VAL:HG22	1.56	0.87
5:c:53:THR:O	5:c:57:LEU:N	2.07	0.87
4:U:114:ILE:HA	4:U:117:LYS:HD3	1.55	0.87
5:V:28:VAL:HA	5:V:32:GLU:HB2	1.56	0.87
1:F:25:ASP:HB2	4:U:147:VAL:CB	2.05	0.87
1:L:133:TYR:CZ	1:L:352:PHE:HE1	1.92	0.87
1:N:305:MET:HE1	1:N:335:ARG:NH2	1.89	0.87
1:H:95:ARG:HH12	3:T:265:ARG:HB2	1.35	0.87
1:L:207:GLU:HA	1:L:210:ARG:HG2	1.56	0.87
1:L:342:GLY:O	1:L:345:ILE:CG2	2.22	0.87
2:Q:264:LYS:C	3:T:121:VAL:CG2	2.47	0.87
5:c:102:ARG:NH1	5:c:102:ARG:O	2.07	0.87
4:U:204:ARG:HH12	2:W:76:LYS:NZ	1.67	0.87
1:I:257:CYS:CB	1:I:258:PRO:HD3	2.04	0.87
4:U:54:LEU:HD11	5:V:97:LEU:CG	2.04	0.87
1:C:133:TYR:CE2	1:C:352:PHE:CE1	2.62	0.86
1:F:252:ASN:CA	1:F:255:PHE:CE2	2.57	0.86
1:H:95:ARG:NH2	3:T:269:ASN:HD21	1.71	0.86
3:T:243:LEU:HD22	4:U:111:ARG:CD	2.05	0.86
2:Q:272:GLU:HG3	3:T:117:GLU:C	1.99	0.86
2:X:279:ASN:HB2	3:a:109:HIS:HE1	1.33	0.86
2:Q:257:GLU:CD	3:T:131:ARG:HB2	2.01	0.86
1:K:252:ASN:CB	1:K:255:PHE:CZ	2.58	0.86
1:M:252:ASN:HA	1:M:255:PHE:CZ	2.11	0.86
1:N:305:MET:HE1	1:N:335:ARG:HE	1.39	0.86
3:T:249:ASP:OD2	4:U:72:LYS:HD2	1.73	0.86
2:Q:281:MET:O	2:S:4:ILE:HD11	1.74	0.86
2:X:273:GLU:CG	3:a:113:ARG:HH22	1.89	0.86
1:B:230:ALA:HB3	1:B:255:PHE:HZ	1.40	0.86
3:T:215:ARG:HG2	4:U:111:ARG:HH21	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:PHE:CZ	1:B:312:ARG:HG2	2.11	0.86
1:I:109:PRO:HD2	1:I:161:HIS:CD2	2.11	0.86
2:Q:250:GLU:HG2	3:T:138:GLN:HB2	1.56	0.86
1:C:133:TYR:CD2	1:C:352:PHE:CZ	2.64	0.85
1:F:25:ASP:HB2	4:U:147:VAL:CG2	2.05	0.85
2:P:282:THR:C	2:S:3:ALA:HB1	2.00	0.85
2:X:257:GLU:CD	3:a:131:ARG:NH1	2.33	0.85
1:M:230:ALA:HB3	1:M:255:PHE:HZ	1.39	0.85
1:L:196:ARG:HD2	1:L:253:GLU:CD	2.01	0.85
3:T:229:LEU:HD13	4:U:93:LEU:HB2	0.86	0.85
1:E:133:TYR:CE1	1:E:355:MET:HB3	2.10	0.85
3:T:221:ILE:CG2	4:U:98:ARG:HG2	2.07	0.85
5:V:46:ARG:HA	5:V:51:ASN:HB3	1.59	0.85
5:V:53:THR:H	5:V:56:GLU:HB2	1.42	0.85
2:Q:276:HIS:HB2	3:T:114:LYS:CG	2.03	0.85
5:V:43:LYS:HA	5:V:46:ARG:HD2	1.59	0.85
3:T:215:ARG:HG2	4:U:111:ARG:NH2	1.91	0.85
3:T:237:TRP:HE1	4:U:81:GLN:C	1.84	0.85
4:U:50:LYS:CD	5:V:156:PHE:CD1	2.51	0.85
2:X:236:GLU:OE2	3:a:149:GLN:NE2	2.10	0.84
3:a:224:LEU:HG	3:a:228:GLN:HG3	1.59	0.84
1:L:143:TYR:HB3	1:L:345:ILE:HG21	1.57	0.84
2:Q:272:GLU:CD	3:T:117:GLU:HB2	2.01	0.84
5:V:138:LYS:HZ3	5:V:144:ASN:HB3	1.41	0.84
2:X:279:ASN:HB2	3:a:109:HIS:ND1	1.91	0.84
1:L:333:PRO:CG	2:Y:6:LYS:HZ1	1.90	0.84
2:Q:260:LEU:HG	3:T:128:GLU:CD	2.02	0.84
1:F:252:ASN:HB2	1:F:255:PHE:HZ	1.37	0.84
5:V:38:THR:HG23	5:V:71:THR:H	1.40	0.84
3:T:215:ARG:HB3	4:U:108:ASP:CG	2.01	0.84
1:H:163:VAL:CG2	1:H:175:ILE:CG2	2.56	0.84
1:I:109:PRO:HD2	1:I:161:HIS:NE2	1.92	0.84
1:B:146:GLY:CA	4:U:209:GLU:CD	2.50	0.84
1:E:289:ILE:HD11	1:G:63:GLY:C	2.02	0.84
3:T:249:ASP:OD2	4:U:72:LYS:CD	2.26	0.84
1:H:133:TYR:CZ	1:H:352:PHE:CZ	2.62	0.84
4:U:45:ARG:HH22	5:V:127:THR:HB	1.42	0.84
5:V:147:ARG:NH1	5:V:147:ARG:O	2.09	0.84
3:a:213:ALA:HA	3:a:216:ARG:HB2	1.59	0.83
2:P:282:THR:C	2:S:3:ALA:CB	2.51	0.83
3:T:250:LEU:CD2	4:U:118:VAL:HG11	2.06	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:240:ILE:HG12	4:U:104:VAL:HA	1.61	0.83
2:W:256:LEU:HD11	2:X:260:LEU:HD13	1.59	0.83
4:b:58:LYS:HG3	5:c:100:LEU:HD21	1.60	0.83
2:P:278:LEU:HD11	2:S:1:MET:HG2	1.61	0.83
1:H:95:ARG:HH22	3:T:269:ASN:HD21	0.85	0.83
3:T:229:LEU:HD12	4:U:93:LEU:CD1	2.09	0.83
5:V:113:ASP:N	5:V:116:GLU:OE1	2.11	0.83
1:D:252:ASN:HA	1:D:255:PHE:CZ	2.13	0.83
1:D:252:ASN:HB2	1:D:255:PHE:CZ	2.13	0.83
3:T:251:GLN:HG2	4:U:114:ILE:HD11	1.57	0.83
1:I:252:ASN:HA	1:I:255:PHE:CE2	2.14	0.83
1:N:109:PRO:HD2	1:N:161:HIS:CE1	2.12	0.83
3:T:215:ARG:O	4:U:108:ASP:OD2	1.96	0.83
1:L:332:PRO:O	1:L:335:ARG:CG	2.27	0.82
4:U:147:VAL:HG13	4:U:148:ARG:HD3	1.60	0.82
2:Q:272:GLU:O	3:T:114:LYS:CD	2.15	0.82
2:W:72:GLU:O	2:W:76:LYS:HG3	1.77	0.82
1:E:109:PRO:HG2	1:E:161:HIS:NE2	1.93	0.82
1:G:252:ASN:HB2	1:G:255:PHE:CZ	2.14	0.82
4:U:45:ARG:NH2	5:V:127:THR:HB	1.94	0.82
1:N:252:ASN:CB	1:N:255:PHE:CZ	2.62	0.82
2:Q:250:GLU:HB3	3:T:139:ARG:HG3	1.59	0.82
2:Q:282:THR:HG22	2:R:1:MET:HE1	0.86	0.82
4:b:69:ARG:NH1	4:b:69:ARG:O	2.13	0.82
2:X:247:THR:CG2	3:a:142:ASN:ND2	2.25	0.82
1:C:133:TYR:CE2	1:C:352:PHE:HE1	1.95	0.82
1:K:133:TYR:CZ	1:K:352:PHE:HZ	1.97	0.82
3:T:236:LEU:CD1	4:U:104:VAL:HG11	2.09	0.82
1:H:95:ARG:NH1	3:T:265:ARG:CB	2.43	0.81
2:X:247:THR:CB	3:a:142:ASN:ND2	2.43	0.81
2:P:142:GLU:HA	2:P:145:GLU:CG	2.09	0.81
3:T:244:GLU:CD	4:U:79:ARG:HB3	2.05	0.81
1:C:253:GLU:HA	1:C:256:ARG:CD	2.10	0.81
1:F:305:MET:HE3	1:F:336:LYS:HD3	1.62	0.81
3:T:212:LEU:HD21	4:U:112:TYR:CB	2.11	0.81
3:T:222:ASP:HA	4:U:94:GLN:CD	2.06	0.81
2:X:257:GLU:OE1	3:a:131:ARG:NH1	2.13	0.81
4:b:46:LYS:HA	4:b:49:LEU:HD12	1.60	0.81
2:P:278:LEU:O	2:P:282:THR:HG23	1.80	0.81
4:U:56:ILE:HG22	5:V:124:THR:HG22	1.61	0.81
1:J:252:ASN:CA	1:J:255:PHE:CE2	2.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:91:ARG:HE	2:X:92:ILE:HD12	1.44	0.81
2:Q:260:LEU:HG	3:T:128:GLU:OE2	1.80	0.81
4:U:48:GLN:HB2	5:V:3:ASP:HB2	1.60	0.81
1:H:133:TYR:CE1	1:H:352:PHE:CE1	2.68	0.81
1:J:252:ASN:HA	1:J:255:PHE:HE2	1.43	0.81
2:Q:261:TYR:HE1	3:T:126:ARG:HH21	1.12	0.81
2:P:53:THR:HA	2:Q:57:LEU:HD11	1.62	0.81
2:Q:253:ILE:O	2:Q:257:GLU:HG2	1.79	0.81
5:V:112:ILE:O	5:V:148:ILE:N	2.13	0.81
1:N:252:ASN:CA	1:N:255:PHE:CE2	2.64	0.81
1:L:257:CYS:CB	1:L:258:PRO:HD3	2.04	0.81
2:P:142:GLU:HA	2:P:145:GLU:OE2	1.81	0.81
3:T:201:ARG:HH21	3:T:205:ARG:HA	1.46	0.81
5:V:101:PHE:HA	5:V:104:PHE:CD1	2.16	0.81
2:W:88:LEU:HD11	2:X:85:VAL:CG1	2.09	0.81
1:N:305:MET:CE	1:N:335:ARG:HE	1.94	0.80
1:M:109:PRO:HD2	1:M:161:HIS:CD2	2.16	0.80
3:T:238:GLN:NE2	3:T:242:ASN:OD1	2.15	0.80
4:U:51:THR:HA	5:V:161:GLU:O	1.81	0.80
4:U:100:LEU:HG	4:U:103:ARG:HH21	1.47	0.80
2:Q:257:GLU:HB3	3:T:132:ALA:HB2	1.64	0.80
2:Q:276:HIS:CB	3:T:110:PHE:HE1	1.94	0.80
5:c:14:GLU:HA	5:c:17:LYS:HD3	1.64	0.80
2:P:284:ILE:HG12	2:S:7:LYS:C	2.07	0.80
3:T:229:LEU:CD1	4:U:93:LEU:CD1	2.60	0.80
3:T:229:LEU:CD1	4:U:93:LEU:HD12	2.11	0.80
1:B:133:TYR:CE2	1:B:352:PHE:CZ	2.68	0.80
1:E:282:ILE:O	1:E:290:ARG:HG2	1.81	0.80
5:V:121:LEU:HD23	5:V:124:THR:HG21	1.64	0.80
1:E:289:ILE:CD1	1:G:63:GLY:O	2.30	0.80
1:G:262:PHE:CZ	1:G:312:ARG:HG2	2.17	0.80
2:Q:273:GLU:N	3:T:114:LYS:CE	2.40	0.80
1:F:109:PRO:HD2	1:F:161:HIS:CD2	2.17	0.79
1:N:109:PRO:CG	1:N:161:HIS:NE2	2.45	0.79
3:T:229:LEU:HD13	4:U:93:LEU:CG	2.11	0.79
1:B:345:ILE:HD13	4:U:208:PHE:CD1	2.18	0.79
1:G:252:ASN:HA	1:G:255:PHE:HE2	1.44	0.79
1:K:133:TYR:CE1	1:K:352:PHE:CZ	2.69	0.79
3:T:118:GLU:O	3:T:121:VAL:CG1	2.29	0.79
4:U:48:GLN:NE2	5:V:3:ASP:OD1	2.15	0.79
3:T:257:GLN:NE2	4:U:125:ILE:HG12	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:271:ASN:OD1	4:U:136:ARG:HG3	1.83	0.79
1:D:148:THR:HG23	4:U:169:LEU:HD11	1.63	0.79
2:P:278:LEU:CD1	2:S:1:MET:HG2	2.12	0.79
3:T:212:LEU:HB3	4:U:109:GLU:OE2	1.83	0.79
5:c:112:ILE:HB	5:c:148:ILE:HB	1.62	0.79
5:V:54:PRO:HA	5:V:57:LEU:HG	1.65	0.79
2:X:272:GLU:HB3	3:a:113:ARG:HE	0.71	0.79
5:V:130:GLU:O	5:V:134:GLU:N	2.16	0.79
3:a:205:ARG:HH22	3:a:209:LYS:HD3	1.46	0.79
4:U:57:ALA:HB1	5:V:100:LEU:HB3	1.65	0.79
2:Q:272:GLU:HG3	3:T:117:GLU:CB	2.13	0.78
4:U:48:GLN:NE2	5:V:3:ASP:OD2	1.96	0.78
5:V:111:TYR:HE1	5:V:113:ASP:HB2	1.47	0.78
1:E:109:PRO:CD	1:E:161:HIS:NE2	2.45	0.78
1:G:252:ASN:CA	1:G:255:PHE:CE2	2.65	0.78
1:N:305:MET:HE1	1:N:335:ARG:NE	1.97	0.78
1:E:207:GLU:HA	1:E:210:ARG:HG2	1.65	0.78
3:T:215:ARG:C	4:U:108:ASP:OD2	2.26	0.78
4:U:147:VAL:CG2	4:U:148:ARG:H	1.96	0.78
5:V:137:MET:O	5:V:141:ASP:N	2.15	0.78
1:D:133:TYR:CZ	1:D:352:PHE:HE1	2.02	0.78
1:A:133:TYR:CG	1:A:352:PHE:CZ	2.67	0.78
1:D:252:ASN:CB	1:D:255:PHE:CZ	2.66	0.78
2:P:142:GLU:HA	2:P:145:GLU:CD	2.07	0.78
1:B:133:TYR:CZ	1:B:352:PHE:CE1	2.71	0.78
3:a:233:ALA:HB1	4:b:100:LEU:HD12	1.65	0.78
3:a:247:LYS:HE3	4:b:79:ARG:HH21	1.48	0.78
2:P:284:ILE:O	2:R:4:ILE:HG21	1.84	0.77
2:Q:272:GLU:CG	3:T:117:GLU:CB	2.62	0.77
2:S:1:MET:HB3	2:S:4:ILE:CG1	2.13	0.77
3:T:208:LYS:CD	4:U:112:TYR:CD2	2.64	0.77
3:T:215:ARG:CZ	4:U:112:TYR:HB2	2.13	0.77
3:a:203:THR:HG22	3:a:207:LYS:HE2	1.65	0.77
1:C:252:ASN:HA	1:C:255:PHE:CZ	2.18	0.77
1:M:301:GLY:O	1:M:336:LYS:HB2	1.84	0.77
1:H:133:TYR:CE2	1:H:352:PHE:CE1	2.68	0.77
1:K:352:PHE:CE1	1:K:355:MET:HG3	2.18	0.77
1:N:305:MET:CE	1:N:335:ARG:NE	2.47	0.77
5:V:143:ASN:HD22	5:V:147:ARG:HH22	1.30	0.77
2:Q:250:GLU:OE2	3:T:138:GLN:C	2.28	0.77
1:B:146:GLY:HA2	4:U:209:GLU:HG2	0.79	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:251:LYS:HD2	3:T:139:ARG:NH2	1.98	0.77
2:Q:257:GLU:OE1	3:T:131:ARG:HB2	1.84	0.77
1:I:169:TYR:OH	1:K:49:GLN:HG3	1.85	0.77
2:S:4:ILE:HG13	2:S:5:LYS:N	2.00	0.77
4:U:147:VAL:HG13	4:U:148:ARG:CD	2.15	0.77
2:Q:261:TYR:HA	3:T:128:GLU:OE1	1.83	0.77
3:T:241:TYR:CE2	4:U:76:LEU:HB3	2.19	0.77
1:L:342:GLY:C	1:L:345:ILE:HG22	2.09	0.77
5:V:50:GLN:NE2	5:V:84:CYS:O	2.16	0.77
5:V:58:GLN:NE2	5:V:62:ASP:OD1	2.18	0.77
2:P:277:ALA:HB1	2:R:1:MET:HG2	1.66	0.77
3:T:221:ILE:HG21	4:U:98:ARG:HA	1.66	0.77
1:E:252:ASN:HA	1:E:255:PHE:CE2	2.20	0.77
1:H:252:ASN:HA	1:H:255:PHE:HE2	1.49	0.77
2:Q:257:GLU:HG3	3:T:132:ALA:N	1.99	0.77
3:T:221:ILE:HD11	4:U:101:HIS:CD2	2.19	0.77
5:c:106:LYS:NZ	5:c:120:MET:SD	2.59	0.76
2:Q:272:GLU:CG	3:T:117:GLU:HB3	2.15	0.76
4:U:63:ARG:NH2	5:V:103:MET:SD	2.59	0.76
4:U:100:LEU:CD2	4:U:103:ARG:HH21	1.99	0.76
2:Q:261:TYR:HD1	3:T:125:ASP:O	1.68	0.76
5:V:140:GLY:HA2	5:V:156:PHE:HB2	1.65	0.76
1:L:143:TYR:CB	1:L:345:ILE:HG21	2.15	0.76
2:P:284:ILE:H	2:S:7:LYS:HB2	1.50	0.76
3:T:240:ILE:HG23	4:U:107:VAL:HG11	1.66	0.76
1:F:109:PRO:CG	1:F:161:HIS:NE2	2.49	0.76
1:N:305:MET:SD	1:N:335:ARG:CZ	2.73	0.76
2:Q:251:LYS:CD	3:T:139:ARG:NH2	2.49	0.76
4:U:61:LEU:CD2	5:V:100:LEU:HD23	2.16	0.76
3:a:220:ALA:HB1	3:a:223:HIS:HE1	1.49	0.76
3:T:257:GLN:HE22	4:U:125:ILE:HG12	1.50	0.76
4:U:56:ILE:HG21	5:V:124:THR:HG23	1.66	0.76
1:D:23:GLY:HA3	4:U:183:LYS:HD2	1.64	0.76
2:R:3:ALA:CB	3:T:106:ILE:HD12	2.16	0.76
5:V:149:ASP:N	5:V:152:GLU:OE1	2.18	0.76
4:b:136:ARG:HD2	4:b:140:LYS:HE3	1.68	0.76
2:P:142:GLU:CA	2:P:145:GLU:HG2	2.16	0.76
1:B:305:MET:HE2	1:B:335:ARG:CB	2.16	0.75
2:Q:250:GLU:O	3:T:135:ALA:HB1	1.86	0.75
1:B:230:ALA:HB3	1:B:255:PHE:CZ	2.20	0.75
1:J:252:ASN:CB	1:J:255:PHE:CZ	2.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:207:GLU:HA	1:M:210:ARG:HG2	1.67	0.75
5:V:101:PHE:HA	5:V:104:PHE:HD1	1.51	0.75
1:A:133:TYR:CZ	1:A:352:PHE:HE1	2.04	0.75
1:D:133:TYR:CE2	1:D:352:PHE:HE1	2.04	0.75
5:V:104:PHE:O	5:V:106:LYS:NZ	2.19	0.75
2:Q:246:VAL:HG12	3:T:142:ASN:HD21	1.51	0.75
3:T:208:LYS:NZ	4:U:112:TYR:CD2	2.40	0.75
5:V:143:ASN:N	5:V:152:GLU:OE2	2.18	0.75
1:M:230:ALA:HB3	1:M:255:PHE:CZ	2.21	0.75
3:T:213:ALA:HA	3:T:216:ARG:HG2	1.69	0.75
5:c:45:MET:HA	5:c:48:LEU:HB2	1.69	0.75
5:c:137:MET:O	5:c:141:ASP:N	2.14	0.75
1:A:151:ILE:HD11	1:A:282:ILE:HG13	1.66	0.75
1:B:305:MET:HE2	1:B:335:ARG:HB2	1.68	0.75
3:T:240:ILE:O	3:T:244:GLU:HG2	1.87	0.75
1:D:305:MET:SD	1:D:335:ARG:CB	2.75	0.74
2:P:278:LEU:CD1	2:S:1:MET:SD	2.72	0.74
4:b:156:GLN:NE2	4:b:166:SER:O	2.19	0.74
1:F:25:ASP:HB3	4:U:147:VAL:CB	2.13	0.74
2:Q:261:TYR:CZ	3:T:126:ARG:NH2	2.54	0.74
4:b:145:ARG:HH21	5:c:60:MET:HG3	1.50	0.74
5:c:135:GLU:HA	5:c:138:LYS:HD2	1.67	0.74
5:V:142:LYS:NZ	5:V:152:GLU:O	2.20	0.74
2:Q:264:LYS:CD	3:T:128:GLU:OE2	2.35	0.74
3:T:236:LEU:HD21	4:U:104:VAL:HG11	1.69	0.74
3:a:247:LYS:NZ	4:b:110:GLU:OE1	2.19	0.74
1:L:333:PRO:CG	2:Y:6:LYS:NZ	2.49	0.74
5:c:45:MET:O	5:c:49:GLY:N	2.21	0.74
4:b:47:LEU:HD21	5:c:4:ILE:HA	1.68	0.74
1:C:253:GLU:CA	1:C:256:ARG:HG2	2.18	0.74
1:E:109:PRO:CG	1:E:161:HIS:NE2	2.50	0.74
3:T:265:ARG:O	3:T:269:ASN:ND2	2.20	0.74
1:F:305:MET:CE	1:F:336:LYS:HD3	2.16	0.74
3:T:208:LYS:HD2	4:U:112:TYR:HE2	0.59	0.74
3:T:267:ARG:HE	5:V:151:ASP:H	1.36	0.74
4:b:55:GLN:HA	4:b:58:LYS:HD2	1.68	0.74
2:X:260:LEU:HD23	2:X:260:LEU:O	1.88	0.73
4:U:54:LEU:HD22	5:V:92:LYS:HD2	1.70	0.73
3:T:221:ILE:HG21	4:U:98:ARG:CG	2.18	0.73
2:X:247:THR:HG22	3:a:138:GLN:CG	2.19	0.73
2:X:254:ASP:OD2	3:a:135:ALA:CB	2.31	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:36:ILE:HG12	5:c:44:VAL:HG21	1.71	0.73
1:L:326:LYS:CD	2:Y:20:ASP:OD2	2.35	0.73
3:T:212:LEU:HD21	4:U:112:TYR:HB3	1.68	0.73
5:V:40:GLU:HA	5:V:43:LYS:HE3	1.69	0.73
2:X:257:GLU:OE1	3:a:131:ARG:CZ	2.36	0.73
1:K:252:ASN:CA	1:K:255:PHE:CE2	2.66	0.73
2:Q:282:THR:CG2	2:R:1:MET:SD	2.72	0.73
5:V:58:GLN:HA	5:V:61:ILE:HD12	1.70	0.73
1:B:146:GLY:O	4:U:209:GLU:CD	2.32	0.73
2:Q:272:GLU:OE2	3:T:117:GLU:HB3	1.89	0.73
5:c:104:PHE:HA	5:c:120:MET:HG3	1.69	0.73
1:E:133:TYR:CE2	1:E:352:PHE:HE1	2.07	0.73
2:P:281:MET:HG3	2:R:1:MET:HB2	1.69	0.73
3:T:213:ALA:O	3:T:216:ARG:NE	2.18	0.73
4:U:47:LEU:O	4:U:51:THR:HG23	1.89	0.73
4:U:48:GLN:HB2	5:V:3:ASP:CB	2.18	0.73
2:X:257:GLU:HB3	3:a:131:ARG:HH11	1.51	0.73
1:O:207:GLU:O	1:O:210:ARG:CG	2.37	0.73
4:U:41:ILE:HD11	5:V:138:LYS:HB2	1.70	0.73
4:U:115:GLU:O	4:U:119:THR:HG23	1.89	0.73
1:A:282:ILE:HG21	1:A:294:TYR:CE2	2.23	0.72
3:T:262:ASN:OD1	3:T:265:ARG:NH1	2.20	0.72
2:W:256:LEU:CD1	2:X:257:GLU:HG2	2.19	0.72
3:a:250:LEU:O	3:a:254:PHE:HB2	1.88	0.72
4:U:52:LEU:HG	5:V:126:GLU:HB2	1.71	0.72
5:V:155:GLU:HA	5:V:158:LYS:HG2	1.71	0.72
3:T:256:GLN:HE21	4:U:68:ARG:HH12	1.31	0.72
3:a:232:LYS:HE2	3:a:236:LEU:HD11	1.71	0.72
3:T:226:GLU:HG3	4:U:88:LEU:O	1.88	0.72
4:U:61:LEU:HD22	5:V:100:LEU:HD23	1.69	0.72
2:X:250:GLU:OE1	3:a:138:GLN:HG2	1.88	0.72
1:D:146:GLY:CA	4:U:173:LEU:HD22	2.19	0.72
4:U:100:LEU:CG	4:U:103:ARG:HH21	2.02	0.72
1:E:166:TYR:CD1	1:E:289:ILE:HG23	2.25	0.72
1:H:133:TYR:CG	1:H:352:PHE:CZ	2.72	0.72
4:U:83:LEU:HB2	4:U:85:LEU:HD23	1.70	0.72
1:L:196:ARG:HD2	1:L:253:GLU:OE2	1.88	0.72
3:T:208:LYS:HG3	4:U:112:TYR:CZ	2.24	0.72
2:X:272:GLU:CB	3:a:117:GLU:OE2	2.37	0.72
1:L:133:TYR:CE2	1:L:352:PHE:HE1	2.08	0.72
1:N:279:TYR:OH	1:N:283:MET:HE3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:264:LYS:HB2	3:T:125:ASP:OD1	1.89	0.72
3:a:214:GLU:OE2	3:a:215:ARG:NH1	2.22	0.72
1:I:189:LEU:HA	1:I:257:CYS:SG	2.29	0.71
2:X:279:ASN:CB	3:a:109:HIS:CE1	2.66	0.71
1:F:252:ASN:HA	1:F:255:PHE:HE2	1.46	0.71
1:N:252:ASN:HA	1:N:255:PHE:HE2	1.50	0.71
3:T:222:ASP:HA	4:U:94:GLN:NE2	2.05	0.71
1:K:305:MET:CG	1:K:335:ARG:CD	2.68	0.71
1:I:257:CYS:CB	1:I:258:PRO:CD	2.68	0.71
2:P:282:THR:O	2:S:4:ILE:N	2.22	0.71
3:T:236:LEU:HD11	4:U:104:VAL:CG1	2.18	0.71
4:U:50:LYS:CG	5:V:156:PHE:CZ	2.70	0.71
5:V:121:LEU:HB3	5:V:128:ILE:HG13	1.72	0.71
2:X:247:THR:HG21	3:a:142:ASN:OD1	1.91	0.71
4:b:132:ILE:HA	4:b:135:LEU:HB2	1.70	0.71
2:P:284:ILE:O	2:P:284:ILE:HG22	1.91	0.71
2:Q:257:GLU:HB2	3:T:132:ALA:CB	2.18	0.71
3:T:256:GLN:NE2	4:U:68:ARG:CZ	2.53	0.71
4:U:141:ARG:NH1	4:U:141:ARG:O	2.24	0.71
1:D:133:TYR:CE2	1:D:352:PHE:CE1	2.78	0.71
2:Q:282:THR:CB	2:R:1:MET:HE1	2.18	0.71
5:V:98:SER:HB2	5:V:150:TYR:CZ	2.26	0.71
5:V:152:GLU:O	5:V:156:PHE:HB3	1.91	0.71
1:E:106:THR:HG21	1:E:140:LEU:HD12	1.73	0.71
1:N:305:MET:HE1	1:N:335:ARG:CZ	2.20	0.71
3:a:264:LEU:HD13	4:b:128:LEU:HB2	1.73	0.71
1:B:305:MET:HE1	1:B:335:ARG:HB2	1.72	0.71
1:M:304:THR:O	1:M:335:ARG:NE	2.24	0.71
1:O:305:MET:HE1	1:O:335:ARG:HE	1.56	0.71
4:b:133:PHE:HD1	4:b:136:ARG:HH12	1.39	0.71
5:c:141:ASP:HB3	5:c:144:ASN:HA	1.73	0.71
1:D:332:PRO:O	1:D:335:ARG:CG	2.35	0.71
3:T:230:ARG:HD3	4:U:86:ALA:HA	1.71	0.71
3:T:234:LYS:CD	4:U:85:LEU:HD21	2.02	0.71
4:U:71:GLU:HG3	4:U:74:ARG:HH21	1.55	0.71
5:V:57:LEU:O	5:V:60:MET:HG2	1.89	0.71
5:V:102:ARG:HA	5:V:105:ASP:HB2	1.71	0.71
1:M:109:PRO:HD2	1:M:161:HIS:NE2	2.05	0.70
1:M:305:MET:SD	1:M:335:ARG:CG	2.79	0.70
5:V:14:GLU:HA	5:V:17:LYS:HE2	1.73	0.70
3:T:233:ALA:CB	4:U:100:LEU:HD12	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:241:TYR:CE1	4:U:76:LEU:C	2.69	0.70
5:c:134:GLU:HG3	5:c:138:LYS:HE3	1.72	0.70
1:E:106:THR:CG2	1:E:135:ALA:HB3	2.21	0.70
2:Q:268:LYS:HB2	3:T:121:VAL:HB	0.83	0.70
2:X:273:GLU:HG2	3:a:113:ARG:HH12	1.57	0.70
4:b:51:THR:O	4:b:55:GLN:NE2	2.24	0.70
5:c:139:ASP:O	5:c:142:LYS:NZ	2.23	0.70
1:E:104:LEU:HD12	1:E:133:TYR:O	1.90	0.70
2:P:149:LYS:HE3	2:P:153:HIS:NE2	2.06	0.70
3:T:268:ILE:HA	3:T:271:ASN:HB2	1.73	0.70
4:U:60:GLU:HG3	4:U:63:ARG:HH21	1.57	0.70
5:V:80:MET:HA	5:V:83:ARG:HB2	1.72	0.70
1:A:230:ALA:HB3	1:A:255:PHE:HZ	1.55	0.70
1:B:133:TYR:CG	1:B:352:PHE:HZ	2.09	0.70
1:K:133:TYR:CZ	1:K:352:PHE:CZ	2.80	0.70
3:T:268:ILE:HA	3:T:271:ASN:HD22	1.56	0.70
4:U:53:LEU:HD13	5:V:121:LEU:CG	2.19	0.70
5:V:131:ASP:O	5:V:135:GLU:N	2.25	0.70
1:F:25:ASP:CB	4:U:147:VAL:HB	2.17	0.70
2:P:284:ILE:N	2:S:7:LYS:HB2	2.07	0.70
2:Q:250:GLU:OE1	3:T:139:ARG:CA	2.39	0.70
5:V:112:ILE:HB	5:V:148:ILE:HB	1.73	0.70
3:T:236:LEU:HD11	4:U:104:VAL:HG21	1.74	0.70
1:B:133:TYR:CE2	1:B:352:PHE:HE1	2.05	0.70
1:H:163:VAL:HG23	1:H:175:ILE:HG21	1.74	0.70
3:T:229:LEU:HD11	4:U:93:LEU:HB2	1.68	0.70
4:U:53:LEU:HD21	5:V:117:LEU:CD1	2.22	0.70
4:U:181:THR:O	4:U:185:ASN:ND2	2.25	0.70
3:a:230:ARG:HE	4:b:86:ALA:HA	1.57	0.70
3:a:237:TRP:NE1	4:b:81:GLN:O	2.24	0.70
1:I:109:PRO:CD	1:I:161:HIS:NE2	2.54	0.69
2:P:57:LEU:N	2:Q:57:LEU:HD21	2.07	0.69
2:Q:272:GLU:HG3	3:T:118:GLU:N	2.07	0.69
2:Q:284:ILE:HG21	2:S:5:LYS:HG3	1.73	0.69
3:T:204:GLU:HA	3:T:207:LYS:HG2	1.74	0.69
3:a:270:ASP:OD2	5:c:111:TYR:OH	2.08	0.69
1:K:352:PHE:CE1	1:K:355:MET:CB	2.74	0.69
3:T:219:LEU:HD23	4:U:101:HIS:HB2	1.73	0.69
4:U:54:LEU:CD1	5:V:157:MET:CG	2.69	0.69
4:b:117:LYS:HA	4:b:120:LYS:HD2	1.75	0.69
1:K:196:ARG:HD2	1:K:253:GLU:CD	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:57:LEU:HA	2:Q:57:LEU:HD23	1.74	0.69
2:Q:257:GLU:HG3	3:T:131:ARG:C	2.16	0.69
2:W:166:ALA:HA	2:X:165:VAL:HG21	1.72	0.69
1:L:334:GLU:O	1:L:338:SER:HB3	1.93	0.69
3:T:208:LYS:HA	3:T:211:ILE:HD12	1.74	0.69
3:T:215:ARG:HH12	4:U:112:TYR:HA	1.54	0.69
3:T:221:ILE:HG21	4:U:98:ARG:CA	2.22	0.69
3:T:221:ILE:HG22	4:U:98:ARG:HG2	1.72	0.69
4:U:66:GLU:OE2	4:U:69:ARG:NE	2.20	0.69
4:b:125:ILE:O	4:b:129:THR:OG1	2.09	0.69
1:N:305:MET:CE	1:N:335:ARG:CZ	2.70	0.69
5:V:143:ASN:ND2	5:V:147:ARG:HH22	1.90	0.69
2:X:257:GLU:CB	3:a:131:ARG:HH11	2.02	0.69
4:b:88:LEU:HD12	4:b:96:LEU:HD12	1.72	0.69
1:E:305:MET:CE	1:E:336:LYS:HD2	2.20	0.69
2:P:279:ASN:HA	2:P:282:THR:HG23	1.75	0.69
4:U:108:ASP:HA	4:U:111:ARG:HG2	1.73	0.69
5:V:94:GLU:HB3	5:V:154:LEU:HD22	1.73	0.69
4:b:145:ARG:H	4:b:148:ARG:HE	1.41	0.69
4:b:159:LEU:HD13	4:b:164:LYS:HG2	1.74	0.69
5:c:83:ARG:NH2	5:c:84:CYS:SG	2.66	0.69
1:M:305:MET:SD	1:M:335:ARG:HG3	2.33	0.69
4:U:147:VAL:C	4:U:148:ARG:HD3	2.17	0.69
5:V:94:GLU:C	5:V:97:LEU:HB2	2.17	0.69
5:c:94:GLU:O	5:c:98:SER:OG	2.08	0.69
1:D:252:ASN:CA	1:D:255:PHE:CE2	2.65	0.69
5:V:94:GLU:O	5:V:97:LEU:CB	2.40	0.69
5:V:97:LEU:HB3	5:V:153:PHE:CE2	2.28	0.69
2:W:256:LEU:HD21	2:X:256:LEU:HB3	1.75	0.69
2:X:260:LEU:HD23	2:X:260:LEU:C	2.17	0.69
1:D:252:ASN:CA	1:D:255:PHE:CZ	2.76	0.68
3:T:253:LYS:HE2	4:U:118:VAL:HG21	1.76	0.68
1:H:328:LYS:NZ	2:X:212:GLU:HG3	2.09	0.68
1:J:252:ASN:HB2	1:J:255:PHE:HZ	1.54	0.68
1:K:305:MET:HG2	1:K:335:ARG:CD	2.23	0.68
2:X:257:GLU:HA	2:X:260:LEU:HB3	1.75	0.68
2:Q:264:LYS:O	3:T:121:VAL:HG21	1.93	0.68
3:T:236:LEU:CG	4:U:104:VAL:HG11	2.23	0.68
1:L:133:TYR:CE2	1:L:352:PHE:CE1	2.81	0.68
5:c:37:SER:O	5:c:41:LEU:N	2.27	0.68
1:D:25:ASP:HB3	4:U:181:THR:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:252:ASN:CB	1:F:255:PHE:CE2	2.76	0.68
4:U:48:GLN:NE2	5:V:3:ASP:CB	2.57	0.68
4:U:54:LEU:CD1	5:V:97:LEU:HG	2.22	0.68
1:C:133:TYR:CZ	1:C:352:PHE:CE1	2.76	0.68
1:D:24:ASP:OD2	1:D:28:ARG:NH2	2.25	0.68
2:P:282:THR:CA	2:S:3:ALA:HB3	2.23	0.68
4:U:60:GLU:OE2	4:U:63:ARG:NE	2.27	0.68
5:c:37:SER:H	5:c:40:GLU:HB2	1.59	0.68
2:P:284:ILE:CA	2:S:4:ILE:HA	2.14	0.68
2:W:91:ARG:HE	2:X:92:ILE:CG1	2.06	0.68
4:b:56:ILE:HG13	5:c:124:THR:HA	1.76	0.68
2:X:268:LYS:O	2:X:272:GLU:CG	2.41	0.68
5:c:55:GLU:O	5:c:59:GLU:HB2	1.94	0.68
5:c:59:GLU:O	5:c:63:GLU:N	2.21	0.68
1:M:332:PRO:O	1:M:335:ARG:HB3	1.95	0.67
5:V:81:MET:O	5:V:85:MET:N	2.27	0.67
2:Q:257:GLU:HG3	3:T:132:ALA:CA	2.25	0.67
4:b:55:GLN:OE1	4:b:58:LYS:NZ	2.27	0.67
1:I:257:CYS:HB2	1:I:258:PRO:CD	2.24	0.67
1:J:326:LYS:HE2	2:W:254:ASP:CG	2.20	0.67
3:T:256:GLN:HE21	4:U:68:ARG:NH1	1.82	0.67
4:U:183:LYS:NZ	4:U:184:GLU:OE2	2.24	0.67
5:V:151:ASP:O	5:V:154:LEU:N	2.27	0.67
1:C:133:TYR:CE1	1:C:355:MET:HB3	2.29	0.67
1:D:333:PRO:C	1:D:335:ARG:H	2.02	0.67
1:K:189:LEU:HB2	1:K:257:CYS:SG	2.34	0.67
3:T:256:GLN:CD	4:U:68:ARG:NH1	2.42	0.67
5:V:36:ILE:HD12	5:V:71:THR:HG23	1.74	0.67
5:c:116:GLU:OE1	5:c:116:GLU:N	2.24	0.67
1:L:207:GLU:O	1:L:210:ARG:HG3	1.94	0.67
2:R:3:ALA:HB1	3:T:106:ILE:HD12	1.76	0.67
5:V:95:GLU:CD	5:V:95:GLU:H	2.02	0.67
1:N:262:PHE:CZ	1:N:312:ARG:HG2	2.30	0.67
2:Q:260:LEU:HG	2:Q:264:LYS:HE2	1.76	0.67
3:T:121:VAL:HG13	3:T:122:SER:N	2.10	0.67
3:T:259:TYR:HA	3:T:262:ASN:ND2	2.10	0.67
1:B:146:GLY:C	4:U:209:GLU:CD	2.62	0.67
3:T:257:GLN:HG3	4:U:121:ASN:ND2	2.10	0.67
5:V:21:LYS:HA	5:V:24:PHE:CD2	2.29	0.67
3:T:243:LEU:HD22	4:U:111:ARG:NE	2.10	0.67
4:U:56:ILE:HB	5:V:124:THR:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:144:LEU:HD22	5:c:86:LYS:HD2	1.76	0.67
1:H:95:ARG:HH12	3:T:265:ARG:CB	2.07	0.67
5:V:121:LEU:HA	5:V:124:THR:HG23	1.77	0.67
2:Q:250:GLU:HG2	3:T:138:GLN:CB	2.25	0.66
2:Q:264:LYS:HD3	3:T:124:LYS:HB2	1.77	0.66
2:Q:269:ALA:HB2	3:T:118:GLU:OE2	1.95	0.66
3:a:263:VAL:HG22	5:c:110:GLY:HA2	1.76	0.66
1:N:109:PRO:HG2	1:N:161:HIS:NE2	2.09	0.66
3:a:212:LEU:O	3:a:216:ARG:N	2.26	0.66
1:A:252:ASN:CA	1:A:255:PHE:CZ	2.79	0.66
2:Q:250:GLU:HB3	3:T:139:ARG:CG	2.26	0.66
3:T:251:GLN:HE21	4:U:114:ILE:HD13	1.61	0.66
4:U:100:LEU:HD23	4:U:103:ARG:CZ	2.25	0.66
3:a:212:LEU:C	3:a:216:ARG:HE	2.03	0.66
1:D:23:GLY:O	4:U:183:LYS:HB3	1.95	0.66
4:b:143:THR:O	4:b:148:ARG:NH2	2.28	0.66
5:c:73:ASP:O	5:c:77:PHE:N	2.29	0.66
1:E:133:TYR:CD2	1:E:352:PHE:CZ	2.84	0.66
3:T:241:TYR:CD2	4:U:76:LEU:HD22	2.31	0.66
4:U:53:LEU:HD21	5:V:117:LEU:HD11	1.77	0.66
1:O:37:ARG:O	1:O:65:LEU:HA	1.96	0.66
1:O:207:GLU:O	1:O:210:ARG:HG2	1.96	0.66
5:V:96:GLU:O	5:V:100:LEU:HG	1.95	0.66
2:W:91:ARG:CZ	2:X:92:ILE:HG13	2.26	0.66
3:a:261:ILE:HA	3:a:264:LEU:HD12	1.77	0.66
2:P:156:GLU:HG2	2:P:160:ARG:NH2	2.10	0.66
2:Q:257:GLU:CB	3:T:132:ALA:CB	2.70	0.66
4:b:145:ARG:HB3	4:b:148:ARG:HG3	1.78	0.66
5:c:53:THR:N	5:c:56:GLU:HB2	2.07	0.66
1:A:143:TYR:CE2	1:C:44:MET:CE	2.73	0.66
1:F:252:ASN:HB2	1:F:255:PHE:CE2	2.30	0.66
1:H:133:TYR:CE1	1:H:355:MET:HB3	2.30	0.66
3:T:210:LYS:HD3	3:T:213:ALA:HB3	1.78	0.66
3:T:226:GLU:CG	4:U:88:LEU:O	2.43	0.66
3:a:265:ARG:HA	3:a:268:ILE:HD12	1.77	0.66
3:a:267:ARG:HD2	5:c:150:TYR:HB3	1.78	0.66
1:F:305:MET:CE	1:F:336:LYS:CD	2.67	0.66
2:P:282:THR:O	2:S:3:ALA:HB3	1.93	0.66
2:Q:261:TYR:OH	3:T:126:ARG:NH2	2.28	0.66
4:U:61:LEU:HB2	5:V:100:LEU:HD23	1.78	0.66
5:V:111:TYR:CE1	5:V:113:ASP:HB2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:137:MET:HG2	5:V:141:ASP:HB3	1.78	0.66
3:a:261:ILE:HG22	3:a:265:ARG:HH12	1.61	0.66
1:M:109:PRO:CG	1:M:161:HIS:NE2	2.59	0.65
3:T:230:ARG:NH2	4:U:88:LEU:O	2.28	0.65
1:A:133:TYR:CD1	1:A:352:PHE:HZ	2.14	0.65
1:J:335:ARG:C	1:J:337:TYR:H	2.03	0.65
3:T:221:ILE:HG21	4:U:98:ARG:HG2	1.77	0.65
4:U:58:LYS:HA	5:V:100:LEU:HD22	1.79	0.65
5:V:61:ILE:HA	5:V:65:ASP:HB2	1.79	0.65
5:V:95:GLU:N	5:V:95:GLU:OE1	2.29	0.65
2:X:261:TYR:HE1	2:X:265:LEU:HD22	1.61	0.65
1:E:133:TYR:CZ	1:E:352:PHE:HE1	2.15	0.65
1:I:305:MET:HE1	1:I:335:ARG:CG	2.26	0.65
3:T:212:LEU:CB	4:U:109:GLU:OE2	2.45	0.65
3:T:267:ARG:O	3:T:271:ASN:N	2.30	0.65
4:U:89:GLY:N	4:U:92:GLU:OE2	2.26	0.65
3:T:226:GLU:OE2	4:U:89:GLY:HA2	1.96	0.65
2:P:142:GLU:CG	2:P:145:GLU:OE2	2.42	0.65
3:T:256:GLN:NE2	4:U:68:ARG:HH22	1.93	0.65
3:a:240:ILE:O	3:a:244:GLU:HG2	1.97	0.65
4:b:52:LEU:HD12	5:c:126:GLU:HB2	1.78	0.65
1:C:133:TYR:CG	1:C:352:PHE:HZ	2.15	0.65
1:C:252:ASN:HB2	1:C:255:PHE:CZ	2.31	0.65
1:E:143:TYR:OH	1:G:45:VAL:N	2.30	0.65
1:F:169:TYR:OH	1:H:49:GLN:HB3	1.97	0.65
5:V:49:GLY:N	5:V:51:ASN:OD1	2.26	0.65
5:V:74:PHE:O	5:V:78:LEU:HB2	1.96	0.65
2:W:88:LEU:HD12	2:X:85:VAL:HA	1.78	0.65
1:J:169:TYR:OH	1:L:49:GLN:HB3	1.97	0.65
1:L:133:TYR:CE1	1:L:355:MET:HB3	2.32	0.65
1:N:279:TYR:OH	1:N:283:MET:CE	2.45	0.65
2:Q:272:GLU:OE1	2:Q:272:GLU:HA	1.95	0.65
2:W:91:ARG:NE	2:X:92:ILE:HD12	2.11	0.65
1:F:25:ASP:N	4:U:147:VAL:HG23	2.12	0.65
3:T:244:GLU:CD	4:U:79:ARG:CB	2.70	0.65
5:V:153:PHE:O	5:V:157:MET:N	2.27	0.65
2:X:261:TYR:CE1	2:X:265:LEU:HD22	2.31	0.65
3:a:209:LYS:O	3:a:216:ARG:NH2	2.28	0.65
4:b:54:LEU:HD21	5:c:157:MET:HG3	1.79	0.65
5:c:79:VAL:O	5:c:83:ARG:CB	2.43	0.65
1:E:106:THR:HG21	1:E:140:LEU:CD1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:109:PRO:CG	1:I:161:HIS:NE2	2.60	0.65
2:Q:250:GLU:OE2	3:T:138:GLN:O	2.15	0.65
4:U:47:LEU:HD23	5:V:4:ILE:HG13	1.78	0.65
1:D:133:TYR:CE1	1:D:355:MET:HB3	2.33	0.64
1:K:196:ARG:HD2	1:K:253:GLU:OE2	1.97	0.64
1:O:207:GLU:O	1:O:210:ARG:HG3	1.96	0.64
1:E:133:TYR:CD2	1:E:352:PHE:HZ	2.16	0.64
1:G:252:ASN:CB	1:G:255:PHE:CZ	2.81	0.64
2:Q:269:ALA:H	3:T:121:VAL:HG21	1.61	0.64
3:T:118:GLU:C	3:T:121:VAL:HG12	2.22	0.64
5:V:53:THR:OG1	5:V:56:GLU:N	2.24	0.64
1:O:305:MET:SD	1:O:335:ARG:NE	2.70	0.64
2:Q:257:GLU:HG3	3:T:132:ALA:HA	1.79	0.64
3:T:210:LYS:HA	3:T:213:ALA:HB3	1.78	0.64
5:V:11:GLN:HA	5:V:89:SER:HB3	1.78	0.64
5:V:28:VAL:HG23	5:V:32:GLU:N	2.08	0.64
2:X:261:TYR:CE1	2:X:265:LEU:HB2	2.32	0.64
3:a:268:ILE:HG12	4:b:131:LYS:HZ2	1.61	0.64
5:c:130:GLU:HA	5:c:133:ILE:HD12	1.79	0.64
1:E:108:ALA:HB1	1:E:161:HIS:CE1	2.31	0.64
1:F:25:ASP:CA	4:U:147:VAL:HG23	2.27	0.64
4:U:150:SER:O	4:U:153:ALA:N	2.29	0.64
3:a:224:LEU:HD23	3:a:229:LEU:HA	1.79	0.64
1:G:333:PRO:C	1:G:335:ARG:H	2.05	0.64
3:T:221:ILE:HD11	4:U:101:HIS:CG	2.33	0.64
3:T:222:ASP:HA	4:U:94:GLN:CG	2.26	0.64
4:U:45:ARG:NH2	5:V:127:THR:O	2.30	0.64
5:V:112:ILE:N	5:V:148:ILE:O	2.31	0.64
2:W:91:ARG:HH21	2:X:92:ILE:CG1	1.97	0.64
4:b:45:ARG:NH2	5:c:132:ASP:OD2	2.31	0.64
2:Q:275:ASP:C	3:T:110:PHE:HD1	2.06	0.64
3:T:266:ASN:ND2	5:V:109:ASP:O	2.24	0.64
4:U:49:LEU:HD22	5:V:132:ASP:HB3	1.79	0.64
1:F:25:ASP:H	4:U:147:VAL:HG23	1.63	0.64
1:H:163:VAL:CG2	1:H:175:ILE:HG21	2.27	0.64
1:M:336:LYS:C	1:M:338:SER:H	2.06	0.64
4:U:125:ILE:O	4:U:129:THR:HG23	1.98	0.64
5:V:142:LYS:HG2	5:V:152:GLU:HG2	1.80	0.64
4:b:72:LYS:HG3	4:b:76:LEU:HD21	1.80	0.64
5:c:115:ASP:HA	5:c:118:LYS:HG2	1.78	0.64
1:D:146:GLY:HA2	4:U:173:LEU:CB	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:207:GLU:HA	1:O:210:ARG:HG2	1.80	0.64
2:W:88:LEU:CD1	2:X:85:VAL:HA	2.27	0.64
1:B:207:GLU:CA	1:B:210:ARG:HG2	2.26	0.64
1:B:252:ASN:CB	1:B:255:PHE:CZ	2.81	0.64
3:T:268:ILE:O	3:T:272:GLN:N	2.31	0.64
1:B:227:MET:HA	1:B:255:PHE:CE1	2.33	0.63
1:F:28:ARG:O	4:U:154:MET:HE3	1.98	0.63
1:F:227:MET:HE3	1:F:255:PHE:HE1	1.60	0.63
2:P:282:THR:HA	2:S:3:ALA:HB3	1.80	0.63
5:V:29:LEU:N	5:V:32:GLU:OE1	2.32	0.63
3:a:267:ARG:HE	4:b:132:ILE:HG21	1.62	0.63
1:D:23:GLY:O	4:U:183:LYS:CB	2.45	0.63
1:M:262:PHE:CZ	1:M:312:ARG:HG2	2.33	0.63
2:Q:250:GLU:CD	3:T:142:ASN:ND2	2.56	0.63
3:T:221:ILE:CG2	4:U:98:ARG:CG	2.75	0.63
4:U:53:LEU:CD2	5:V:117:LEU:HD11	2.27	0.63
2:X:247:THR:HG22	3:a:138:GLN:HG3	1.79	0.63
4:b:159:LEU:HB2	4:b:163:ALA:HA	1.80	0.63
2:Q:257:GLU:OE2	3:T:131:ARG:CB	2.30	0.63
3:T:236:LEU:CD2	4:U:104:VAL:HG11	2.28	0.63
4:U:125:ILE:HD12	4:U:126:ALA:N	2.13	0.63
3:a:219:LEU:HD21	4:b:101:HIS:CG	2.34	0.63
3:a:228:GLN:NE2	3:a:231:GLU:OE1	2.32	0.63
1:E:133:TYR:CE2	1:E:352:PHE:CE1	2.86	0.63
2:Q:251:LYS:CD	3:T:139:ARG:HH22	2.07	0.63
2:Q:272:GLU:HB3	3:T:114:LYS:HD2	1.81	0.63
4:U:56:ILE:HG12	5:V:123:ALA:C	2.23	0.63
3:a:257:GLN:NE2	4:b:118:VAL:O	2.29	0.63
1:I:169:TYR:OH	1:K:49:GLN:CG	2.47	0.63
1:L:207:GLU:CA	1:L:210:ARG:HG2	2.28	0.63
1:N:262:PHE:CE2	1:N:312:ARG:HG2	2.33	0.63
3:T:236:LEU:HD21	4:U:101:HIS:HA	1.78	0.63
2:W:256:LEU:HG	2:X:260:LEU:CD1	2.29	0.63
3:a:204:GLU:HA	3:a:207:LYS:HE3	1.79	0.63
1:K:352:PHE:CD1	1:K:355:MET:CG	2.80	0.63
1:L:109:PRO:HD2	1:L:161:HIS:CD2	2.34	0.63
2:Q:275:ASP:C	3:T:110:PHE:CD1	2.76	0.63
3:T:261:ILE:CG1	4:U:124:GLU:OE2	2.41	0.63
5:V:89:SER:OG	5:V:161:GLU:OE2	2.12	0.63
3:a:252:GLU:HA	3:a:255:LYS:HE2	1.79	0.63
1:B:146:GLY:HA3	4:U:209:GLU:CG	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:TYR:CD2	1:D:352:PHE:CZ	2.87	0.63
1:K:257:CYS:HB2	1:K:258:PRO:CD	2.27	0.63
2:P:142:GLU:C	2:P:145:GLU:HG2	2.24	0.63
2:Q:261:TYR:CD1	3:T:125:ASP:O	2.51	0.63
3:T:256:GLN:NE2	4:U:68:ARG:NH2	2.47	0.63
4:b:60:GLU:HB3	5:c:103:MET:HG3	1.81	0.63
1:F:334:GLU:O	1:F:338:SER:HB3	1.99	0.63
3:T:243:LEU:HD22	4:U:111:ARG:HD3	1.78	0.63
4:b:156:GLN:HA	4:b:163:ALA:HB1	1.80	0.63
3:T:248:PHE:CE1	4:U:71:GLU:HB3	2.34	0.63
4:U:50:LYS:HD2	5:V:156:PHE:CE1	2.29	0.63
5:V:12:LEU:HD13	5:V:78:LEU:HG	1.80	0.63
5:c:101:PHE:HA	5:c:104:PHE:HB2	1.81	0.63
2:Q:281:MET:O	2:S:4:ILE:CD1	2.44	0.62
2:S:1:MET:CB	2:S:4:ILE:HG12	2.25	0.62
2:W:162:TYR:CD1	2:X:165:VAL:HG11	2.34	0.62
1:D:23:GLY:CA	4:U:183:LYS:HD2	2.29	0.62
2:P:282:THR:C	2:S:3:ALA:HB3	2.24	0.62
1:G:332:PRO:O	1:G:335:ARG:HG2	1.99	0.62
1:L:305:MET:HE1	1:L:335:ARG:CB	2.28	0.62
4:U:118:VAL:O	4:U:122:ILE:HG12	1.98	0.62
5:V:94:GLU:HB3	5:V:154:LEU:HD13	1.81	0.62
3:a:209:LYS:HE3	3:a:216:ARG:HH22	1.64	0.62
3:a:256:GLN:HE22	5:c:102:ARG:HG2	1.64	0.62
5:c:104:PHE:O	5:c:116:GLU:HB3	1.99	0.62
1:J:303:THR:O	1:J:306:TYR:CD1	2.53	0.62
1:O:109:PRO:CB	1:O:163:VAL:HG21	2.29	0.62
1:C:192:ILE:CD1	1:C:256:ARG:CD	2.61	0.62
2:Q:276:HIS:CB	3:T:110:PHE:CE1	2.77	0.62
2:W:256:LEU:HD11	2:X:257:GLU:HG2	1.79	0.62
5:c:5:TYR:CZ	5:c:83:ARG:HG3	2.34	0.62
3:T:257:GLN:HG3	4:U:121:ASN:CG	2.24	0.62
5:V:86:LYS:N	5:V:86:LYS:HD2	2.13	0.62
5:c:31:ALA:HB2	5:c:43:LYS:HZ1	1.65	0.62
5:c:44:VAL:O	5:c:48:LEU:N	2.33	0.62
1:B:169:TYR:OH	1:D:49:GLN:HB3	2.00	0.62
2:Q:272:GLU:OE1	3:T:117:GLU:HB2	1.99	0.62
3:T:226:GLU:OE2	4:U:90:PHE:CD2	2.52	0.62
3:a:219:LEU:HD13	4:b:98:ARG:HA	1.82	0.62
3:a:247:LYS:HB2	4:b:111:ARG:HB3	1.81	0.62
5:c:17:LYS:HG3	5:c:78:LEU:HD22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:50:LYS:CD	5:V:156:PHE:CZ	2.80	0.62
5:V:105:ASP:HA	5:V:116:GLU:HG2	1.82	0.62
5:c:112:ILE:O	5:c:148:ILE:N	2.30	0.62
1:D:146:GLY:CA	4:U:173:LEU:CG	2.78	0.62
3:T:236:LEU:HD21	4:U:104:VAL:CG1	2.29	0.62
5:c:60:MET:O	5:c:64:VAL:N	2.33	0.62
1:N:109:PRO:CD	1:N:161:HIS:CE1	2.81	0.62
1:N:333:PRO:C	1:N:335:ARG:H	2.08	0.62
2:Q:261:TYR:CE1	3:T:125:ASP:HB3	2.34	0.62
3:T:240:ILE:HG12	4:U:104:VAL:CA	2.30	0.62
5:V:94:GLU:HA	5:V:97:LEU:HD22	1.81	0.62
2:X:252:SER:O	2:X:256:LEU:HG	1.99	0.62
2:X:253:ILE:HA	2:X:256:LEU:HB2	1.82	0.62
5:c:46:ARG:HB3	5:c:51:ASN:HD21	1.64	0.62
1:E:305:MET:HE3	1:E:336:LYS:CD	2.26	0.61
4:U:89:GLY:O	4:U:93:LEU:HG	2.00	0.61
5:V:4:ILE:HG23	5:V:79:VAL:HG21	1.81	0.61
5:c:105:ASP:CG	5:c:110:GLY:H	2.08	0.61
1:D:146:GLY:HA2	4:U:173:LEU:CD1	2.13	0.61
1:H:227:MET:HB3	1:H:255:PHE:CE1	2.35	0.61
1:N:334:GLU:O	1:N:338:SER:HB3	2.00	0.61
1:H:163:VAL:CG2	1:H:175:ILE:HG23	2.25	0.61
3:a:215:ARG:HD3	4:b:111:ARG:NH2	2.14	0.61
1:I:262:PHE:CZ	1:I:312:ARG:HG2	2.35	0.61
1:O:196:ARG:HD2	1:O:253:GLU:CD	2.25	0.61
2:Q:272:GLU:CG	3:T:117:GLU:HB2	2.29	0.61
3:T:219:LEU:HD13	3:T:232:LYS:HE3	1.83	0.61
3:T:226:GLU:HA	4:U:93:LEU:HD12	1.73	0.61
3:T:230:ARG:NE	4:U:87:GLY:H	1.98	0.61
3:T:250:LEU:HD23	3:T:253:LYS:HZ1	1.64	0.61
4:U:56:ILE:CG2	5:V:124:THR:CG2	2.55	0.61
5:V:82:VAL:O	5:V:86:LYS:HG3	2.00	0.61
1:E:334:GLU:O	1:E:338:SER:HB3	2.01	0.61
1:K:252:ASN:HA	1:K:255:PHE:HE2	1.59	0.61
3:T:215:ARG:NH1	4:U:112:TYR:N	2.45	0.61
3:T:219:LEU:HD22	3:T:232:LYS:HZ1	1.64	0.61
3:T:248:PHE:CZ	4:U:71:GLU:HB2	2.36	0.61
5:c:41:LEU:HD23	5:c:57:LEU:HA	1.83	0.61
5:c:140:GLY:HA2	5:c:152:GLU:O	2.00	0.61
2:P:282:THR:O	2:S:3:ALA:HB1	1.91	0.61
3:T:222:ASP:CB	4:U:94:GLN:NE2	2.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:21:LYS:HA	5:V:24:PHE:CG	2.36	0.61
2:Q:264:LYS:HE3	3:T:124:LYS:HB3	1.82	0.61
3:a:261:ILE:HG22	3:a:265:ARG:NH1	2.16	0.61
1:E:109:PRO:HD2	1:E:161:HIS:CE1	2.36	0.60
2:Q:253:ILE:HG22	3:T:135:ALA:CB	2.27	0.60
5:V:150:TYR:CE2	5:V:154:LEU:HD11	2.37	0.60
4:b:58:LYS:HE2	5:c:90:LYS:NZ	2.16	0.60
1:E:133:TYR:HE1	1:E:355:MET:HB3	1.65	0.60
1:O:252:ASN:HA	1:O:255:PHE:CZ	2.36	0.60
5:V:72:VAL:HG13	5:V:77:PHE:CG	2.35	0.60
5:V:105:ASP:HB3	5:V:109:ASP:H	1.66	0.60
1:H:133:TYR:CE1	1:H:352:PHE:HE1	2.08	0.60
1:I:301:GLY:O	1:I:336:LYS:CB	2.49	0.60
1:M:305:MET:SD	1:M:335:ARG:NE	2.74	0.60
3:T:216:ARG:HG3	3:T:216:ARG:O	2.00	0.60
3:T:251:GLN:C	3:T:255:LYS:HZ3	2.09	0.60
5:V:15:GLU:OE1	5:V:15:GLU:N	2.32	0.60
5:V:97:LEU:HB3	5:V:153:PHE:HE2	1.65	0.60
1:B:207:GLU:O	1:B:210:ARG:HG3	2.02	0.60
1:C:133:TYR:CE2	1:C:352:PHE:CZ	2.89	0.60
1:M:196:ARG:HD2	1:M:253:GLU:CD	2.26	0.60
2:P:284:ILE:HG12	2:S:8:MET:N	2.15	0.60
2:Q:269:ALA:O	2:Q:273:GLU:HB2	2.01	0.60
3:T:240:ILE:CB	4:U:80:CYS:SG	2.83	0.60
5:V:5:TYR:HD1	5:V:79:VAL:HG21	1.67	0.60
1:H:133:TYR:CE1	1:H:352:PHE:CZ	2.89	0.60
1:L:305:MET:HE2	1:L:335:ARG:CB	2.19	0.60
5:c:94:GLU:O	5:c:98:SER:CB	2.49	0.60
3:T:271:ASN:CB	4:U:135:LEU:HD22	2.25	0.60
3:a:268:ILE:HG13	4:b:132:ILE:HD11	1.83	0.60
5:c:140:GLY:O	5:c:142:LYS:N	2.34	0.60
1:J:219:VAL:HG11	1:J:312:ARG:HG2	1.83	0.60
1:M:109:PRO:CD	1:M:161:HIS:NE2	2.63	0.60
1:N:252:ASN:HB2	1:N:255:PHE:HZ	1.62	0.60
1:O:163:VAL:HG13	1:O:175:ILE:HG12	1.84	0.60
2:R:4:ILE:O	2:R:4:ILE:HG22	2.01	0.60
3:T:225:ASN:ND2	3:T:226:GLU:OE1	2.35	0.60
4:U:198:LEU:HD23	4:U:201:MET:HB2	1.84	0.60
5:V:38:THR:HG23	5:V:71:THR:N	2.14	0.60
2:X:279:ASN:CB	3:a:109:HIS:ND1	2.64	0.60
1:B:146:GLY:O	4:U:209:GLU:OE1	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:160:THR:HG22	1:H:162:ASN:ND2	2.17	0.60
4:U:41:ILE:HB	4:U:46:LYS:HD3	1.84	0.60
5:V:48:LEU:HD21	5:V:85:MET:SD	2.42	0.60
5:V:97:LEU:O	5:V:101:PHE:HB2	2.02	0.60
1:H:252:ASN:CA	1:H:255:PHE:CE2	2.79	0.59
1:J:113:LYS:O	1:J:116:ARG:HG2	2.01	0.59
1:O:230:ALA:HB3	1:O:255:PHE:CZ	2.37	0.59
1:O:287:ILE:HD12	1:O:290:ARG:HD2	1.83	0.59
2:X:257:GLU:CG	3:a:131:ARG:NH1	2.65	0.59
1:A:162:ASN:ND2	1:A:281:SER:OG	2.35	0.59
1:G:133:TYR:CE2	1:G:352:PHE:HE1	2.20	0.59
1:K:252:ASN:HA	1:K:255:PHE:CZ	2.34	0.59
1:K:352:PHE:CE1	1:K:355:MET:CG	2.85	0.59
1:H:95:ARG:NH1	3:T:265:ARG:CD	2.63	0.59
1:H:305:MET:SD	1:H:336:LYS:HD2	2.42	0.59
1:M:252:ASN:CA	1:M:255:PHE:CZ	2.85	0.59
3:T:221:ILE:HG21	4:U:98:ARG:CD	2.32	0.59
3:T:251:GLN:HG2	4:U:114:ILE:CD1	2.27	0.59
4:U:48:GLN:OE1	5:V:6:LYS:CE	2.49	0.59
4:U:57:ALA:HB2	5:V:104:PHE:CZ	2.37	0.59
5:V:150:TYR:CZ	5:V:154:LEU:HD21	2.37	0.59
2:W:256:LEU:HG	2:X:260:LEU:HD12	1.85	0.59
5:c:60:MET:HA	5:c:63:GLU:HB2	1.84	0.59
1:L:109:PRO:HD2	1:L:161:HIS:NE2	2.17	0.59
4:U:111:ARG:HA	4:U:114:ILE:HG22	1.85	0.59
2:X:257:GLU:CD	3:a:131:ARG:CZ	2.75	0.59
4:b:132:ILE:HG22	4:b:136:ARG:HG2	1.84	0.59
5:c:60:MET:HE2	5:c:80:MET:HE2	1.84	0.59
1:A:227:MET:HA	1:A:255:PHE:CE1	2.37	0.59
3:T:230:ARG:NH2	4:U:88:LEU:H	1.96	0.59
4:U:159:LEU:O	4:U:162:ARG:HG3	2.02	0.59
5:c:9:VAL:HA	5:c:17:LYS:HE2	1.84	0.59
1:L:133:TYR:CD2	1:L:352:PHE:CZ	2.91	0.59
1:M:230:ALA:CB	1:M:255:PHE:CZ	2.84	0.59
3:T:217:LYS:O	4:U:101:HIS:CE1	2.56	0.59
3:T:219:LEU:HD21	4:U:97:CYS:SG	2.41	0.59
3:T:226:GLU:CG	4:U:93:LEU:CD1	2.69	0.59
1:H:326:LYS:NZ	2:X:219:ASP:HB2	2.18	0.59
2:P:281:MET:CG	2:R:1:MET:HB2	2.32	0.59
3:T:216:ARG:CB	4:U:105:ASP:CG	2.75	0.59
3:a:261:ILE:HG12	3:a:264:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:244:GLU:HB3	4:U:79:ARG:HD2	1.85	0.59
5:V:140:GLY:O	5:V:152:GLU:HB3	2.03	0.59
1:C:252:ASN:CB	1:C:255:PHE:CZ	2.86	0.59
4:U:201:MET:HB3	2:W:80:ASP:CG	2.28	0.59
1:D:334:GLU:O	1:D:338:SER:HB3	2.03	0.59
4:U:54:LEU:HD13	5:V:157:MET:CG	2.33	0.59
3:a:216:ARG:HG3	4:b:105:ASP:CG	2.28	0.59
4:b:77:SER:O	4:b:81:GLN:HA	2.03	0.59
1:D:301:GLY:O	1:D:336:LYS:HA	2.02	0.58
2:P:277:ALA:CB	2:R:1:MET:HG2	2.32	0.58
5:V:82:VAL:HA	5:V:86:LYS:HA	1.84	0.58
1:A:133:TYR:CE1	1:A:352:PHE:CZ	2.90	0.58
1:J:306:TYR:HB2	1:J:309:ILE:HB	1.85	0.58
1:K:305:MET:SD	1:K:336:LYS:HD3	2.42	0.58
3:T:248:PHE:CZ	4:U:71:GLU:CB	2.86	0.58
1:A:133:TYR:HE2	1:A:346:LEU:HD21	1.68	0.58
1:E:333:PRO:C	1:E:335:ARG:H	2.11	0.58
1:K:352:PHE:CD1	1:M:45:VAL:HG21	2.38	0.58
1:N:305:MET:SD	1:N:335:ARG:CD	2.91	0.58
2:P:278:LEU:CD1	2:S:1:MET:CG	2.76	0.58
5:c:43:LYS:HE3	5:c:44:VAL:HG23	1.85	0.58
2:Q:282:THR:O	3:T:106:ILE:HD11	2.03	0.58
5:V:3:ASP:HB3	5:V:6:LYS:HE3	1.85	0.58
5:V:75:ASP:N	5:V:75:ASP:OD1	2.33	0.58
4:b:46:LYS:NZ	5:c:3:ASP:OD2	2.28	0.58
1:L:143:TYR:HB3	1:L:345:ILE:HD13	1.86	0.58
2:Q:261:TYR:CD1	3:T:125:ASP:HB3	2.39	0.58
2:Q:264:LYS:HD2	3:T:128:GLU:OE2	2.02	0.58
3:T:212:LEU:CD2	4:U:112:TYR:CB	2.81	0.58
4:U:54:LEU:HB2	5:V:157:MET:SD	2.43	0.58
4:U:141:ARG:HH12	4:U:144:LEU:HD11	1.68	0.58
2:X:261:TYR:CE1	2:X:265:LEU:CD2	2.87	0.58
4:b:60:GLU:HG3	5:c:103:MET:SD	2.44	0.58
1:C:304:THR:HB	1:C:335:ARG:HD2	1.86	0.58
1:E:283:MET:O	1:E:290:ARG:CZ	2.51	0.58
1:F:109:PRO:HD2	1:F:161:HIS:NE2	2.19	0.58
1:K:169:TYR:OH	1:M:49:GLN:HB3	2.03	0.58
2:P:142:GLU:O	2:P:145:GLU:HG2	2.03	0.58
2:Q:257:GLU:HB3	3:T:128:GLU:O	2.02	0.58
3:T:200:LYS:O	3:T:204:GLU:N	2.20	0.58
3:T:215:ARG:HB3	4:U:108:ASP:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:102:ARG:C	5:V:103:MET:HE2	2.29	0.58
1:B:331:ALA:O	1:B:335:ARG:NH1	2.36	0.58
1:E:283:MET:HA	1:E:290:ARG:CD	2.30	0.58
5:V:11:GLN:HB3	5:V:88:ASP:HA	1.86	0.58
5:V:95:GLU:HG2	5:V:96:GLU:H	1.69	0.58
3:a:215:ARG:HD2	3:a:243:LEU:HD21	1.84	0.58
3:a:219:LEU:HD22	3:a:232:LYS:HZ1	1.69	0.58
5:c:73:ASP:N	5:c:76:GLU:HB2	2.19	0.58
1:K:257:CYS:CB	1:K:258:PRO:CD	2.81	0.58
1:O:333:PRO:C	1:O:335:ARG:H	2.11	0.58
2:P:284:ILE:CG2	2:S:8:MET:HG3	2.23	0.58
2:Q:268:LYS:C	3:T:118:GLU:OE1	2.47	0.58
2:Q:273:GLU:OE1	3:T:114:LYS:NZ	2.37	0.58
2:S:1:MET:HB3	2:S:4:ILE:CD1	2.34	0.58
3:T:208:LYS:CG	4:U:112:TYR:CD2	2.83	0.58
3:T:255:LYS:HA	3:T:258:LYS:HZ3	1.68	0.58
3:a:229:LEU:HD22	4:b:94:GLN:HA	1.85	0.58
5:V:94:GLU:O	5:V:150:TYR:OH	2.20	0.58
5:V:120:MET:O	5:V:124:THR:HG23	2.03	0.58
5:c:121:LEU:HB3	5:c:128:ILE:HD12	1.85	0.58
1:C:252:ASN:CA	1:C:255:PHE:CZ	2.87	0.58
1:L:109:PRO:CG	1:L:161:HIS:NE2	2.67	0.58
2:W:256:LEU:CD1	2:X:260:LEU:CD1	2.77	0.58
2:X:273:GLU:CG	3:a:113:ARG:NH2	2.55	0.58
5:c:97:LEU:HD22	5:c:153:PHE:CZ	2.39	0.58
1:K:102:PRO:O	1:K:129:VAL:HG21	2.03	0.57
1:O:305:MET:CE	1:O:335:ARG:HE	2.16	0.57
2:P:278:LEU:O	2:P:282:THR:CG2	2.52	0.57
3:T:250:LEU:HA	3:T:253:LYS:HZ1	1.69	0.57
4:U:100:LEU:HD23	4:U:103:ARG:NH2	2.19	0.57
1:A:133:TYR:CE1	1:A:352:PHE:CE1	2.92	0.57
1:N:257:CYS:HB3	1:N:258:PRO:HD3	1.86	0.57
2:Q:250:GLU:CD	3:T:139:ARG:HA	2.27	0.57
3:T:215:ARG:NH2	4:U:112:TYR:HD1	2.02	0.57
4:U:60:GLU:HB3	5:V:103:MET:HB3	1.85	0.57
4:U:141:ARG:O	4:U:141:ARG:CZ	2.52	0.57
4:U:175:GLN:HA	4:U:178:LYS:HG2	1.84	0.57
4:U:185:ASN:N	4:U:187:GLU:OE2	2.37	0.57
1:G:133:TYR:CZ	1:G:352:PHE:HE1	2.22	0.57
1:K:230:ALA:HB3	1:K:255:PHE:HZ	1.69	0.57
2:P:282:THR:CA	2:S:3:ALA:CB	2.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:157:ASP:OD2	2:Q:161:LYS:NZ	2.37	0.57
5:V:94:GLU:HG3	5:V:158:LYS:HZ3	1.68	0.57
5:c:113:ASP:HA	5:c:147:ARG:HA	1.84	0.57
1:H:133:TYR:OH	1:H:352:PHE:HE1	1.87	0.57
1:J:305:MET:HE1	1:J:335:ARG:HE	1.70	0.57
1:K:252:ASN:CA	1:K:255:PHE:CZ	2.85	0.57
4:b:45:ARG:HH12	4:b:49:LEU:HG	1.68	0.57
1:D:146:GLY:CA	4:U:173:LEU:CD2	2.82	0.57
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.87	0.57
1:L:230:ALA:HB3	1:L:255:PHE:HZ	1.68	0.57
2:X:132:SER:O	2:X:136:LYS:HG2	2.04	0.57
1:H:133:TYR:CD1	1:H:352:PHE:CZ	2.92	0.57
2:P:284:ILE:HG22	2:R:4:ILE:HG21	1.87	0.57
5:V:7:ALA:O	5:V:11:GLN:HG2	2.04	0.57
3:a:199:GLY:O	3:a:202:GLN:NE2	2.38	0.57
3:a:264:LEU:HD23	3:a:267:ARG:CZ	2.34	0.57
4:b:58:LYS:HE2	5:c:90:LYS:HZ1	1.68	0.57
5:c:97:LEU:HD23	5:c:100:LEU:HD12	1.86	0.57
1:B:230:ALA:CB	1:B:255:PHE:CZ	2.87	0.57
1:B:345:ILE:CD1	4:U:208:PHE:CD1	2.88	0.57
2:P:162:TYR:CE1	2:Q:165:VAL:HG11	2.40	0.57
2:W:91:ARG:HE	2:X:92:ILE:HG13	1.69	0.57
2:W:162:TYR:CE1	2:X:165:VAL:HG11	2.39	0.57
1:A:305:MET:SD	1:A:335:ARG:HB2	2.45	0.57
1:H:253:GLU:HA	1:H:256:ARG:HB2	1.86	0.57
1:I:109:PRO:HD2	1:I:161:HIS:CE1	2.39	0.57
2:P:278:LEU:O	2:P:282:THR:N	2.37	0.57
2:S:4:ILE:HG13	2:S:5:LYS:H	1.67	0.57
4:U:57:ALA:HB2	5:V:104:PHE:CE2	2.40	0.57
2:W:256:LEU:HD23	2:X:256:LEU:HD13	1.85	0.57
1:E:282:ILE:O	1:E:290:ARG:CG	2.53	0.57
2:P:283:SER:CA	2:S:7:LYS:HD2	2.28	0.57
2:Q:260:LEU:CG	2:Q:264:LYS:HE2	2.34	0.57
4:b:43:ALA:HA	5:c:3:ASP:HB3	1.87	0.57
5:c:65:ASP:HB3	5:c:68:GLY:HA2	1.86	0.57
1:K:189:LEU:HD13	1:K:257:CYS:SG	2.45	0.57
2:R:7:LYS:HG2	2:S:8:MET:HE3	1.86	0.57
3:T:213:ALA:O	3:T:218:VAL:HG22	2.05	0.57
4:U:122:ILE:HA	4:U:125:ILE:HG13	1.87	0.57
5:V:27:PHE:O	5:V:29:LEU:N	2.38	0.57
5:V:138:LYS:NZ	5:V:144:ASN:HB3	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:74:ARG:O	4:b:78:THR:HG23	2.05	0.57
1:A:331:ALA:O	1:A:335:ARG:NH1	2.37	0.56
5:V:40:GLU:O	5:V:43:LYS:HG2	2.05	0.56
2:W:166:ALA:CA	2:X:165:VAL:HG21	2.35	0.56
4:b:45:ARG:HH22	4:b:49:LEU:HD21	1.70	0.56
1:A:133:TYR:CD1	1:A:352:PHE:CZ	2.92	0.56
1:E:109:PRO:HD2	1:E:161:HIS:CD2	2.39	0.56
1:L:342:GLY:HA2	1:L:345:ILE:HG22	1.88	0.56
3:T:229:LEU:CD1	4:U:93:LEU:HB3	2.12	0.56
4:U:186:ARG:NH1	4:U:189:GLY:HA3	2.20	0.56
3:a:211:ILE:HG22	3:a:215:ARG:HH22	1.70	0.56
3:a:257:GLN:NE2	4:b:122:ILE:HG13	2.20	0.56
4:b:72:LYS:HE3	4:b:76:LEU:HD11	1.86	0.56
4:b:103:ARG:HA	4:b:106:LYS:HD2	1.87	0.56
1:B:332:PRO:O	1:B:335:ARG:CG	2.31	0.56
1:E:207:GLU:O	1:E:210:ARG:HG3	2.06	0.56
1:J:51:ASP:OD1	1:J:51:ASP:N	2.38	0.56
1:J:219:VAL:CG1	1:J:312:ARG:HG2	2.35	0.56
1:L:252:ASN:HB2	1:L:255:PHE:CZ	2.40	0.56
2:P:56:GLU:C	2:Q:57:LEU:HD21	2.30	0.56
3:T:208:LYS:NZ	3:T:212:LEU:HD11	2.20	0.56
3:T:226:GLU:OE1	4:U:90:PHE:CD2	2.58	0.56
4:U:50:LYS:HD3	5:V:156:PHE:HE1	1.53	0.56
2:W:256:LEU:HD13	2:X:257:GLU:HG2	1.88	0.56
3:a:267:ARG:HH21	4:b:132:ILE:HB	1.70	0.56
4:b:136:ARG:HH11	4:b:140:LYS:HD2	1.70	0.56
5:c:23:ALA:HA	5:c:26:ILE:HD12	1.87	0.56
5:c:101:PHE:HE2	5:c:110:GLY:HA2	1.70	0.56
5:c:105:ASP:OD1	5:c:107:ASN:ND2	2.37	0.56
2:Q:276:HIS:CA	3:T:110:PHE:CD1	2.58	0.56
3:T:215:ARG:HB3	4:U:108:ASP:HB3	1.88	0.56
3:T:262:ASN:O	3:T:266:ASN:ND2	2.37	0.56
5:V:93:SER:OG	5:V:94:GLU:N	2.35	0.56
5:V:114:LEU:HG	5:V:146:GLY:O	2.05	0.56
3:a:230:ARG:HG2	4:b:85:LEU:HB3	1.85	0.56
4:b:63:ARG:HA	4:b:66:GLU:HG3	1.87	0.56
5:c:52:PRO:HB2	5:c:57:LEU:HD23	1.88	0.56
2:Q:276:HIS:C	3:T:110:PHE:CE1	2.77	0.56
3:T:230:ARG:NH2	4:U:88:LEU:N	2.49	0.56
3:a:249:ASP:OD2	4:b:72:LYS:NZ	2.38	0.56
5:c:36:ILE:HB	5:c:72:VAL:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ASN:HA	1:D:255:PHE:HE2	1.60	0.56
1:J:80:ASP:OD2	1:J:84:LYS:NZ	2.39	0.56
1:K:257:CYS:HB2	1:K:258:PRO:HD3	1.87	0.56
2:Q:268:LYS:O	3:T:118:GLU:OE1	2.23	0.56
5:V:155:GLU:HA	5:V:158:LYS:HE2	1.86	0.56
4:b:69:ARG:HD2	4:b:72:LYS:HB3	1.87	0.56
5:c:142:LYS:O	5:c:144:ASN:ND2	2.37	0.56
1:E:305:MET:CE	1:E:336:LYS:CD	2.81	0.56
1:L:342:GLY:CA	1:L:345:ILE:HG22	2.36	0.56
1:M:109:PRO:HD2	1:M:161:HIS:CE1	2.41	0.56
3:T:241:TYR:C	4:U:76:LEU:HD23	2.30	0.56
4:U:154:MET:N	4:U:154:MET:SD	2.79	0.56
5:V:113:ASP:HA	5:V:147:ARG:HA	1.87	0.56
5:V:150:TYR:CE1	5:V:154:LEU:HD21	2.41	0.56
3:a:229:LEU:HD11	4:b:94:GLN:HG3	1.88	0.56
1:H:326:LYS:HZ1	2:X:219:ASP:HB2	1.71	0.56
1:I:189:LEU:CA	1:I:257:CYS:SG	2.93	0.56
3:T:200:LYS:O	3:T:203:THR:OG1	2.23	0.56
3:T:222:ASP:CA	4:U:94:GLN:NE2	2.69	0.56
2:W:91:ARG:NE	2:X:92:ILE:HG13	2.20	0.56
3:a:240:ILE:HD11	4:b:100:LEU:O	2.05	0.56
1:F:51:ASP:OD1	1:F:51:ASP:N	2.39	0.56
1:J:334:GLU:O	1:J:338:SER:HB3	2.06	0.56
1:B:345:ILE:HD13	4:U:208:PHE:CE1	2.40	0.55
1:K:230:ALA:HB3	1:K:255:PHE:CZ	2.41	0.55
1:N:196:ARG:HD2	1:N:253:GLU:OE2	2.06	0.55
3:T:216:ARG:HB3	4:U:105:ASP:CB	2.36	0.55
5:V:105:ASP:C	5:V:108:ALA:H	2.15	0.55
3:a:224:LEU:HB3	3:a:229:LEU:HG	1.87	0.55
4:b:145:ARG:HG2	4:b:147:VAL:HG22	1.88	0.55
4:U:55:GLN:HA	4:U:58:LYS:HG2	1.88	0.55
1:B:146:GLY:HA2	4:U:209:GLU:CB	2.21	0.55
1:F:333:PRO:C	1:F:335:ARG:H	2.14	0.55
1:J:222:ASP:OD1	1:J:315:LYS:NZ	2.40	0.55
1:M:109:PRO:HG2	1:M:161:HIS:NE2	2.20	0.55
3:T:212:LEU:O	3:T:216:ARG:N	2.32	0.55
3:T:217:LYS:HD3	4:U:104:VAL:HG21	1.87	0.55
3:T:234:LYS:HZ2	3:T:237:TRP:CD1	2.25	0.55
3:T:263:VAL:HG22	5:V:150:TYR:HB2	1.87	0.55
3:T:267:ARG:O	3:T:271:ASN:ND2	2.39	0.55
5:V:152:GLU:O	5:V:156:PHE:CB	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:110:GLU:O	4:b:114:ILE:HG12	2.06	0.55
2:P:214:TYR:CD2	2:Q:211:ALA:HB1	2.42	0.55
5:V:5:TYR:CZ	5:V:76:GLU:HG2	2.41	0.55
1:K:305:MET:HG3	1:K:335:ARG:CD	2.28	0.55
3:T:212:LEU:CA	3:T:215:ARG:HB2	2.31	0.55
4:U:53:LEU:HD13	5:V:121:LEU:CD2	2.36	0.55
4:b:61:LEU:HD22	5:c:99:ASP:HB3	1.88	0.55
1:I:301:GLY:O	1:I:336:LYS:HB3	2.07	0.55
3:T:236:LEU:O	3:T:239:SER:OG	2.12	0.55
1:A:80:ASP:OD2	1:A:84:LYS:NZ	2.40	0.55
1:B:187:ASP:OD2	1:B:191:LYS:NZ	2.39	0.55
2:Q:272:GLU:HG3	3:T:117:GLU:HB2	1.89	0.55
3:T:229:LEU:HD13	4:U:93:LEU:CD1	2.30	0.55
3:T:259:TYR:OH	5:V:105:ASP:OD2	2.16	0.55
5:V:80:MET:SD	5:V:83:ARG:NE	2.80	0.55
5:V:102:ARG:HB3	5:V:102:ARG:CZ	2.36	0.55
3:a:219:LEU:HD22	3:a:232:LYS:NZ	2.21	0.55
1:E:313:MET:CG	1:E:329:ILE:HD13	2.36	0.55
1:K:51:ASP:OD1	1:K:51:ASP:N	2.40	0.55
1:D:257:CYS:HB3	1:D:258:PRO:HD3	1.89	0.55
1:F:25:ASP:HB3	4:U:147:VAL:HG21	0.56	0.55
4:U:41:ILE:HG21	5:V:135:GLU:HG2	1.88	0.55
4:U:100:LEU:CD2	4:U:103:ARG:NH2	2.68	0.55
3:a:215:ARG:HD3	4:b:111:ARG:HH21	1.71	0.55
5:c:102:ARG:HG3	5:c:103:MET:HE2	1.89	0.55
2:Q:257:GLU:CG	3:T:132:ALA:N	2.69	0.55
3:T:208:LYS:HZ1	3:T:212:LEU:HD11	1.72	0.55
5:V:5:TYR:CD1	5:V:79:VAL:HG21	2.42	0.55
2:X:257:GLU:O	2:X:261:TYR:N	2.38	0.55
4:b:54:LEU:HD13	5:c:92:LYS:HZ2	1.72	0.55
1:L:333:PRO:C	1:L:335:ARG:H	2.15	0.54
2:Q:250:GLU:CD	3:T:138:GLN:C	2.75	0.54
3:T:234:LYS:HA	3:T:237:TRP:HB3	1.89	0.54
4:U:51:THR:HB	5:V:161:GLU:HB2	1.89	0.54
4:U:61:LEU:CD2	5:V:100:LEU:CD2	2.85	0.54
4:U:78:THR:O	4:U:81:GLN:NE2	2.39	0.54
1:F:227:MET:HE3	1:F:255:PHE:CE1	2.42	0.54
1:H:227:MET:HB3	1:H:255:PHE:HE1	1.73	0.54
1:D:23:GLY:C	4:U:183:LYS:HD2	2.32	0.54
1:D:51:ASP:OD1	1:D:51:ASP:N	2.39	0.54
1:M:257:CYS:HB3	1:M:258:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:284:ILE:N	2:S:4:ILE:HA	2.22	0.54
3:T:227:ASP:O	3:T:231:GLU:HG3	2.08	0.54
3:T:247:LYS:HG2	4:U:111:ARG:HA	1.88	0.54
5:V:14:GLU:HG3	5:V:18:ASN:ND2	2.22	0.54
1:F:169:TYR:OH	1:H:49:GLN:CG	2.55	0.54
4:U:136:ARG:HA	4:U:139:PHE:CD2	2.42	0.54
5:V:11:GLN:NE2	5:V:161:GLU:OE2	2.32	0.54
2:X:261:TYR:OH	2:X:265:LEU:HD23	2.08	0.54
5:c:5:TYR:HD2	5:c:82:VAL:HG23	1.72	0.54
5:c:9:VAL:HG13	5:c:17:LYS:HE2	1.87	0.54
3:T:241:TYR:HA	4:U:80:CYS:HB3	1.89	0.54
4:U:83:LEU:HD11	4:U:100:LEU:HD21	1.86	0.54
4:U:196:ASP:OD2	4:U:199:SER:N	2.39	0.54
5:V:112:ILE:HD13	5:V:117:LEU:HD13	1.89	0.54
5:V:137:MET:SD	5:V:144:ASN:HA	2.48	0.54
2:X:257:GLU:CB	3:a:131:ARG:HH12	2.09	0.54
3:a:257:GLN:HB3	4:b:121:ASN:HB3	1.89	0.54
3:a:267:ARG:HD2	5:c:150:TYR:HD2	1.72	0.54
1:A:252:ASN:CB	1:A:255:PHE:CZ	2.91	0.54
1:A:301:GLY:C	1:A:336:LYS:HA	2.33	0.54
1:B:257:CYS:HB3	1:B:258:PRO:HD3	1.90	0.54
1:D:230:ALA:HB3	1:D:255:PHE:CZ	2.43	0.54
1:D:230:ALA:HB3	1:D:255:PHE:HZ	1.71	0.54
1:E:207:GLU:CA	1:E:210:ARG:HG2	2.37	0.54
1:N:335:ARG:C	1:N:337:TYR:H	2.15	0.54
2:Q:282:THR:HG21	2:R:1:MET:CE	2.22	0.54
4:b:137:GLY:C	4:b:139:PHE:H	2.15	0.54
1:F:169:TYR:OH	1:H:49:GLN:CB	2.56	0.54
2:R:4:ILE:O	2:R:4:ILE:CG2	2.55	0.54
3:T:250:LEU:HD13	4:U:115:GLU:CA	2.38	0.54
5:c:4:ILE:HG13	5:c:5:TYR:N	2.22	0.54
1:A:51:ASP:OD1	1:A:51:ASP:N	2.39	0.54
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.90	0.54
1:D:133:TYR:CD2	1:D:352:PHE:HZ	2.26	0.54
2:Q:251:LYS:HA	3:T:139:ARG:HH21	0.58	0.54
2:Q:264:LYS:HD2	3:T:128:GLU:CD	2.33	0.54
3:T:227:ASP:OD2	3:T:227:ASP:N	2.41	0.54
3:T:238:GLN:NE2	3:T:241:TYR:HB3	2.23	0.54
4:U:46:LYS:HE3	5:V:139:ASP:OD1	2.07	0.54
5:c:90:LYS:HE3	5:c:161:GLU:HG3	1.88	0.54
1:H:154:ASP:O	1:H:156:GLY:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:260:LEU:CD1	2:Q:264:LYS:HE2	2.38	0.54
3:T:226:GLU:OE1	4:U:90:PHE:HD2	1.90	0.54
5:V:100:LEU:O	5:V:103:MET:HB2	2.07	0.54
5:V:101:PHE:CE1	5:V:112:ILE:HG13	2.43	0.54
1:F:169:TYR:OH	1:H:49:GLN:HG3	2.08	0.54
4:U:88:LEU:HB3	4:U:92:GLU:OE2	2.08	0.54
4:b:88:LEU:HD22	4:b:92:GLU:HB3	1.90	0.54
5:c:27:PHE:HE2	5:c:77:PHE:CZ	2.26	0.54
1:E:313:MET:O	1:E:317:ILE:HD12	2.09	0.53
1:G:257:CYS:HB2	1:G:258:PRO:HD3	1.89	0.53
4:U:46:LYS:HD2	5:V:139:ASP:HB2	1.89	0.53
5:V:117:LEU:HG	5:V:121:LEU:HD12	1.89	0.53
3:a:208:LYS:HB2	4:b:112:TYR:HE2	1.73	0.53
3:a:227:ASP:HA	3:a:230:ARG:HD2	1.90	0.53
5:c:61:ILE:O	5:c:65:ASP:N	2.41	0.53
5:c:64:VAL:HG21	5:c:72:VAL:HG13	1.89	0.53
1:B:109:PRO:CD	1:B:161:HIS:CD2	2.87	0.53
1:B:222:ASP:OD1	1:B:315:LYS:NZ	2.42	0.53
1:L:207:GLU:O	1:L:210:ARG:CG	2.56	0.53
3:T:216:ARG:HD2	4:U:101:HIS:NE2	2.23	0.53
4:U:54:LEU:HD11	5:V:97:LEU:CD1	2.38	0.53
4:b:134:ASP:HB3	4:b:138:LYS:HE3	1.89	0.53
5:c:101:PHE:CE2	5:c:110:GLY:HA2	2.43	0.53
5:c:140:GLY:N	5:c:156:PHE:HB2	2.23	0.53
1:O:164:PRO:HG2	1:O:171:LEU:HB2	1.90	0.53
1:O:257:CYS:HB3	1:O:258:PRO:HD3	1.91	0.53
3:T:250:LEU:HA	3:T:253:LYS:NZ	2.23	0.53
3:T:255:LYS:HG2	3:T:258:LYS:HZ1	1.72	0.53
3:T:259:TYR:CD2	5:V:102:ARG:HB2	2.43	0.53
4:U:150:SER:HB2	4:U:154:MET:SD	2.48	0.53
1:E:335:ARG:C	1:E:337:TYR:H	2.16	0.53
4:U:60:GLU:HG2	5:V:120:MET:SD	2.48	0.53
5:V:26:ILE:HG12	5:V:27:PHE:HA	1.90	0.53
4:b:89:GLY:N	4:b:92:GLU:OE1	2.22	0.53
4:b:128:LEU:HA	4:b:131:LYS:HB3	1.91	0.53
1:H:333:PRO:C	1:H:335:ARG:H	2.15	0.53
1:N:305:MET:HE3	1:N:335:ARG:NH2	2.22	0.53
2:Q:250:GLU:CD	3:T:139:ARG:N	2.67	0.53
2:Q:265:LEU:HB2	3:T:125:ASP:OD2	2.09	0.53
3:a:201:ARG:HH21	3:a:204:GLU:CD	2.16	0.53
3:a:216:ARG:HA	4:b:105:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:194:ASN:C	4:U:195:ILE:HD13	2.33	0.53
2:W:256:LEU:HD12	2:X:260:LEU:HD13	1.84	0.53
3:a:243:LEU:HA	3:a:246:GLU:CD	2.34	0.53
2:P:149:LYS:HG2	2:P:153:HIS:CD2	2.43	0.53
2:P:256:LEU:HD11	2:Q:257:GLU:OE2	2.09	0.53
2:P:256:LEU:HD21	3:T:131:ARG:CD	2.38	0.53
4:U:119:THR:O	4:U:123:THR:HG23	2.09	0.53
4:U:147:VAL:O	4:U:148:ARG:NH1	2.42	0.53
5:V:94:GLU:HG3	5:V:158:LYS:NZ	2.24	0.53
5:V:118:LYS:O	5:V:122:GLN:HG2	2.08	0.53
3:a:244:GLU:OE1	4:b:79:ARG:NE	2.42	0.53
5:c:38:THR:O	5:c:57:LEU:HD13	2.09	0.53
1:F:109:PRO:CD	1:F:161:HIS:NE2	2.72	0.53
1:H:257:CYS:HB3	1:H:258:PRO:HD3	1.91	0.53
1:L:222:ASP:OD1	1:L:315:LYS:NZ	2.41	0.53
1:O:230:ALA:CB	1:O:255:PHE:CE2	2.92	0.53
2:Q:165:VAL:O	2:Q:169:LEU:N	2.42	0.53
2:Q:254:ASP:OD1	3:T:132:ALA:HB1	2.08	0.53
3:T:234:LYS:HZ2	3:T:237:TRP:CG	2.27	0.53
3:T:271:ASN:HB3	4:U:135:LEU:HD23	1.88	0.53
5:V:10:GLU:HB3	5:V:11:GLN:HE21	1.73	0.53
5:c:44:VAL:HA	5:c:47:MET:HE3	1.91	0.53
5:c:52:PRO:HG2	5:c:60:MET:HE1	1.90	0.53
1:A:352:PHE:CD1	1:A:355:MET:HG3	2.44	0.53
5:V:48:LEU:HG	5:V:50:GLN:H	1.74	0.53
2:X:247:THR:HG22	3:a:138:GLN:HG2	1.91	0.53
5:c:28:VAL:HG13	5:c:34:GLY:HA2	1.91	0.53
5:c:89:SER:OG	5:c:161:GLU:OE1	2.20	0.53
1:B:305:MET:HE2	1:B:335:ARG:C	2.34	0.53
1:F:326:LYS:CE	2:W:177:GLU:OE2	2.52	0.53
1:L:305:MET:CE	1:L:335:ARG:CB	2.65	0.53
1:M:51:ASP:N	1:M:51:ASP:OD1	2.41	0.53
1:M:301:GLY:O	1:M:336:LYS:CB	2.55	0.53
2:P:146:ILE:HG23	2:P:147:GLN:N	2.23	0.53
4:U:121:ASN:O	4:U:124:GLU:HG3	2.09	0.53
5:V:105:ASP:HA	5:V:107:ASN:OD1	2.09	0.53
1:N:187:ASP:OD2	1:N:191:LYS:NZ	2.42	0.52
2:P:284:ILE:HG12	2:S:8:MET:HA	1.91	0.52
3:T:212:LEU:HD22	4:U:109:GLU:CA	2.32	0.52
3:T:256:GLN:HE22	4:U:68:ARG:HH22	1.55	0.52
4:U:170:ARG:NH1	4:U:173:LEU:HD11	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:264:LEU:HD11	4:b:125:ILE:HA	1.90	0.52
1:A:133:TYR:CE2	1:A:352:PHE:CE1	2.83	0.52
1:B:154:ASP:OD2	1:B:161:HIS:HB2	2.09	0.52
1:B:305:MET:CE	1:B:335:ARG:CB	2.76	0.52
1:C:230:ALA:HB3	1:C:255:PHE:HZ	1.75	0.52
1:G:133:TYR:CD2	1:G:352:PHE:CZ	2.97	0.52
1:L:252:ASN:HA	1:L:255:PHE:CZ	2.43	0.52
1:L:252:ASN:CB	1:L:255:PHE:CZ	2.92	0.52
5:V:126:GLU:O	5:V:128:ILE:HG12	2.09	0.52
1:B:207:GLU:HA	1:B:210:ARG:CG	2.32	0.52
1:G:196:ARG:HD2	1:G:253:GLU:CD	2.34	0.52
1:I:305:MET:HE1	1:I:335:ARG:HG2	1.90	0.52
4:U:128:LEU:HD23	4:U:131:LYS:HG3	1.91	0.52
5:V:101:PHE:O	5:V:105:ASP:N	2.22	0.52
1:K:113:LYS:O	1:K:116:ARG:HG2	2.08	0.52
1:L:133:TYR:CD2	1:L:352:PHE:HZ	2.25	0.52
1:M:301:GLY:N	1:M:336:LYS:HB2	2.24	0.52
1:O:227:MET:HA	1:O:255:PHE:CE1	2.44	0.52
2:R:3:ALA:HB3	3:T:106:ILE:HD12	1.91	0.52
3:T:238:GLN:HE22	3:T:241:TYR:HD2	1.58	0.52
3:T:267:ARG:HH21	5:V:151:ASP:HB3	1.75	0.52
5:V:58:GLN:NE2	5:V:58:GLN:O	2.43	0.52
5:V:82:VAL:HG12	5:V:87:ASP:H	1.74	0.52
1:H:227:MET:HA	1:H:255:PHE:HZ	1.75	0.52
1:L:207:GLU:HA	1:L:210:ARG:CG	2.32	0.52
1:M:252:ASN:CB	1:M:255:PHE:CZ	2.92	0.52
2:P:282:THR:O	2:S:3:ALA:CA	2.58	0.52
4:U:136:ARG:HA	4:U:139:PHE:HB2	1.91	0.52
5:V:59:GLU:HA	5:V:62:ASP:OD2	2.08	0.52
1:G:133:TYR:CE2	1:G:352:PHE:CE1	2.97	0.52
3:T:221:ILE:CG2	4:U:98:ARG:CD	2.87	0.52
4:U:113:ASP:OD1	4:U:114:ILE:N	2.43	0.52
3:a:232:LYS:HD3	4:b:97:CYS:SG	2.50	0.52
1:B:227:MET:HA	1:B:255:PHE:HE1	1.75	0.52
1:B:301:GLY:C	1:B:336:LYS:HA	2.35	0.52
1:G:335:ARG:C	1:G:337:TYR:H	2.18	0.52
2:Q:273:GLU:N	3:T:114:LYS:CD	2.66	0.52
4:U:127:ASP:O	4:U:131:LYS:HG2	2.10	0.52
5:V:20:PHE:O	5:V:23:ALA:HB3	2.10	0.52
1:B:333:PRO:C	1:B:335:ARG:H	2.17	0.52
1:H:196:ARG:HD2	1:H:253:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:333:PRO:C	1:J:335:ARG:H	2.18	0.52
2:Q:272:GLU:OE1	3:T:117:GLU:CB	2.56	0.52
5:V:14:GLU:HA	5:V:17:LYS:HG2	1.91	0.52
5:V:45:MET:CE	5:V:50:GLN:HG2	2.40	0.52
1:H:95:ARG:CZ	3:T:265:ARG:HB2	2.34	0.52
1:N:257:CYS:CB	1:N:258:PRO:HD3	2.40	0.52
2:Q:264:LYS:HD2	3:T:128:GLU:OE1	2.10	0.52
3:T:263:VAL:N	5:V:110:GLY:HA3	2.25	0.52
5:V:40:GLU:O	5:V:44:VAL:HG23	2.10	0.52
3:a:212:LEU:HA	4:b:108:ASP:OD1	2.10	0.52
3:a:248:PHE:HB3	4:b:72:LYS:HD2	1.92	0.52
4:b:43:ALA:HB1	5:c:3:ASP:O	2.10	0.52
1:B:305:MET:HE2	1:B:335:ARG:O	2.10	0.52
1:E:283:MET:O	1:E:290:ARG:NE	2.43	0.52
1:H:51:ASP:N	1:H:51:ASP:OD1	2.41	0.52
5:V:141:ASP:HB2	5:V:148:ILE:HG12	1.92	0.52
5:V:142:LYS:H	5:V:152:GLU:HG2	1.75	0.52
4:b:60:GLU:OE2	4:b:63:ARG:NH2	2.43	0.52
4:b:76:LEU:HD23	4:b:79:ARG:HH12	1.75	0.52
5:c:80:MET:HA	5:c:83:ARG:HE	1.74	0.52
1:C:133:TYR:CG	1:C:352:PHE:CZ	2.96	0.51
1:D:146:GLY:HA2	4:U:173:LEU:CG	2.37	0.51
1:I:51:ASP:OD1	1:I:51:ASP:N	2.40	0.51
2:Q:221:TYR:O	2:Q:225:ILE:N	2.38	0.51
3:T:222:ASP:HA	4:U:94:GLN:HG2	1.91	0.51
3:a:204:GLU:HA	3:a:207:LYS:HB2	1.93	0.51
3:a:238:GLN:HE21	3:a:242:ASN:HD21	1.58	0.51
3:T:226:GLU:CD	4:U:90:PHE:CD2	2.88	0.51
4:U:50:LYS:HG2	5:V:156:PHE:HZ	1.69	0.51
5:V:154:LEU:HB3	5:V:158:LYS:HZ3	1.76	0.51
3:a:88:ASP:OD1	3:a:88:ASP:N	2.42	0.51
5:c:24:PHE:CE2	5:c:35:CYS:HA	2.44	0.51
1:I:337:TYR:O	1:I:341:ILE:HD12	2.11	0.51
3:T:221:ILE:HG21	4:U:98:ARG:HD2	1.91	0.51
3:T:237:TRP:CD1	4:U:81:GLN:O	2.59	0.51
5:V:69:SER:OG	5:V:70:GLY:N	2.43	0.51
4:b:102:ALA:O	4:b:106:LYS:HG3	2.10	0.51
1:D:133:TYR:CD2	1:D:352:PHE:CE1	2.99	0.51
1:G:335:ARG:CG	1:G:335:ARG:HH11	2.23	0.51
4:U:73:GLY:HA2	4:U:76:LEU:HD12	1.93	0.51
5:V:75:ASP:CG	5:V:76:GLU:HG3	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:109:ASP:HB3	5:V:111:TYR:CE2	2.46	0.51
4:b:53:LEU:HB3	5:c:104:PHE:CZ	2.45	0.51
5:c:32:GLU:OE1	5:c:39:LYS:NZ	2.29	0.51
1:K:133:TYR:CD1	1:K:352:PHE:HZ	2.28	0.51
2:Q:251:LYS:HD3	3:T:139:ARG:NH2	2.24	0.51
4:U:144:LEU:H	4:U:144:LEU:HD12	1.74	0.51
5:V:57:LEU:HA	5:V:60:MET:SD	2.51	0.51
5:V:99:ASP:O	5:V:103:MET:HG2	2.10	0.51
2:X:235:ALA:O	2:X:239:ALA:N	2.43	0.51
5:c:92:LYS:HA	5:c:96:GLU:HB3	1.93	0.51
1:A:332:PRO:O	1:A:335:ARG:CG	2.33	0.51
1:B:305:MET:CE	1:B:335:ARG:O	2.59	0.51
1:E:257:CYS:HB2	1:E:258:PRO:HD3	1.92	0.51
1:L:51:ASP:OD1	1:L:51:ASP:N	2.44	0.51
1:L:109:PRO:CD	1:L:161:HIS:NE2	2.74	0.51
2:Q:240:GLU:O	2:Q:244:ARG:HG3	2.11	0.51
2:Q:276:HIS:CG	3:T:110:PHE:CE1	2.99	0.51
3:T:216:ARG:HB3	4:U:105:ASP:HA	1.93	0.51
3:T:260:GLU:HG3	5:V:98:SER:OG	2.11	0.51
4:U:88:LEU:C	4:U:93:LEU:HD21	2.35	0.51
5:V:53:THR:HG23	5:V:56:GLU:HG2	1.92	0.51
3:a:221:ILE:O	3:a:229:LEU:HD21	2.10	0.51
4:b:50:LYS:HD3	5:c:160:VAL:HG11	1.91	0.51
5:c:64:VAL:CG2	5:c:76:GLU:HB3	2.40	0.51
1:J:305:MET:HE1	1:J:335:ARG:NE	2.25	0.51
1:K:305:MET:HG2	1:K:335:ARG:NE	2.26	0.51
1:L:216:LEU:HG	1:L:238:LYS:CD	2.32	0.51
2:P:284:ILE:HA	2:S:4:ILE:O	2.11	0.51
4:U:61:LEU:HD23	5:V:100:LEU:CD2	2.40	0.51
4:U:141:ARG:HH22	4:U:144:LEU:HD13	1.76	0.51
2:W:218:GLU:OE2	2:X:217:LYS:HB2	2.10	0.51
3:a:257:GLN:HA	4:b:125:ILE:HD11	1.93	0.51
5:c:121:LEU:HA	5:c:124:THR:HG23	1.93	0.51
1:E:207:GLU:O	1:E:210:ARG:CG	2.59	0.51
1:H:95:ARG:NH1	3:T:265:ARG:CG	2.73	0.51
1:H:196:ARG:HD2	1:H:253:GLU:CD	2.36	0.51
1:H:326:LYS:CE	2:X:215:SER:HB3	2.31	0.51
1:O:163:VAL:HG22	1:O:175:ILE:HG23	1.91	0.51
2:Q:268:LYS:O	2:Q:269:ALA:C	2.51	0.51
3:T:202:GLN:NE2	3:T:206:GLU:OE2	2.44	0.51
3:T:243:LEU:CB	4:U:111:ARG:HD3	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:105:ASP:O	5:V:108:ALA:N	2.38	0.51
4:b:48:GLN:HB2	5:c:126:GLU:CD	2.36	0.51
1:B:207:GLU:O	1:B:210:ARG:CG	2.59	0.51
1:J:326:LYS:HE2	2:W:254:ASP:CB	2.40	0.51
1:L:230:ALA:HB3	1:L:255:PHE:CZ	2.46	0.51
3:T:217:LYS:HB2	3:T:236:LEU:HD13	1.92	0.51
3:T:247:LYS:HD2	4:U:110:GLU:HB3	1.93	0.51
3:T:250:LEU:HD13	4:U:115:GLU:HA	1.92	0.51
3:T:260:GLU:O	3:T:263:VAL:HB	2.10	0.51
2:X:265:LEU:HD12	2:X:265:LEU:O	2.10	0.51
3:a:206:GLU:O	3:a:210:LYS:HD3	2.11	0.51
4:b:108:ASP:O	4:b:112:TYR:HB2	2.11	0.51
5:c:5:TYR:CG	5:c:79:VAL:HG13	2.46	0.51
1:A:252:ASN:HB2	1:A:255:PHE:CZ	2.45	0.51
1:F:154:ASP:OD2	1:F:161:HIS:HB3	2.11	0.51
1:I:109:PRO:HG2	1:I:161:HIS:NE2	2.25	0.51
1:J:335:ARG:C	1:J:337:TYR:N	2.69	0.51
2:P:57:LEU:N	2:Q:57:LEU:CD2	2.74	0.51
2:Q:253:ILE:HG22	3:T:135:ALA:HB1	1.93	0.51
2:Q:273:GLU:CB	3:T:114:LYS:HE2	2.38	0.51
5:V:94:GLU:OE1	5:V:158:LYS:HA	2.11	0.51
1:H:160:THR:HG22	1:H:162:ASN:CG	2.36	0.50
1:H:252:ASN:HB2	1:H:255:PHE:CZ	2.47	0.50
1:O:230:ALA:HB3	1:O:255:PHE:HZ	1.75	0.50
2:X:253:ILE:O	2:X:257:GLU:N	2.43	0.50
3:a:226:GLU:O	3:a:230:ARG:HG3	2.11	0.50
1:A:230:ALA:HB3	1:A:255:PHE:CZ	2.42	0.50
1:C:230:ALA:HB3	1:C:255:PHE:CZ	2.46	0.50
1:H:216:LEU:O	1:H:254:ARG:HG2	2.10	0.50
1:N:51:ASP:OD1	1:N:51:ASP:N	2.44	0.50
1:O:230:ALA:CB	1:O:255:PHE:HE2	2.23	0.50
2:W:88:LEU:CD1	2:X:85:VAL:HG13	2.15	0.50
2:X:272:GLU:HB2	3:a:113:ARG:HH21	1.76	0.50
1:E:143:TYR:OH	1:G:45:VAL:O	2.22	0.50
2:Q:246:VAL:HG11	3:T:141:ARG:NH2	2.25	0.50
3:T:121:VAL:CG1	3:T:122:SER:N	2.73	0.50
3:T:205:ARG:NH2	3:T:208:LYS:HB3	2.26	0.50
5:V:17:LYS:HA	5:V:20:PHE:HB2	1.92	0.50
2:W:84:ASP:OD1	2:W:84:ASP:O	2.30	0.50
5:c:136:LEU:HD22	5:c:156:PHE:HE1	1.77	0.50
1:L:133:TYR:CG	1:L:352:PHE:HZ	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:133:TYR:CE1	1:M:352:PHE:HZ	2.29	0.50
3:T:244:GLU:OE2	4:U:79:ARG:C	2.54	0.50
4:U:55:GLN:O	4:U:59:GLN:HG2	2.11	0.50
4:U:83:LEU:HD11	4:U:100:LEU:CD2	2.42	0.50
5:V:106:LYS:NZ	5:V:116:GLU:HA	2.26	0.50
5:V:141:ASP:OD2	5:V:146:GLY:N	2.44	0.50
5:c:61:ILE:HA	5:c:64:VAL:HG22	1.92	0.50
2:Q:265:LEU:O	2:Q:269:ALA:HB3	2.11	0.50
3:T:200:LYS:HE3	3:T:204:GLU:HB2	1.94	0.50
3:T:248:PHE:HA	3:T:251:GLN:CD	2.36	0.50
3:T:254:PHE:CE1	4:U:121:ASN:CB	2.88	0.50
4:U:48:GLN:CD	5:V:3:ASP:CG	2.69	0.50
2:W:91:ARG:HG2	2:X:92:ILE:HD12	1.92	0.50
2:W:194:GLU:OE2	2:W:198:LYS:NZ	2.44	0.50
5:c:53:THR:O	5:c:56:GLU:N	2.44	0.50
1:A:352:PHE:CE1	1:A:355:MET:CB	2.95	0.50
1:C:331:ALA:O	1:C:335:ARG:NH1	2.44	0.50
1:I:167:GLU:O	1:I:169:TYR:CD1	2.65	0.50
1:L:109:PRO:HG2	1:L:161:HIS:NE2	2.27	0.50
5:V:81:MET:HE3	5:V:85:MET:HB3	1.94	0.50
3:a:247:LYS:HE3	4:b:79:ARG:NH2	2.22	0.50
5:c:5:TYR:CD1	5:c:79:VAL:HG13	2.46	0.50
1:M:133:TYR:CD1	1:M:352:PHE:HZ	2.30	0.50
1:O:334:GLU:O	1:O:338:SER:HB3	2.11	0.50
3:T:250:LEU:CD1	4:U:114:ILE:HG23	2.41	0.50
2:X:261:TYR:OH	2:X:265:LEU:CD2	2.60	0.50
1:N:305:MET:HE3	1:N:335:ARG:HH21	1.69	0.50
2:Q:250:GLU:OE1	3:T:139:ARG:HG2	2.12	0.50
2:Q:279:ASN:OD1	3:T:107:GLU:OE1	2.30	0.50
3:T:267:ARG:NE	5:V:151:ASP:H	2.06	0.50
3:T:269:ASN:HA	3:T:272:GLN:HB2	1.93	0.50
1:D:24:ASP:O	4:U:180:ASP:HB3	2.11	0.50
1:O:207:GLU:CA	1:O:210:ARG:HG2	2.42	0.50
3:T:245:ALA:HB2	4:U:76:LEU:HG	1.93	0.50
1:A:333:PRO:C	1:A:335:ARG:H	2.20	0.49
1:C:80:ASP:OD2	1:C:84:LYS:NZ	2.45	0.49
1:E:80:ASP:OD2	1:E:84:LYS:NZ	2.45	0.49
1:I:260:THR:HA	1:I:263:GLN:O	2.12	0.49
1:O:222:ASP:OD1	1:O:315:LYS:NZ	2.44	0.49
5:V:5:TYR:HD1	5:V:79:VAL:CG2	2.25	0.49
5:V:81:MET:C	5:V:84:CYS:H	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:107:ASN:OD1	5:V:107:ASN:N	2.32	0.49
2:X:252:SER:O	2:X:256:LEU:N	2.45	0.49
5:c:28:VAL:HA	5:c:31:ALA:HB3	1.94	0.49
5:c:97:LEU:HD22	5:c:153:PHE:CE2	2.47	0.49
5:c:151:ASP:O	5:c:155:GLU:HG3	2.12	0.49
1:K:305:MET:SD	1:K:336:LYS:CD	2.99	0.49
3:T:212:LEU:CD2	4:U:112:TYR:HB2	2.42	0.49
3:T:212:LEU:HD23	3:T:215:ARG:CD	2.42	0.49
3:T:261:ILE:HD11	4:U:125:ILE:HG22	0.69	0.49
4:U:64:GLU:OE1	4:U:68:ARG:NH2	2.45	0.49
5:V:121:LEU:HD22	5:V:128:ILE:CD1	2.42	0.49
2:W:166:ALA:HA	2:X:165:VAL:CG2	2.42	0.49
3:a:230:ARG:HA	4:b:85:LEU:HD12	1.93	0.49
1:A:168:GLY:CA	1:C:47:MET:HE2	2.42	0.49
1:G:333:PRO:C	1:G:335:ARG:N	2.70	0.49
1:K:333:PRO:C	1:K:335:ARG:H	2.18	0.49
1:K:352:PHE:HD1	1:M:45:VAL:HG21	1.75	0.49
3:T:236:LEU:HD11	4:U:104:VAL:CG2	2.41	0.49
3:T:252:GLU:O	3:T:256:GLN:HG3	2.12	0.49
4:U:134:ASP:O	4:U:138:LYS:HD3	2.12	0.49
4:U:147:VAL:HG13	4:U:148:ARG:HD2	1.92	0.49
5:V:10:GLU:CB	5:V:11:GLN:HE21	2.25	0.49
1:G:24:ASP:CG	4:b:146:ARG:HG3	2.37	0.49
1:H:216:LEU:O	1:H:254:ARG:NE	2.36	0.49
1:J:306:TYR:C	1:J:308:GLY:H	2.19	0.49
1:M:207:GLU:O	1:M:210:ARG:CG	2.61	0.49
1:O:227:MET:HA	1:O:255:PHE:CZ	2.47	0.49
2:Q:246:VAL:CG1	3:T:142:ASN:HD21	2.23	0.49
2:Q:260:LEU:HB3	3:T:128:GLU:HG2	1.94	0.49
2:Q:260:LEU:HD11	2:Q:264:LYS:HE2	1.94	0.49
3:T:200:LYS:HG3	3:T:204:GLU:HB2	1.95	0.49
4:U:41:ILE:HD11	5:V:138:LYS:CB	2.39	0.49
5:V:121:LEU:O	5:V:124:THR:OG1	2.20	0.49
5:V:130:GLU:CD	5:V:133:ILE:HB	2.37	0.49
2:Y:4:ILE:O	2:Y:5:LYS:C	2.53	0.49
1:D:148:THR:CG2	4:U:169:LEU:HD11	2.37	0.49
2:P:284:ILE:HG12	2:S:8:MET:CA	2.43	0.49
5:V:104:PHE:CD1	5:V:112:ILE:HD11	2.48	0.49
5:V:107:ASN:ND2	5:V:115:ASP:OD2	2.45	0.49
3:a:237:TRP:NE1	4:b:80:CYS:SG	2.85	0.49
1:E:133:TYR:CD2	1:E:352:PHE:CE1	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:262:PHE:CE2	1:L:312:ARG:HG3	2.47	0.49
1:L:345:ILE:HG23	1:L:346:LEU:N	2.27	0.49
1:M:257:CYS:CB	1:M:258:PRO:HD3	2.43	0.49
2:P:162:TYR:HE1	2:Q:165:VAL:HG11	1.78	0.49
2:P:277:ALA:HB1	2:R:1:MET:CG	2.40	0.49
3:T:259:TYR:CG	5:V:102:ARG:HB2	2.47	0.49
4:b:44:SER:OG	4:b:48:GLN:OE1	2.27	0.49
4:b:146:ARG:HH22	5:c:50:GLN:CD	2.21	0.49
5:c:143:ASN:ND2	5:c:152:GLU:HG3	2.27	0.49
5:c:149:ASP:O	5:c:153:PHE:N	2.41	0.49
1:F:257:CYS:CB	1:F:258:PRO:HD3	2.42	0.49
1:H:334:GLU:O	1:H:338:SER:HB3	2.12	0.49
1:J:335:ARG:O	1:J:337:TYR:N	2.45	0.49
2:Q:246:VAL:O	2:Q:250:GLU:N	2.45	0.49
3:T:205:ARG:HG3	3:T:209:LYS:CE	2.41	0.49
3:T:247:LYS:HZ1	4:U:110:GLU:HG2	1.78	0.49
3:T:250:LEU:HD13	4:U:115:GLU:N	2.28	0.49
5:V:104:PHE:O	5:V:106:LYS:HG2	2.12	0.49
4:b:53:LEU:HB3	5:c:104:PHE:HZ	1.78	0.49
1:F:335:ARG:C	1:F:337:TYR:H	2.19	0.49
1:G:24:ASP:OD1	4:b:146:ARG:CG	2.54	0.49
3:T:241:TYR:HA	4:U:80:CYS:CB	2.42	0.49
4:U:46:LYS:CD	5:V:139:ASP:HB2	2.42	0.49
5:V:45:MET:O	5:V:48:LEU:HB3	2.12	0.49
3:a:266:ASN:ND2	5:c:110:GLY:HA3	2.28	0.49
5:c:54:PRO:O	5:c:58:GLN:CB	2.61	0.49
5:c:92:LYS:HZ1	5:c:161:GLU:HG3	1.77	0.49
1:A:143:TYR:CD2	1:C:44:MET:CE	2.96	0.49
3:T:257:GLN:O	3:T:261:ILE:HG12	2.13	0.49
4:U:183:LYS:HG2	4:U:184:GLU:OE2	2.13	0.49
5:V:19:GLU:H	5:V:19:GLU:CD	2.21	0.49
5:V:92:LYS:HD2	5:V:160:VAL:O	2.13	0.49
4:b:51:THR:OG1	4:b:55:GLN:NE2	2.43	0.49
4:b:77:SER:O	4:b:82:PRO:HD3	2.12	0.49
5:c:132:ASP:O	5:c:136:LEU:HG	2.13	0.49
5:c:137:MET:HA	5:c:148:ILE:HD11	1.95	0.49
1:E:107:GLU:HG3	1:E:134:VAL:HG12	1.94	0.49
1:H:328:LYS:HZ3	2:X:212:GLU:HG3	1.76	0.49
1:J:187:ASP:OD2	1:J:191:LYS:NZ	2.45	0.49
1:L:189:LEU:HB2	1:L:257:CYS:SG	2.52	0.49
3:T:222:ASP:HB3	4:U:94:GLN:HE21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:89:GLY:C	4:U:93:LEU:HG	2.38	0.49
5:V:121:LEU:HD23	5:V:124:THR:CG2	2.39	0.49
3:a:261:ILE:HG21	4:b:124:GLU:CD	2.38	0.49
5:c:35:CYS:SG	5:c:36:ILE:N	2.83	0.49
5:c:63:GLU:HB3	5:c:83:ARG:HD2	1.95	0.49
1:C:162:ASN:ND2	1:C:281:SER:OG	2.45	0.48
1:D:302:GLY:C	1:D:304:THR:H	2.21	0.48
1:D:305:MET:SD	1:D:335:ARG:NE	2.86	0.48
2:Q:257:GLU:CB	3:T:132:ALA:CA	2.91	0.48
2:Q:276:HIS:CD2	3:T:110:PHE:CE1	2.94	0.48
4:U:46:LYS:CE	5:V:139:ASP:CG	2.86	0.48
4:U:53:LEU:CD1	5:V:121:LEU:HG	2.33	0.48
4:U:178:LYS:HA	4:U:181:THR:OG1	2.13	0.48
4:U:202:GLU:OE2	4:U:202:GLU:N	2.42	0.48
5:c:54:PRO:O	5:c:58:GLN:HB3	2.12	0.48
1:L:109:PRO:HB2	1:L:161:HIS:NE2	2.28	0.48
1:O:109:PRO:HB2	1:O:163:VAL:HG21	1.94	0.48
5:c:121:LEU:O	5:c:124:THR:OG1	2.22	0.48
1:K:129:VAL:CG2	1:K:130:PRO:HD2	2.42	0.48
1:N:230:ALA:HB3	1:N:255:PHE:CZ	2.49	0.48
5:V:109:ASP:HB3	5:V:111:TYR:CZ	2.48	0.48
2:X:70:LYS:O	2:X:74:ALA:N	2.42	0.48
2:X:261:TYR:CE1	2:X:265:LEU:CB	2.96	0.48
3:a:219:LEU:HD11	4:b:101:HIS:HB3	1.95	0.48
3:a:244:GLU:OE2	4:b:103:ARG:NH2	2.46	0.48
4:b:58:LYS:O	4:b:62:GLU:HG2	2.12	0.48
5:c:96:GLU:O	5:c:100:LEU:HG	2.13	0.48
1:C:107:GLU:OE1	1:C:116:ARG:HB3	2.13	0.48
1:I:336:LYS:HE2	1:I:337:TYR:CE2	2.49	0.48
2:P:39:LEU:O	2:P:43:LEU:N	2.46	0.48
4:U:56:ILE:CB	5:V:124:THR:HA	2.43	0.48
5:V:131:ASP:HB3	5:V:135:GLU:HG3	1.96	0.48
3:a:200:LYS:HG3	3:a:201:ARG:NH2	2.28	0.48
5:c:13:THR:HB	5:c:15:GLU:OE1	2.13	0.48
5:c:97:LEU:O	5:c:101:PHE:HB2	2.13	0.48
1:H:95:ARG:HH12	3:T:265:ARG:CG	2.26	0.48
2:P:284:ILE:CG1	2:S:7:LYS:C	2.81	0.48
2:Q:11:LEU:N	2:Q:14:ASP:OD2	2.47	0.48
3:T:256:GLN:HG2	5:V:102:ARG:CZ	2.43	0.48
4:U:48:GLN:HG2	5:V:3:ASP:OD2	2.14	0.48
1:A:302:GLY:C	1:A:304:THR:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:240:ILE:HG23	4:U:107:VAL:CG1	2.41	0.48
4:U:204:ARG:HH12	2:W:76:LYS:CD	2.27	0.48
5:V:73:ASP:O	5:V:77:PHE:HB3	2.13	0.48
2:X:127:MET:O	2:X:131:GLU:N	2.45	0.48
3:a:240:ILE:HG13	4:b:104:VAL:HG22	1.96	0.48
3:a:255:LYS:HB2	4:b:68:ARG:HH21	1.78	0.48
4:b:81:GLN:CD	4:b:81:GLN:H	2.21	0.48
4:b:152:ASP:O	4:b:156:GLN:HG2	2.13	0.48
1:A:133:TYR:CE2	1:A:346:LEU:HD21	2.48	0.48
1:E:252:ASN:HA	1:E:255:PHE:HE2	1.76	0.48
1:I:154:ASP:OD2	1:I:161:HIS:HB3	2.13	0.48
1:M:109:PRO:HB2	1:M:161:HIS:NE2	2.29	0.48
3:T:226:GLU:HB3	3:T:230:ARG:HH12	1.79	0.48
4:U:45:ARG:NH1	5:V:126:GLU:OE2	2.34	0.48
4:b:148:ARG:HA	5:c:84:CYS:O	2.13	0.48
5:c:36:ILE:HA	5:c:40:GLU:HB3	1.95	0.48
1:C:187:ASP:OD2	1:C:191:LYS:NZ	2.46	0.48
1:E:289:ILE:O	1:E:293:LEU:HG	2.13	0.48
1:H:352:PHE:CE1	1:H:355:MET:HB2	2.48	0.48
2:Q:250:GLU:CD	3:T:139:ARG:CA	2.87	0.48
2:Q:257:GLU:O	3:T:128:GLU:HB3	2.13	0.48
3:T:232:LYS:NZ	3:T:236:LEU:HB2	2.28	0.48
5:V:104:PHE:C	5:V:116:GLU:HB3	2.39	0.48
5:c:36:ILE:HD13	5:c:44:VAL:HG11	1.95	0.48
5:c:43:LYS:HA	5:c:46:ARG:HG3	1.95	0.48
1:B:146:GLY:HA3	4:U:209:GLU:CD	2.32	0.48
1:L:110:LEU:H	1:L:161:HIS:HE1	1.61	0.48
5:V:117:LEU:HB3	5:V:133:ILE:HG23	1.96	0.48
3:a:209:LYS:HD2	3:a:209:LYS:HA	1.63	0.48
4:b:53:LEU:HD21	5:c:121:LEU:HG	1.95	0.48
5:c:101:PHE:CE1	5:c:112:ILE:HG13	2.49	0.48
5:c:113:ASP:OD1	5:c:114:LEU:N	2.43	0.48
1:M:162:ASN:ND2	1:M:281:SER:OG	2.46	0.48
1:M:352:PHE:CD1	1:M:355:MET:HG3	2.48	0.48
4:b:134:ASP:HA	4:b:138:LYS:HG3	1.95	0.48
5:c:60:MET:HG2	5:c:83:ARG:NH1	2.29	0.48
1:B:302:GLY:C	1:B:304:THR:H	2.22	0.47
1:E:106:THR:CG2	1:E:140:LEU:CD1	2.92	0.47
1:F:196:ARG:HD2	1:F:253:GLU:CD	2.39	0.47
1:I:300:SER:OG	1:I:338:SER:OG	2.26	0.47
1:N:252:ASN:CA	1:N:255:PHE:CZ	2.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:236:LEU:CG	4:U:104:VAL:CG1	2.90	0.47
3:T:250:LEU:HD12	4:U:114:ILE:HG23	1.95	0.47
4:U:47:LEU:CD2	5:V:4:ILE:HG13	2.44	0.47
5:V:88:ASP:C	5:V:90:LYS:H	2.21	0.47
3:a:252:GLU:OE1	3:a:255:LYS:NZ	2.26	0.47
1:I:169:TYR:OH	1:K:49:GLN:CB	2.61	0.47
1:O:207:GLU:C	1:O:210:ARG:HG2	2.39	0.47
3:T:205:ARG:HG3	3:T:209:LYS:HE3	1.95	0.47
3:T:213:ALA:CA	3:T:216:ARG:HG2	2.41	0.47
4:U:60:GLU:HG2	5:V:120:MET:HE1	1.95	0.47
5:V:81:MET:O	5:V:84:CYS:N	2.40	0.47
5:V:129:THR:N	5:V:132:ASP:OD2	2.25	0.47
2:X:247:THR:CG2	3:a:138:GLN:HG3	2.44	0.47
2:X:266:LYS:O	2:X:270:ILE:HG13	2.14	0.47
5:c:17:LYS:N	5:c:17:LYS:HD2	2.30	0.47
1:B:133:TYR:HE2	1:B:346:LEU:HD21	1.78	0.47
5:V:105:ASP:CB	5:V:109:ASP:H	2.27	0.47
5:V:137:MET:CG	5:V:141:ASP:HB3	2.45	0.47
3:a:210:LYS:HA	3:a:213:ALA:HB3	1.95	0.47
3:a:264:LEU:HD22	4:b:128:LEU:HB2	1.97	0.47
4:b:56:ILE:O	4:b:59:GLN:NE2	2.47	0.47
4:b:91:ALA:HA	4:b:94:GLN:OE1	2.14	0.47
1:B:211:ASP:OD1	1:B:215:LYS:NZ	2.46	0.47
1:C:107:GLU:OE2	1:C:116:ARG:NE	2.43	0.47
1:C:335:ARG:C	1:C:337:TYR:H	2.23	0.47
1:I:169:TYR:OH	1:K:49:GLN:HB3	2.15	0.47
1:K:352:PHE:CE1	1:K:355:MET:HB3	2.48	0.47
2:S:4:ILE:CG1	2:S:5:LYS:N	2.76	0.47
5:V:14:GLU:HG3	5:V:18:ASN:HD21	1.77	0.47
5:c:5:TYR:CD2	5:c:82:VAL:HG23	2.49	0.47
1:A:227:MET:HA	1:A:255:PHE:HE1	1.78	0.47
1:C:252:ASN:O	1:C:256:ARG:HG2	2.13	0.47
1:L:133:TYR:HE1	1:L:355:MET:HB3	1.78	0.47
3:T:266:ASN:CG	5:V:111:TYR:HD2	2.22	0.47
4:U:204:ARG:NH2	2:W:73:LEU:CD2	2.78	0.47
1:E:133:TYR:CG	1:E:352:PHE:CZ	3.02	0.47
1:O:335:ARG:C	1:O:337:TYR:H	2.22	0.47
5:V:11:GLN:CD	5:V:89:SER:H	2.22	0.47
5:V:109:ASP:N	5:V:109:ASP:OD1	2.45	0.47
2:W:218:GLU:HG2	2:X:221:TYR:CE1	2.49	0.47
2:W:221:TYR:HB3	2:X:221:TYR:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:157:ASP:OD2	2:X:161:LYS:NZ	2.41	0.47
3:a:205:ARG:NH1	3:a:209:LYS:HG2	2.29	0.47
3:a:226:GLU:HG2	4:b:93:LEU:HD12	1.96	0.47
3:a:245:ALA:HA	4:b:72:LYS:HE3	1.95	0.47
4:b:60:GLU:O	5:c:103:MET:HE3	2.13	0.47
1:A:133:TYR:CZ	1:A:352:PHE:HZ	2.17	0.47
1:A:352:PHE:CE1	1:A:355:MET:HB2	2.50	0.47
1:D:154:ASP:O	1:D:155:SER:C	2.58	0.47
1:E:289:ILE:O	1:E:289:ILE:HG22	2.15	0.47
1:G:133:TYR:CD2	1:G:352:PHE:CE1	3.02	0.47
1:M:133:TYR:CZ	1:M:352:PHE:HZ	2.33	0.47
1:M:207:GLU:O	1:M:210:ARG:HG3	2.15	0.47
1:N:196:ARG:HD2	1:N:253:GLU:CD	2.39	0.47
2:P:53:THR:CA	2:Q:57:LEU:HD11	2.39	0.47
2:P:142:GLU:CA	2:P:145:GLU:OE2	2.58	0.47
3:T:212:LEU:HA	3:T:215:ARG:HD2	1.97	0.47
3:T:215:ARG:HH11	4:U:112:TYR:HB2	1.64	0.47
4:U:49:LEU:HD11	5:V:132:ASP:OD1	2.15	0.47
5:V:92:LYS:HZ3	5:V:161:GLU:CD	2.22	0.47
2:W:256:LEU:CD2	2:X:256:LEU:HB3	2.44	0.47
2:X:236:GLU:OE2	3:a:149:GLN:OE1	2.30	0.47
3:a:226:GLU:HB2	4:b:90:PHE:CE2	2.50	0.47
3:a:247:LYS:NZ	4:b:79:ARG:HE	2.12	0.47
3:a:266:ASN:HD22	5:c:110:GLY:HA3	1.79	0.47
1:E:106:THR:CG2	1:E:140:LEU:HD11	2.45	0.47
1:G:252:ASN:HB2	1:G:255:PHE:HZ	1.77	0.47
1:L:133:TYR:CZ	1:L:352:PHE:CE1	2.85	0.47
3:T:247:LYS:HA	4:U:114:ILE:HG21	1.97	0.47
4:U:48:GLN:CD	5:V:6:LYS:NZ	2.68	0.47
5:V:45:MET:HE2	5:V:50:GLN:HG2	1.97	0.47
5:V:93:SER:C	5:V:97:LEU:HD13	2.40	0.47
5:V:101:PHE:CZ	5:V:150:TYR:HA	2.50	0.47
2:X:268:LYS:C	2:X:272:GLU:HG2	2.37	0.47
3:a:248:PHE:O	3:a:252:GLU:HG2	2.15	0.47
5:c:80:MET:HA	5:c:83:ARG:NE	2.29	0.47
1:A:164:PRO:HD3	1:A:281:SER:HB3	1.96	0.47
1:B:154:ASP:OD2	1:B:161:HIS:CB	2.63	0.47
1:G:188:TYR:CD2	1:G:257:CYS:HA	2.50	0.47
1:K:252:ASN:CB	1:K:255:PHE:HZ	2.21	0.47
3:T:247:LYS:NZ	4:U:110:GLU:HG2	2.29	0.47
3:T:256:GLN:O	3:T:259:TYR:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:263:VAL:HG13	3:T:267:ARG:HD2	1.95	0.47
3:T:271:ASN:HD21	4:U:136:ARG:HE	1.63	0.47
4:U:99:GLN:O	4:U:103:ARG:HG3	2.15	0.47
5:V:12:LEU:HD12	5:V:87:ASP:HB2	1.97	0.47
5:V:84:CYS:C	5:V:86:LYS:HZ2	2.23	0.47
5:V:103:MET:HE2	5:V:103:MET:N	2.30	0.47
5:V:156:PHE:CE2	5:V:157:MET:HE2	2.50	0.47
5:c:64:VAL:HB	5:c:76:GLU:HB3	1.97	0.47
1:A:282:ILE:CG2	1:A:294:TYR:CZ	2.98	0.47
1:C:333:PRO:C	1:C:335:ARG:H	2.23	0.47
1:E:301:GLY:C	1:E:336:LYS:HA	2.40	0.47
1:H:282:ILE:O	1:H:290:ARG:HG2	2.15	0.47
1:K:80:ASP:OD2	1:K:84:LYS:NZ	2.48	0.47
1:K:352:PHE:CE1	1:K:355:MET:HB2	2.50	0.47
2:P:279:ASN:CA	2:P:282:THR:HG23	2.43	0.47
3:T:212:LEU:CD2	4:U:112:TYR:HB3	2.41	0.47
5:V:14:GLU:CA	5:V:17:LYS:HE2	2.43	0.47
5:V:113:ASP:HA	5:V:147:ARG:HB2	1.96	0.47
5:V:121:LEU:HB3	5:V:128:ILE:HG21	1.96	0.47
5:V:134:GLU:OE2	5:V:137:MET:HB3	2.15	0.47
2:W:218:GLU:OE2	2:X:214:TYR:HA	2.15	0.47
2:X:257:GLU:OE1	3:a:131:ARG:HD3	2.15	0.47
3:a:248:PHE:CD2	4:b:72:LYS:HB2	2.50	0.47
5:c:93:SER:O	5:c:97:LEU:N	2.48	0.47
5:c:145:ASP:HB2	5:c:147:ARG:O	2.15	0.47
1:A:133:TYR:CE1	1:A:352:PHE:HZ	2.33	0.46
1:B:308:GLY:O	1:B:312:ARG:HB3	2.14	0.46
1:L:133:TYR:HE2	1:L:346:LEU:HD21	1.81	0.46
2:P:85:VAL:O	2:P:89:ASN:N	2.45	0.46
3:T:232:LYS:NZ	3:T:236:LEU:HD22	2.30	0.46
4:U:100:LEU:HD23	4:U:103:ARG:HH21	1.71	0.46
4:U:201:MET:HB3	2:W:80:ASP:OD1	2.15	0.46
5:V:157:MET:SD	5:V:160:VAL:HB	2.56	0.46
3:a:248:PHE:HA	3:a:251:GLN:CD	2.40	0.46
1:E:108:ALA:HB1	1:E:161:HIS:ND1	2.30	0.46
3:T:240:ILE:CG1	4:U:104:VAL:HB	2.45	0.46
3:T:241:TYR:N	4:U:80:CYS:SG	2.89	0.46
5:V:43:LYS:O	5:V:46:ARG:HB2	2.15	0.46
5:V:140:GLY:O	5:V:142:LYS:N	2.48	0.46
5:V:149:ASP:O	5:V:152:GLU:HB2	2.15	0.46
3:a:247:LYS:HG2	3:a:251:GLN:NE2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:247:LYS:HD3	4:b:110:GLU:HB3	1.97	0.46
5:c:74:PHE:O	5:c:78:LEU:HG	2.15	0.46
5:c:104:PHE:HB3	5:c:112:ILE:HG12	1.96	0.46
5:c:112:ILE:N	5:c:148:ILE:O	2.45	0.46
1:D:116:ARG:NH2	1:D:375:PHE:CE1	2.83	0.46
2:Q:272:GLU:HG3	3:T:117:GLU:HB3	1.89	0.46
2:Q:276:HIS:CG	3:T:110:PHE:CZ	2.98	0.46
5:V:129:THR:O	5:V:133:ILE:HG12	2.15	0.46
3:a:224:LEU:HD21	3:a:232:LYS:HB3	1.98	0.46
3:a:225:ASN:N	3:a:228:GLN:HB3	2.31	0.46
1:B:262:PHE:CE2	1:B:312:ARG:HG2	2.49	0.46
1:E:143:TYR:CE2	1:G:44:MET:HE2	2.51	0.46
1:L:335:ARG:C	1:L:337:TYR:H	2.23	0.46
3:T:251:GLN:O	3:T:255:LYS:HG3	2.16	0.46
5:V:10:GLU:OE1	5:V:161:GLU:HG3	2.14	0.46
5:V:92:LYS:HE2	5:V:161:GLU:HA	1.96	0.46
5:V:105:ASP:CG	5:V:109:ASP:H	2.23	0.46
3:a:248:PHE:CD1	4:b:72:LYS:HA	2.49	0.46
3:a:260:GLU:HG3	5:c:98:SER:HB3	1.98	0.46
1:J:326:LYS:NZ	2:W:254:ASP:HA	2.30	0.46
1:K:129:VAL:HG22	1:K:130:PRO:HD2	1.97	0.46
1:L:109:PRO:HD2	1:L:161:HIS:CE1	2.50	0.46
2:P:78:ALA:O	2:P:82:GLU:N	2.47	0.46
4:U:198:LEU:HD23	4:U:198:LEU:O	2.15	0.46
5:V:38:THR:C	5:V:39:LYS:HD3	2.41	0.46
5:V:106:LYS:HE3	5:V:119:ILE:HB	1.96	0.46
2:W:84:ASP:OD1	2:W:88:LEU:CG	2.42	0.46
2:X:261:TYR:HA	2:X:264:LYS:HB3	1.97	0.46
3:a:261:ILE:HD11	4:b:125:ILE:HG13	1.98	0.46
5:c:94:GLU:O	5:c:98:SER:HB2	2.15	0.46
5:c:107:ASN:ND2	5:c:116:GLU:OE2	2.47	0.46
1:B:133:TYR:CG	1:B:352:PHE:CZ	2.96	0.46
1:B:133:TYR:CE1	1:B:355:MET:HB3	2.50	0.46
1:M:133:TYR:CE1	1:M:352:PHE:CZ	3.03	0.46
1:M:133:TYR:CG	1:M:352:PHE:HZ	2.33	0.46
1:O:154:ASP:O	1:O:156:GLY:N	2.49	0.46
2:P:193:LEU:O	2:P:197:LEU:N	2.45	0.46
3:T:216:ARG:CG	4:U:105:ASP:OD1	2.64	0.46
3:T:222:ASP:CG	4:U:94:GLN:NE2	2.74	0.46
3:T:226:GLU:HG2	4:U:88:LEU:O	2.16	0.46
3:a:113:ARG:NH2	3:a:117:GLU:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:244:GLU:CD	4:b:79:ARG:HG3	2.40	0.46
1:D:80:ASP:OD2	1:D:84:LYS:NZ	2.48	0.46
1:K:305:MET:HG2	1:K:335:ARG:HE	1.81	0.46
1:M:133:TYR:CZ	1:M:352:PHE:CZ	3.03	0.46
1:N:336:LYS:HG2	1:N:337:TYR:CD1	2.51	0.46
3:T:236:LEU:HD11	4:U:104:VAL:CB	2.45	0.46
5:V:38:THR:HA	5:V:41:LEU:HD12	1.97	0.46
5:V:106:LYS:HZ1	5:V:116:GLU:HA	1.79	0.46
3:a:267:ARG:NH2	4:b:136:ARG:HH21	2.14	0.46
5:c:36:ILE:HB	5:c:72:VAL:O	2.16	0.46
1:E:110:LEU:H	1:E:161:HIS:HE1	1.63	0.46
1:I:154:ASP:O	1:I:156:GLY:N	2.48	0.46
2:P:56:GLU:C	2:Q:57:LEU:CD2	2.88	0.46
2:Q:40:GLU:HA	2:Q:40:GLU:OE1	2.16	0.46
3:T:210:LYS:HD2	3:T:214:GLU:OE2	2.16	0.46
3:T:248:PHE:CZ	4:U:71:GLU:HB3	2.51	0.46
4:U:83:LEU:CD1	4:U:100:LEU:CD2	2.84	0.46
1:A:230:ALA:CB	1:A:255:PHE:CZ	2.98	0.46
1:N:300:SER:OG	1:N:338:SER:OG	2.31	0.46
5:V:121:LEU:HA	5:V:124:THR:CG2	2.45	0.46
2:X:260:LEU:C	2:X:260:LEU:CD2	2.86	0.46
3:a:240:ILE:HG23	4:b:107:VAL:HG21	1.98	0.46
3:a:267:ARG:HD2	5:c:150:TYR:CD2	2.51	0.46
4:b:125:ILE:O	4:b:129:THR:CB	2.63	0.46
5:c:95:GLU:H	5:c:95:GLU:CD	2.24	0.46
1:C:252:ASN:CA	1:C:255:PHE:CE2	2.77	0.46
1:H:328:LYS:HZ1	2:X:212:GLU:HG3	1.81	0.46
1:H:352:PHE:CE1	1:H:355:MET:CB	2.99	0.46
1:I:257:CYS:HB3	1:I:258:PRO:HD3	1.95	0.46
1:L:257:CYS:CB	1:L:258:PRO:CD	2.68	0.46
2:P:149:LYS:HG2	2:P:153:HIS:NE2	2.30	0.46
3:T:249:ASP:CG	4:U:72:LYS:CD	2.89	0.46
4:U:58:LYS:NZ	5:V:161:GLU:OXT	2.49	0.46
5:V:141:ASP:HA	5:V:152:GLU:CD	2.41	0.46
5:V:158:LYS:HA	5:V:158:LYS:HD3	1.70	0.46
4:b:101:HIS:O	4:b:104:VAL:HB	2.16	0.46
5:c:24:PHE:HE2	5:c:35:CYS:HA	1.81	0.46
1:D:333:PRO:C	1:D:335:ARG:N	2.70	0.45
1:L:336:LYS:HE2	1:L:336:LYS:HB3	1.67	0.45
3:T:222:ASP:HB2	3:T:223:HIS:CE1	2.51	0.45
4:U:204:ARG:HH12	2:W:76:LYS:CE	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:12:LEU:HD23	5:V:17:LYS:NZ	2.31	0.45
2:X:278:LEU:O	2:X:279:ASN:C	2.54	0.45
3:a:219:LEU:HD21	4:b:101:HIS:CB	2.45	0.45
5:c:9:VAL:HA	5:c:17:LYS:CE	2.46	0.45
5:c:135:GLU:HG3	5:c:136:LEU:N	2.29	0.45
1:B:80:ASP:OD2	1:B:84:LYS:NZ	2.49	0.45
1:N:56:ASP:OD1	1:N:56:ASP:N	2.48	0.45
3:T:239:SER:O	3:T:243:LEU:HG	2.16	0.45
3:T:253:LYS:HE2	3:T:253:LYS:HB2	1.65	0.45
4:U:48:GLN:CD	5:V:6:LYS:HZ3	2.05	0.45
5:V:38:THR:N	5:V:70:GLY:HA2	2.30	0.45
5:V:114:LEU:HD13	5:V:133:ILE:HG22	1.97	0.45
3:a:255:LYS:HB2	4:b:68:ARG:NH2	2.31	0.45
5:c:104:PHE:C	5:c:112:ILE:HG12	2.41	0.45
1:C:230:ALA:CB	1:C:255:PHE:CE2	2.99	0.45
1:C:250:ILE:HG23	1:C:253:GLU:HB2	1.99	0.45
1:H:257:CYS:CB	1:H:258:PRO:HD3	2.46	0.45
1:K:230:ALA:CB	1:K:255:PHE:CZ	2.99	0.45
2:Q:214:TYR:O	2:Q:218:GLU:HG3	2.16	0.45
3:T:200:LYS:HD2	3:T:203:THR:OG1	2.16	0.45
3:T:232:LYS:HA	3:T:235:GLU:OE1	2.16	0.45
3:T:241:TYR:HD1	4:U:80:CYS:HB3	1.81	0.45
4:b:133:PHE:O	4:b:137:GLY:HA3	2.16	0.45
1:A:133:TYR:HE2	1:A:346:LEU:CD2	2.28	0.45
1:B:108:ALA:HB1	1:B:161:HIS:CE1	2.52	0.45
1:F:109:PRO:CD	1:F:161:HIS:CD2	2.95	0.45
1:J:162:ASN:HD21	1:J:278:THR:HA	1.82	0.45
1:K:169:TYR:OH	1:M:49:GLN:CB	2.65	0.45
3:T:210:LYS:HD2	3:T:214:GLU:CD	2.41	0.45
3:T:267:ARG:HD2	5:V:150:TYR:HB3	1.98	0.45
5:V:60:MET:HG3	5:V:65:ASP:OD1	2.16	0.45
3:a:225:ASN:O	3:a:229:LEU:N	2.33	0.45
4:b:57:ALA:HB1	5:c:100:LEU:HA	1.98	0.45
5:c:36:ILE:O	5:c:72:VAL:N	2.24	0.45
5:c:101:PHE:CE2	5:c:150:TYR:HB2	2.52	0.45
1:C:51:ASP:OD1	1:C:51:ASP:N	2.49	0.45
1:J:302:GLY:C	1:J:304:THR:H	2.25	0.45
1:M:207:GLU:CA	1:M:210:ARG:HG2	2.42	0.45
1:N:333:PRO:C	1:N:335:ARG:N	2.75	0.45
2:Q:246:VAL:O	2:Q:250:GLU:HG3	2.16	0.45
2:Q:276:HIS:HA	3:T:110:PHE:HE1	0.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:54:LEU:HB2	5:V:157:MET:HE3	1.99	0.45
3:a:227:ASP:OD1	3:a:228:GLN:N	2.50	0.45
1:A:116:ARG:NH2	1:A:375:PHE:CE1	2.84	0.45
1:B:146:GLY:CA	4:U:209:GLU:HB3	2.08	0.45
1:E:133:TYR:CG	1:E:352:PHE:HZ	2.34	0.45
1:H:352:PHE:CD1	1:H:355:MET:HG3	2.51	0.45
1:I:304:THR:OG1	1:I:335:ARG:HD2	2.16	0.45
1:L:133:TYR:CG	1:L:352:PHE:CZ	3.05	0.45
2:Q:127:MET:O	2:Q:131:GLU:N	2.45	0.45
2:Q:261:TYR:CA	3:T:128:GLU:OE1	2.59	0.45
2:Q:272:GLU:HB2	3:T:118:GLU:OE1	2.17	0.45
4:U:56:ILE:HD12	4:U:59:GLN:HG3	1.99	0.45
5:V:45:MET:HG3	5:V:48:LEU:HD23	1.97	0.45
2:W:256:LEU:CG	2:X:260:LEU:CD1	2.94	0.45
3:a:254:PHE:CZ	4:b:117:LYS:HB3	2.52	0.45
3:a:267:ARG:NE	4:b:132:ILE:HD13	2.32	0.45
5:c:64:VAL:O	5:c:66:GLU:HG3	2.17	0.45
1:M:133:TYR:CE2	1:M:352:PHE:HZ	2.35	0.45
1:N:109:PRO:CD	1:N:161:HIS:CD2	2.87	0.45
2:W:204:LEU:O	2:W:208:GLU:N	2.49	0.45
4:b:145:ARG:HH12	5:c:56:GLU:HA	1.81	0.45
2:P:101:ARG:O	2:P:105:ARG:HG3	2.16	0.45
5:V:88:ASP:OD2	5:V:89:SER:N	2.50	0.45
5:V:91:GLY:HA2	5:V:159:GLY:HA3	1.99	0.45
5:V:117:LEU:HA	5:V:117:LEU:HD12	1.65	0.45
5:V:118:LYS:HD3	5:V:133:ILE:HG13	1.97	0.45
5:V:129:THR:OG1	5:V:131:ASP:HB2	2.17	0.45
2:X:272:GLU:CB	3:a:113:ARG:CZ	2.94	0.45
3:a:211:ILE:O	3:a:214:GLU:HG3	2.17	0.45
3:a:240:ILE:HG22	4:b:80:CYS:HB2	1.98	0.45
1:F:196:ARG:HD2	1:F:253:GLU:OE2	2.16	0.45
1:M:227:MET:HA	1:M:255:PHE:CE1	2.51	0.45
1:O:51:ASP:OD1	1:O:51:ASP:N	2.50	0.45
2:P:162:TYR:HE1	2:Q:165:VAL:CG1	2.30	0.45
3:a:217:LYS:O	4:b:101:HIS:NE2	2.50	0.45
3:a:250:LEU:HD22	4:b:115:GLU:HA	1.98	0.45
3:a:263:VAL:O	3:a:267:ARG:HD3	2.17	0.45
4:b:69:ARG:NE	4:b:72:LYS:HE2	2.32	0.45
4:b:146:ARG:HH12	5:c:50:GLN:HG2	1.81	0.45
5:c:58:GLN:O	5:c:61:ILE:HB	2.16	0.45
1:A:143:TYR:CZ	1:C:44:MET:CE	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ALA:CB	1:A:255:PHE:HZ	2.27	0.45
2:P:274:LEU:HD13	2:Q:274:LEU:HB3	1.98	0.45
2:P:282:THR:HB	2:S:3:ALA:CB	2.47	0.45
3:T:241:TYR:O	4:U:76:LEU:HD23	2.16	0.45
4:U:46:LYS:HE3	5:V:139:ASP:HB2	1.97	0.45
4:U:50:LYS:CG	5:V:156:PHE:HE1	2.18	0.45
4:U:54:LEU:HB3	5:V:161:GLU:O	2.17	0.45
5:V:30:GLY:N	5:V:32:GLU:OE1	2.50	0.45
5:V:73:ASP:O	5:V:77:PHE:N	2.42	0.45
3:a:255:LYS:HE3	4:b:68:ARG:HH21	1.82	0.45
4:b:58:LYS:HG3	5:c:100:LEU:CD2	2.40	0.45
4:b:63:ARG:O	4:b:66:GLU:HG3	2.17	0.45
4:b:145:ARG:N	4:b:148:ARG:HE	2.12	0.45
1:L:133:TYR:CE1	1:L:352:PHE:HE1	2.35	0.44
2:P:210:GLN:O	2:P:214:TYR:CG	2.70	0.44
3:T:228:GLN:HE21	3:T:232:LYS:HB2	1.82	0.44
3:T:250:LEU:HD13	4:U:115:GLU:HG3	1.89	0.44
2:X:247:THR:HB	3:a:142:ASN:ND2	2.29	0.44
3:a:237:TRP:HB3	4:b:83:LEU:HD11	1.99	0.44
3:a:254:PHE:HA	3:a:257:GLN:OE1	2.16	0.44
5:c:104:PHE:HB3	5:c:112:ILE:CD1	2.47	0.44
1:J:113:LYS:O	1:J:116:ARG:CG	2.64	0.44
1:K:56:ASP:OD1	1:K:56:ASP:N	2.50	0.44
1:N:108:ALA:HB1	1:N:161:HIS:ND1	2.32	0.44
3:T:247:LYS:HZ1	4:U:110:GLU:CD	2.25	0.44
5:V:36:ILE:HG21	5:V:72:VAL:H	1.82	0.44
5:V:154:LEU:HB3	5:V:158:LYS:NZ	2.31	0.44
3:a:226:GLU:O	4:b:93:LEU:HD13	2.18	0.44
4:b:133:PHE:HB2	5:c:94:GLU:OE2	2.17	0.44
1:H:352:PHE:O	1:H:352:PHE:CG	2.70	0.44
1:I:332:PRO:C	1:I:334:GLU:H	2.24	0.44
1:N:252:ASN:CB	1:N:255:PHE:HZ	2.23	0.44
3:T:241:TYR:CD2	4:U:76:LEU:CD2	2.99	0.44
5:V:111:TYR:CD1	5:V:147:ARG:HB2	2.52	0.44
5:V:112:ILE:CG2	5:V:117:LEU:HB2	2.48	0.44
5:V:151:ASP:OD1	5:V:152:GLU:N	2.50	0.44
3:a:207:LYS:O	3:a:211:ILE:HG13	2.18	0.44
3:a:209:LYS:HA	3:a:212:LEU:HD12	1.98	0.44
3:a:225:ASN:OD1	3:a:226:GLU:N	2.51	0.44
5:c:64:VAL:HG12	5:c:79:VAL:HG12	1.99	0.44
1:B:219:VAL:O	1:B:220:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:ILE:HG12	4:U:180:ASP:OD2	2.17	0.44
1:K:252:ASN:HB2	1:K:255:PHE:CE1	2.50	0.44
2:P:143:ILE:O	2:P:146:ILE:HG22	2.17	0.44
4:U:54:LEU:HB2	5:V:157:MET:CE	2.46	0.44
5:V:111:TYR:CB	5:V:149:ASP:HA	2.46	0.44
3:a:121:VAL:O	3:a:125:ASP:N	2.47	0.44
4:b:68:ARG:HA	4:b:71:GLU:OE1	2.18	0.44
5:c:24:PHE:HA	5:c:27:PHE:CD2	2.52	0.44
5:c:27:PHE:CD2	5:c:36:ILE:HD11	2.52	0.44
5:c:60:MET:HE3	5:c:83:ARG:HH22	1.82	0.44
5:c:120:MET:HE3	5:c:120:MET:HB3	1.80	0.44
1:D:25:ASP:CB	4:U:181:THR:HA	2.46	0.44
1:H:352:PHE:CD1	1:H:355:MET:HB2	2.53	0.44
1:J:169:TYR:OH	1:L:49:GLN:CB	2.64	0.44
1:M:109:PRO:CD	1:M:161:HIS:CD2	2.94	0.44
2:Q:143:ILE:O	2:Q:147:GLN:HG3	2.18	0.44
3:T:226:GLU:CA	4:U:93:LEU:HD12	2.37	0.44
3:T:264:LEU:HD23	3:T:264:LEU:HA	1.77	0.44
3:a:226:GLU:HA	3:a:229:LEU:HD12	2.00	0.44
4:b:41:ILE:HD11	5:c:131:ASP:CG	2.43	0.44
5:c:33:ASP:OD1	5:c:40:GLU:HG2	2.17	0.44
5:c:156:PHE:CZ	5:c:157:MET:HE2	2.53	0.44
1:E:282:ILE:O	1:E:290:ARG:CD	2.65	0.44
1:J:252:ASN:CA	1:J:255:PHE:CZ	2.95	0.44
1:K:352:PHE:O	1:K:352:PHE:CG	2.71	0.44
2:R:7:LYS:HG2	2:S:8:MET:CE	2.46	0.44
3:a:219:LEU:HA	3:a:219:LEU:HD23	1.48	0.44
3:a:254:PHE:O	3:a:258:LYS:HE2	2.17	0.44
4:b:75:ALA:O	4:b:79:ARG:HG2	2.18	0.44
4:b:143:THR:O	4:b:144:LEU:HD23	2.18	0.44
1:M:133:TYR:CD2	1:M:352:PHE:HZ	2.36	0.44
3:T:229:LEU:HD22	4:U:93:LEU:C	2.42	0.44
5:V:46:ARG:N	5:V:52:PRO:HD2	2.33	0.44
5:V:112:ILE:O	5:V:112:ILE:HG22	2.17	0.44
5:V:149:ASP:C	5:V:149:ASP:OD1	2.61	0.44
3:a:229:LEU:CD2	4:b:94:GLN:HA	2.47	0.44
5:c:40:GLU:HG3	5:c:43:LYS:HE2	1.98	0.44
5:c:127:THR:O	5:c:128:ILE:HD13	2.17	0.44
1:B:308:GLY:O	1:B:312:ARG:CB	2.66	0.44
1:C:192:ILE:CD1	1:C:256:ARG:HG3	2.47	0.44
1:D:56:ASP:OD1	1:D:56:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:MET:O	1:E:290:ARG:NH2	2.50	0.44
1:G:252:ASN:CA	1:G:255:PHE:CZ	3.01	0.44
1:I:108:ALA:HB1	1:I:161:HIS:ND1	2.33	0.44
1:M:352:PHE:CD2	1:M:352:PHE:O	2.71	0.44
2:P:218:GLU:OE1	2:Q:214:TYR:CE1	2.71	0.44
1:C:334:GLU:HG2	1:C:341:ILE:HD13	2.00	0.44
1:M:227:MET:HB2	1:M:255:PHE:HE1	1.83	0.44
1:N:335:ARG:O	1:N:337:TYR:N	2.46	0.44
3:T:222:ASP:OD2	3:T:222:ASP:N	2.51	0.44
3:T:233:ALA:CB	4:U:100:LEU:CD1	2.74	0.44
4:U:46:LYS:HD2	5:V:139:ASP:CB	2.48	0.44
4:U:130:GLN:O	4:U:133:PHE:HB2	2.17	0.44
5:V:50:GLN:OE1	5:V:85:MET:HG3	2.18	0.44
5:V:112:ILE:HG21	5:V:117:LEU:HD13	2.00	0.44
3:a:250:LEU:O	3:a:254:PHE:CB	2.63	0.44
1:E:283:MET:CA	1:E:290:ARG:HD3	2.38	0.43
3:T:207:LYS:HD3	3:T:207:LYS:N	2.33	0.43
3:T:236:LEU:HD12	3:T:236:LEU:HA	1.67	0.43
3:T:256:GLN:HE21	4:U:68:ARG:CZ	2.25	0.43
4:U:53:LEU:HA	5:V:124:THR:HG21	2.00	0.43
5:V:145:ASP:C	5:V:147:ARG:H	2.25	0.43
2:W:84:ASP:O	2:W:85:VAL:C	2.60	0.43
5:c:140:GLY:HA3	5:c:148:ILE:HG12	1.99	0.43
1:E:227:MET:HB3	1:E:255:PHE:CZ	2.53	0.43
1:F:275:HIS:ND1	1:F:275:HIS:N	2.64	0.43
1:H:335:ARG:H	1:H:335:ARG:HG2	1.63	0.43
1:L:110:LEU:H	1:L:161:HIS:CE1	2.36	0.43
2:P:214:TYR:HB3	2:Q:214:TYR:CB	2.47	0.43
3:T:216:ARG:CB	4:U:105:ASP:OD1	2.66	0.43
5:V:113:ASP:O	5:V:116:GLU:N	2.51	0.43
5:V:130:GLU:OE2	5:V:133:ILE:HB	2.17	0.43
5:V:151:ASP:O	5:V:152:GLU:C	2.61	0.43
4:b:145:ARG:NH2	5:c:56:GLU:O	2.49	0.43
1:F:25:ASP:CG	4:U:147:VAL:HG21	2.32	0.43
1:F:109:PRO:HB2	1:F:161:HIS:CE1	2.53	0.43
1:G:262:PHE:CE2	1:G:312:ARG:HG2	2.53	0.43
1:I:169:TYR:HH	1:K:49:GLN:HG3	1.82	0.43
2:P:214:TYR:HB3	2:Q:214:TYR:HB2	2.00	0.43
4:U:100:LEU:O	4:U:104:VAL:HG12	2.18	0.43
4:U:170:ARG:HD2	4:U:173:LEU:HD21	2.00	0.43
3:a:221:ILE:O	3:a:224:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:265:ARG:HA	3:a:268:ILE:HB	1.99	0.43
5:c:67:ASP:N	5:c:67:ASP:OD1	2.51	0.43
1:C:302:GLY:C	1:C:304:THR:H	2.26	0.43
1:G:302:GLY:C	1:G:304:THR:H	2.26	0.43
2:Q:257:GLU:OE1	2:Q:257:GLU:HA	2.18	0.43
4:U:61:LEU:HD23	5:V:100:LEU:HD21	2.01	0.43
5:V:36:ILE:HB	5:V:71:THR:HA	1.99	0.43
5:V:72:VAL:HG13	5:V:77:PHE:CD2	2.53	0.43
5:c:40:GLU:HA	5:c:43:LYS:HG3	2.00	0.43
1:O:163:VAL:HG22	1:O:175:ILE:CG2	2.48	0.43
2:Q:260:LEU:HD23	3:T:128:GLU:HG2	1.98	0.43
5:V:94:GLU:CB	5:V:154:LEU:HD22	2.47	0.43
3:a:208:LYS:HE2	4:b:112:TYR:HE2	1.83	0.43
4:b:44:SER:HA	4:b:47:LEU:HB2	2.01	0.43
4:b:61:LEU:O	4:b:64:GLU:HG2	2.18	0.43
1:I:304:THR:CB	1:I:335:ARG:HD2	2.48	0.43
1:L:133:TYR:CD2	1:L:352:PHE:CE1	3.07	0.43
1:L:260:THR:HA	1:L:263:GLN:O	2.18	0.43
1:M:110:LEU:H	1:M:161:HIS:HE1	1.66	0.43
2:Q:277:ALA:O	2:Q:281:MET:N	2.40	0.43
3:T:248:PHE:O	3:T:252:GLU:HG2	2.19	0.43
3:T:254:PHE:CE1	4:U:121:ASN:ND2	2.87	0.43
4:U:61:LEU:HB2	5:V:100:LEU:CD2	2.46	0.43
5:V:156:PHE:HE2	5:V:157:MET:HE2	1.84	0.43
2:X:154:ILE:O	2:X:155:ALA:C	2.59	0.43
1:G:219:VAL:O	1:G:220:ALA:HB3	2.18	0.43
1:I:337:TYR:O	1:I:341:ILE:CD1	2.67	0.43
3:T:229:LEU:HD22	4:U:93:LEU:O	2.19	0.43
4:U:46:LYS:HE3	5:V:139:ASP:CG	2.43	0.43
4:U:64:GLU:HG2	4:U:68:ARG:NE	2.34	0.43
5:V:74:PHE:O	5:V:78:LEU:HD13	2.19	0.43
2:X:261:TYR:CZ	2:X:265:LEU:HD23	2.52	0.43
2:X:273:GLU:HG2	3:a:113:ARG:NH1	2.29	0.43
4:b:147:VAL:C	5:c:50:GLN:HE22	2.27	0.43
5:c:41:LEU:HB3	5:c:57:LEU:HB3	2.00	0.43
1:A:305:MET:SD	1:A:335:ARG:CB	3.07	0.43
1:D:25:ASP:HB3	4:U:181:THR:CA	2.47	0.43
1:D:25:ASP:OD2	4:U:181:THR:HG22	2.17	0.43
1:I:283:MET:O	1:I:290:ARG:NE	2.52	0.43
1:O:305:MET:CE	1:O:335:ARG:HH21	2.31	0.43
3:T:247:LYS:NZ	4:U:110:GLU:CG	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:7:ALA:O	5:V:10:GLU:N	2.51	0.43
5:V:46:ARG:HG3	5:V:52:PRO:HD2	2.00	0.43
5:V:137:MET:SD	5:V:141:ASP:HB3	2.58	0.43
2:X:272:GLU:HB3	3:a:113:ARG:CD	2.41	0.43
3:a:208:LYS:HB2	4:b:112:TYR:CE2	2.54	0.43
4:b:148:ARG:O	4:b:149:ILE:HD13	2.18	0.43
1:A:151:ILE:HG13	1:A:282:ILE:CD1	2.49	0.43
1:B:331:ALA:HB1	1:B:335:ARG:HD3	2.00	0.43
1:G:335:ARG:CG	1:G:335:ARG:NH1	2.80	0.43
1:J:167:GLU:O	1:J:169:TYR:CD1	2.72	0.43
1:M:227:MET:HA	1:M:255:PHE:CZ	2.54	0.43
2:Q:237:THR:O	2:Q:241:PHE:N	2.46	0.43
4:U:201:MET:SD	4:U:201:MET:C	3.02	0.43
4:U:202:GLU:CD	4:U:205:LYS:HZ2	2.27	0.43
5:V:70:GLY:O	5:V:71:THR:OG1	2.36	0.43
5:V:117:LEU:HD22	5:V:148:ILE:HD11	2.00	0.43
3:a:217:LYS:HB2	4:b:101:HIS:CE1	2.54	0.43
5:c:45:MET:HG3	5:c:52:PRO:HD2	1.99	0.43
1:B:334:GLU:OE1	1:B:334:GLU:N	2.51	0.43
1:D:23:GLY:O	4:U:183:LYS:HB2	2.18	0.43
1:D:230:ALA:CB	1:D:255:PHE:CE2	3.02	0.43
1:E:335:ARG:O	1:E:337:TYR:N	2.44	0.43
1:F:182:GLY:O	1:F:213:LYS:NZ	2.52	0.43
1:N:361:GLU:OE2	1:N:373:LYS:NZ	2.52	0.43
2:P:53:THR:HG22	2:Q:57:LEU:HD12	2.01	0.43
2:P:146:ILE:CG2	2:P:147:GLN:N	2.82	0.43
5:V:101:PHE:O	5:V:104:PHE:HB2	2.18	0.43
2:X:277:ALA:O	2:X:281:MET:HG3	2.19	0.43
3:a:221:ILE:HG22	4:b:97:CYS:HB3	2.00	0.43
1:I:169:TYR:CZ	1:K:49:GLN:HG3	2.54	0.42
1:I:301:GLY:O	1:I:336:LYS:HB2	2.19	0.42
4:U:54:LEU:HD11	5:V:97:LEU:HD11	2.00	0.42
4:U:146:ARG:HD3	4:U:149:ILE:HD11	2.01	0.42
3:a:237:TRP:NE1	4:b:80:CYS:HG	2.16	0.42
4:b:105:ASP:O	4:b:108:ASP:HB3	2.19	0.42
1:L:56:ASP:OD1	1:L:56:ASP:N	2.51	0.42
1:L:312:ARG:HA	1:L:312:ARG:HD2	1.91	0.42
1:M:154:ASP:O	1:M:156:GLY:N	2.52	0.42
2:P:156:GLU:CD	2:P:160:ARG:NH2	2.77	0.42
4:U:201:MET:SD	4:U:203:GLY:N	2.92	0.42
5:V:5:TYR:O	5:V:9:VAL:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:112:TYR:O	4:b:115:GLU:HG3	2.20	0.42
4:b:139:PHE:C	4:b:141:ARG:N	2.77	0.42
5:c:102:ARG:CZ	5:c:108:ALA:HB2	2.48	0.42
5:c:114:LEU:HD12	5:c:133:ILE:HG22	2.01	0.42
1:E:79:TRP:HZ3	1:E:83:GLU:OE1	2.02	0.42
1:E:207:GLU:HA	1:E:210:ARG:CG	2.45	0.42
1:F:335:ARG:H	1:F:335:ARG:HG2	1.57	0.42
1:G:188:TYR:CE1	1:G:266:PHE:HB3	2.54	0.42
1:H:217:CYS:SG	1:H:254:ARG:O	2.77	0.42
1:I:244:ASP:OD1	1:I:244:ASP:N	2.49	0.42
1:K:352:PHE:O	1:K:352:PHE:CD2	2.73	0.42
2:X:254:ASP:O	2:X:258:ASP:HB3	2.19	0.42
4:b:154:MET:HE2	4:b:154:MET:N	2.35	0.42
5:c:38:THR:HG23	5:c:57:LEU:HB2	2.01	0.42
5:c:136:LEU:HB3	5:c:156:PHE:CE1	2.54	0.42
1:C:301:GLY:C	1:C:336:LYS:HA	2.45	0.42
1:K:189:LEU:CB	1:K:257:CYS:SG	3.07	0.42
1:M:196:ARG:HD2	1:M:253:GLU:OE2	2.19	0.42
2:Q:265:LEU:CB	3:T:125:ASP:OD2	2.67	0.42
3:T:118:GLU:CD	3:T:121:VAL:HG11	2.44	0.42
5:V:45:MET:HG2	5:V:52:PRO:HD3	2.00	0.42
2:W:154:ILE:O	2:W:158:ALA:N	2.42	0.42
4:b:45:ARG:CZ	5:c:127:THR:HG23	2.49	0.42
1:A:133:TYR:CE1	1:A:352:PHE:HE1	2.35	0.42
1:E:154:ASP:O	1:E:156:GLY:N	2.52	0.42
1:E:219:VAL:O	1:E:220:ALA:HB3	2.20	0.42
1:E:302:GLY:C	1:E:304:THR:H	2.26	0.42
1:I:301:GLY:C	1:I:336:LYS:HB2	2.45	0.42
1:I:305:MET:HE3	1:I:337:TYR:CE1	2.54	0.42
1:M:109:PRO:CB	1:M:161:HIS:NE2	2.82	0.42
1:M:219:VAL:O	1:M:220:ALA:HB3	2.19	0.42
3:T:226:GLU:CB	4:U:93:LEU:HD11	2.47	0.42
3:a:217:LYS:N	4:b:101:HIS:CE1	2.88	0.42
3:a:252:GLU:O	4:b:68:ARG:NH2	2.53	0.42
4:b:145:ARG:NH2	5:c:60:MET:HG3	2.27	0.42
1:B:3:ASP:OD1	1:B:3:ASP:N	2.50	0.42
1:G:133:TYR:CE1	1:G:355:MET:HB3	2.54	0.42
1:L:154:ASP:O	1:L:156:GLY:N	2.51	0.42
2:Q:257:GLU:HB3	3:T:132:ALA:CB	2.40	0.42
3:T:248:PHE:HA	3:T:251:GLN:OE1	2.19	0.42
5:V:105:ASP:HB3	5:V:108:ALA:CA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:145:ARG:H	4:b:148:ARG:NE	2.13	0.42
5:c:27:PHE:O	5:c:43:LYS:NZ	2.52	0.42
5:c:97:LEU:HD12	5:c:154:LEU:HD23	2.00	0.42
5:c:114:LEU:CD1	5:c:133:ILE:HG22	2.49	0.42
5:c:140:GLY:O	5:c:152:GLU:HG2	2.19	0.42
1:A:352:PHE:CG	1:A:352:PHE:O	2.71	0.42
1:E:335:ARG:H	1:E:335:ARG:HG2	1.55	0.42
1:I:110:LEU:H	1:I:161:HIS:HE1	1.68	0.42
1:K:154:ASP:O	1:K:156:GLY:N	2.53	0.42
2:P:284:ILE:HG12	2:S:7:LYS:O	2.19	0.42
2:S:4:ILE:O	2:S:8:MET:HG3	2.19	0.42
3:T:100:ASN:OD1	3:T:100:ASN:N	2.52	0.42
3:T:254:PHE:CD1	4:U:118:VAL:HA	2.54	0.42
4:U:50:LYS:HD2	5:V:156:PHE:CD1	2.48	0.42
4:U:136:ARG:HA	4:U:139:PHE:CG	2.55	0.42
4:U:142:PRO:O	4:U:145:ARG:NE	2.47	0.42
5:V:78:LEU:O	5:V:82:VAL:HG13	2.20	0.42
4:b:49:LEU:HD22	5:c:121:LEU:HD22	2.00	0.42
4:b:50:LYS:CD	5:c:160:VAL:HG11	2.49	0.42
4:b:76:LEU:HD23	4:b:79:ARG:NH1	2.35	0.42
4:b:98:ARG:NH2	4:b:99:GLN:HB3	2.34	0.42
1:D:230:ALA:CB	1:D:255:PHE:CZ	3.02	0.42
1:J:303:THR:O	1:J:306:TYR:HD1	2.01	0.42
1:K:230:ALA:CB	1:K:255:PHE:CE2	3.03	0.42
1:L:332:PRO:HA	1:L:333:PRO:HD3	1.91	0.42
1:M:352:PHE:O	1:M:352:PHE:CG	2.72	0.42
1:O:196:ARG:HD2	1:O:253:GLU:OE2	2.19	0.42
2:Q:50:LEU:O	2:Q:54:GLU:N	2.52	0.42
2:S:8:MET:HE2	2:S:8:MET:HB3	1.85	0.42
3:T:110:PHE:CD1	3:T:110:PHE:C	2.94	0.42
3:T:226:GLU:N	3:T:229:LEU:HD12	2.34	0.42
4:U:52:LEU:CG	5:V:126:GLU:HB2	2.45	0.42
4:U:55:GLN:HG3	4:U:58:LYS:HZ3	1.84	0.42
5:V:134:GLU:CD	5:V:137:MET:HB3	2.45	0.42
5:c:14:GLU:N	5:c:14:GLU:OE1	2.52	0.42
1:D:252:ASN:CB	1:D:255:PHE:HZ	2.27	0.42
2:P:241:PHE:CD2	2:P:241:PHE:C	2.95	0.42
2:Q:54:GLU:O	2:Q:57:LEU:HB2	2.20	0.42
3:T:210:LYS:HD3	3:T:210:LYS:HA	1.66	0.42
3:T:253:LYS:O	3:T:257:GLN:CB	2.68	0.42
4:U:54:LEU:HD13	5:V:157:MET:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:108:ASP:OD1	4:U:111:ARG:NE	2.42	0.42
5:V:21:LYS:C	5:V:21:LYS:HD3	2.45	0.42
5:V:96:GLU:OE2	5:V:97:LEU:HD12	2.20	0.42
5:V:153:PHE:HA	5:V:156:PHE:HB3	2.01	0.42
5:V:155:GLU:CA	5:V:158:LYS:HE2	2.50	0.42
3:a:260:GLU:O	3:a:263:VAL:HB	2.20	0.42
4:b:48:GLN:NE2	5:c:126:GLU:OE2	2.53	0.42
4:b:72:LYS:O	4:b:76:LEU:HG	2.19	0.42
4:b:152:ASP:OD1	4:b:166:SER:HB3	2.20	0.42
5:c:92:LYS:NZ	5:c:161:GLU:HA	2.35	0.42
1:D:133:TYR:CG	1:D:352:PHE:HZ	2.37	0.42
1:H:227:MET:HA	1:H:255:PHE:CZ	2.54	0.42
1:H:352:PHE:HB2	1:J:45:VAL:HG21	2.00	0.42
1:M:230:ALA:CB	1:M:255:PHE:CE2	3.03	0.42
1:O:163:VAL:HA	1:O:164:PRO:HD3	1.94	0.42
2:Q:269:ALA:N	3:T:118:GLU:OE1	2.51	0.42
3:T:243:LEU:CD2	4:U:111:ARG:HD3	2.49	0.42
4:U:46:LYS:CE	5:V:139:ASP:OD1	2.67	0.42
4:U:49:LEU:HD21	5:V:127:THR:O	2.20	0.42
5:V:11:GLN:HE22	5:V:161:GLU:CD	2.25	0.42
5:V:97:LEU:HA	5:V:100:LEU:HD12	2.02	0.42
5:V:114:LEU:HD11	5:V:137:MET:HB2	2.01	0.42
3:a:263:VAL:HG13	5:c:150:TYR:HB2	2.01	0.42
4:b:63:ARG:HH11	4:b:67:GLU:CD	2.28	0.42
4:b:147:VAL:HG12	5:c:52:PRO:HB3	2.00	0.42
5:c:28:VAL:HA	5:c:34:GLY:HA2	2.02	0.42
1:H:302:GLY:C	1:H:304:THR:H	2.27	0.41
1:N:279:TYR:CZ	1:N:283:MET:HE2	2.55	0.41
3:T:236:LEU:CD1	4:U:104:VAL:HG21	2.45	0.41
4:U:48:GLN:CD	5:V:3:ASP:CB	2.93	0.41
4:U:196:ASP:OD2	4:U:196:ASP:C	2.63	0.41
5:V:21:LYS:O	5:V:24:PHE:N	2.54	0.41
5:V:64:VAL:HA	5:V:66:GLU:OE1	2.20	0.41
5:V:142:LYS:HE2	5:V:155:GLU:HG3	2.01	0.41
5:V:142:LYS:HZ1	5:V:156:PHE:HB2	1.84	0.41
2:W:256:LEU:CG	2:X:260:LEU:HD13	2.48	0.41
2:X:272:GLU:C	3:a:113:ARG:CZ	2.93	0.41
2:X:275:ASP:O	3:a:109:HIS:CE1	2.72	0.41
5:c:7:ALA:O	5:c:11:GLN:N	2.28	0.41
1:A:352:PHE:CD1	1:A:355:MET:HB2	2.54	0.41
1:I:109:PRO:HB2	1:I:161:HIS:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:162:ASN:ND2	1:J:277:THR:O	2.52	0.41
1:L:342:GLY:HA2	1:L:345:ILE:CG2	2.49	0.41
1:O:333:PRO:C	1:O:335:ARG:N	2.78	0.41
2:P:156:GLU:CD	2:P:160:ARG:HH22	2.28	0.41
2:Q:272:GLU:HG3	3:T:117:GLU:CA	2.50	0.41
3:T:214:GLU:HG3	3:T:218:VAL:CG2	2.50	0.41
3:T:254:PHE:O	3:T:258:LYS:HG3	2.20	0.41
4:U:173:LEU:HD12	4:U:174:LYS:HD3	2.02	0.41
5:V:11:GLN:HB3	5:V:88:ASP:CA	2.49	0.41
2:X:276:HIS:CE1	3:a:110:PHE:CB	2.89	0.41
5:c:71:THR:OG1	5:c:72:VAL:N	2.53	0.41
5:c:112:ILE:O	5:c:137:MET:HE1	2.20	0.41
1:G:133:TYR:CG	1:G:352:PHE:CZ	3.08	0.41
1:H:219:VAL:O	1:H:220:ALA:HB3	2.21	0.41
1:J:182:GLY:O	1:J:213:LYS:NZ	2.53	0.41
1:K:51:ASP:CG	1:K:52:SER:N	2.78	0.41
1:M:110:LEU:H	1:M:161:HIS:CE1	2.38	0.41
1:M:207:GLU:O	1:M:210:ARG:HG2	2.20	0.41
3:T:216:ARG:HB3	4:U:105:ASP:CA	2.49	0.41
4:U:42:SER:O	4:U:46:LYS:N	2.21	0.41
4:U:55:GLN:HG3	5:V:161:GLU:OXT	2.20	0.41
5:V:60:MET:O	5:V:64:VAL:HG23	2.20	0.41
5:V:104:PHE:HB3	5:V:116:GLU:HB3	2.01	0.41
5:V:145:ASP:HB2	5:V:147:ARG:HD3	2.01	0.41
2:W:210:GLN:HB3	2:W:214:TYR:CE1	2.55	0.41
3:a:234:LYS:HA	4:b:83:LEU:CD1	2.50	0.41
4:b:112:TYR:HA	4:b:115:GLU:HG3	2.01	0.41
5:c:6:LYS:NZ	5:c:9:VAL:HG21	2.35	0.41
5:c:48:LEU:HD11	5:c:77:PHE:HE1	1.85	0.41
5:c:73:ASP:HB2	5:c:76:GLU:HG3	2.02	0.41
1:E:335:ARG:C	1:E:337:TYR:N	2.79	0.41
1:G:133:TYR:CD2	1:G:352:PHE:HZ	2.37	0.41
1:H:51:ASP:CG	1:H:52:SER:N	2.79	0.41
1:I:227:MET:HA	1:I:255:PHE:HZ	1.86	0.41
1:M:352:PHE:CE1	1:M:355:MET:CB	3.03	0.41
2:Q:162:TYR:O	2:Q:166:ALA:N	2.52	0.41
2:Q:272:GLU:CB	3:T:114:LYS:HD2	2.46	0.41
3:T:241:TYR:CZ	4:U:76:LEU:HB3	2.56	0.41
5:V:131:ASP:O	5:V:134:GLU:N	2.53	0.41
5:V:145:ASP:HB2	5:V:147:ARG:NH1	2.35	0.41
5:V:145:ASP:HB2	5:V:147:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:272:GLU:HB2	3:a:113:ARG:NH2	2.35	0.41
5:c:37:SER:H	5:c:40:GLU:CB	2.28	0.41
1:A:33:SER:O	1:A:70:PRO:HD2	2.21	0.41
1:A:154:ASP:O	1:A:155:SER:C	2.63	0.41
1:E:285:CYS:O	1:E:290:ARG:NE	2.49	0.41
2:P:142:GLU:O	2:P:146:ILE:HG22	2.19	0.41
2:P:152:LYS:NZ	5:c:54:PRO:HB3	2.35	0.41
3:T:238:GLN:O	3:T:242:ASN:ND2	2.53	0.41
3:T:248:PHE:CE1	4:U:71:GLU:CB	3.03	0.41
3:T:256:GLN:HB3	5:V:99:ASP:OD1	2.21	0.41
4:U:114:ILE:O	4:U:118:VAL:HG12	2.19	0.41
2:X:247:THR:OG1	3:a:142:ASN:ND2	2.53	0.41
4:b:138:LYS:HA	4:b:141:ARG:HH22	1.84	0.41
5:c:60:MET:O	5:c:64:VAL:HG13	2.20	0.41
5:c:106:LYS:HD3	5:c:106:LYS:HA	1.79	0.41
1:D:335:ARG:C	1:D:337:TYR:H	2.28	0.41
1:F:167:GLU:O	1:F:169:TYR:CD1	2.74	0.41
1:H:164:PRO:HG2	1:H:171:LEU:HB2	2.02	0.41
1:M:51:ASP:CG	1:M:52:SER:N	2.78	0.41
1:N:335:ARG:C	1:N:337:TYR:N	2.79	0.41
1:O:3:ASP:OD1	1:O:3:ASP:N	2.49	0.41
2:P:156:GLU:CG	2:P:160:ARG:NH2	2.81	0.41
2:Q:254:ASP:HB2	3:T:135:ALA:HB3	2.02	0.41
3:T:222:ASP:CB	4:U:94:GLN:HE21	2.32	0.41
3:T:256:GLN:HA	5:V:102:ARG:NH1	2.36	0.41
4:U:44:SER:HB2	5:V:2:ASP:OD1	2.20	0.41
4:U:155:MET:HG3	4:U:156:GLN:CD	2.45	0.41
5:V:88:ASP:C	5:V:90:LYS:N	2.79	0.41
2:W:260:LEU:HD11	2:X:263:GLN:OE1	2.20	0.41
5:c:72:VAL:HG11	5:c:80:MET:HE3	2.02	0.41
5:c:121:LEU:C	5:c:128:ILE:HG13	2.46	0.41
5:c:136:LEU:O	5:c:148:ILE:HD11	2.20	0.41
1:M:336:LYS:C	1:M:338:SER:N	2.72	0.41
2:P:267:TYR:HB2	2:Q:267:TYR:HB3	2.02	0.41
3:T:204:GLU:OE2	3:T:208:LYS:HB2	2.21	0.41
3:T:205:ARG:HA	3:T:205:ARG:NE	2.36	0.41
3:T:244:GLU:HB3	4:U:79:ARG:HB2	2.02	0.41
2:W:260:LEU:CD1	2:X:263:GLN:OE1	2.69	0.41
3:a:259:TYR:CD1	5:c:108:ALA:C	2.98	0.41
4:b:45:ARG:NH1	4:b:49:LEU:HG	2.34	0.41
1:E:227:MET:CB	1:E:255:PHE:HZ	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:336:LYS:HG2	1:L:337:TYR:CD1	2.56	0.41
1:O:161:HIS:HB3	1:O:163:VAL:HG23	2.03	0.41
1:O:335:ARG:H	1:O:335:ARG:HG2	1.50	0.41
3:T:263:VAL:HG13	5:V:150:TYR:HB3	2.02	0.41
4:U:46:LYS:CE	5:V:139:ASP:HB2	2.50	0.41
5:V:91:GLY:CA	5:V:159:GLY:HA3	2.51	0.41
3:a:220:ALA:HB1	3:a:223:HIS:CE1	2.40	0.41
4:b:68:ARG:O	4:b:71:GLU:HB2	2.20	0.41
1:A:282:ILE:HG21	1:A:294:TYR:CZ	2.56	0.41
1:D:133:TYR:CG	1:D:352:PHE:CZ	3.09	0.41
1:E:50:LYS:NZ	1:E:57:GLU:OE2	2.54	0.41
1:F:154:ASP:O	1:F:155:SER:C	2.63	0.41
1:F:252:ASN:CB	1:F:255:PHE:HZ	2.18	0.41
1:H:133:TYR:HE1	1:H:355:MET:HB3	1.81	0.41
1:H:163:VAL:HG22	1:H:175:ILE:CB	2.40	0.41
2:P:256:LEU:HD21	3:T:131:ARG:HD2	2.02	0.41
2:P:278:LEU:HD11	2:S:1:MET:CE	2.47	0.41
2:P:284:ILE:HA	2:S:8:MET:HG3	2.03	0.41
2:Q:263:GLN:O	2:Q:267:TYR:HB2	2.21	0.41
2:S:13:LEU:O	2:S:14:ASP:C	2.59	0.41
3:T:206:GLU:HA	3:T:209:LYS:HG2	2.03	0.41
3:T:271:ASN:OD1	4:U:136:ARG:CG	2.59	0.41
5:V:58:GLN:O	5:V:61:ILE:HB	2.21	0.41
5:V:79:VAL:O	5:V:83:ARG:N	2.54	0.41
5:V:81:MET:CE	5:V:85:MET:HB3	2.51	0.41
5:V:140:GLY:HA3	5:V:148:ILE:HD13	2.03	0.41
4:b:60:GLU:CB	5:c:103:MET:HG3	2.50	0.41
5:c:5:TYR:O	5:c:9:VAL:HG23	2.21	0.41
5:c:14:GLU:O	5:c:17:LYS:HB2	2.21	0.41
5:c:85:MET:HB3	5:c:87:ASP:OD1	2.21	0.41
5:c:90:LYS:NZ	5:c:92:LYS:HE2	2.35	0.41
5:c:102:ARG:HA	5:c:102:ARG:HD2	1.92	0.41
5:c:121:LEU:HD22	5:c:128:ILE:HD12	2.03	0.41
5:c:126:GLU:HG2	5:c:127:THR:H	1.85	0.41
1:J:56:ASP:OD1	1:J:56:ASP:N	2.52	0.41
1:L:219:VAL:O	1:L:220:ALA:HB3	2.21	0.41
1:O:108:ALA:HA	1:O:109:PRO:HD3	1.94	0.41
2:Q:282:THR:HB	3:T:106:ILE:HD11	2.02	0.41
3:T:212:LEU:HD23	3:T:215:ARG:HD2	2.03	0.41
3:T:228:GLN:NE2	3:T:232:LYS:HB2	2.36	0.41
3:T:247:LYS:HZ1	4:U:110:GLU:CG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:50:GLN:HB3	5:V:85:MET:SD	2.61	0.41
5:V:88:ASP:OD2	5:V:91:GLY:N	2.45	0.41
5:V:130:GLU:C	5:V:133:ILE:H	2.29	0.41
2:X:252:SER:O	2:X:256:LEU:CB	2.69	0.41
2:X:253:ILE:O	2:X:256:LEU:HB2	2.21	0.41
3:a:232:LYS:O	3:a:235:GLU:HG3	2.21	0.41
3:a:247:LYS:O	3:a:251:GLN:HG3	2.21	0.41
4:b:100:LEU:HD23	4:b:100:LEU:HA	1.91	0.41
5:c:154:LEU:O	5:c:158:LYS:HB2	2.20	0.41
1:A:51:ASP:CG	1:A:52:SER:N	2.79	0.40
1:D:51:ASP:CG	1:D:52:SER:N	2.79	0.40
1:I:196:ARG:HD2	1:I:253:GLU:CD	2.46	0.40
1:O:230:ALA:HB3	1:O:255:PHE:CE2	2.56	0.40
3:T:222:ASP:HB3	4:U:94:GLN:NE2	2.33	0.40
3:T:255:LYS:HA	3:T:258:LYS:NZ	2.36	0.40
5:V:131:ASP:HB3	5:V:135:GLU:CD	2.46	0.40
3:a:121:VAL:O	3:a:122:SER:C	2.63	0.40
3:a:255:LYS:HB2	3:a:255:LYS:HE3	1.76	0.40
4:b:47:LEU:O	4:b:51:THR:HG22	2.20	0.40
1:A:219:VAL:O	1:A:220:ALA:HB3	2.21	0.40
1:C:192:ILE:CD1	1:C:256:ARG:CG	2.99	0.40
1:F:169:TYR:HE1	1:H:49:GLN:CD	2.29	0.40
3:T:202:GLN:O	3:T:206:GLU:HG2	2.22	0.40
3:T:263:VAL:HG13	5:V:150:TYR:CB	2.51	0.40
3:a:89:ASP:OD1	3:a:89:ASP:N	2.51	0.40
4:b:148:ARG:HB3	5:c:86:LYS:HG3	2.04	0.40
1:G:336:LYS:HG2	1:G:337:TYR:CD1	2.56	0.40
1:J:51:ASP:CG	1:J:52:SER:N	2.79	0.40
2:P:154:ILE:O	2:P:158:ALA:N	2.42	0.40
3:T:205:ARG:O	3:T:209:LYS:HG2	2.21	0.40
3:T:240:ILE:HG22	4:U:80:CYS:HB2	2.03	0.40
3:T:260:GLU:O	3:T:264:LEU:HG	2.21	0.40
2:X:266:LYS:O	2:X:270:ILE:CG1	2.69	0.40
3:a:257:GLN:HE21	4:b:122:ILE:N	2.19	0.40
5:c:135:GLU:HG3	5:c:136:LEU:HD23	2.03	0.40
1:B:333:PRO:C	1:B:335:ARG:N	2.79	0.40
1:E:282:ILE:O	1:E:290:ARG:HD3	2.21	0.40
1:G:230:ALA:HB3	1:G:255:PHE:CZ	2.56	0.40
1:L:333:PRO:C	1:L:335:ARG:N	2.80	0.40
1:N:124:PHE:CD1	1:N:362:TYR:CD1	3.09	0.40
4:U:45:ARG:HH22	5:V:127:THR:CB	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:58:LYS:HA	5:V:100:LEU:CD2	2.47	0.40
5:V:32:GLU:HB3	5:V:35:CYS:SG	2.62	0.40
5:V:104:PHE:N	5:V:120:MET:HE2	2.36	0.40
5:V:154:LEU:O	5:V:158:LYS:N	2.54	0.40
5:c:4:ILE:HD11	5:c:5:TYR:CZ	2.57	0.40
5:c:117:LEU:HD21	5:c:136:LEU:HB2	2.02	0.40
5:c:118:LYS:HB3	5:c:133:ILE:HG21	2.03	0.40
1:B:257:CYS:CB	1:B:258:PRO:HD3	2.50	0.40
1:C:56:ASP:OD1	1:C:56:ASP:N	2.50	0.40
1:E:289:ILE:CD1	1:G:63:GLY:C	2.85	0.40
1:F:67:LEU:HG	1:F:203:THR:HG21	2.03	0.40
1:G:260:THR:HA	1:G:263:GLN:O	2.22	0.40
1:N:279:TYR:CZ	1:N:283:MET:CE	3.04	0.40
2:Q:257:GLU:CG	3:T:132:ALA:CA	2.96	0.40
5:V:28:VAL:C	5:V:30:GLY:H	2.29	0.40
5:V:94:GLU:HB3	5:V:154:LEU:CD2	2.47	0.40
5:V:99:ASP:CG	5:V:102:ARG:HH22	2.30	0.40
5:V:120:MET:O	5:V:123:ALA:HB3	2.22	0.40
2:X:253:ILE:CA	2:X:256:LEU:HB2	2.50	0.40
4:b:69:ARG:NH1	4:b:73:GLY:H	2.18	0.40
4:b:132:ILE:C	4:b:134:ASP:N	2.78	0.40
5:c:80:MET:HE3	5:c:80:MET:HB2	1.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	373/375 (100%)	362 (97%)	9 (2%)	2 (0%)	24	63
1	B	373/375 (100%)	359 (96%)	14 (4%)	0	100	100
1	C	373/375 (100%)	362 (97%)	10 (3%)	1 (0%)	36	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	373/375 (100%)	360 (96%)	11 (3%)	2 (0%)	24	63
1	E	373/375 (100%)	359 (96%)	13 (4%)	1 (0%)	36	72
1	F	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	72
1	G	373/375 (100%)	359 (96%)	12 (3%)	2 (0%)	24	63
1	H	373/375 (100%)	360 (96%)	11 (3%)	2 (0%)	24	63
1	I	373/375 (100%)	362 (97%)	10 (3%)	1 (0%)	36	72
1	J	373/375 (100%)	360 (96%)	10 (3%)	3 (1%)	16	54
1	K	373/375 (100%)	358 (96%)	12 (3%)	3 (1%)	16	54
1	L	373/375 (100%)	359 (96%)	11 (3%)	3 (1%)	16	54
1	M	373/375 (100%)	358 (96%)	13 (4%)	2 (0%)	24	63
1	N	373/375 (100%)	362 (97%)	10 (3%)	1 (0%)	36	72
1	O	373/375 (100%)	358 (96%)	14 (4%)	1 (0%)	36	72
2	P	272/286 (95%)	272 (100%)	0	0	100	100
2	Q	272/286 (95%)	272 (100%)	0	0	100	100
2	R	27/286 (9%)	27 (100%)	0	0	100	100
2	S	27/286 (9%)	27 (100%)	0	0	100	100
2	W	272/286 (95%)	272 (100%)	0	0	100	100
2	X	272/286 (95%)	270 (99%)	2 (1%)	0	100	100
2	Y	27/286 (9%)	27 (100%)	0	0	100	100
2	Z	27/286 (9%)	27 (100%)	0	0	100	100
3	T	122/186 (66%)	114 (93%)	8 (7%)	0	100	100
3	a	134/186 (72%)	130 (97%)	4 (3%)	0	100	100
4	U	168/170 (99%)	150 (89%)	18 (11%)	0	100	100
4	b	124/170 (73%)	104 (84%)	20 (16%)	0	100	100
5	V	158/160 (99%)	116 (73%)	41 (26%)	1 (1%)	21	59
5	c	158/160 (99%)	139 (88%)	19 (12%)	0	100	100
All	All	7655/8945 (86%)	7346 (96%)	283 (4%)	26 (0%)	37	72

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	155	SER
1	H	155	SER

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Mol	Chain	Res	Type
1	I	155	SER
1	K	155	SER
1	L	155	SER
1	M	155	SER
1	O	155	SER
1	A	155	SER
1	G	336	LYS
1	J	336	LYS
1	F	155	SER
1	J	220	ALA
1	N	155	SER
1	A	49	GLN
1	C	49	GLN
1	D	334	GLU
1	G	49	GLN
1	K	103	THR
1	L	336	LYS
1	M	49	GLN
1	D	49	GLN
1	H	49	GLN
1	J	49	GLN
1	K	49	GLN
1	L	49	GLN
5	V	28	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/318 (100%)	315 (99%)	3 (1%)	70	79
1	B	318/318 (100%)	315 (99%)	3 (1%)	70	79
1	C	318/318 (100%)	317 (100%)	1 (0%)	86	86
1	D	318/318 (100%)	314 (99%)	4 (1%)	61	74
1	E	318/318 (100%)	314 (99%)	4 (1%)	61	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	318/318 (100%)	315 (99%)	3 (1%)	70	79
1	G	318/318 (100%)	315 (99%)	3 (1%)	70	79
1	H	318/318 (100%)	315 (99%)	3 (1%)	70	79
1	I	318/318 (100%)	318 (100%)	0	100	100
1	J	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	K	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	L	318/318 (100%)	315 (99%)	3 (1%)	70	79
1	M	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	N	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	O	318/318 (100%)	315 (99%)	3 (1%)	70	79
2	P	236/246 (96%)	236 (100%)	0	100	100
2	Q	236/246 (96%)	236 (100%)	0	100	100
2	R	24/246 (10%)	24 (100%)	0	100	100
2	S	24/246 (10%)	24 (100%)	0	100	100
2	W	236/246 (96%)	235 (100%)	1 (0%)	84	84
2	X	236/246 (96%)	233 (99%)	3 (1%)	61	74
2	Y	24/246 (10%)	24 (100%)	0	100	100
2	Z	24/246 (10%)	24 (100%)	0	100	100
3	T	117/169 (69%)	116 (99%)	1 (1%)	70	79
3	a	129/169 (76%)	129 (100%)	0	100	100
4	U	145/145 (100%)	144 (99%)	1 (1%)	76	81
4	b	106/145 (73%)	105 (99%)	1 (1%)	70	79
5	V	141/141 (100%)	135 (96%)	6 (4%)	26	47
5	c	141/141 (100%)	141 (100%)	0	100	100
All	All	6589/7648 (86%)	6538 (99%)	51 (1%)	70	80

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	SER
1	A	282	ILE
1	A	336	LYS
1	B	163	VAL
1	B	287	ILE

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Mol	Chain	Res	Type
1	B	336	LYS
1	C	336	LYS
1	D	163	VAL
1	D	287	ILE
1	D	335	ARG
1	D	336	LYS
1	E	107	GLU
1	E	287	ILE
1	E	313	MET
1	E	336	LYS
1	F	287	ILE
1	F	305	MET
1	F	336	LYS
1	G	287	ILE
1	G	335	ARG
1	G	336	LYS
1	H	163	VAL
1	H	254	ARG
1	H	336	LYS
1	J	305	MET
1	J	336	LYS
1	K	163	VAL
1	K	336	LYS
1	L	177	ARG
1	L	287	ILE
1	L	335	ARG
1	M	47	MET
1	M	336	LYS
1	N	335	ARG
1	N	336	LYS
1	O	37	ARG
1	O	335	ARG
1	O	336	LYS
3	T	223	HIS
4	U	52	LEU
5	V	12	LEU
5	V	28	VAL
5	V	64	VAL
5	V	87	ASP
5	V	107	ASN
5	V	109	ASP
2	W	274	LEU

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Mol	Chain	Res	Type
2	X	165	VAL
2	X	261	TYR
2	X	264	LYS
4	b	108	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	B	92	ASN
1	B	111	ASN
1	C	162	ASN
1	D	40	HIS
1	D	111	ASN
1	E	137	GLN
1	G	263	GLN
1	H	59	GLN
1	I	162	ASN
1	J	49	GLN
1	J	162	ASN
1	L	92	ASN
1	L	128	ASN
1	L	263	GLN
1	M	162	ASN
1	M	371	HIS
1	N	87	HIS
1	N	121	GLN
1	N	263	GLN
1	N	296	ASN
1	O	371	HIS
2	Q	47	GLN
2	Q	276	HIS
2	Q	279	ASN
3	T	142	ASN
3	T	225	ASN
3	T	238	GLN
3	T	242	ASN
3	T	251	GLN
3	T	256	GLN
3	T	269	ASN
3	T	271	ASN
5	V	58	GLN

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Mol	Chain	Res	Type
5	V	143	ASN
2	W	47	GLN
2	X	153	HIS
2	X	210	GLN
2	X	276	HIS
3	a	138	GLN
3	a	142	ASN
3	a	223	HIS
3	a	238	GLN
3	a	262	ASN
3	a	266	ASN
3	a	269	ASN
4	b	48	GLN
4	b	59	GLN
4	b	156	GLN
5	c	51	ASN
5	c	143	ASN

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.

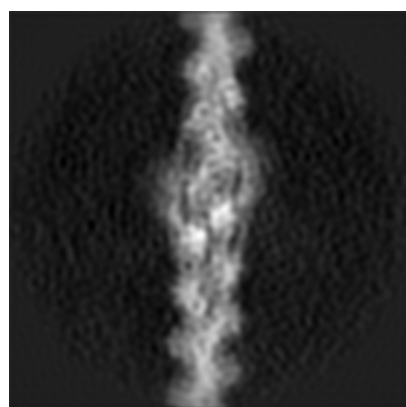
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22978. These allow visual inspection of the internal detail of the map and identification of artifacts.

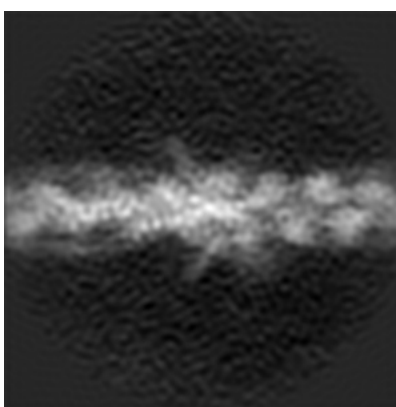
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

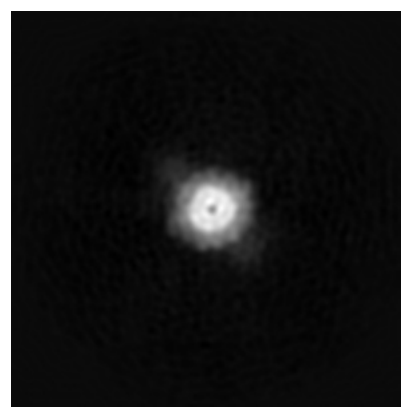
6.1.1 Primary map



X



Y

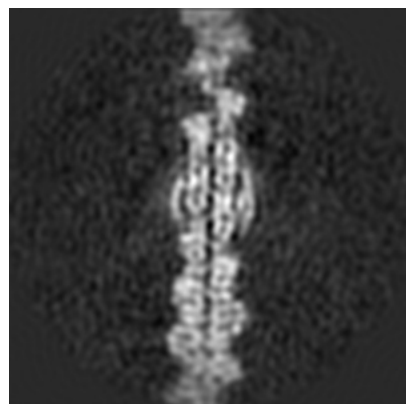


Z

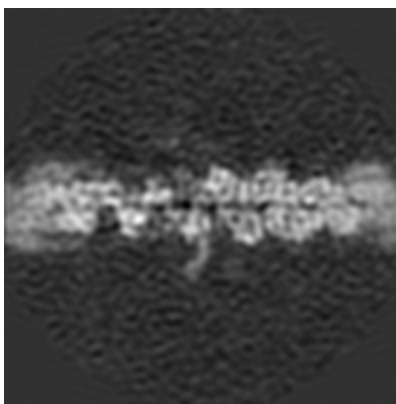
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

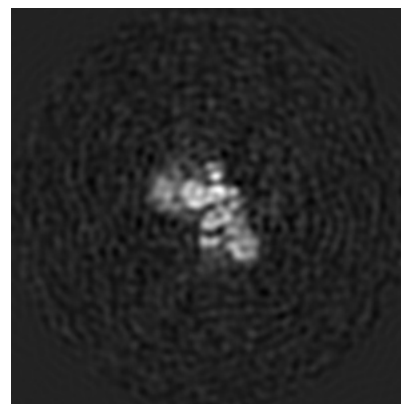
6.2.1 Primary map



X Index: 81



Y Index: 81

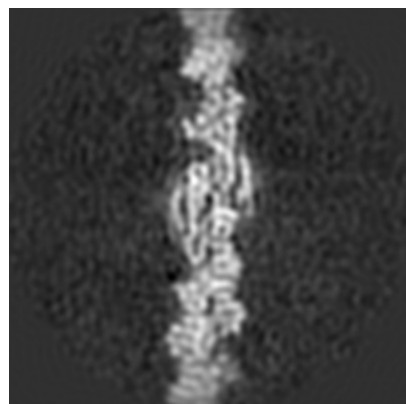


Z Index: 81

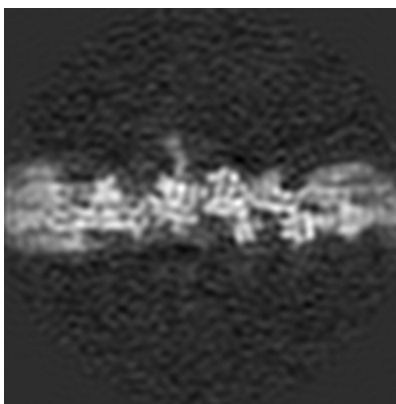
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

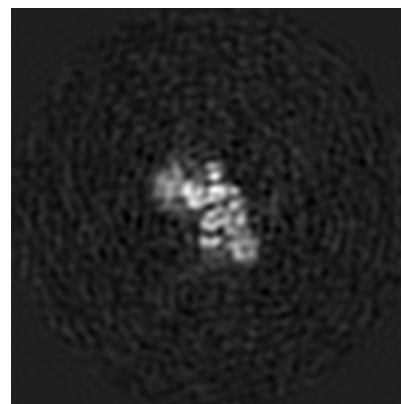
6.3.1 Primary map



X Index: 79



Y Index: 78

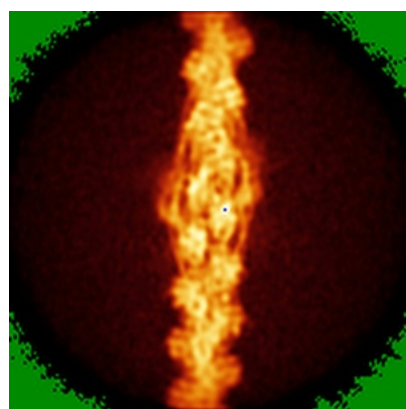


Z Index: 82

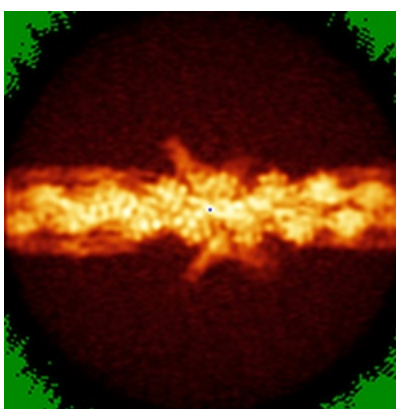
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

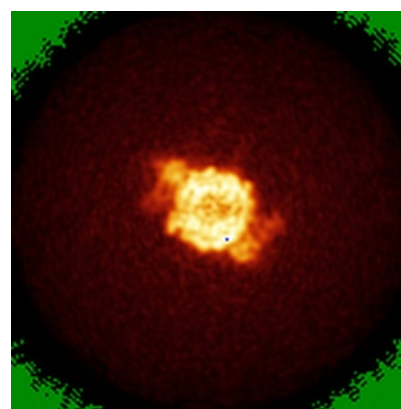
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.031. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

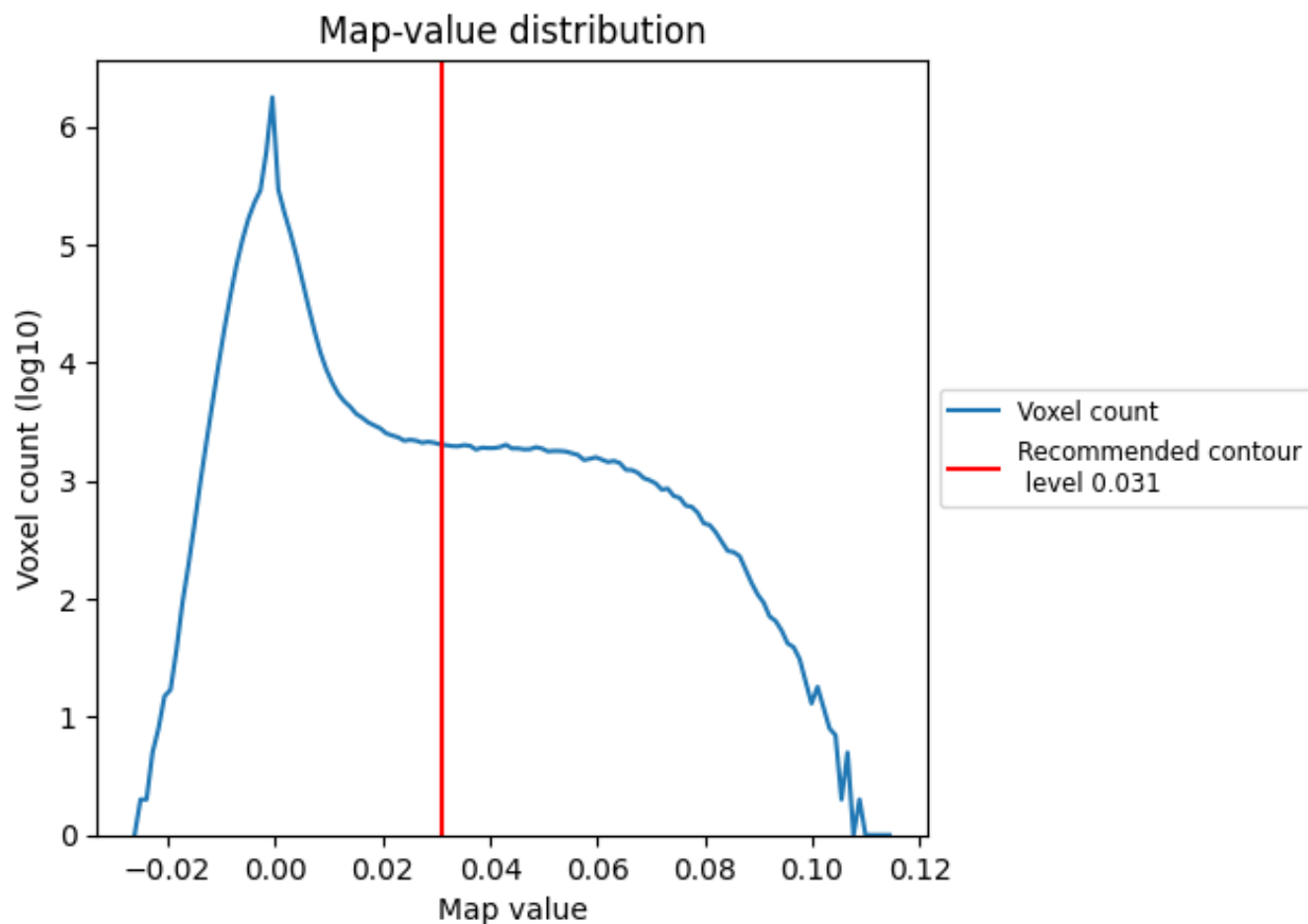
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

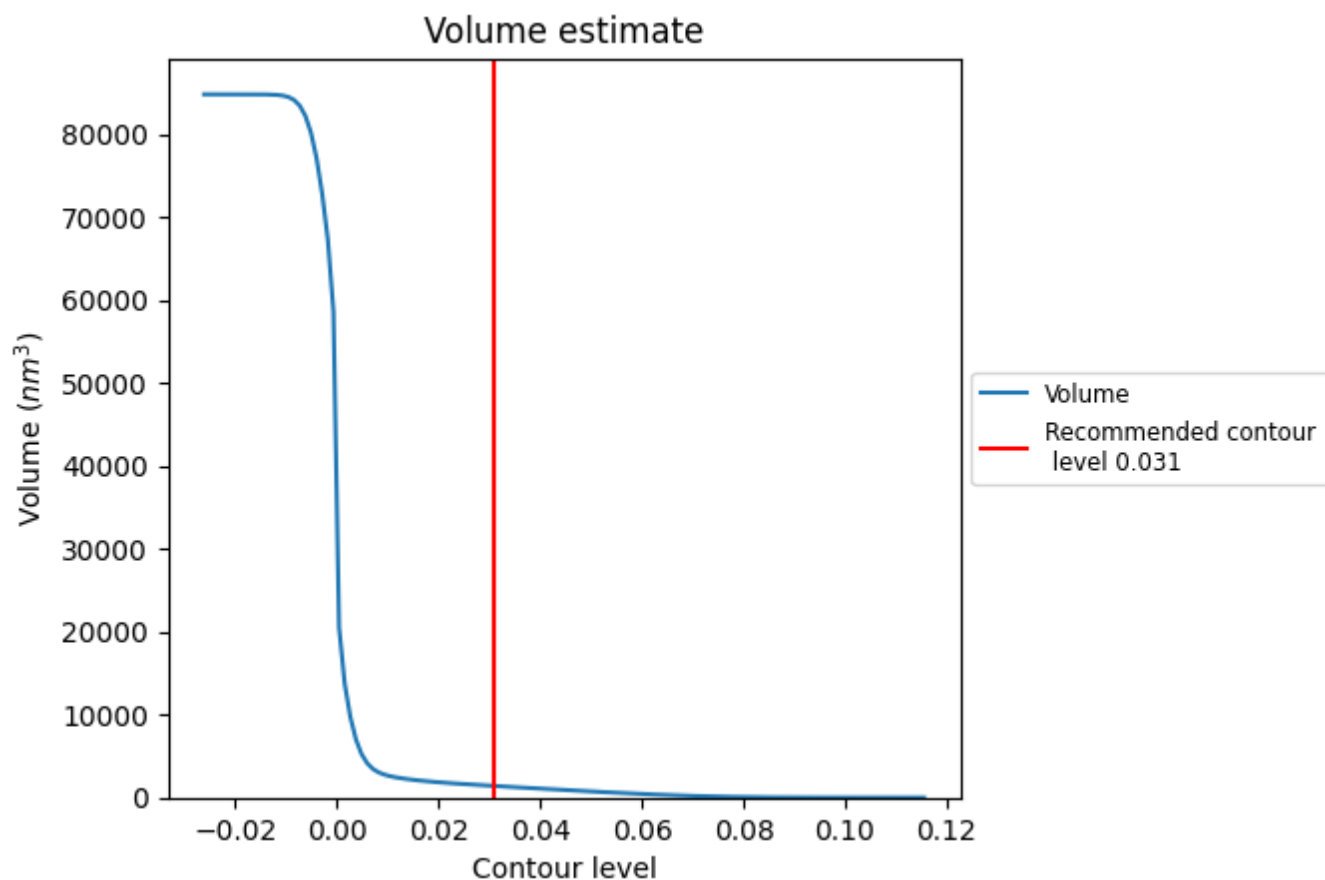
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

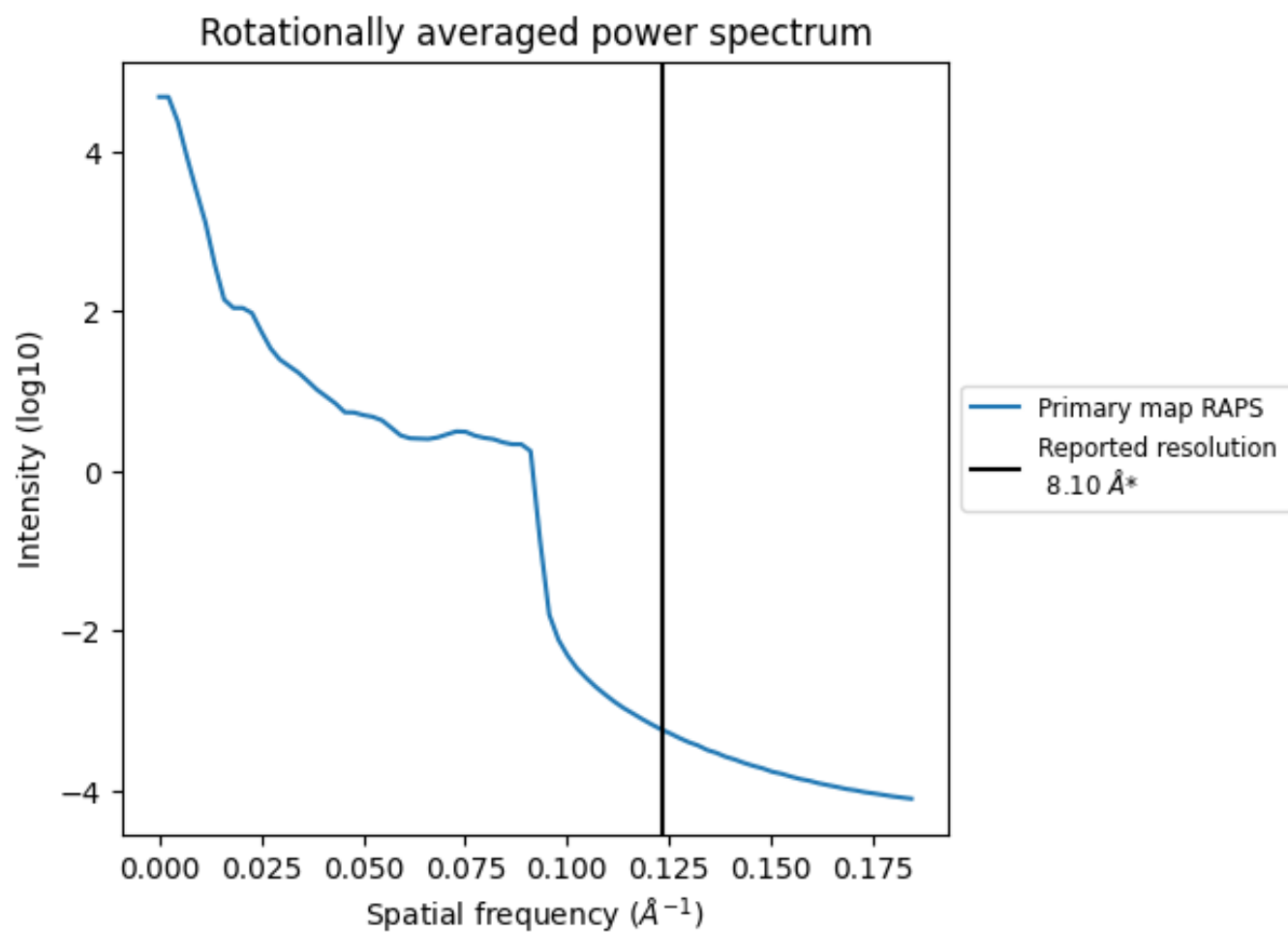
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1395 nm³; this corresponds to an approximate mass of 1260 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

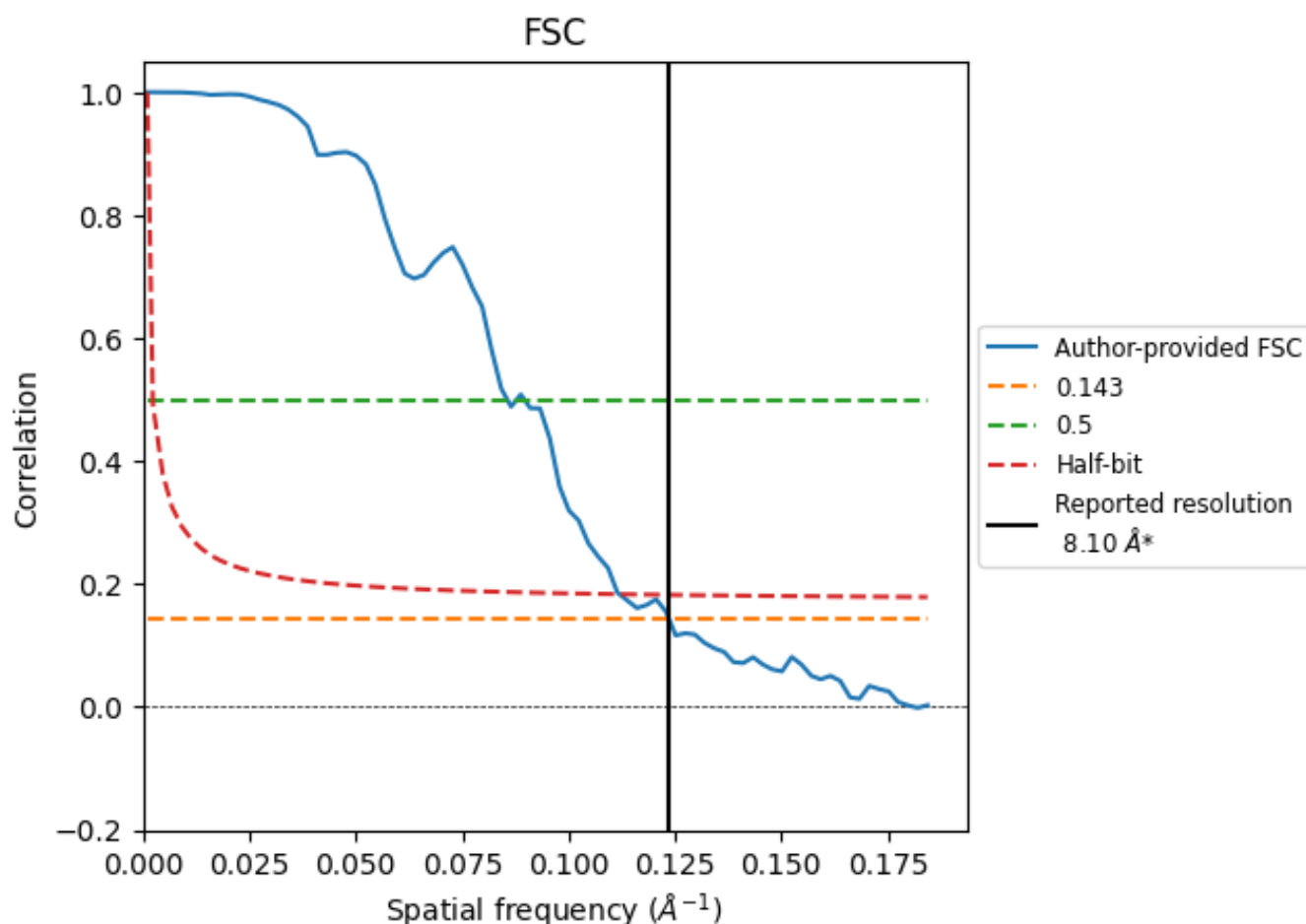


*Reported resolution corresponds to spatial frequency of 0.123 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.123 Å⁻¹

8.2 Resolution estimates [i](#)

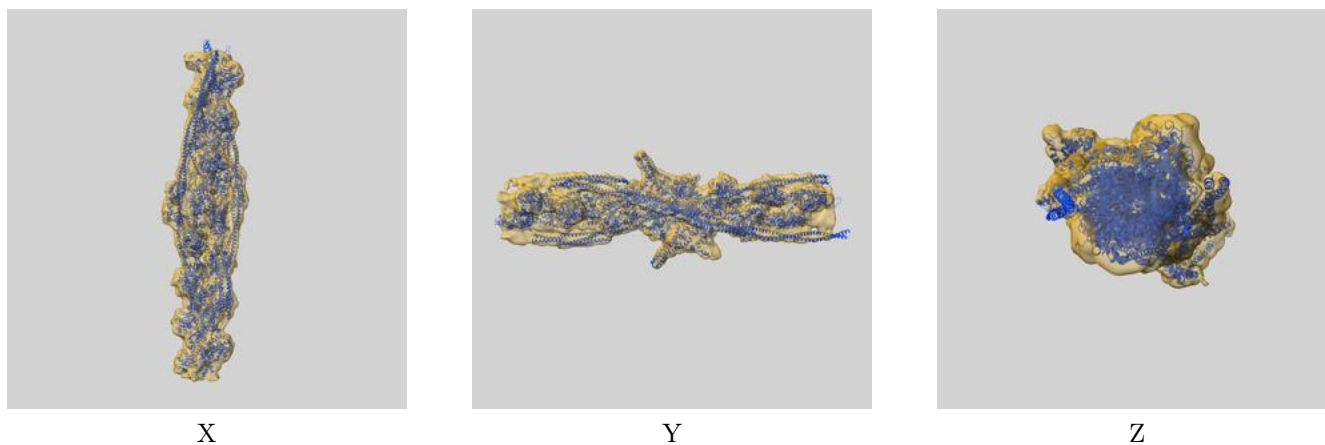
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.10	-	-
Author-provided FSC curve	8.09	11.68	8.93
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22978 and PDB model 7KON. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



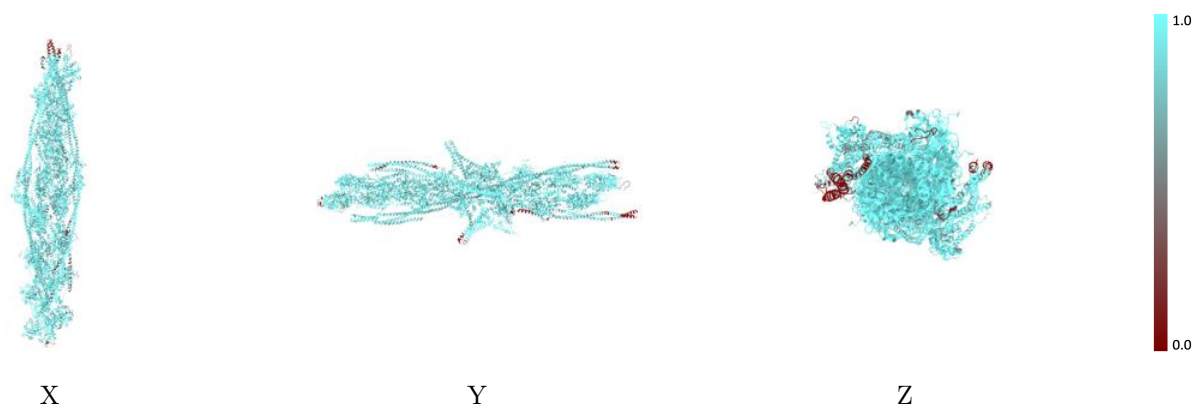
The images above show the 3D surface view of the map at the recommended contour level 0.031 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



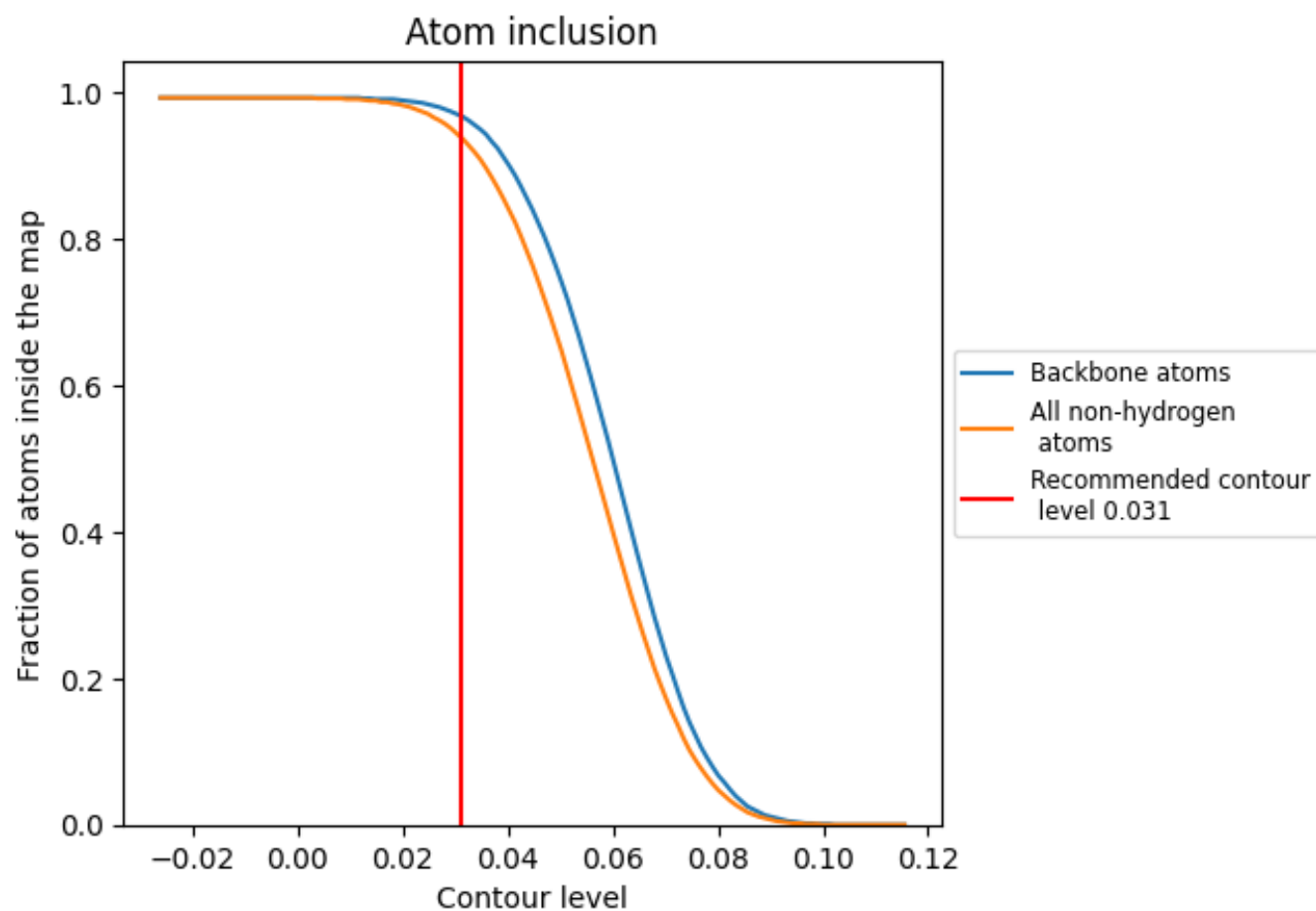
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.031).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9390	 0.1120
A	 0.9360	 0.0860
B	 0.9890	 0.1030
C	 0.9910	 0.1040
D	 0.9830	 0.1050
E	 0.9750	 0.1010
F	 0.9680	 0.1060
G	 0.9840	 0.1090
H	 0.9830	 0.1050
I	 0.9770	 0.1080
J	 0.9800	 0.1070
K	 0.9850	 0.1070
L	 0.9780	 0.1040
M	 0.9810	 0.0920
N	 0.9680	 0.0930
O	 0.9040	 0.0700
P	 0.9050	 0.1540
Q	 0.8970	 0.1500
R	 0.9300	 0.1650
S	 0.9390	 0.1740
T	 0.8490	 0.1720
U	 0.6870	 0.1370
V	 0.9530	 0.1750
W	 0.7860	 0.1270
X	 0.8080	 0.1100
Y	 0.7820	 0.0010
Z	 0.9260	 0.1630
a	 0.7830	 0.1610
b	 0.9710	 0.1500
c	 0.9220	 0.1190

