



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:25 AM UTC

PDB ID : 7KO4 / pdb_00007ko4
EMDB ID : EMD-22964
Title : Structure of cardiac native thin filament at pCa=5.8 having upper and lower troponins in Ca²⁺ free state
Authors : Galkin, V.E.; Risi, C.M.
Deposited on : 2020-11-06
Resolution : 8.00 Å(reported)
Based on initial model : 6KN7

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:

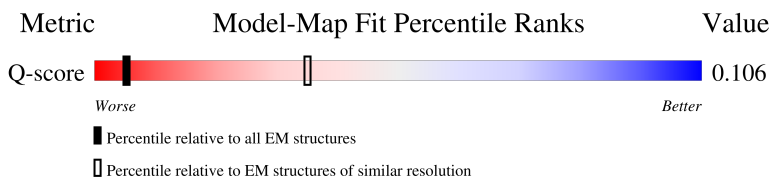
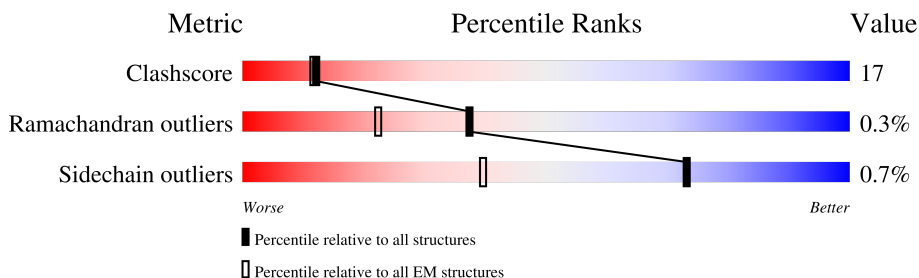
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 8.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



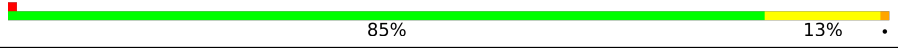
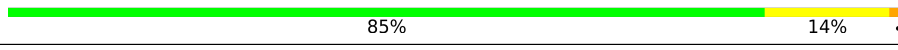
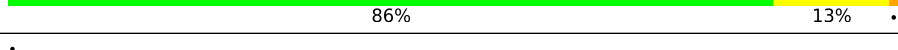
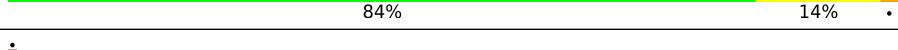
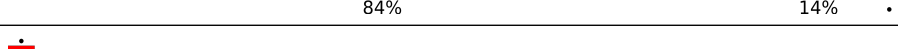
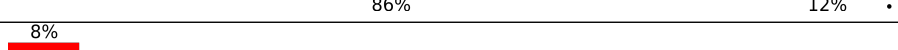
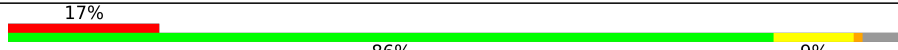
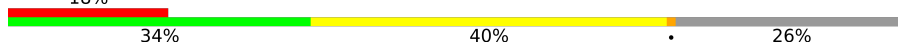
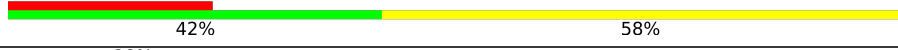
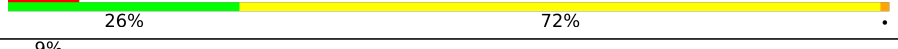
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

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	 84% 13% .
1	B	375	 82% 16% .
1	C	375	 85% 14% .
1	D	375	 85% 13% .

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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 61463 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 Isoform 4 of Troponin T, cardiac muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	138	Total	C	N	O	S	0	0
			1211	740	241	229	1		
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	170	Total	C	N	O	S	0	0
			1374	848	263	258	5		

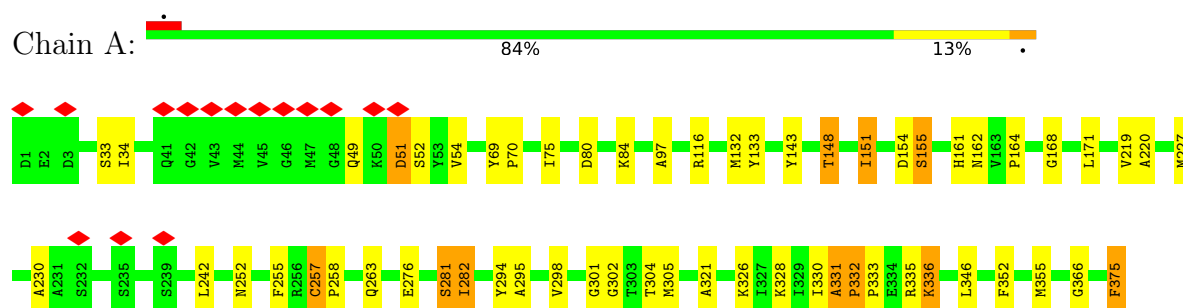
- Molecule 5 is a protein called Troponin C.

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		

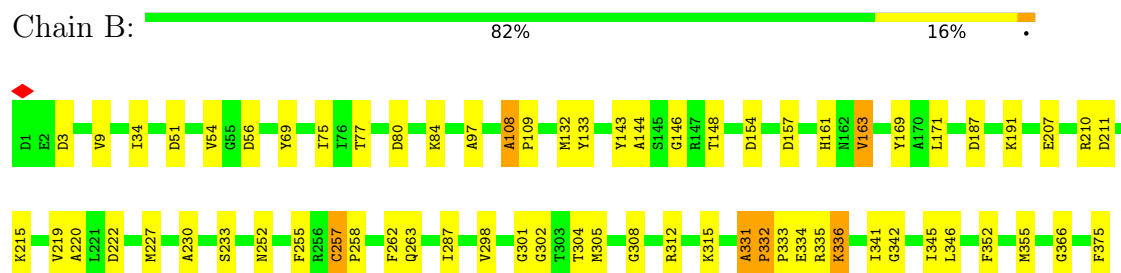
3 Residue-property plots

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.

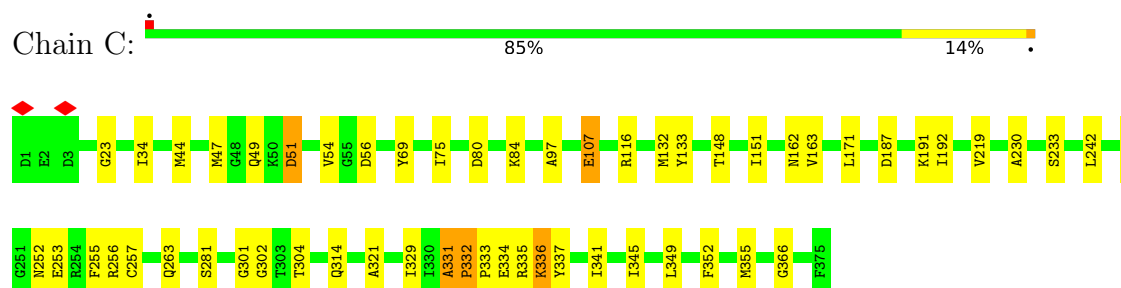
- Molecule 1: Actin, alpha skeletal muscle



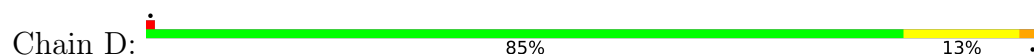
- Molecule 1: Actin, alpha skeletal muscle

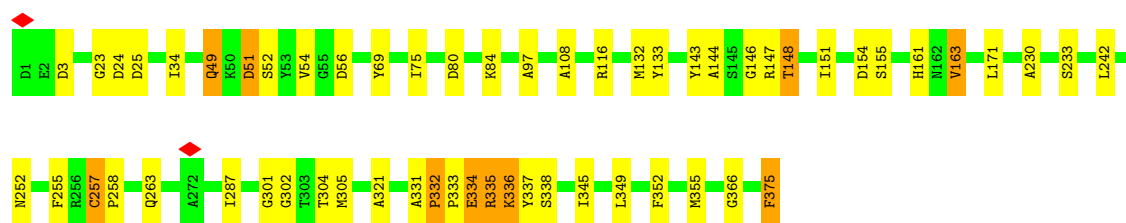


- Molecule 1: Actin, alpha skeletal muscle



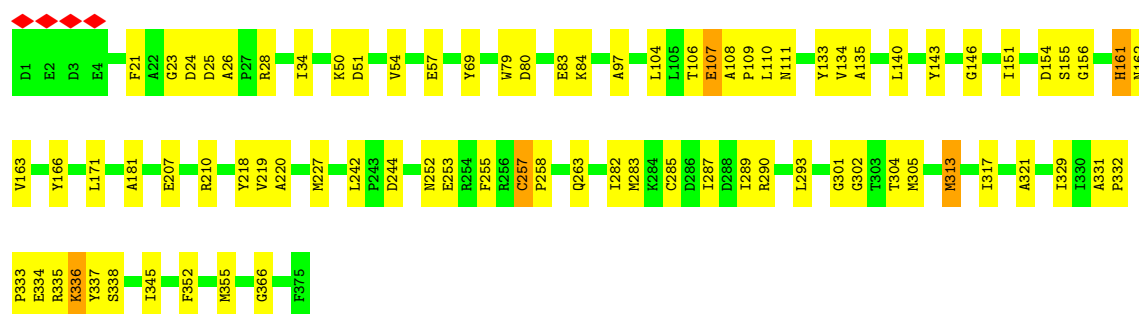
- Molecule 1: Actin, alpha skeletal muscle





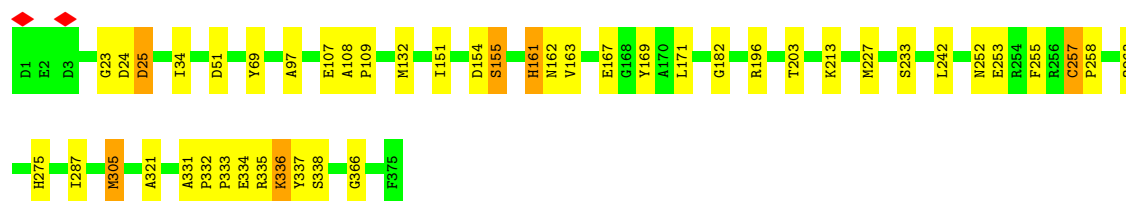
- Molecule 1: Actin, alpha skeletal muscle

Chain E: 78% 20% .



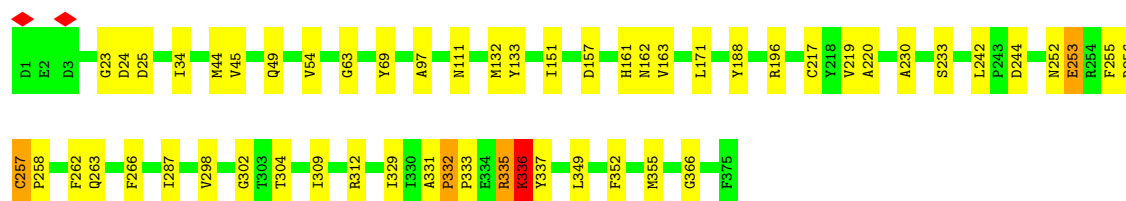
- Molecule 1: Actin, alpha skeletal muscle

Chain F: 88% 11% .



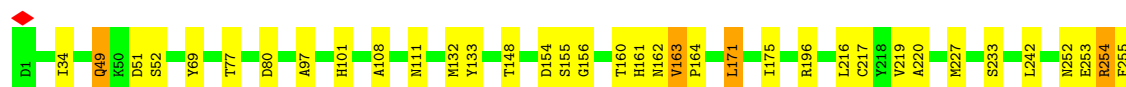
- Molecule 1: Actin, alpha skeletal muscle

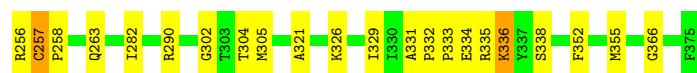
Chain G: 85% 13% .



- Molecule 1: Actin, alpha skeletal muscle

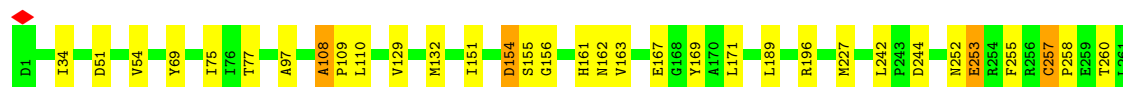
Chain H: 85% 14% .





- Molecule 1: Actin, alpha skeletal muscle

Chain I: 86% 13%



- Molecule 1: Actin, alpha skeletal muscle

Chain J: 85% 13%



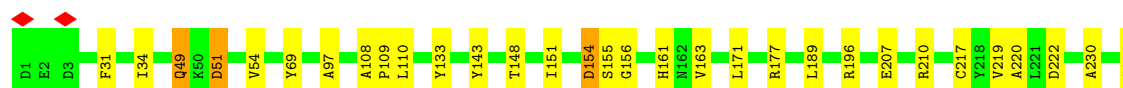
- Molecule 1: Actin, alpha skeletal muscle

Chain K: 86% 13%



- Molecule 1: Actin, alpha skeletal muscle

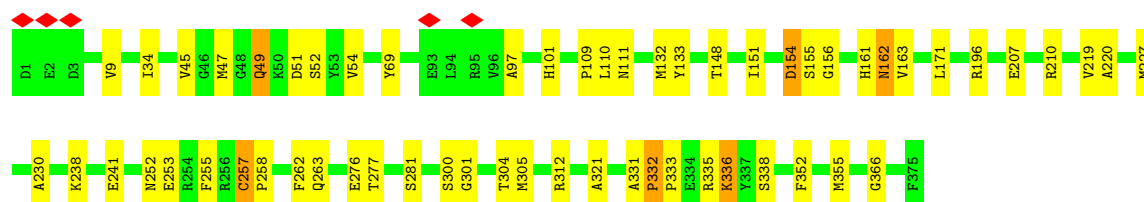
Chain L: 84% 14%



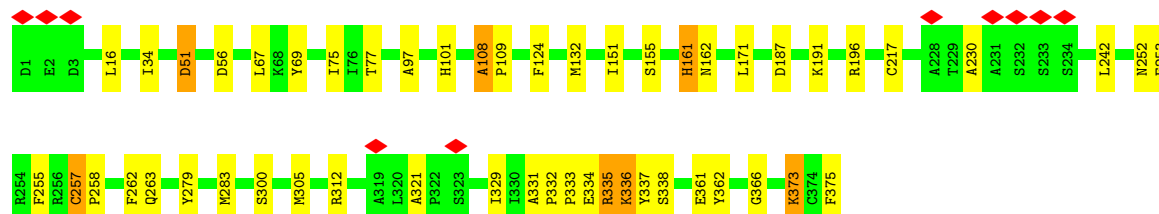
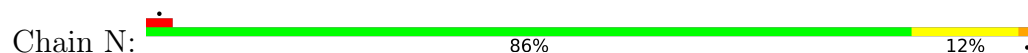
- Molecule 1: Actin, alpha skeletal muscle

Chain M: 84% 14%

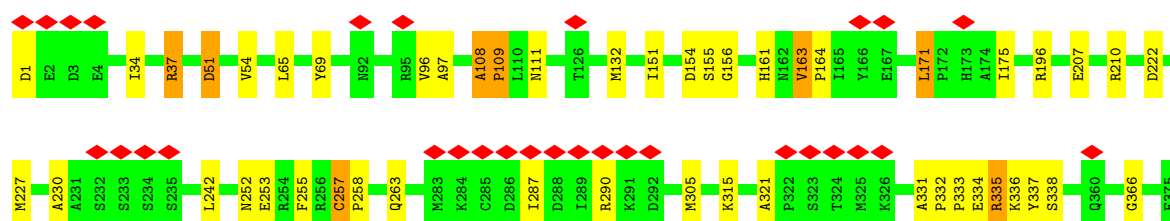
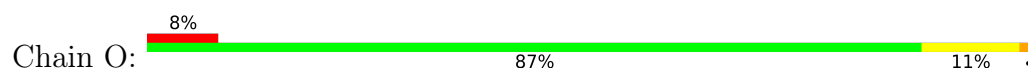




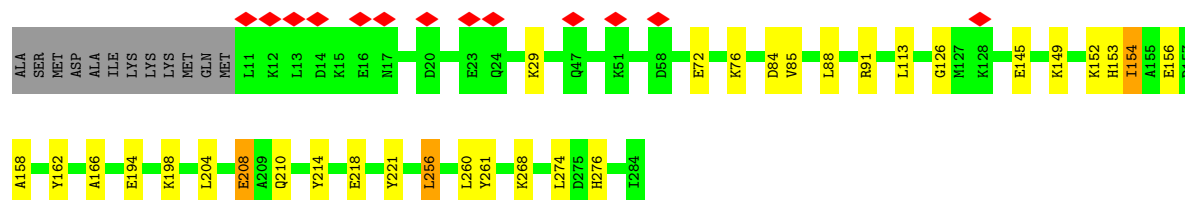
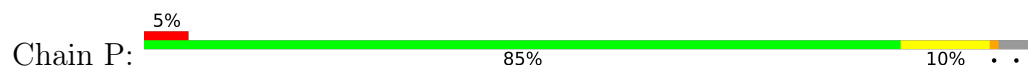
- Molecule 1: Actin, alpha skeletal muscle



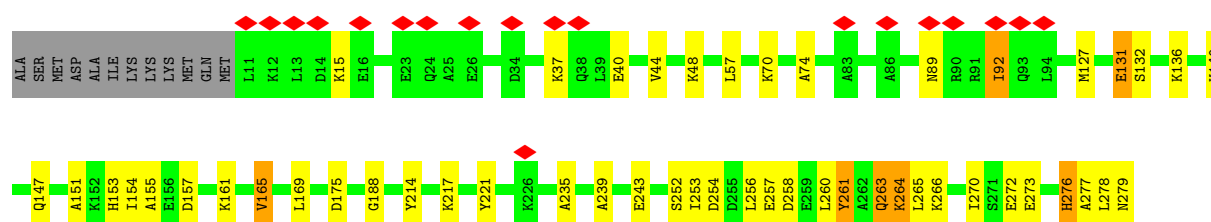
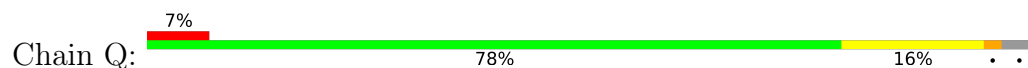
- Molecule 1: Actin, alpha skeletal muscle

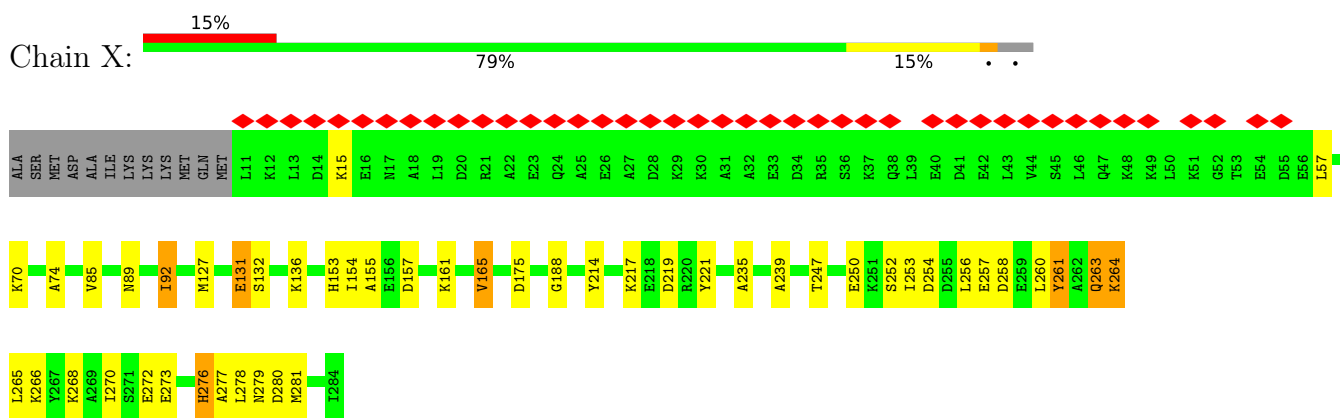


- Molecule 2: Tropomyosin alpha-1 chain

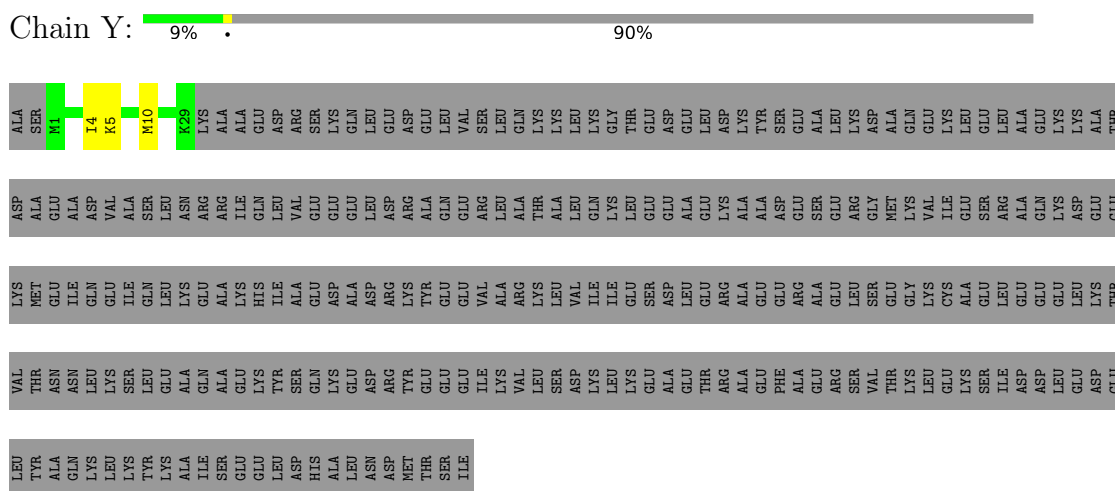


- Molecule 2: Tropomyosin alpha-1 chain

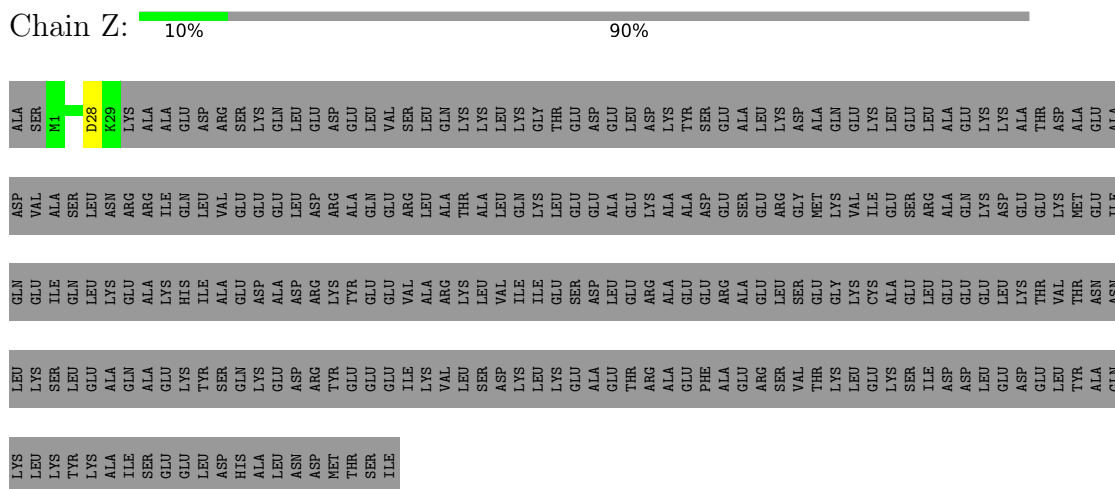




- Molecule 2: Tropomyosin alpha-1 chain

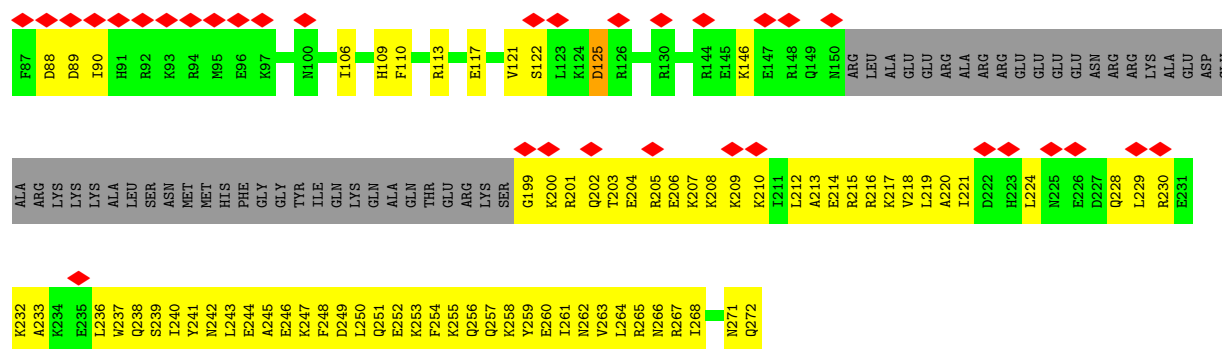


- Molecule 2: Tropomyosin alpha-1 chain

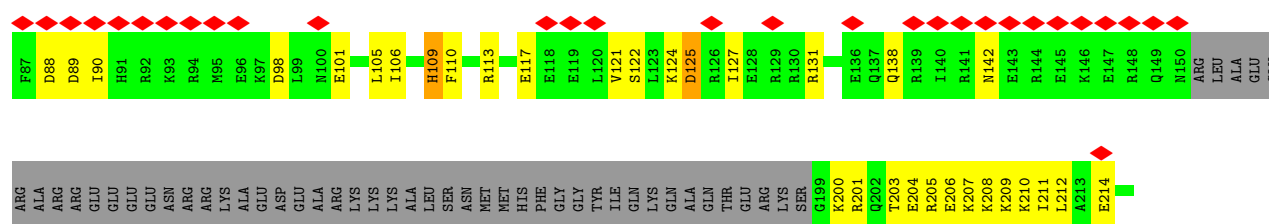
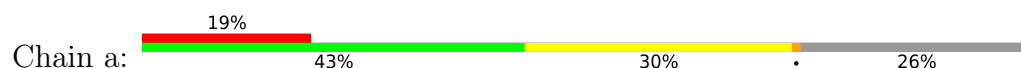


- Molecule 3: Isoform 4 of Troponin T, cardiac muscle

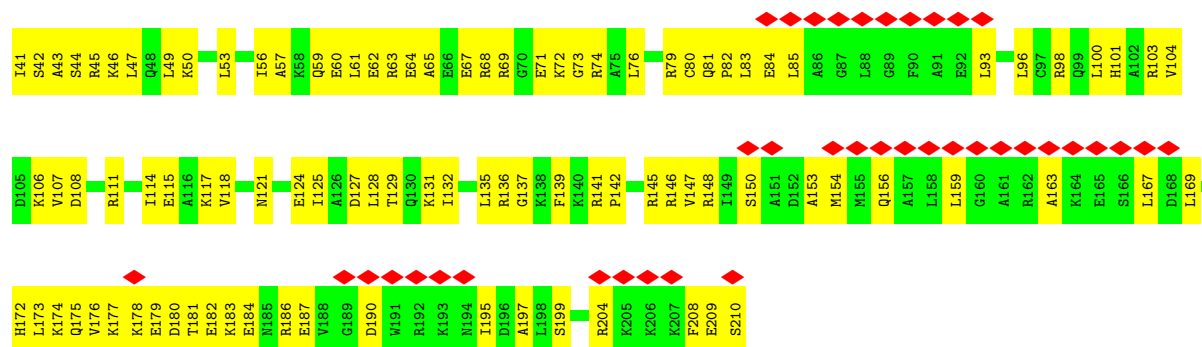




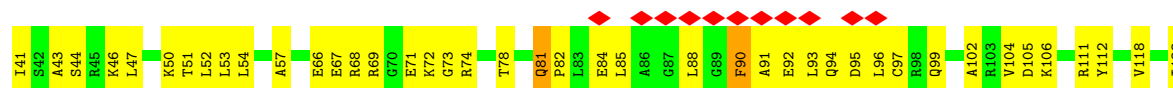
• Molecule 3: Isoform 4 of Troponin T, cardiac muscle

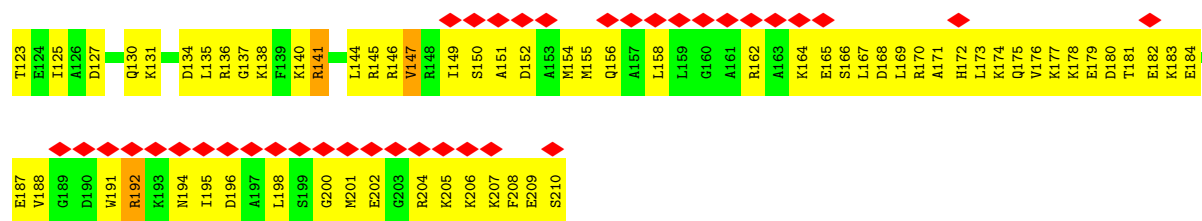


• Molecule 4: Troponin I, cardiac muscle

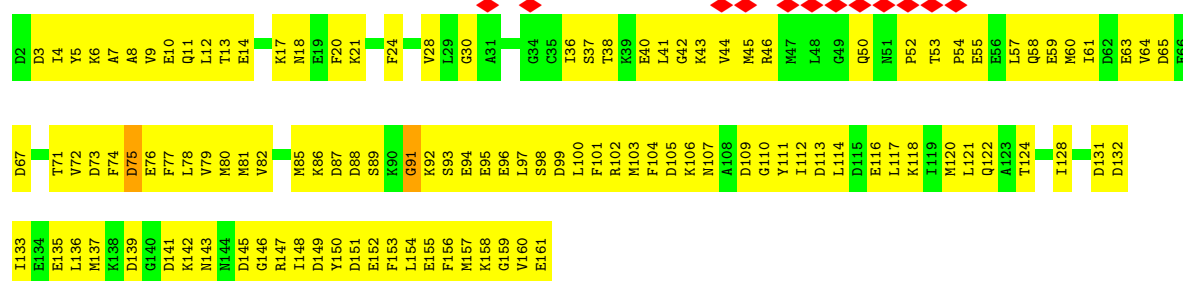


• Molecule 4: Troponin I, cardiac muscle

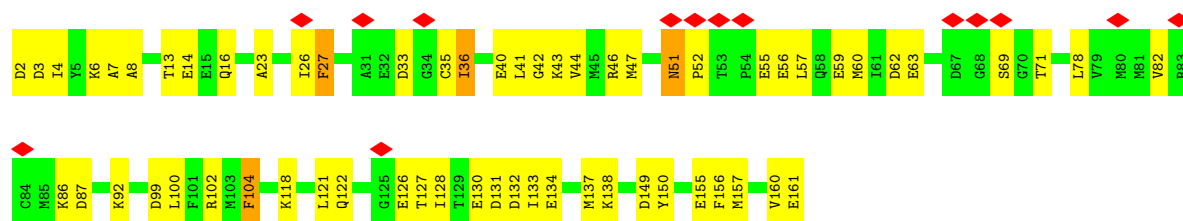




• Molecule 5: Troponin C



• 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	11933	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	0.109	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	439.344, 439.344, 439.344	wwPDB
Map dimensions	162, 162, 162	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	32/4058 (0.8%)
1	C	0.93	0/2996	1.32	37/4058 (0.9%)
1	D	0.92	1/2996 (0.0%)	1.32	36/4058 (0.9%)
1	E	0.92	0/2996	1.33	33/4058 (0.8%)
1	F	0.89	0/2996	1.32	37/4058 (0.9%)
1	G	0.94	2/2996 (0.1%)	1.33	36/4058 (0.9%)
1	H	0.90	1/2996 (0.0%)	1.33	34/4058 (0.8%)
1	I	0.91	0/2996	1.31	34/4058 (0.8%)
1	J	0.90	0/2996	1.33	33/4058 (0.8%)
1	K	0.91	1/2996 (0.0%)	1.31	35/4058 (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	37/4058 (0.9%)
1	O	0.90	0/2996	1.31	32/4058 (0.8%)
2	P	1.30	1/2215 (0.0%)	1.27	7/2954 (0.2%)
2	Q	1.32	2/2215 (0.1%)	1.30	9/2954 (0.3%)
2	R	1.22	0/230	1.09	0/301
2	S	1.16	0/230	1.14	1/301 (0.3%)
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	1.17	0/230	1.14	1/301 (0.3%)
3	T	0.81	1/1220 (0.1%)	0.93	4/1613 (0.2%)
3	a	1.02	1/1220 (0.1%)	1.13	5/1613 (0.3%)
4	U	0.21	0/1384	0.49	0/1840
4	b	0.93	0/1384	1.11	9/1840 (0.5%)
5	V	0.24	0/1286	0.56	0/1719
5	c	0.95	0/1286	1.20	7/1719 (0.4%)
All	All	0.97	15/62500 (0.0%)	1.27	576/84234 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	V	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	161	HIS	CB-CG	-6.01	1.41	1.50
2	P	256	LEU	CB-CG	-5.88	1.41	1.53
2	W	256	LEU	CB-CG	-5.87	1.41	1.53
1	K	161	HIS	CB-CG	-5.83	1.42	1.50
2	Q	57	LEU	CG-CD2	-5.78	1.33	1.52
2	X	57	LEU	CG-CD2	-5.75	1.33	1.52
1	D	161	HIS	CB-CG	-5.70	1.42	1.50
2	X	276	HIS	CB-CG	-5.47	1.42	1.50
2	Q	276	HIS	CB-CG	-5.40	1.42	1.50
1	G	161	HIS	CG-CD2	-5.33	1.29	1.35
3	a	109	HIS	CB-CG	-5.27	1.42	1.50
1	G	256	ARG	NE-CZ	5.26	1.38	1.33
1	N	67	LEU	CB-CG	5.23	1.64	1.53
3	T	109	HIS	CB-CG	-5.13	1.43	1.50
1	A	161	HIS	CB-CG	-5.09	1.43	1.50

All (576) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	125	ASP	N-CA-C	-9.27	101.25	111.36
3	T	125	ASP	N-CA-C	-9.22	101.31	111.36
1	J	163	VAL	N-CA-C	9.09	116.54	107.55
1	K	163	VAL	N-CA-C	8.94	117.92	107.73
1	O	163	VAL	N-CA-C	8.68	117.09	109.02
1	C	163	VAL	N-CA-C	8.56	117.48	107.73
1	D	163	VAL	N-CA-C	8.49	117.40	107.73
1	N	263	GLN	CA-C-N	8.41	128.06	119.82
1	N	263	GLN	C-N-CA	8.41	128.06	119.82
1	F	69	TYR	CA-C-N	8.29	128.01	119.56
1	F	69	TYR	C-N-CA	8.29	128.01	119.56
1	O	263	GLN	CA-C-N	8.29	127.93	119.56
1	O	263	GLN	C-N-CA	8.29	127.93	119.56
1	B	69	TYR	CA-C-N	8.26	127.90	119.56
1	B	69	TYR	C-N-CA	8.26	127.90	119.56
1	E	163	VAL	N-CA-C	8.24	116.87	107.89
1	H	263	GLN	CA-C-N	8.22	127.94	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	263	GLN	C-N-CA	8.22	127.94	119.56
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
1	K	111	ASN	CA-CB-CG	8.15	120.75	112.60
1	O	69	TYR	CA-C-N	8.12	127.84	119.56
1	O	69	TYR	C-N-CA	8.12	127.84	119.56
1	G	163	VAL	N-CA-C	8.10	117.25	107.61
1	E	69	TYR	CA-C-N	8.06	127.78	119.56
1	E	69	TYR	C-N-CA	8.06	127.78	119.56
1	L	163	VAL	N-CA-C	8.05	116.67	107.89
1	B	366	GLY	CA-C-N	8.00	127.72	119.56
1	B	366	GLY	C-N-CA	8.00	127.72	119.56
1	K	366	GLY	CA-C-N	7.98	127.70	119.56
1	K	366	GLY	C-N-CA	7.98	127.70	119.56
1	A	263	GLN	CA-C-N	7.98	127.62	119.56
1	A	263	GLN	C-N-CA	7.98	127.62	119.56
1	F	263	GLN	CA-C-N	7.92	127.64	119.56
1	F	263	GLN	C-N-CA	7.92	127.64	119.56
1	N	69	TYR	CA-C-N	7.89	128.08	119.87
1	N	69	TYR	C-N-CA	7.89	128.08	119.87
1	J	366	GLY	CA-C-N	7.86	127.58	119.56
1	J	366	GLY	C-N-CA	7.86	127.58	119.56
4	b	81	GLN	CA-C-N	7.86	127.88	119.78
4	b	81	GLN	C-N-CA	7.86	127.88	119.78
1	N	34	ILE	N-CA-C	7.86	120.17	108.46
1	H	366	GLY	CA-C-N	7.85	127.51	119.82
1	H	366	GLY	C-N-CA	7.85	127.51	119.82
1	E	263	GLN	CA-C-N	7.84	127.56	119.56
1	E	263	GLN	C-N-CA	7.84	127.56	119.56
1	K	69	TYR	CA-C-N	7.82	127.54	119.56
1	K	69	TYR	C-N-CA	7.82	127.54	119.56
1	D	263	GLN	CA-C-N	7.78	127.42	119.56
1	D	263	GLN	C-N-CA	7.78	127.42	119.56
5	c	104	PHE	CA-CB-CG	7.76	121.56	113.80
1	J	219	VAL	N-CA-C	7.75	118.55	110.72
1	E	111	ASN	CA-CB-CG	7.72	120.32	112.60
1	G	366	GLY	CA-C-N	7.70	127.42	119.56
1	G	366	GLY	C-N-CA	7.70	127.42	119.56
1	J	263	GLN	CA-C-N	7.70	127.41	119.56
1	J	263	GLN	C-N-CA	7.70	127.41	119.56
5	c	27	PHE	CA-CB-CG	7.70	121.50	113.80
1	A	69	TYR	CA-C-N	7.67	127.85	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	TYR	C-N-CA	7.67	127.85	119.87
1	G	69	TYR	CA-C-N	7.67	127.38	119.56
1	G	69	TYR	C-N-CA	7.67	127.38	119.56
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	E	366	GLY	CA-C-N	7.64	127.35	119.56
1	E	366	GLY	C-N-CA	7.64	127.35	119.56
1	L	69	TYR	CA-C-N	7.61	127.32	119.56
1	L	69	TYR	C-N-CA	7.61	127.32	119.56
1	C	69	TYR	CA-C-N	7.61	127.32	119.56
1	C	69	TYR	C-N-CA	7.61	127.32	119.56
1	M	69	TYR	CA-C-N	7.60	127.31	119.56
1	M	69	TYR	C-N-CA	7.60	127.31	119.56
1	J	69	TYR	CA-C-N	7.58	128.23	120.04
1	J	69	TYR	C-N-CA	7.58	128.23	120.04
1	L	366	GLY	CA-C-N	7.57	127.28	119.56
1	L	366	GLY	C-N-CA	7.57	127.28	119.56
1	B	263	GLN	CA-C-N	7.49	127.12	119.56
1	B	263	GLN	C-N-CA	7.49	127.12	119.56
1	D	366	GLY	CA-C-N	7.48	127.19	119.56
1	D	366	GLY	C-N-CA	7.48	127.19	119.56
1	M	366	GLY	CA-C-N	7.46	127.16	119.56
1	M	366	GLY	C-N-CA	7.46	127.16	119.56
1	G	263	GLN	CA-C-N	7.40	127.03	119.56
1	G	263	GLN	C-N-CA	7.40	127.03	119.56
1	H	97	ALA	CA-C-N	7.40	127.11	119.56
1	H	97	ALA	C-N-CA	7.40	127.11	119.56
1	F	366	GLY	CA-C-N	7.39	128.04	119.47
1	F	366	GLY	C-N-CA	7.39	128.04	119.47
1	L	332	PRO	CA-C-N	7.37	127.08	119.56
1	L	332	PRO	C-N-CA	7.37	127.08	119.56
1	B	148	THR	N-CA-C	-7.37	104.81	114.31
1	C	263	GLN	CA-C-N	7.34	127.04	119.56
1	C	263	GLN	C-N-CA	7.34	127.04	119.56
1	D	34	ILE	N-CA-C	7.27	119.29	108.46
1	M	263	GLN	CA-C-N	7.26	126.90	119.56
1	M	263	GLN	C-N-CA	7.26	126.90	119.56
1	L	263	GLN	CA-C-N	7.26	126.89	119.56
1	L	263	GLN	C-N-CA	7.26	126.89	119.56
1	L	171	LEU	CA-C-N	7.25	126.95	119.56
1	L	171	LEU	C-N-CA	7.25	126.95	119.56
1	E	34	ILE	N-CA-C	7.23	119.24	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	331	ALA	CA-C-N	7.23	127.83	120.38
1	F	331	ALA	C-N-CA	7.23	127.83	120.38
1	D	69	TYR	CA-C-N	7.21	127.83	120.04
1	D	69	TYR	C-N-CA	7.21	127.83	120.04
1	J	97	ALA	CA-C-N	7.16	126.86	119.56
1	J	97	ALA	C-N-CA	7.16	126.86	119.56
1	B	331	ALA	CA-C-N	7.15	127.74	120.38
1	B	331	ALA	C-N-CA	7.15	127.74	120.38
1	O	151	ILE	CB-CA-C	-7.14	102.05	110.91
1	L	34	ILE	N-CA-C	7.14	118.10	108.11
1	C	366	GLY	CA-C-N	7.13	126.84	119.56
1	C	366	GLY	C-N-CA	7.13	126.84	119.56
1	N	329	ILE	N-CA-C	7.13	118.15	108.17
1	O	97	ALA	CA-C-N	7.11	126.81	119.56
1	O	97	ALA	C-N-CA	7.11	126.81	119.56
1	A	97	ALA	CA-C-N	7.10	126.80	119.56
1	A	97	ALA	C-N-CA	7.10	126.80	119.56
1	A	366	GLY	CA-C-N	7.09	126.80	119.56
1	A	366	GLY	C-N-CA	7.09	126.80	119.56
1	O	171	LEU	CA-C-N	7.09	126.80	119.56
1	O	171	LEU	C-N-CA	7.09	126.80	119.56
1	O	366	GLY	CA-C-N	7.08	126.78	119.56
1	O	366	GLY	C-N-CA	7.08	126.78	119.56
1	I	263	GLN	CA-C-N	7.07	126.70	119.56
1	I	263	GLN	C-N-CA	7.07	126.70	119.56
1	I	171	LEU	CA-C-N	7.04	126.74	119.56
1	I	171	LEU	C-N-CA	7.04	126.74	119.56
1	F	25	ASP	CA-CB-CG	7.04	119.64	112.60
1	J	321	ALA	CA-C-N	7.00	126.99	119.78
1	J	321	ALA	C-N-CA	7.00	126.99	119.78
1	H	171	LEU	CA-C-N	7.00	126.70	119.56
1	H	171	LEU	C-N-CA	7.00	126.70	119.56
1	C	171	LEU	CA-C-N	7.00	126.70	119.56
1	C	171	LEU	C-N-CA	7.00	126.70	119.56
1	J	148	THR	N-CA-C	-7.00	105.29	114.31
5	c	51	ASN	CA-C-N	6.98	126.90	119.85
5	c	51	ASN	C-N-CA	6.98	126.90	119.85
1	N	257	CYS	CA-C-N	6.97	127.56	119.47
1	N	257	CYS	C-N-CA	6.97	127.56	119.47
1	M	171	LEU	CA-C-N	6.95	126.65	119.56
1	M	171	LEU	C-N-CA	6.95	126.65	119.56
1	A	171	LEU	CA-C-N	6.93	126.63	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	LEU	C-N-CA	6.93	126.63	119.56
1	D	97	ALA	CA-C-N	6.93	126.63	119.56
1	D	97	ALA	C-N-CA	6.93	126.63	119.56
1	I	69	TYR	CA-C-N	6.91	126.61	119.56
1	I	69	TYR	C-N-CA	6.91	126.61	119.56
1	N	366	GLY	CA-C-N	6.89	126.59	119.56
1	N	366	GLY	C-N-CA	6.89	126.59	119.56
1	I	97	ALA	CA-C-N	6.89	126.59	119.56
1	I	97	ALA	C-N-CA	6.89	126.59	119.56
1	I	366	GLY	CA-C-N	6.89	126.59	119.56
1	I	366	GLY	C-N-CA	6.89	126.59	119.56
1	A	75	ILE	N-CA-C	6.89	117.81	108.17
1	E	161	HIS	N-CA-C	6.87	120.13	111.69
1	G	171	LEU	CA-C-N	6.84	126.54	119.56
1	G	171	LEU	C-N-CA	6.84	126.54	119.56
1	E	332	PRO	CA-C-N	6.83	126.53	119.56
1	E	332	PRO	C-N-CA	6.83	126.53	119.56
2	P	126	GLY	N-CA-C	-6.81	104.60	112.50
1	G	332	PRO	CA-C-N	6.80	126.50	119.56
1	G	332	PRO	C-N-CA	6.80	126.50	119.56
1	O	34	ILE	N-CA-C	6.79	117.89	108.12
1	F	257	CYS	CA-C-N	6.77	127.32	119.47
1	F	257	CYS	C-N-CA	6.77	127.32	119.47
2	W	126	GLY	N-CA-C	-6.76	104.66	112.50
1	J	171	LEU	CA-C-N	6.76	126.46	119.56
1	J	171	LEU	C-N-CA	6.76	126.46	119.56
1	N	151	ILE	CA-C-N	-6.76	114.33	123.12
1	N	151	ILE	C-N-CA	-6.76	114.33	123.12
2	W	208	GLU	N-CA-C	-6.76	103.84	111.14
1	A	331	ALA	CA-C-N	6.76	127.34	120.38
1	A	331	ALA	C-N-CA	6.76	127.34	120.38
1	B	132	MET	N-CA-C	6.76	119.44	109.24
1	I	151	ILE	CA-C-N	-6.76	114.08	122.93
1	I	151	ILE	C-N-CA	-6.76	114.08	122.93
1	I	331	ALA	CA-C-N	6.72	127.30	120.38
1	I	331	ALA	C-N-CA	6.72	127.30	120.38
1	L	31	PHE	CA-C-N	6.72	126.68	119.76
1	L	31	PHE	C-N-CA	6.72	126.68	119.76
1	M	111	ASN	CA-CB-CG	6.69	119.29	112.60
1	A	257	CYS	CA-C-N	6.69	127.23	119.47
1	A	257	CYS	C-N-CA	6.69	127.23	119.47
2	P	208	GLU	N-CA-C	-6.68	103.93	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	171	LEU	CA-C-N	6.67	126.37	119.56
1	F	171	LEU	C-N-CA	6.67	126.37	119.56
2	X	263	GLN	N-CA-C	-6.67	103.70	110.97
1	E	257	CYS	CA-C-N	6.65	127.18	119.47
1	E	257	CYS	C-N-CA	6.65	127.18	119.47
1	N	331	ALA	CA-C-N	6.62	127.20	120.38
1	N	331	ALA	C-N-CA	6.62	127.20	120.38
1	B	171	LEU	CA-C-N	6.61	126.30	119.56
1	B	171	LEU	C-N-CA	6.61	126.30	119.56
2	Q	263	GLN	N-CA-C	-6.60	103.78	110.97
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
3	a	109	HIS	CA-CB-CG	6.58	120.38	113.80
1	D	171	LEU	CA-C-N	6.58	126.27	119.56
1	D	171	LEU	C-N-CA	6.58	126.27	119.56
1	C	148	THR	N-CA-C	-6.55	105.85	114.31
1	C	331	ALA	CA-C-N	6.53	127.11	120.38
1	C	331	ALA	C-N-CA	6.53	127.11	120.38
1	N	97	ALA	CA-C-N	6.53	127.04	119.47
1	N	97	ALA	C-N-CA	6.53	127.04	119.47
3	T	109	HIS	CA-CB-CG	6.52	120.32	113.80
1	C	329	ILE	N-CA-C	6.51	117.67	108.36
3	T	90	ILE	N-CA-C	-6.49	104.16	110.72
1	I	257	CYS	CA-C-N	6.48	126.99	119.47
1	I	257	CYS	C-N-CA	6.48	126.99	119.47
1	C	34	ILE	N-CA-C	6.48	118.12	108.46
1	J	298	VAL	N-CA-C	6.48	117.18	108.11
1	H	108	ALA	CA-C-N	6.45	126.14	119.82
1	H	108	ALA	C-N-CA	6.45	126.14	119.82
1	C	332	PRO	CA-C-N	6.44	126.13	119.82
1	C	332	PRO	C-N-CA	6.44	126.13	119.82
1	K	332	PRO	CA-C-N	6.44	126.13	119.56
1	K	332	PRO	C-N-CA	6.44	126.13	119.56
1	O	321	ALA	CA-C-N	6.43	126.40	120.03
1	O	321	ALA	C-N-CA	6.43	126.40	120.03
1	M	257	CYS	CA-C-N	6.43	126.92	119.47
1	M	257	CYS	C-N-CA	6.43	126.92	119.47
1	F	151	ILE	CA-C-N	-6.42	114.68	122.90
1	F	151	ILE	C-N-CA	-6.42	114.68	122.90
1	M	148	THR	N-CA-C	-6.40	105.22	114.12
1	I	34	ILE	N-CA-C	6.40	118.00	108.46
1	N	171	LEU	CA-C-N	6.39	126.02	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	171	LEU	C-N-CA	6.39	126.02	119.56
1	G	329	ILE	N-CA-C	6.39	117.11	108.17
1	B	34	ILE	N-CA-C	6.38	117.31	108.12
1	J	108	ALA	CA-C-N	6.36	126.05	119.56
1	J	108	ALA	C-N-CA	6.36	126.05	119.56
3	a	90	ILE	N-CA-C	-6.35	104.31	110.72
1	K	151	ILE	CA-C-N	-6.33	114.80	122.90
1	K	151	ILE	C-N-CA	-6.33	114.80	122.90
1	G	257	CYS	CA-C-N	6.33	126.81	119.47
1	G	257	CYS	C-N-CA	6.33	126.81	119.47
1	K	34	ILE	N-CA-C	6.29	116.92	108.11
1	O	257	CYS	CA-C-N	6.29	126.77	119.47
1	O	257	CYS	C-N-CA	6.29	126.77	119.47
1	H	148	THR	N-CA-C	-6.28	106.20	114.31
1	A	332	PRO	CA-C-N	6.28	125.96	119.56
1	A	332	PRO	C-N-CA	6.28	125.96	119.56
1	F	132	MET	N-CA-C	6.27	118.95	109.23
1	N	75	ILE	N-CA-C	6.26	116.94	108.17
1	O	108	ALA	CA-C-N	6.26	126.46	119.32
1	O	108	ALA	C-N-CA	6.26	126.46	119.32
1	L	217	CYS	N-CA-C	6.25	119.72	110.48
1	I	163	VAL	N-CA-C	6.24	114.84	107.73
1	D	75	ILE	N-CA-C	6.23	116.90	108.17
1	B	332	PRO	CA-C-N	6.23	126.70	119.47
1	B	332	PRO	C-N-CA	6.23	126.70	119.47
1	D	148	THR	N-CA-C	-6.19	106.32	114.31
1	M	163	VAL	N-CA-C	6.19	114.97	107.61
1	H	257	CYS	CA-C-N	6.18	126.64	119.47
1	H	257	CYS	C-N-CA	6.18	126.64	119.47
4	b	105	ASP	CA-CB-CG	6.18	118.78	112.60
1	C	242	LEU	CA-C-N	6.18	125.86	119.56
1	C	242	LEU	C-N-CA	6.18	125.86	119.56
1	J	332	PRO	CA-C-N	6.18	125.80	119.56
1	J	332	PRO	C-N-CA	6.18	125.80	119.56
1	M	34	ILE	N-CA-C	6.17	117.00	108.12
1	G	217	CYS	N-CA-C	6.15	118.85	110.55
1	H	332	PRO	CA-C-N	6.14	125.76	119.56
1	H	332	PRO	C-N-CA	6.14	125.76	119.56
1	F	332	PRO	CA-C-N	6.13	125.81	119.56
1	F	332	PRO	C-N-CA	6.13	125.81	119.56
1	E	151	ILE	CA-C-N	-6.11	114.93	122.93
1	E	151	ILE	C-N-CA	-6.11	114.93	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	CYS	CA-C-N	6.10	126.55	119.47
1	D	257	CYS	C-N-CA	6.10	126.55	119.47
2	Q	15	LYS	N-CA-C	-6.10	104.74	111.82
2	S	28	ASP	CA-CB-CG	6.10	118.70	112.60
1	E	331	ALA	CA-C-N	6.09	126.66	120.38
1	E	331	ALA	C-N-CA	6.09	126.66	120.38
1	H	132	MET	N-CA-C	6.09	118.67	109.23
1	D	332	PRO	CA-C-N	6.08	125.76	119.56
1	D	332	PRO	C-N-CA	6.08	125.76	119.56
1	M	151	ILE	CA-C-N	-6.07	115.13	122.90
1	M	151	ILE	C-N-CA	-6.07	115.13	122.90
1	B	75	ILE	N-CA-C	6.05	116.63	108.17
1	G	242	LEU	N-CA-C	-6.05	101.95	110.29
1	A	148	THR	N-CA-C	-6.04	106.52	114.31
1	K	97	ALA	CA-C-N	6.03	127.38	119.84
1	K	97	ALA	C-N-CA	6.03	127.38	119.84
1	J	331	ALA	CA-C-N	6.03	126.59	120.38
1	J	331	ALA	C-N-CA	6.03	126.59	120.38
1	G	309	ILE	N-CA-C	6.01	116.79	110.72
1	H	331	ALA	CA-C-N	6.00	126.56	120.38
1	H	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	M	162	ASN	CA-C-N	-5.98	118.13	123.33
1	M	162	ASN	C-N-CA	-5.98	118.13	123.33
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
2	Z	28	ASP	CA-CB-CG	5.97	118.57	112.60
2	X	15	LYS	N-CA-C	-5.95	104.92	111.82
1	F	163	VAL	N-CA-C	5.95	114.69	107.61
1	K	101	HIS	CA-C-N	5.93	127.26	119.84
1	K	101	HIS	C-N-CA	5.93	127.26	119.84
1	A	34	ILE	N-CA-C	5.92	117.29	108.46
2	P	154	ILE	N-CA-C	-5.92	104.73	110.42
1	K	154	ASP	CA-C-N	5.92	132.85	121.54
1	K	154	ASP	C-N-CA	5.92	132.85	121.54
1	A	276	GLU	N-CA-C	-5.92	105.14	112.90
1	L	54	VAL	N-CA-C	5.92	117.00	108.48
1	I	75	ILE	N-CA-C	5.92	117.00	108.48
1	O	51	ASP	CA-CB-CG	-5.92	106.68	112.60
1	M	154	ASP	CA-C-N	5.92	132.84	121.54
1	M	154	ASP	C-N-CA	5.92	132.84	121.54
1	N	217	CYS	N-CA-C	5.91	119.26	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	321	ALA	CA-C-N	5.89	125.86	120.21
1	N	321	ALA	C-N-CA	5.89	125.86	120.21
2	W	154	ILE	N-CA-C	-5.89	104.77	110.42
1	D	331	ALA	CA-C-N	5.89	126.44	120.38
1	D	331	ALA	C-N-CA	5.89	126.44	120.38
1	O	332	PRO	CA-C-N	5.88	126.30	119.47
1	O	332	PRO	C-N-CA	5.88	126.30	119.47
1	N	332	PRO	CA-C-N	5.87	126.28	119.47
1	N	332	PRO	C-N-CA	5.87	126.28	119.47
1	K	163	VAL	CA-C-N	5.86	126.32	119.99
1	K	163	VAL	C-N-CA	5.86	126.32	119.99
1	O	151	ILE	N-CA-CB	5.85	117.10	110.72
1	B	257	CYS	CA-C-N	5.84	126.25	119.47
1	B	257	CYS	C-N-CA	5.84	126.25	119.47
1	N	162	ASN	N-CA-C	5.84	119.29	111.24
3	a	106	ILE	N-CA-C	-5.84	104.82	110.42
1	A	298	VAL	N-CA-C	5.83	116.26	107.80
1	J	34	ILE	N-CA-C	5.83	116.51	108.12
1	N	242	LEU	CA-C-N	5.83	126.23	119.47
1	N	242	LEU	C-N-CA	5.83	126.23	119.47
5	c	149	ASP	CA-CB-CG	5.82	118.42	112.60
1	D	375	PHE	CA-CB-CG	5.81	119.61	113.80
1	F	161	HIS	N-CA-C	5.81	118.84	111.69
1	M	101	HIS	CA-C-N	5.81	125.76	119.78
1	M	101	HIS	C-N-CA	5.81	125.76	119.78
1	A	375	PHE	CA-CB-CG	5.80	119.60	113.80
1	K	242	LEU	CA-C-N	5.80	126.19	119.47
1	K	242	LEU	C-N-CA	5.80	126.19	119.47
1	A	54	VAL	N-CA-C	5.79	116.21	108.11
1	N	161	HIS	N-CA-C	5.78	117.67	111.36
1	M	9	VAL	N-CA-C	5.75	116.16	108.11
1	C	321	ALA	CA-C-N	5.74	125.70	119.78
1	C	321	ALA	C-N-CA	5.74	125.70	119.78
1	E	242	LEU	CA-C-N	5.74	126.13	119.47
1	E	242	LEU	C-N-CA	5.74	126.13	119.47
1	L	148	THR	N-CA-C	-5.73	106.63	113.97
1	H	34	ILE	N-CA-C	5.73	117.00	108.46
1	O	132	MET	N-CA-C	5.73	118.55	109.50
3	T	106	ILE	N-CA-C	-5.73	104.92	110.42
1	L	97	ALA	CA-C-N	5.72	126.10	119.47
1	L	97	ALA	C-N-CA	5.72	126.10	119.47
1	C	54	VAL	N-CA-C	5.72	116.71	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	331	ALA	CA-C-N	5.72	126.27	120.38
1	M	331	ALA	C-N-CA	5.72	126.27	120.38
1	G	132	MET	N-CA-C	5.71	118.09	109.23
1	H	329	ILE	N-CA-C	5.71	116.17	108.17
1	E	97	ALA	CA-C-N	5.71	125.39	119.56
1	E	97	ALA	C-N-CA	5.71	125.39	119.56
1	C	75	ILE	N-CA-C	5.71	116.16	108.17
1	A	242	LEU	CA-C-N	5.71	126.09	119.47
1	A	242	LEU	C-N-CA	5.71	126.09	119.47
1	B	163	VAL	CA-C-N	5.70	126.18	120.14
1	B	163	VAL	C-N-CA	5.70	126.18	120.14
1	L	298	VAL	N-CA-C	5.69	116.05	107.80
1	C	97	ALA	CA-C-N	5.69	126.07	119.47
1	C	97	ALA	C-N-CA	5.69	126.07	119.47
4	b	147	VAL	N-CA-C	5.69	117.86	108.99
1	E	181	ALA	N-CA-C	5.68	116.58	108.74
1	C	151	ILE	CB-CA-C	-5.68	103.20	110.98
2	X	89	ASN	N-CA-C	-5.67	105.18	111.36
2	Q	89	ASN	N-CA-C	-5.67	105.18	111.36
1	C	107	GLU	N-CA-C	5.66	117.13	108.52
1	G	54	VAL	N-CA-C	5.66	116.04	108.11
1	D	321	ALA	CA-C-N	5.66	125.61	119.78
1	D	321	ALA	C-N-CA	5.66	125.61	119.78
5	c	99	ASP	CA-CB-CG	5.66	118.26	112.60
2	W	154	ILE	N-CA-CB	5.65	117.17	110.55
1	B	157	ASP	CA-CB-CG	5.65	118.25	112.60
1	K	298	VAL	N-CA-C	5.65	115.99	107.80
1	I	132	MET	N-CA-C	5.63	117.96	109.23
1	E	321	ALA	CA-C-N	5.63	125.58	119.78
1	E	321	ALA	C-N-CA	5.63	125.58	119.78
1	C	51	ASP	CA-CB-CG	-5.62	106.98	112.60
1	M	54	VAL	N-CA-C	5.62	116.57	108.48
1	H	233	SER	N-CA-C	5.61	118.62	108.69
1	H	321	ALA	CA-C-N	5.60	125.57	120.03
1	H	321	ALA	C-N-CA	5.60	125.57	120.03
1	M	132	MET	N-CA-C	5.60	117.91	109.23
1	G	331	ALA	CA-C-N	5.60	126.14	120.38
1	G	331	ALA	C-N-CA	5.60	126.14	120.38
1	A	132	MET	N-CA-C	5.59	117.90	109.23
1	C	257	CYS	CA-C-N	5.59	125.27	119.56
1	C	257	CYS	C-N-CA	5.59	125.27	119.56
1	J	257	CYS	CA-C-N	5.59	125.26	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	257	CYS	C-N-CA	5.59	125.26	119.56
1	D	151	ILE	CA-C-N	-5.57	115.41	122.37
1	D	151	ILE	C-N-CA	-5.57	115.41	122.37
2	P	154	ILE	N-CA-CB	5.57	117.06	110.55
1	B	108	ALA	CA-C-N	5.56	125.92	119.47
1	B	108	ALA	C-N-CA	5.56	125.92	119.47
1	C	132	MET	N-CA-C	5.55	117.62	109.24
1	M	276	GLU	N-CA-C	-5.55	105.63	112.90
1	K	309	ILE	N-CA-C	5.55	116.32	110.72
1	N	108	ALA	CA-C-N	5.55	125.91	119.47
1	N	108	ALA	C-N-CA	5.55	125.91	119.47
1	F	108	ALA	CA-C-N	5.54	125.90	119.47
1	F	108	ALA	C-N-CA	5.54	125.90	119.47
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	I	108	ALA	CA-C-N	5.53	125.88	119.47
1	I	108	ALA	C-N-CA	5.53	125.88	119.47
1	G	162	ASN	CA-C-N	-5.52	118.53	123.33
1	G	162	ASN	C-N-CA	-5.52	118.53	123.33
1	F	242	LEU	CA-C-N	5.51	125.86	119.47
1	F	242	LEU	C-N-CA	5.51	125.86	119.47
1	N	132	MET	N-CA-C	5.51	117.77	109.23
1	K	132	MET	N-CA-C	5.50	117.76	109.23
1	D	54	VAL	N-CA-C	5.50	116.40	108.48
1	B	77	THR	N-CA-C	-5.47	107.15	113.88
1	K	331	ALA	CA-C-N	5.47	126.02	120.38
1	K	331	ALA	C-N-CA	5.47	126.02	120.38
1	G	97	ALA	CA-C-N	5.47	126.67	119.84
1	G	97	ALA	C-N-CA	5.47	126.67	119.84
2	Q	276	HIS	CA-CB-CG	-5.46	108.33	113.80
1	G	34	ILE	N-CA-C	5.46	116.59	108.46
1	O	242	LEU	CA-C-N	5.46	125.80	119.47
1	O	242	LEU	C-N-CA	5.46	125.80	119.47
1	F	162	ASN	CA-C-N	-5.46	118.58	123.33
1	F	162	ASN	C-N-CA	-5.46	118.58	123.33
1	E	171	LEU	CA-C-N	5.45	125.12	119.56
1	E	171	LEU	C-N-CA	5.45	125.12	119.56
1	C	314	GLN	N-CA-C	-5.45	104.99	111.69
4	b	141	ARG	CA-C-N	5.44	125.11	119.56
4	b	141	ARG	C-N-CA	5.44	125.11	119.56
1	D	108	ALA	CA-C-N	5.43	125.77	119.47
1	D	108	ALA	C-N-CA	5.43	125.77	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	77	THR	N-CA-C	-5.43	107.02	113.97
1	J	132	MET	N-CA-C	5.42	117.64	109.23
1	M	97	ALA	CA-C-N	5.42	126.61	119.84
1	M	97	ALA	C-N-CA	5.42	126.61	119.84
1	C	163	VAL	CA-C-N	5.41	125.84	119.99
1	C	163	VAL	C-N-CA	5.41	125.84	119.99
1	N	373	LYS	N-CA-C	5.41	120.53	113.88
1	L	154	ASP	CA-C-N	5.40	131.86	121.54
1	L	154	ASP	C-N-CA	5.40	131.86	121.54
3	a	226	GLU	N-CA-C	5.40	117.17	111.28
1	J	222	ASP	CA-CB-CG	5.40	118.00	112.60
1	H	80	ASP	N-CA-C	-5.39	105.06	111.69
1	M	277	THR	N-CA-C	-5.39	105.31	111.07
1	N	51	ASP	CA-CB-CG	-5.38	107.22	112.60
1	G	233	SER	N-CA-C	5.37	117.42	108.99
2	X	188	GLY	N-CA-C	-5.37	106.27	112.50
1	I	54	VAL	N-CA-C	5.36	116.20	108.48
1	I	162	ASN	N-CA-C	5.35	118.63	111.24
1	K	108	ALA	CA-C-N	5.35	125.42	119.32
1	K	108	ALA	C-N-CA	5.35	125.42	119.32
1	O	111	ASN	CA-C-N	5.35	125.35	119.90
1	O	111	ASN	C-N-CA	5.35	125.35	119.90
1	D	242	LEU	CA-C-N	5.34	125.01	119.56
1	D	242	LEU	C-N-CA	5.34	125.01	119.56
1	E	253	GLU	CA-C-N	5.34	127.97	120.28
1	E	253	GLU	C-N-CA	5.34	127.97	120.28
1	E	54	VAL	N-CA-C	5.34	116.17	108.48
1	F	107	GLU	N-CA-C	5.34	117.30	109.24
2	Q	131	GLU	N-CA-C	-5.33	105.54	111.36
1	K	233	SER	N-CA-C	5.33	117.36	108.99
2	Q	188	GLY	N-CA-C	-5.33	106.32	112.50
1	L	242	LEU	CA-C-N	5.33	125.65	119.47
1	L	242	LEU	C-N-CA	5.33	125.65	119.47
1	B	97	ALA	CA-C-N	5.33	125.65	119.47
1	B	97	ALA	C-N-CA	5.33	125.65	119.47
2	X	131	GLU	N-CA-C	-5.32	105.56	111.36
1	N	101	HIS	CA-CB-CG	5.31	119.11	113.80
2	W	113	LEU	N-CA-C	-5.31	105.57	111.36
1	G	244	ASP	N-CA-C	-5.31	106.31	114.16
1	J	54	VAL	N-CA-C	5.30	116.36	108.46
1	K	321	ALA	CA-C-N	5.30	125.24	119.78
1	K	321	ALA	C-N-CA	5.30	125.24	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	VAL	N-CA-C	5.30	115.48	107.80
1	F	321	ALA	CA-C-N	5.30	125.24	119.78
1	F	321	ALA	C-N-CA	5.30	125.24	119.78
2	P	113	LEU	N-CA-C	-5.29	105.59	111.36
2	X	276	HIS	CA-CB-CG	-5.29	108.51	113.80
1	D	242	LEU	N-CA-C	-5.29	102.52	110.24
1	F	34	ILE	N-CA-C	5.29	115.73	108.12
1	I	275	HIS	CA-CB-CG	-5.28	108.52	113.80
2	Q	175	ASP	CA-CB-CG	5.28	117.88	112.60
1	F	203	THR	N-CA-C	5.27	117.44	111.11
2	X	175	ASP	CA-CB-CG	5.27	117.87	112.60
2	X	92	ILE	CB-CA-C	-5.26	105.23	111.97
1	N	16	LEU	N-CA-C	5.25	118.15	109.85
1	H	101	HIS	CA-C-N	5.25	125.19	119.78
1	H	101	HIS	C-N-CA	5.25	125.19	119.78
1	C	151	ILE	CA-C-N	-5.23	116.08	122.93
1	C	151	ILE	C-N-CA	-5.23	116.08	122.93
1	B	9	VAL	N-CA-C	5.23	115.65	108.12
1	I	242	LEU	CA-C-N	5.23	125.53	119.47
1	I	242	LEU	C-N-CA	5.23	125.53	119.47
1	O	331	ALA	CA-C-N	5.22	125.76	120.38
1	O	331	ALA	C-N-CA	5.22	125.76	120.38
1	D	233	SER	N-CA-C	5.22	117.19	108.99
1	E	151	ILE	CB-CA-C	-5.22	103.83	110.98
2	P	29	LYS	N-CA-C	-5.22	105.77	111.82
1	F	233	SER	N-CA-C	5.21	117.92	109.06
1	M	332	PRO	CA-C-N	5.21	125.51	119.47
1	M	332	PRO	C-N-CA	5.21	125.51	119.47
4	b	192	ARG	N-CA-C	5.20	116.95	111.28
1	E	51	ASP	CA-CB-CG	-5.20	107.40	112.60
2	W	29	LYS	N-CA-C	-5.20	105.79	111.82
1	H	242	LEU	CA-C-N	5.20	125.50	119.47
1	H	242	LEU	C-N-CA	5.20	125.50	119.47
1	J	75	ILE	N-CA-C	5.20	116.85	108.85
1	J	148	THR	CA-C-O	5.18	124.52	118.77
1	I	253	GLU	CA-C-N	5.17	127.72	120.28
1	I	253	GLU	C-N-CA	5.17	127.72	120.28
1	B	375	PHE	CA-CB-CG	5.17	118.97	113.80
1	E	162	ASN	N-CA-C	5.16	118.36	111.24
2	Q	92	ILE	CB-CA-C	-5.16	105.36	111.97
1	L	151	ILE	CA-C-N	-5.16	115.93	122.37
1	L	151	ILE	C-N-CA	-5.16	115.93	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	77	THR	N-CA-C	-5.15	107.37	113.97
1	D	163	VAL	CA-C-N	5.15	125.55	119.99
1	D	163	VAL	C-N-CA	5.15	125.55	119.99
1	H	161	HIS	CA-CB-CG	5.14	118.94	113.80
1	D	132	MET	N-CA-C	5.13	117.19	109.23
5	c	33	ASP	CA-CB-CG	-5.13	107.47	112.60
4	b	90	PHE	CA-CB-CG	5.13	118.93	113.80
1	C	233	SER	N-CA-C	5.12	117.02	108.99
1	L	51	ASP	CA-CB-CG	-5.11	107.49	112.60
1	F	151	ILE	CB-CA-C	-5.11	103.98	110.98
1	H	77	THR	N-CA-C	-5.11	107.43	113.97
1	G	111	ASN	CA-C-N	5.11	125.11	119.90
1	G	111	ASN	C-N-CA	5.11	125.11	119.90
1	F	163	VAL	CA-C-N	5.11	125.26	119.90
1	F	163	VAL	C-N-CA	5.11	125.26	119.90
1	G	157	ASP	N-CA-C	-5.10	106.21	112.90
1	G	253	GLU	CA-C-N	5.09	127.62	120.28
1	G	253	GLU	C-N-CA	5.09	127.62	120.28
1	L	257	CYS	CA-C-N	5.09	125.38	119.47
1	L	257	CYS	C-N-CA	5.09	125.38	119.47
1	O	54	VAL	N-CA-C	5.09	115.81	108.48
1	N	375	PHE	CA-CB-CG	5.08	118.88	113.80
1	J	51	ASP	CA-CB-CG	-5.07	107.53	112.60
1	B	54	VAL	N-CA-C	5.07	115.21	108.11
2	Q	153	HIS	N-CA-C	-5.07	105.65	111.07
1	L	233	SER	N-CA-C	5.06	116.94	108.99
1	D	51	ASP	CA-CB-CG	-5.06	107.54	112.60
2	P	261	TYR	N-CA-C	-5.06	105.85	111.36
1	J	101	HIS	CA-C-N	5.06	124.99	119.78
1	J	101	HIS	C-N-CA	5.06	124.99	119.78
1	L	321	ALA	CA-C-N	5.05	125.03	120.03
1	L	321	ALA	C-N-CA	5.05	125.03	120.03
1	O	109	PRO	N-CA-C	5.05	121.27	113.75
1	M	321	ALA	CA-C-N	5.04	124.97	119.78
1	M	321	ALA	C-N-CA	5.04	124.97	119.78
1	G	298	VAL	N-CA-C	5.03	115.10	107.80
1	H	111	ASN	CA-C-N	5.03	126.13	119.84
1	H	111	ASN	C-N-CA	5.03	126.13	119.84
1	B	51	ASP	CA-CB-CG	-5.03	107.57	112.60
1	A	51	ASP	CA-CB-CG	-5.03	107.57	112.60
1	A	151	ILE	CA-C-N	-5.03	116.34	122.93
1	A	151	ILE	C-N-CA	-5.03	116.34	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	163	VAL	CB-CA-C	-5.03	104.99	110.37
2	W	261	TYR	N-CA-C	-5.03	105.88	111.36
1	C	219	VAL	N-CA-C	5.02	116.47	111.00
1	I	129	VAL	CA-C-N	5.01	124.62	119.56
1	I	129	VAL	C-N-CA	5.01	124.62	119.56
1	A	321	ALA	CA-C-N	5.01	124.99	120.03
1	A	321	ALA	C-N-CA	5.01	124.99	120.03
1	B	233	SER	N-CA-C	5.01	117.32	108.75
4	b	90	PHE	N-CA-C	5.01	117.13	111.02
1	I	151	ILE	CB-CA-C	-5.01	104.12	110.98
1	L	108	ALA	CA-C-N	5.00	125.27	119.47
1	L	108	ALA	C-N-CA	5.00	125.27	119.47
2	X	153	HIS	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	V	91	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2933	0	2894	105	0
1	B	2933	0	2894	89	0
1	C	2933	0	2894	75	0
1	D	2933	0	2894	81	0
1	E	2933	0	2894	106	0
1	F	2933	0	2894	65	0
1	G	2933	0	2894	56	0
1	H	2933	0	2894	74	0
1	I	2933	0	2894	52	0
1	J	2933	0	2894	37	0
1	K	2933	0	2894	63	0
1	L	2933	0	2894	75	0
1	M	2933	0	2894	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	2933	0	2894	56	0
1	O	2933	0	2894	41	0
2	P	2207	0	2200	60	0
2	Q	2207	0	2200	152	0
2	R	231	0	245	3	0
2	S	231	0	245	0	0
2	W	2207	0	2200	91	0
2	X	2207	0	2200	162	0
2	Y	231	0	245	2	0
2	Z	231	0	245	0	0
3	T	1211	0	1226	139	0
3	a	1211	0	1226	179	0
4	U	1374	0	1436	244	0
4	b	1374	0	1436	360	0
5	V	1273	0	1201	157	0
5	c	1273	0	1201	169	0
All	All	61463	0	60916	2105	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (2105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ILE:HG22	4:U:208:PHE:CZ	1.36	1.61
4:b:43:ALA:CB	5:c:4:ILE:HG12	1.45	1.46
2:X:272:GLU:CG	3:a:113:ARG:NE	1.79	1.45
2:X:272:GLU:CG	3:a:113:ARG:HE	1.26	1.45
1:G:25:ASP:HB3	4:b:145:ARG:CZ	1.52	1.38
1:H:163:VAL:HG22	1:H:175:ILE:CG1	1.50	1.37
1:B:341:ILE:CG2	4:U:208:PHE:CZ	2.09	1.34
2:Q:272:GLU:HG3	3:T:113:ARG:NH2	1.42	1.32
2:X:272:GLU:CB	3:a:113:ARG:HE	1.45	1.29
2:X:272:GLU:O	3:a:113:ARG:CD	1.80	1.29
2:X:272:GLU:HG2	3:a:113:ARG:NE	0.99	1.29
1:C:345:ILE:HG23	4:b:209:GLU:CG	1.64	1.27
1:C:349:LEU:HD21	4:b:209:GLU:OE2	1.32	1.27
1:A:330:ILE:HD12	2:Q:37:LYS:NZ	1.49	1.26
4:b:44:SER:N	5:c:4:ILE:HB	1.49	1.25
2:X:272:GLU:C	3:a:113:ARG:NE	1.93	1.25
1:J:306:TYR:O	1:J:309:ILE:HG22	1.31	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TYR:CD2	1:A:352:PHE:HZ	1.55	1.24
1:H:133:TYR:CD2	1:H:352:PHE:HZ	1.54	1.23
4:b:43:ALA:C	5:c:4:ILE:HB	1.61	1.23
1:B:252:ASN:HA	1:B:255:PHE:CZ	1.73	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
1:E:313:MET:SD	1:E:329:ILE:HD13	1.79	1.22
4:U:159:LEU:CD2	2:X:136:LYS:HD2	1.69	1.22
3:a:268:ILE:HG12	4:b:131:LYS:NZ	1.55	1.21
1:B:332:PRO:O	1:B:335:ARG:HG3	1.36	1.21
1:C:23:GLY:CA	4:b:208:PHE:CD1	2.23	1.21
4:b:205:LYS:HD2	4:b:206:LYS:HD2	1.22	1.20
1:L:305:MET:CE	1:L:335:ARG:HB2	1.70	1.20
1:B:146:GLY:HA2	4:U:209:GLU:CG	1.71	1.20
1:E:313:MET:SD	1:E:329:ILE:CD1	2.30	1.19
4:b:50:LYS:CG	5:c:160:VAL:HG21	1.72	1.19
4:b:44:SER:HB2	5:c:3:ASP:H	1.05	1.19
1:A:326:LYS:HB3	2:Q:48:LYS:CE	1.70	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
1:H:133:TYR:CZ	1:H:352:PHE:CE1	2.31	1.18
1:J:252:ASN:HA	1:J:255:PHE:CE2	1.78	1.18
1:B:252:ASN:HA	1:B:255:PHE:CE2	1.78	1.18
1:A:332:PRO:O	1:A:335:ARG:HG3	1.38	1.17
1:A:133:TYR:CE2	1:A:352:PHE:CZ	2.32	1.17
4:U:159:LEU:HD23	2:X:136:LYS:CD	1.75	1.17
1:C:23:GLY:HA2	4:b:208:PHE:CD1	1.79	1.16
1:G:252:ASN:HA	1:G:255:PHE:CE2	1.80	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
4:b:50:LYS:CD	5:c:160:VAL:CG2	2.24	1.16
4:b:50:LYS:CD	5:c:160:VAL:HG21	1.74	1.16
1:A:148:THR:HB	1:C:47:MET:HE1	1.20	1.15
1:B:341:ILE:CG2	4:U:208:PHE:HZ	1.51	1.15
1:B:144:ALA:HA	4:U:208:PHE:CE1	1.82	1.15
2:W:88:LEU:HD11	2:X:85:VAL:HG13	1.21	1.15
1:A:133:TYR:CD2	1:A:352:PHE:CZ	2.34	1.15
4:b:43:ALA:HB3	5:c:4:ILE:HG12	1.26	1.15
2:Q:272:GLU:CB	3:T:113:ARG:HH22	1.61	1.14
4:b:53:LEU:HG	5:c:157:MET:HE2	1.28	1.14
1:A:326:LYS:CB	2:Q:48:LYS:CE	2.26	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:GLY:O	1:B:345:ILE:HG22	1.48	1.13
1:N:252:ASN:HA	1:N:255:PHE:CE2	1.82	1.13
4:b:43:ALA:O	5:c:4:ILE:HD13	1.47	1.13
2:P:91:ARG:HH21	2:Q:92:ILE:HG13	1.07	1.13
2:X:272:GLU:O	3:a:113:ARG:HD2	1.43	1.13
1:H:133:TYR:CE2	1:H:352:PHE:CZ	2.37	1.12
4:U:197:ALA:HA	2:W:87:SER:CB	1.79	1.12
2:Q:272:GLU:CG	3:T:113:ARG:NH2	2.12	1.12
4:b:43:ALA:CB	5:c:4:ILE:CG1	2.27	1.11
1:D:332:PRO:O	1:D:335:ARG:HG2	1.46	1.11
1:M:252:ASN:HA	1:M:255:PHE:CE2	1.86	1.11
4:b:43:ALA:HB1	5:c:4:ILE:CG1	1.79	1.11
1:C:345:ILE:HG23	4:b:209:GLU:HG3	1.15	1.11
1:C:252:ASN:HA	1:C:255:PHE:CE2	1.84	1.11
1:L:332:PRO:O	1:L:335:ARG:HG2	1.50	1.11
1:N:305:MET:SD	1:N:335:ARG:NE	2.24	1.11
1:L:257:CYS:HB3	1:L:258:PRO:HD3	1.14	1.10
1:L:305:MET:HE2	1:L:335:ARG:HB2	1.30	1.10
2:Q:161:LYS:O	2:Q:165:VAL:HG12	1.50	1.10
3:a:127:ILE:HG22	3:a:131:ARG:NH1	1.62	1.10
4:b:145:ARG:HH11	4:b:147:VAL:HG11	1.14	1.10
5:c:8:ALA:HA	5:c:82:VAL:HG21	1.22	1.10
1:C:332:PRO:O	1:C:335:ARG:HG3	1.52	1.10
2:Q:276:HIS:ND1	3:T:110:PHE:CE1	2.20	1.10
4:U:197:ALA:CB	2:W:87:SER:HB2	1.81	1.10
2:X:265:LEU:HD13	3:a:121:VAL:HG12	1.32	1.10
2:X:272:GLU:CD	3:a:117:GLU:HB2	1.75	1.10
1:B:144:ALA:HA	4:U:208:PHE:HE1	1.05	1.09
1:L:342:GLY:O	1:L:345:ILE:HG22	1.52	1.09
2:X:161:LYS:O	2:X:165:VAL:HG12	1.50	1.09
4:b:43:ALA:HB1	5:c:4:ILE:HG12	1.11	1.09
4:b:177:LYS:O	4:b:181:THR:HG23	1.52	1.09
5:V:59:GLU:OE2	2:W:153:HIS:CE1	2.04	1.09
1:F:252:ASN:HA	1:F:255:PHE:CE2	1.88	1.09
1:H:163:VAL:CG2	1:H:175:ILE:HD13	1.81	1.09
4:b:146:ARG:NH2	5:c:51:ASN:HB3	1.66	1.09
1:B:133:TYR:CD2	1:B:352:PHE:HZ	1.70	1.08
2:X:272:GLU:OE1	3:a:117:GLU:HB2	1.51	1.08
4:b:44:SER:HB2	5:c:3:ASP:N	1.67	1.08
1:E:25:ASP:HB2	4:b:181:THR:HG22	1.33	1.08
2:W:84:ASP:OD1	2:W:88:LEU:HG	1.50	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:91:ARG:HH21	2:X:92:ILE:HG13	1.07	1.08
2:X:276:HIS:HE1	3:a:110:PHE:HB2	1.17	1.08
1:B:146:GLY:HA2	4:U:209:GLU:HG3	1.10	1.08
1:C:23:GLY:O	4:b:208:PHE:HD1	1.32	1.08
1:D:146:GLY:HA2	4:U:177:LYS:HZ3	0.93	1.08
2:P:145:GLU:OE2	2:P:149:LYS:HE3	1.50	1.08
4:b:47:LEU:HD13	5:c:7:ALA:HB2	1.27	1.08
2:Q:272:GLU:HG3	3:T:113:ARG:CZ	1.82	1.08
3:a:259:TYR:CB	5:c:102:ARG:HD2	1.84	1.08
1:C:345:ILE:CG2	4:b:209:GLU:CG	2.31	1.07
1:H:133:TYR:CD2	1:H:352:PHE:CZ	2.42	1.07
4:b:50:LYS:HD3	5:c:160:VAL:CG2	1.82	1.07
1:F:305:MET:HE3	1:F:336:LYS:CD	1.83	1.07
2:Q:272:GLU:OE2	3:T:117:GLU:HB2	1.53	1.07
3:a:259:TYR:HB3	5:c:102:ARG:HD2	1.30	1.07
1:C:192:ILE:CD1	1:C:256:ARG:HD3	1.83	1.07
4:b:50:LYS:HG2	5:c:160:VAL:HG21	1.28	1.07
1:A:148:THR:CB	1:C:47:MET:HE1	1.84	1.07
2:X:272:GLU:HG3	3:a:113:ARG:HG2	1.16	1.06
1:M:238:LYS:NZ	2:P:276:HIS:NE2	2.01	1.06
1:H:163:VAL:HG22	1:H:175:ILE:HG12	1.09	1.06
2:Q:276:HIS:ND1	3:T:110:PHE:CD1	2.23	1.06
2:X:272:GLU:HG3	3:a:113:ARG:CG	1.84	1.06
1:N:109:PRO:HD2	1:N:161:HIS:NE2	1.70	1.05
1:C:192:ILE:HD12	1:C:256:ARG:CD	1.86	1.05
2:X:272:GLU:HG2	3:a:113:ARG:CD	1.86	1.05
4:b:53:LEU:HG	5:c:157:MET:CE	1.85	1.05
4:U:197:ALA:HB1	2:W:87:SER:HB2	1.38	1.04
1:A:143:TYR:CZ	1:C:44:MET:HE2	1.91	1.04
1:F:305:MET:HE3	1:F:336:LYS:HD2	1.33	1.04
1:C:345:ILE:CG2	4:b:209:GLU:HG2	1.86	1.04
1:N:252:ASN:HB2	1:N:255:PHE:CZ	1.93	1.04
4:b:135:LEU:HD23	4:b:138:LYS:HD2	1.39	1.03
1:A:143:TYR:CE2	1:C:44:MET:HE2	1.94	1.03
2:Q:272:GLU:CG	3:T:113:ARG:HH22	1.69	1.03
4:b:53:LEU:CG	5:c:157:MET:HE2	1.88	1.03
1:D:146:GLY:HA2	4:U:177:LYS:NZ	1.74	1.02
1:F:25:ASP:N	4:U:147:VAL:HG21	1.73	1.02
4:U:159:LEU:HD23	2:X:136:LYS:HD2	1.03	1.02
4:b:44:SER:HA	5:c:4:ILE:N	1.73	1.02
1:H:163:VAL:CG2	1:H:175:ILE:CD1	2.35	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:305:MET:SD	1:I:335:ARG:NE	2.32	1.02
2:Q:272:GLU:HG2	2:Q:276:HIS:NE2	1.73	1.02
3:a:268:ILE:CG1	4:b:131:LYS:HZ1	1.71	1.02
4:b:106:LYS:HA	4:b:106:LYS:HE3	1.41	1.02
1:H:163:VAL:HG21	1:H:175:ILE:HD13	1.39	1.02
1:E:289:ILE:HD11	1:G:63:GLY:O	1.58	1.02
1:A:133:TYR:CG	1:A:352:PHE:HZ	1.78	1.01
1:J:252:ASN:HB2	1:J:255:PHE:CZ	1.95	1.01
4:b:57:ALA:HB1	5:c:100:LEU:HD22	1.39	1.01
1:H:252:ASN:HA	1:H:255:PHE:CE2	1.94	1.01
1:A:330:ILE:CD1	2:Q:37:LYS:NZ	2.23	1.01
1:A:148:THR:HB	1:C:47:MET:CE	1.91	1.00
2:P:91:ARG:HE	2:Q:92:ILE:CD1	1.74	1.00
2:P:91:ARG:NH2	2:Q:92:ILE:HG13	1.75	1.00
2:X:276:HIS:CE1	3:a:110:PHE:HB2	1.96	1.00
4:b:146:ARG:HH21	5:c:51:ASN:CB	1.75	1.00
2:W:91:ARG:NH2	2:X:92:ILE:HG13	1.75	1.00
1:I:305:MET:HE2	1:I:335:ARG:CG	1.91	1.00
1:K:305:MET:HG3	1:K:335:ARG:HD2	1.44	1.00
4:b:50:LYS:HD3	5:c:160:VAL:HG21	1.40	1.00
4:b:155:MET:HA	4:b:155:MET:HE2	1.42	1.00
2:W:91:ARG:HE	2:X:92:ILE:CD1	1.74	0.99
3:a:105:LEU:HB3	3:a:109:HIS:CE1	1.96	0.99
2:X:265:LEU:CD1	3:a:121:VAL:HG12	1.91	0.99
1:L:257:CYS:HB3	1:L:258:PRO:CD	1.91	0.99
1:D:146:GLY:CA	4:U:177:LYS:HZ3	1.76	0.99
1:G:23:GLY:O	4:b:145:ARG:CB	2.11	0.99
1:E:305:MET:HE3	1:E:336:LYS:HD2	1.44	0.99
1:I:305:MET:HE2	1:I:335:ARG:HG3	1.00	0.99
1:D:305:MET:SD	1:D:335:ARG:HB2	2.02	0.98
1:A:326:LYS:HB3	2:Q:48:LYS:NZ	1.78	0.98
1:H:163:VAL:HG23	1:H:175:ILE:CG2	1.93	0.98
1:F:25:ASP:HB2	4:U:147:VAL:CG2	1.94	0.98
2:X:272:GLU:CG	3:a:113:ARG:CG	2.40	0.98
1:K:133:TYR:CE1	1:K:352:PHE:HZ	1.81	0.98
1:F:25:ASP:HB3	4:U:148:ARG:HE	1.25	0.98
1:N:305:MET:HE1	1:N:335:ARG:HH21	1.29	0.97
1:K:305:MET:CG	1:K:335:ARG:HD2	1.93	0.97
1:A:326:LYS:CB	2:Q:48:LYS:HE3	1.93	0.97
4:b:198:LEU:HB3	4:b:201:MET:HG2	1.46	0.97
1:F:24:ASP:HA	4:U:147:VAL:CG1	1.94	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:305:MET:CE	1:I:335:ARG:CG	2.43	0.97
3:a:210:LYS:HA	3:a:210:LYS:HE3	1.47	0.97
1:L:305:MET:HE1	1:L:335:ARG:HB2	1.47	0.97
1:C:192:ILE:HD12	1:C:256:ARG:HD3	0.98	0.97
2:P:256:LEU:CD1	2:Q:260:LEU:HD13	1.95	0.96
1:E:313:MET:SD	1:E:329:ILE:HD11	2.05	0.96
1:K:252:ASN:HB2	1:K:255:PHE:CZ	2.00	0.96
1:C:349:LEU:CD2	4:b:209:GLU:OE2	2.14	0.96
1:E:109:PRO:HD2	1:E:161:HIS:NE2	1.81	0.96
1:H:163:VAL:CG2	1:H:175:ILE:CG1	2.43	0.96
1:C:253:GLU:HA	1:C:256:ARG:HG2	1.48	0.95
1:M:300:SER:HA	1:M:336:LYS:HA	1.46	0.95
2:X:272:GLU:HG2	3:a:113:ARG:CZ	1.96	0.95
1:B:133:TYR:CD2	1:B:352:PHE:CZ	2.54	0.95
1:A:252:ASN:HA	1:A:255:PHE:CE2	2.00	0.95
1:C:253:GLU:HA	1:C:256:ARG:CG	1.96	0.95
2:X:272:GLU:CG	3:a:113:ARG:CD	2.44	0.95
1:A:330:ILE:HD12	2:Q:37:LYS:CE	1.96	0.95
1:H:133:TYR:CG	1:H:352:PHE:HZ	1.84	0.95
5:c:78:LEU:O	5:c:82:VAL:HG23	1.65	0.95
1:L:252:ASN:HA	1:L:255:PHE:CE2	2.01	0.95
2:W:256:LEU:CD1	2:X:260:LEU:HD13	1.95	0.95
1:A:252:ASN:HA	1:A:255:PHE:CZ	2.02	0.94
5:c:118:LYS:HZ3	5:c:128:ILE:HG22	1.30	0.94
1:E:106:THR:HG22	1:E:135:ALA:HB3	1.50	0.94
1:G:25:ASP:CB	4:b:145:ARG:CZ	2.45	0.94
1:A:133:TYR:CZ	1:A:352:PHE:CE1	2.55	0.94
3:a:127:ILE:CG2	3:a:131:ARG:NH1	2.31	0.94
1:N:305:MET:CE	1:N:335:ARG:HH21	1.81	0.94
4:b:174:LYS:HZ2	4:b:178:LYS:HE2	1.32	0.93
4:b:149:ILE:HG13	5:c:51:ASN:HD21	1.34	0.93
4:U:197:ALA:CB	2:W:87:SER:CB	2.46	0.93
2:X:272:GLU:CG	3:a:113:ARG:HG2	1.99	0.93
1:H:133:TYR:CE2	1:H:352:PHE:HZ	1.82	0.93
1:H:163:VAL:CG2	1:H:175:ILE:HG12	1.98	0.93
4:b:50:LYS:HG2	5:c:160:VAL:CG2	1.99	0.93
1:A:330:ILE:HD12	2:Q:37:LYS:HZ1	1.03	0.92
1:B:305:MET:CE	1:B:335:ARG:HB2	1.98	0.92
2:Q:272:GLU:OE2	3:T:117:GLU:CB	2.16	0.92
1:O:252:ASN:HA	1:O:255:PHE:CE2	2.04	0.92
2:Q:272:GLU:O	2:Q:276:HIS:CD2	2.23	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:197:ALA:CA	2:W:87:SER:CB	2.46	0.92
1:K:352:PHE:CD1	1:K:355:MET:HG3	2.05	0.92
1:C:133:TYR:CD2	1:C:352:PHE:HZ	1.86	0.92
1:H:163:VAL:HG23	1:H:175:ILE:HG23	1.48	0.92
4:b:44:SER:CB	5:c:4:ILE:H	1.81	0.92
1:M:241:GLU:OE2	2:P:268:LYS:HE2	1.69	0.92
1:E:28:ARG:NE	4:b:191:TRP:CH2	2.38	0.92
1:F:25:ASP:HB3	4:U:148:ARG:NE	1.84	0.92
4:U:197:ALA:HA	2:W:87:SER:OG	1.70	0.91
1:N:109:PRO:HD2	1:N:161:HIS:CD2	2.04	0.91
1:N:109:PRO:CD	1:N:161:HIS:NE2	2.34	0.91
1:B:207:GLU:HA	1:B:210:ARG:HG2	1.50	0.91
1:C:23:GLY:HA3	4:b:208:PHE:CE1	2.05	0.91
2:Q:276:HIS:HD1	3:T:110:PHE:HD1	0.92	0.91
1:D:146:GLY:N	4:U:177:LYS:CE	2.33	0.91
1:G:23:GLY:C	4:b:145:ARG:HB3	1.96	0.90
1:A:133:TYR:CE2	1:A:352:PHE:HZ	1.79	0.90
4:b:47:LEU:CD1	5:c:7:ALA:HB2	1.99	0.90
1:C:133:TYR:CZ	1:C:352:PHE:HE1	1.89	0.90
1:C:345:ILE:HG21	4:b:209:GLU:HG2	1.51	0.90
2:Q:272:GLU:HG3	3:T:113:ARG:HH22	1.29	0.90
3:a:268:ILE:HG12	4:b:131:LYS:HZ1	0.78	0.90
1:B:133:TYR:CE2	1:B:352:PHE:CE1	2.60	0.90
1:E:28:ARG:CZ	4:b:191:TRP:CZ3	2.54	0.90
1:F:252:ASN:CB	1:F:255:PHE:CZ	2.55	0.90
1:G:25:ASP:HB3	4:b:145:ARG:NH1	1.87	0.90
2:X:279:ASN:HB3	3:a:109:HIS:ND1	1.85	0.90
4:b:47:LEU:HD22	5:c:7:ALA:H	1.33	0.90
4:b:170:ARG:HA	4:b:173:LEU:HD21	1.52	0.90
1:C:23:GLY:O	4:b:208:PHE:CD1	2.23	0.90
1:D:143:TYR:O	4:U:177:LYS:NZ	2.04	0.90
4:U:73:GLY:HA2	4:U:76:LEU:HD12	1.53	0.90
2:X:272:GLU:O	3:a:113:ARG:NE	1.96	0.90
4:b:174:LYS:HA	4:b:177:LYS:HZ3	1.36	0.90
1:A:326:LYS:HE2	2:Q:44:VAL:CG2	2.01	0.89
1:B:133:TYR:CZ	1:B:352:PHE:HE1	1.90	0.89
1:F:24:ASP:HA	4:U:147:VAL:HG11	1.52	0.89
4:b:135:LEU:HA	4:b:138:LYS:HG3	1.53	0.89
1:B:342:GLY:O	1:B:345:ILE:CG2	2.21	0.89
5:V:118:LYS:HG3	5:V:128:ILE:HG13	1.54	0.89
4:b:174:LYS:HG2	4:b:178:LYS:CE	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ASN:CA	1:B:255:PHE:CZ	2.56	0.89
1:N:305:MET:CE	1:N:335:ARG:NH2	2.36	0.89
1:A:133:TYR:CZ	1:A:352:PHE:CZ	2.61	0.89
1:I:257:CYS:HB2	1:I:258:PRO:HD3	1.54	0.89
1:E:28:ARG:NH2	4:b:191:TRP:CZ3	2.40	0.88
1:A:148:THR:CG2	1:C:47:MET:HE1	2.02	0.88
1:G:23:GLY:O	4:b:145:ARG:HB2	1.73	0.88
4:b:53:LEU:CD2	5:c:157:MET:HE2	2.03	0.88
1:E:283:MET:HA	1:E:290:ARG:HD3	1.54	0.88
1:F:109:PRO:HG2	1:F:161:HIS:NE2	1.88	0.88
1:B:109:PRO:HD2	1:B:161:HIS:CD2	2.08	0.88
1:F:25:ASP:CB	4:U:148:ARG:HE	1.86	0.88
2:Q:276:HIS:ND1	3:T:110:PHE:HE1	1.71	0.88
4:b:43:ALA:C	5:c:4:ILE:CB	2.47	0.88
4:b:205:LYS:HE2	4:b:206:LYS:HZ2	1.39	0.88
4:b:146:ARG:HH21	5:c:51:ASN:HB3	1.29	0.88
1:L:133:TYR:CZ	1:L:352:PHE:HE1	1.92	0.87
1:L:207:GLU:HA	1:L:210:ARG:HG2	1.56	0.87
1:C:133:TYR:CE2	1:C:352:PHE:CE1	2.62	0.87
1:L:342:GLY:O	1:L:345:ILE:CG2	2.22	0.87
2:X:279:ASN:OD1	2:X:280:ASP:N	2.08	0.87
1:F:252:ASN:CA	1:F:255:PHE:CE2	2.57	0.87
1:O:1:ASP:HA	1:O:96:VAL:HG22	1.56	0.86
1:N:305:MET:HE1	1:N:335:ARG:NH2	1.88	0.86
2:Q:243:GLU:OE1	3:T:146:LYS:NZ	2.09	0.86
2:X:279:ASN:CB	3:a:109:HIS:ND1	2.38	0.86
1:I:257:CYS:CB	1:I:258:PRO:HD3	2.04	0.86
2:X:272:GLU:OE2	3:a:117:GLU:HB2	1.74	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
4:b:85:LEU:HD23	4:b:96:LEU:HD13	1.58	0.86
1:B:341:ILE:CG2	4:U:208:PHE:CE2	2.58	0.86
2:Q:273:GLU:HA	2:Q:276:HIS:HD2	1.40	0.86
1:M:230:ALA:HB3	1:M:255:PHE:HZ	1.39	0.86
4:b:43:ALA:HB1	5:c:4:ILE:CD1	2.05	0.86
4:b:145:ARG:NH1	4:b:147:VAL:HG11	1.90	0.86
1:C:23:GLY:C	4:b:208:PHE:HD1	1.83	0.86
1:E:133:TYR:CE1	1:E:355:MET:HB3	2.10	0.86
1:B:262:PHE:CZ	1:B:312:ARG:HG2	2.12	0.85
1:I:109:PRO:HD2	1:I:161:HIS:CD2	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ALA:HB3	1:B:255:PHE:HZ	1.40	0.85
1:F:25:ASP:HB2	4:U:147:VAL:HG21	1.58	0.85
4:b:170:ARG:HA	4:b:173:LEU:CD2	2.05	0.85
1:H:133:TYR:CZ	1:H:352:PHE:CZ	2.62	0.85
1:C:133:TYR:CD2	1:C:352:PHE:CZ	2.64	0.85
1:G:25:ASP:CG	4:b:145:ARG:NH1	2.34	0.85
1:E:28:ARG:CZ	4:b:191:TRP:CH2	2.60	0.85
1:L:196:ARG:HD2	1:L:253:GLU:CD	2.01	0.85
1:F:252:ASN:HB2	1:F:255:PHE:HZ	1.37	0.85
3:a:208:LYS:HB3	4:b:112:TYR:CD2	2.11	0.84
4:b:135:LEU:HD23	4:b:138:LYS:CD	2.06	0.84
4:b:205:LYS:HG2	4:b:207:LYS:NZ	1.92	0.84
1:E:146:GLY:CA	4:b:173:LEU:HD13	2.06	0.84
4:b:44:SER:CB	5:c:3:ASP:N	2.39	0.84
2:P:256:LEU:HD11	2:Q:260:LEU:HD13	1.59	0.84
2:X:272:GLU:CA	3:a:113:ARG:HE	1.91	0.84
1:L:143:TYR:HB3	1:L:345:ILE:HG21	1.57	0.84
1:B:146:GLY:CA	4:U:209:GLU:CG	2.54	0.84
1:F:24:ASP:CA	4:U:147:VAL:HG11	2.07	0.84
1:H:163:VAL:CG2	1:H:175:ILE:CG2	2.56	0.84
5:c:118:LYS:NZ	5:c:128:ILE:HG22	1.93	0.84
1:I:109:PRO:HD2	1:I:161:HIS:NE2	1.92	0.83
2:P:72:GLU:O	2:P:76:LYS:HG3	1.78	0.83
2:Q:272:GLU:CD	3:T:117:GLU:OE1	2.22	0.83
2:W:72:GLU:O	2:W:76:LYS:HG3	1.77	0.83
1:E:289:ILE:HD11	1:G:63:GLY:C	2.03	0.83
5:V:137:MET:O	5:V:141:ASP:N	2.10	0.83
4:b:44:SER:CB	5:c:3:ASP:H	1.89	0.83
1:A:326:LYS:CB	2:Q:48:LYS:HE2	2.04	0.83
2:W:256:LEU:HD11	2:X:260:LEU:HD13	1.59	0.83
1:N:109:PRO:HD2	1:N:161:HIS:CE1	2.12	0.83
4:b:198:LEU:HB3	4:b:201:MET:CG	2.08	0.83
1:A:328:LYS:NZ	2:Q:40:GLU:CD	2.36	0.83
4:U:142:PRO:O	4:U:145:ARG:NH1	2.11	0.83
3:a:217:LYS:NZ	3:a:239:SER:HB3	1.93	0.83
3:a:263:VAL:HG11	5:c:150:TYR:CD1	2.12	0.83
2:P:145:GLU:OE2	2:P:149:LYS:CE	2.27	0.83
4:b:74:ARG:O	4:b:78:THR:HG23	1.77	0.83
1:D:252:ASN:HA	1:D:255:PHE:CZ	2.13	0.83
1:E:109:PRO:HG2	1:E:161:HIS:NE2	1.93	0.83
2:X:273:GLU:OE1	3:a:113:ARG:NH1	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:134:GLU:OE2	5:c:138:LYS:HG2	1.78	0.83
1:B:144:ALA:CA	4:U:208:PHE:HE1	1.88	0.82
1:C:23:GLY:C	4:b:208:PHE:CD1	2.57	0.82
1:D:252:ASN:HB2	1:D:255:PHE:CZ	2.13	0.82
1:L:332:PRO:O	1:L:335:ARG:CG	2.27	0.82
4:b:146:ARG:NE	4:b:146:ARG:HA	1.93	0.82
1:A:326:LYS:HB3	2:Q:48:LYS:HE2	1.56	0.82
1:G:252:ASN:HB2	1:G:255:PHE:CZ	2.14	0.82
5:c:46:ARG:HE	5:c:57:LEU:HD21	1.43	0.82
2:X:250:GLU:OE1	3:a:138:GLN:HG2	1.80	0.82
4:b:205:LYS:HG3	4:b:207:LYS:HD2	1.59	0.82
1:I:252:ASN:HA	1:I:255:PHE:CE2	2.14	0.82
1:N:252:ASN:CB	1:N:255:PHE:CZ	2.62	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
2:P:91:ARG:HE	2:Q:92:ILE:HD12	1.44	0.82
4:b:53:LEU:CD2	5:c:157:MET:CE	2.58	0.82
1:E:345:ILE:HD11	4:b:177:LYS:HB3	1.60	0.82
5:V:59:GLU:OE2	2:W:153:HIS:NE2	2.13	0.82
2:X:276:HIS:HB2	3:a:113:ARG:HH11	1.44	0.82
3:a:217:LYS:HZ3	3:a:239:SER:HB3	1.44	0.82
4:b:43:ALA:O	5:c:4:ILE:CD1	2.27	0.82
1:J:252:ASN:HA	1:J:255:PHE:HE2	1.43	0.82
1:F:305:MET:HE3	1:F:336:LYS:HD3	1.62	0.81
4:b:179:GLU:C	4:b:183:LYS:HZ2	1.88	0.81
4:b:180:ASP:HA	4:b:183:LYS:HG2	1.62	0.81
1:A:326:LYS:HE2	2:Q:44:VAL:CG1	2.10	0.81
1:E:146:GLY:HA2	4:b:173:LEU:HD13	1.60	0.81
5:V:59:GLU:OE2	2:W:153:HIS:HE1	1.62	0.81
1:F:24:ASP:HA	4:U:147:VAL:CB	2.10	0.81
1:C:253:GLU:HA	1:C:256:ARG:CD	2.10	0.81
4:b:44:SER:CA	5:c:4:ILE:N	2.44	0.81
1:J:252:ASN:CA	1:J:255:PHE:CE2	2.61	0.81
1:N:305:MET:CE	1:N:335:ARG:HE	1.93	0.81
5:c:44:VAL:HA	5:c:47:MET:HG2	1.63	0.81
1:A:330:ILE:CD1	2:Q:37:LYS:HZ1	1.86	0.81
2:P:145:GLU:CD	2:P:149:LYS:HE3	2.06	0.81
4:b:47:LEU:CD2	5:c:7:ALA:N	2.44	0.81
1:L:257:CYS:CB	1:L:258:PRO:HD3	2.04	0.81
3:a:113:ARG:NH2	3:a:117:GLU:OE1	2.14	0.81
1:C:23:GLY:CA	4:b:208:PHE:CE1	2.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:252:ASN:CA	1:N:255:PHE:CE2	2.64	0.80
4:b:43:ALA:HB3	5:c:4:ILE:CG1	2.05	0.80
3:a:127:ILE:HG22	3:a:131:ARG:HH11	1.44	0.80
4:b:85:LEU:HD23	4:b:96:LEU:CD1	2.10	0.80
1:B:133:TYR:CE2	1:B:352:PHE:CZ	2.68	0.80
1:H:133:TYR:CE1	1:H:352:PHE:CE1	2.68	0.80
1:M:109:PRO:HD2	1:M:161:HIS:CD2	2.16	0.80
1:A:328:LYS:NZ	2:Q:40:GLU:OE1	2.13	0.80
2:W:88:LEU:HD11	2:X:85:VAL:CG1	2.09	0.80
3:a:224:LEU:HD13	3:a:232:LYS:HZ3	1.46	0.80
1:E:289:ILE:CD1	1:G:63:GLY:O	2.30	0.80
2:W:91:ARG:HE	2:X:92:ILE:HD12	1.44	0.80
1:E:282:ILE:O	1:E:290:ARG:HG2	1.81	0.79
2:Q:272:GLU:CA	3:T:113:ARG:HH22	1.95	0.79
4:b:174:LYS:HA	4:b:177:LYS:NZ	1.97	0.79
1:N:109:PRO:CG	1:N:161:HIS:NE2	2.45	0.79
1:K:133:TYR:CE1	1:K:352:PHE:CZ	2.69	0.79
1:M:241:GLU:OE2	2:P:268:LYS:CE	2.29	0.79
4:b:145:ARG:HH11	4:b:147:VAL:CG1	1.94	0.79
1:G:23:GLY:C	4:b:145:ARG:CB	2.55	0.79
1:G:262:PHE:CZ	1:G:312:ARG:HG2	2.17	0.79
4:b:50:LYS:CD	5:c:160:VAL:HG22	2.11	0.79
3:a:105:LEU:HB3	3:a:109:HIS:NE2	1.98	0.79
4:b:174:LYS:C	4:b:178:LYS:HE3	2.06	0.79
1:F:109:PRO:HD2	1:F:161:HIS:CD2	2.17	0.79
4:U:184:GLU:OE1	4:U:187:GLU:CG	2.31	0.79
5:c:59:GLU:HA	5:c:62:ASP:OD2	1.83	0.79
4:b:174:LYS:HG2	4:b:178:LYS:HE3	1.64	0.79
1:G:252:ASN:HA	1:G:255:PHE:HE2	1.44	0.79
1:G:252:ASN:CA	1:G:255:PHE:CE2	2.65	0.79
1:H:326:LYS:NZ	2:X:219:ASP:OD1	2.16	0.79
3:a:205:ARG:HH11	3:a:209:LYS:HG3	1.48	0.79
4:b:173:LEU:O	4:b:176:VAL:HG22	1.83	0.79
4:U:159:LEU:HD23	2:X:136:LYS:CG	2.12	0.78
1:A:326:LYS:HG2	2:Q:44:VAL:CG1	2.12	0.78
1:D:146:GLY:CA	4:U:177:LYS:HE2	2.12	0.78
1:D:147:ARG:N	4:U:173:LEU:HD13	1.98	0.78
1:E:21:PHE:HZ	4:b:184:GLU:HB3	1.49	0.78
1:E:109:PRO:CD	1:E:161:HIS:NE2	2.45	0.78
1:N:305:MET:HE1	1:N:335:ARG:NE	1.97	0.78
4:b:170:ARG:O	4:b:173:LEU:HG	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:GLY:C	1:B:345:ILE:HG22	2.08	0.78
2:Q:272:GLU:CB	3:T:113:ARG:NH2	2.38	0.78
1:D:133:TYR:CZ	1:D:352:PHE:HE1	2.02	0.78
1:D:252:ASN:CB	1:D:255:PHE:CZ	2.66	0.78
3:a:267:ARG:HD2	5:c:150:TYR:CD2	2.19	0.78
1:G:25:ASP:CB	4:b:145:ARG:NH1	2.47	0.78
5:V:142:LYS:NZ	5:V:152:GLU:O	2.17	0.78
2:X:272:GLU:C	3:a:113:ARG:CZ	2.57	0.78
4:b:47:LEU:HD22	5:c:7:ALA:N	1.98	0.78
1:B:133:TYR:CZ	1:B:352:PHE:CE1	2.71	0.78
1:B:143:TYR:HB3	1:B:345:ILE:HD13	1.65	0.78
1:C:252:ASN:HA	1:C:255:PHE:CZ	2.18	0.77
1:E:207:GLU:HA	1:E:210:ARG:HG2	1.65	0.77
4:b:44:SER:CA	5:c:4:ILE:HB	2.14	0.77
1:H:133:TYR:CE2	1:H:352:PHE:CE1	2.68	0.77
1:N:305:MET:CE	1:N:335:ARG:NE	2.47	0.77
4:b:145:ARG:HD2	4:b:147:VAL:CG1	2.13	0.77
5:c:118:LYS:HZ3	5:c:128:ILE:CG2	1.97	0.77
1:B:146:GLY:HA3	4:U:209:GLU:HB3	1.67	0.77
1:K:352:PHE:CE1	1:K:355:MET:HG3	2.18	0.77
1:L:342:GLY:C	1:L:345:ILE:HG22	2.08	0.77
4:b:171:ALA:HB1	4:b:175:GLN:NE2	2.00	0.77
4:b:175:GLN:HA	4:b:178:LYS:CG	2.14	0.77
1:M:301:GLY:O	1:M:336:LYS:HB2	1.83	0.77
4:b:44:SER:HB3	5:c:4:ILE:H	1.49	0.77
1:A:133:TYR:CG	1:A:352:PHE:CZ	2.67	0.77
1:H:252:ASN:HA	1:H:255:PHE:HE2	1.49	0.77
3:T:267:ARG:HD2	5:V:150:TYR:HB3	1.67	0.77
4:b:118:VAL:O	4:b:122:ILE:HG12	1.84	0.77
1:I:169:TYR:OH	1:K:49:GLN:HG3	1.85	0.77
1:E:252:ASN:HA	1:E:255:PHE:CE2	2.20	0.77
1:L:143:TYR:CB	1:L:345:ILE:HG21	2.15	0.77
4:b:205:LYS:CD	4:b:206:LYS:HD2	2.11	0.77
1:A:326:LYS:HB2	2:Q:48:LYS:CE	2.15	0.76
5:c:46:ARG:HH21	5:c:57:LEU:HD13	1.49	0.76
4:b:50:LYS:HD2	5:c:160:VAL:HG22	1.67	0.76
4:b:205:LYS:HE2	4:b:206:LYS:NZ	2.00	0.76
3:T:200:LYS:HZ3	3:T:203:THR:HB	1.50	0.76
1:E:345:ILE:CD1	4:b:177:LYS:HB3	2.16	0.76
4:b:95:ASP:O	4:b:99:GLN:HG2	1.86	0.76
1:B:230:ALA:HB3	1:B:255:PHE:CZ	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:305:MET:SD	1:N:335:ARG:CZ	2.73	0.76
4:U:60:GLU:HG3	5:V:120:MET:HE1	1.65	0.76
4:b:44:SER:HA	5:c:4:ILE:CA	2.15	0.76
4:b:44:SER:CA	5:c:4:ILE:H	1.97	0.76
1:F:109:PRO:CG	1:F:161:HIS:NE2	2.49	0.76
5:V:59:GLU:CG	2:W:153:HIS:HE1	1.98	0.76
5:c:130:GLU:OE1	5:c:133:ILE:HD11	1.86	0.76
1:B:341:ILE:HG23	4:U:208:PHE:CE2	2.20	0.76
3:a:101:GLU:HG3	3:a:105:LEU:CD1	2.15	0.76
4:U:184:GLU:OE1	4:U:187:GLU:CD	2.28	0.76
4:b:50:LYS:CG	5:c:160:VAL:CG2	2.51	0.76
1:D:133:TYR:CE2	1:D:352:PHE:HE1	2.04	0.76
1:A:326:LYS:CG	2:Q:48:LYS:HE3	2.16	0.75
3:T:240:ILE:HA	4:U:107:VAL:HG11	1.67	0.75
1:B:305:MET:HE2	1:B:335:ARG:CB	2.16	0.75
1:J:252:ASN:CB	1:J:255:PHE:CZ	2.69	0.75
1:M:230:ALA:HB3	1:M:255:PHE:CZ	2.21	0.75
4:b:178:LYS:O	4:b:182:GLU:HG3	1.87	0.75
1:A:151:ILE:HD11	1:A:282:ILE:HG13	1.66	0.75
1:E:21:PHE:HZ	4:b:184:GLU:CB	2.00	0.75
1:M:207:GLU:HA	1:M:210:ARG:HG2	1.67	0.75
4:b:54:LEU:HD21	5:c:92:LYS:HE2	1.69	0.75
4:b:81:GLN:HG3	4:b:82:PRO:HD2	1.69	0.75
1:D:305:MET:SD	1:D:335:ARG:CB	2.75	0.75
1:A:133:TYR:CZ	1:A:352:PHE:HE1	2.05	0.75
5:V:59:GLU:O	5:V:63:GLU:N	2.15	0.75
5:V:107:ASN:ND2	5:V:116:GLU:OE2	2.19	0.74
1:B:305:MET:HE2	1:B:335:ARG:HB2	1.68	0.74
2:X:272:GLU:CA	3:a:113:ARG:NE	2.48	0.74
1:A:328:LYS:HZ3	2:Q:40:GLU:CD	1.92	0.74
4:U:47:LEU:HA	4:U:50:LYS:HE3	1.70	0.74
5:V:5:TYR:CD1	5:V:79:VAL:HG11	2.22	0.74
3:a:210:LYS:HA	3:a:210:LYS:CE	2.12	0.74
4:b:47:LEU:CD2	5:c:7:ALA:H	1.99	0.74
1:D:146:GLY:CA	4:U:177:LYS:CE	2.65	0.74
1:E:109:PRO:CG	1:E:161:HIS:NE2	2.50	0.74
3:T:204:GLU:HA	3:T:207:LYS:HD2	1.70	0.74
1:F:24:ASP:HA	4:U:147:VAL:HB	1.69	0.74
2:X:260:LEU:HD23	2:X:260:LEU:O	1.88	0.74
1:C:253:GLU:CA	1:C:256:ARG:HG2	2.18	0.74
1:K:252:ASN:CA	1:K:255:PHE:CE2	2.66	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:145:GLU:CG	2:P:149:LYS:HE3	2.17	0.74
2:X:272:GLU:OE2	3:a:113:ARG:CA	2.35	0.74
2:Q:260:LEU:O	2:Q:260:LEU:HD23	1.88	0.73
2:Q:273:GLU:HA	2:Q:276:HIS:CD2	2.23	0.73
3:T:240:ILE:O	3:T:244:GLU:HG2	1.88	0.73
1:D:148:THR:HG21	4:U:169:LEU:HD11	1.70	0.73
4:U:186:ARG:NH1	4:U:186:ARG:O	2.22	0.73
4:U:197:ALA:HA	2:W:87:SER:HB3	1.71	0.73
4:b:57:ALA:CB	5:c:100:LEU:HD22	2.16	0.73
1:A:282:ILE:HG21	1:A:294:TYR:CE2	2.23	0.73
1:F:305:MET:CE	1:F:336:LYS:HD3	2.17	0.73
1:M:238:LYS:HZ3	2:P:276:HIS:CD2	2.07	0.73
2:P:149:LYS:O	2:P:153:HIS:CD2	2.41	0.73
3:a:127:ILE:CG2	3:a:131:ARG:HH11	1.98	0.73
4:U:80:CYS:SG	4:U:103:ARG:NH2	2.62	0.73
4:U:199:SER:HB3	2:W:84:ASP:OD2	1.87	0.73
3:a:105:LEU:HD22	3:a:109:HIS:HE2	1.53	0.73
4:b:50:LYS:O	5:c:160:VAL:HG11	1.89	0.73
1:E:133:TYR:CE2	1:E:352:PHE:HE1	2.06	0.72
1:O:207:GLU:O	1:O:210:ARG:CG	2.37	0.72
5:V:59:GLU:CD	2:W:153:HIS:HE1	1.97	0.72
3:a:259:TYR:HB2	5:c:102:ARG:HD2	1.69	0.72
1:L:196:ARG:HD2	1:L:253:GLU:OE2	1.89	0.72
5:V:42:GLY:HA2	5:V:57:LEU:HD22	1.71	0.72
2:X:272:GLU:OE1	3:a:117:GLU:CB	2.35	0.72
1:D:146:GLY:N	4:U:177:LYS:HE2	2.03	0.72
1:E:166:TYR:CD1	1:E:289:ILE:HG23	2.25	0.72
1:I:189:LEU:HA	1:I:257:CYS:SG	2.29	0.72
2:P:256:LEU:CD1	2:Q:257:GLU:HG2	2.19	0.72
1:G:349:LEU:HD22	4:b:141:ARG:HG3	1.70	0.72
1:N:279:TYR:OH	1:N:283:MET:HE3	1.90	0.72
2:W:256:LEU:CD1	2:X:257:GLU:HG2	2.19	0.72
2:X:276:HIS:CE1	3:a:110:PHE:CB	2.73	0.72
5:c:62:ASP:OD1	5:c:63:GLU:HG2	1.90	0.72
1:F:25:ASP:N	4:U:147:VAL:CG2	2.51	0.72
1:L:133:TYR:CE2	1:L:352:PHE:HE1	2.08	0.72
1:F:252:ASN:HA	1:F:255:PHE:HE2	1.46	0.71
1:G:24:ASP:C	4:b:145:ARG:HD3	2.13	0.71
1:K:305:MET:CG	1:K:335:ARG:CD	2.68	0.71
2:X:265:LEU:CD1	3:a:121:VAL:CG1	2.68	0.71
1:E:26:ALA:HB3	4:b:188:VAL:HG12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:257:CYS:CB	1:I:258:PRO:CD	2.68	0.71
4:U:108:ASP:OD1	4:U:111:ARG:NH2	2.22	0.71
2:X:276:HIS:HE1	3:a:110:PHE:CB	1.98	0.71
4:b:175:GLN:HA	4:b:178:LYS:CD	2.20	0.71
1:A:330:ILE:CD1	2:Q:37:LYS:CE	2.68	0.71
1:H:133:TYR:CG	1:H:352:PHE:CZ	2.72	0.71
4:b:205:LYS:HG2	4:b:207:LYS:HZ2	1.54	0.71
1:E:25:ASP:CB	4:b:181:THR:HG22	2.16	0.71
5:V:94:GLU:O	5:V:150:TYR:OH	2.03	0.71
1:B:305:MET:HE1	1:B:335:ARG:HB2	1.72	0.71
1:N:305:MET:HE1	1:N:335:ARG:CZ	2.20	0.71
1:E:106:THR:HG21	1:E:140:LEU:HD12	1.73	0.71
1:M:109:PRO:HD2	1:M:161:HIS:NE2	2.05	0.71
3:T:214:GLU:O	3:T:217:LYS:NZ	2.23	0.71
3:a:224:LEU:HD11	3:a:232:LYS:HD2	1.72	0.71
1:C:23:GLY:HA2	4:b:208:PHE:CG	2.25	0.71
1:E:305:MET:CE	1:E:336:LYS:HD2	2.21	0.71
4:b:135:LEU:CD2	4:b:138:LYS:HD2	2.20	0.71
1:N:252:ASN:HA	1:N:255:PHE:HE2	1.50	0.71
3:T:219:LEU:HG	3:T:236:LEU:HD12	1.71	0.71
2:X:272:GLU:OE2	3:a:113:ARG:O	2.08	0.71
1:D:133:TYR:CE2	1:D:352:PHE:CE1	2.78	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
3:T:258:LYS:O	3:T:262:ASN:ND2	2.24	0.71
2:W:166:ALA:HA	2:X:165:VAL:HG21	1.72	0.71
4:b:106:LYS:HA	4:b:106:LYS:CE	2.18	0.71
4:b:135:LEU:HD23	4:b:138:LYS:CE	2.20	0.71
4:b:135:LEU:HA	4:b:138:LYS:CG	2.20	0.71
4:b:149:ILE:CG1	5:c:51:ASN:HD21	2.03	0.71
1:M:305:MET:SD	1:M:335:ARG:CG	2.79	0.71
2:Q:276:HIS:CG	3:T:110:PHE:HE1	2.09	0.71
1:D:332:PRO:O	1:D:335:ARG:CG	2.35	0.70
1:E:106:THR:CG2	1:E:135:ALA:HB3	2.21	0.70
1:F:25:ASP:HB3	4:U:148:ARG:CD	2.21	0.70
5:c:43:LYS:HG2	5:c:46:ARG:HH12	1.54	0.70
1:A:326:LYS:HG2	2:Q:48:LYS:HE3	1.71	0.70
3:a:200:LYS:NZ	3:a:204:GLU:HG3	2.06	0.70
4:b:166:SER:O	4:b:169:LEU:HG	1.90	0.70
2:Q:276:HIS:ND1	3:T:110:PHE:HD1	1.78	0.70
4:b:135:LEU:CA	4:b:138:LYS:HG3	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:146:ARG:HH21	5:c:51:ASN:CG	2.00	0.70
4:b:146:ARG:HA	4:b:146:ARG:CZ	2.22	0.70
4:b:173:LEU:HD12	4:b:177:LYS:NZ	2.06	0.70
2:X:272:GLU:C	3:a:113:ARG:CD	2.52	0.70
1:B:133:TYR:CE2	1:B:352:PHE:HE1	2.05	0.70
4:b:175:GLN:HA	4:b:178:LYS:HG2	1.72	0.70
1:K:352:PHE:CE1	1:K:355:MET:CB	2.74	0.70
2:Q:265:LEU:HD13	3:T:121:VAL:HB	1.72	0.70
3:T:252:GLU:HA	3:T:255:LYS:HE2	1.71	0.70
1:E:104:LEU:HD12	1:E:133:TYR:O	1.90	0.70
1:I:109:PRO:CD	1:I:161:HIS:NE2	2.54	0.70
5:c:23:ALA:O	5:c:26:ILE:HG12	1.92	0.70
1:C:345:ILE:HG12	4:b:209:GLU:HA	1.72	0.70
1:G:25:ASP:HB3	4:b:145:ARG:NE	2.05	0.70
1:A:230:ALA:HB3	1:A:255:PHE:HZ	1.56	0.69
1:D:147:ARG:CA	4:U:173:LEU:HD13	2.21	0.69
1:L:334:GLU:O	1:L:338:SER:HB3	1.92	0.69
4:U:197:ALA:O	2:W:84:ASP:HB2	1.91	0.69
4:b:54:LEU:HD22	5:c:160:VAL:O	1.92	0.69
4:b:172:HIS:O	4:b:176:VAL:HG13	1.92	0.69
5:c:43:LYS:HA	5:c:46:ARG:NH1	2.07	0.69
1:K:196:ARG:HD2	1:K:253:GLU:CD	2.17	0.69
1:H:163:VAL:HG23	1:H:175:ILE:HG21	1.74	0.69
1:D:252:ASN:CA	1:D:255:PHE:CE2	2.65	0.69
1:N:305:MET:CE	1:N:335:ARG:CZ	2.70	0.69
2:Q:260:LEU:HD23	2:Q:260:LEU:C	2.17	0.69
4:b:196:ASP:OD2	4:b:198:LEU:HD23	1.92	0.69
1:M:305:MET:SD	1:M:335:ARG:HG3	2.33	0.69
2:P:166:ALA:HA	2:Q:165:VAL:HG21	1.72	0.69
3:T:245:ALA:HB2	4:U:76:LEU:HD21	1.73	0.69
5:V:104:PHE:O	5:V:106:LYS:NZ	2.26	0.69
4:b:53:LEU:CG	5:c:157:MET:CE	2.57	0.69
1:J:252:ASN:HB2	1:J:255:PHE:HZ	1.54	0.69
2:P:91:ARG:HE	2:Q:92:ILE:CG1	2.06	0.69
3:T:267:ARG:HE	5:V:151:ASP:HB2	1.58	0.69
2:X:257:GLU:HA	2:X:260:LEU:HB3	1.75	0.69
3:a:257:GLN:OE1	4:b:125:ILE:HG13	1.92	0.69
1:E:146:GLY:HA3	4:b:173:LEU:HD13	1.75	0.69
3:T:224:LEU:HD13	3:T:229:LEU:HD13	1.75	0.69
1:F:252:ASN:CB	1:F:255:PHE:CE2	2.75	0.68
4:b:198:LEU:CB	4:b:201:MET:HG2	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:205:LYS:CG	4:b:207:LYS:HD2	2.23	0.68
1:B:133:TYR:CG	1:B:352:PHE:HZ	2.09	0.68
1:D:252:ASN:CA	1:D:255:PHE:CZ	2.76	0.68
2:X:260:LEU:HD23	2:X:260:LEU:C	2.17	0.68
1:K:305:MET:HG2	1:K:335:ARG:CD	2.23	0.68
3:T:237:TRP:HA	3:T:240:ILE:HD12	1.76	0.68
4:U:41:ILE:HG23	4:U:45:ARG:HG2	1.75	0.68
5:c:43:LYS:O	5:c:47:MET:HE3	1.92	0.68
1:G:24:ASP:C	4:b:145:ARG:CD	2.67	0.68
1:L:133:TYR:CE2	1:L:352:PHE:CE1	2.81	0.68
1:D:148:THR:CG2	4:U:169:LEU:HD11	2.23	0.68
4:U:197:ALA:CA	2:W:87:SER:HB2	2.18	0.68
2:W:91:ARG:HE	2:X:92:ILE:CG1	2.06	0.68
1:B:143:TYR:HB3	1:B:345:ILE:HG21	1.75	0.68
5:V:59:GLU:CD	2:W:153:HIS:CE1	2.71	0.68
2:W:256:LEU:HD21	2:X:256:LEU:HB3	1.75	0.68
1:K:189:LEU:HB2	1:K:257:CYS:SG	2.34	0.68
4:b:137:GLY:O	4:b:141:ARG:HG2	1.94	0.68
3:T:200:LYS:HZ1	3:T:204:GLU:HG2	1.56	0.68
5:V:4:ILE:HG23	5:V:79:VAL:HG21	1.75	0.68
2:P:256:LEU:HD21	2:Q:256:LEU:HB3	1.75	0.68
1:B:146:GLY:CA	4:U:209:GLU:CB	2.72	0.68
1:G:349:LEU:CD2	4:b:141:ARG:HG3	2.23	0.67
1:I:257:CYS:HB2	1:I:258:PRO:CD	2.24	0.67
3:a:234:LYS:HA	3:a:234:LYS:HE3	1.77	0.67
1:N:109:PRO:HG2	1:N:161:HIS:NE2	2.09	0.67
5:V:152:GLU:O	5:V:156:PHE:HB2	1.94	0.67
4:b:155:MET:HE2	4:b:155:MET:CA	2.23	0.67
1:D:333:PRO:C	1:D:335:ARG:H	2.02	0.67
1:M:332:PRO:O	1:M:335:ARG:HB3	1.95	0.67
4:b:145:ARG:HD2	4:b:147:VAL:HG11	1.77	0.67
4:U:56:ILE:HB	5:V:124:THR:HG22	1.75	0.67
4:U:184:GLU:OE1	4:U:187:GLU:HG2	1.93	0.67
1:A:143:TYR:CE2	1:C:44:MET:CE	2.73	0.67
1:N:262:PHE:CZ	1:N:312:ARG:HG2	2.30	0.67
2:Q:257:GLU:HA	2:Q:260:LEU:HB3	1.74	0.67
3:T:258:LYS:HG3	4:U:121:ASN:HD21	1.57	0.67
2:X:279:ASN:HD22	3:a:109:HIS:CB	2.08	0.67
1:L:207:GLU:O	1:L:210:ARG:HG3	1.94	0.67
5:V:64:VAL:HG12	5:V:65:ASP:H	1.58	0.67
1:B:146:GLY:HA2	4:U:209:GLU:CB	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:133:TYR:CZ	1:K:352:PHE:CZ	2.80	0.67
4:U:71:GLU:HG3	4:U:74:ARG:HH21	1.60	0.67
1:E:21:PHE:CZ	4:b:184:GLU:CB	2.78	0.67
1:F:25:ASP:CB	4:U:147:VAL:CG2	2.73	0.67
4:b:179:GLU:O	4:b:183:LYS:HG2	1.95	0.67
1:C:133:TYR:CE1	1:C:355:MET:HB3	2.29	0.67
3:T:215:ARG:NH1	4:U:108:ASP:O	2.28	0.67
4:b:200:GLY:C	4:b:201:MET:HE2	2.19	0.67
1:C:133:TYR:CZ	1:C:352:PHE:CE1	2.76	0.66
3:a:205:ARG:HH11	3:a:209:LYS:CG	2.06	0.66
5:V:17:LYS:HA	5:V:20:PHE:HB2	1.76	0.66
2:W:91:ARG:HH21	2:X:92:ILE:CG1	1.97	0.66
4:b:43:ALA:C	5:c:4:ILE:HD13	2.21	0.66
4:b:54:LEU:HD21	5:c:92:LYS:CE	2.24	0.66
4:b:106:LYS:HE3	4:b:106:LYS:CA	2.17	0.66
1:A:252:ASN:CA	1:A:255:PHE:CZ	2.78	0.66
2:P:145:GLU:HG3	2:P:149:LYS:HE3	1.78	0.66
4:b:81:GLN:HE21	4:b:82:PRO:HD2	1.60	0.66
4:b:174:LYS:O	4:b:178:LYS:HG2	1.95	0.66
4:b:201:MET:HE2	4:b:201:MET:N	2.10	0.66
1:F:252:ASN:HB2	1:F:255:PHE:CE2	2.30	0.66
2:P:91:ARG:NE	2:Q:92:ILE:HD12	2.11	0.66
5:V:112:ILE:HG22	5:V:117:LEU:HG	1.78	0.66
4:b:50:LYS:HG2	5:c:160:VAL:HG11	1.77	0.66
1:J:335:ARG:C	1:J:337:TYR:H	2.03	0.66
4:U:174:LYS:HA	4:U:177:LYS:HD2	1.77	0.66
4:U:204:ARG:HB2	2:W:76:LYS:HZ3	1.59	0.66
2:X:272:GLU:OE2	3:a:113:ARG:HB3	1.95	0.66
1:E:28:ARG:NH2	4:b:191:TRP:CE3	2.62	0.66
5:V:55:GLU:OE1	2:W:153:HIS:CE1	2.48	0.66
1:H:133:TYR:CE1	1:H:355:MET:HB3	2.30	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
4:b:150:SER:C	4:b:154:MET:HE2	2.20	0.66
1:E:133:TYR:CD2	1:E:352:PHE:CZ	2.84	0.66
4:U:45:ARG:NH2	5:V:131:ASP:OD1	2.29	0.66
1:C:252:ASN:HB2	1:C:255:PHE:CZ	2.31	0.65
3:T:215:ARG:HD3	4:U:108:ASP:HB3	1.77	0.65
1:A:326:LYS:HE2	2:Q:44:VAL:HG22	1.75	0.65
1:I:305:MET:HE1	1:I:335:ARG:CG	2.26	0.65
4:U:57:ALA:HB1	5:V:100:LEU:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:91:ARG:CZ	2:X:92:ILE:HG13	2.26	0.65
3:a:217:LYS:HE2	3:a:239:SER:CB	2.26	0.65
3:a:256:GLN:HE22	3:a:259:TYR:HE2	1.44	0.65
2:Q:261:TYR:CE1	2:Q:265:LEU:HD22	2.31	0.65
2:Q:261:TYR:HE1	2:Q:265:LEU:HD22	1.61	0.65
2:X:261:TYR:CE1	2:X:265:LEU:HD22	2.31	0.65
1:A:133:TYR:CD1	1:A:352:PHE:HZ	2.14	0.65
1:B:143:TYR:CB	1:B:345:ILE:HG21	2.26	0.65
2:W:91:ARG:NE	2:X:92:ILE:HD12	2.11	0.65
1:E:21:PHE:HE2	4:b:187:GLU:OE1	1.79	0.65
1:M:109:PRO:CG	1:M:161:HIS:NE2	2.59	0.65
4:b:146:ARG:NH2	5:c:51:ASN:CB	2.40	0.65
4:b:175:GLN:O	4:b:179:GLU:HG3	1.95	0.65
2:Q:272:GLU:HA	3:T:113:ARG:HH22	1.60	0.65
2:X:273:GLU:N	3:a:113:ARG:CZ	2.59	0.65
1:C:133:TYR:CG	1:C:352:PHE:HZ	2.15	0.65
1:N:279:TYR:OH	1:N:283:MET:CE	2.45	0.65
1:O:207:GLU:O	1:O:210:ARG:HG3	1.96	0.65
2:X:272:GLU:HG2	3:a:113:ARG:CG	2.17	0.65
1:E:133:TYR:CZ	1:E:352:PHE:HE1	2.14	0.65
1:L:133:TYR:CE1	1:L:355:MET:HB3	2.32	0.65
2:Q:261:TYR:CE1	2:Q:265:LEU:HB2	2.32	0.65
4:b:136:ARG:HG2	4:b:140:LYS:HD3	1.79	0.65
4:b:149:ILE:HD11	5:c:51:ASN:OD1	1.97	0.65
1:I:109:PRO:CG	1:I:161:HIS:NE2	2.60	0.65
3:T:271:ASN:HD21	4:U:136:ARG:HH21	1.43	0.65
4:b:43:ALA:HB3	5:c:4:ILE:HG21	1.79	0.65
1:E:106:THR:HG21	1:E:140:LEU:CD1	2.26	0.65
1:E:143:TYR:OH	1:G:45:VAL:N	2.30	0.65
1:F:305:MET:CE	1:F:336:LYS:CD	2.67	0.65
1:J:169:TYR:OH	1:L:49:GLN:HB3	1.97	0.65
5:V:43:LYS:HA	5:V:46:ARG:HE	1.61	0.65
2:X:279:ASN:HB2	3:a:109:HIS:ND1	2.10	0.65
1:D:133:TYR:CE1	1:D:355:MET:HB3	2.33	0.64
1:F:169:TYR:OH	1:H:49:GLN:HB3	1.97	0.64
3:T:218:VAL:HA	4:U:101:HIS:CE1	2.31	0.64
1:D:146:GLY:O	4:U:173:LEU:HD12	1.98	0.64
1:K:196:ARG:HD2	1:K:253:GLU:OE2	1.97	0.64
1:O:305:MET:SD	1:O:335:ARG:NE	2.70	0.64
2:P:256:LEU:HD11	2:Q:257:GLU:HG2	1.79	0.64
4:U:47:LEU:HD12	4:U:50:LYS:HE3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:50:LYS:HD2	5:V:160:VAL:HG21	1.79	0.64
2:W:88:LEU:HD12	2:X:85:VAL:HA	1.78	0.64
5:c:43:LYS:O	5:c:47:MET:HG2	1.97	0.64
1:E:133:TYR:CD2	1:E:352:PHE:HZ	2.16	0.64
2:W:88:LEU:CD1	2:X:85:VAL:HA	2.27	0.64
2:X:261:TYR:CE1	2:X:265:LEU:HB2	2.32	0.64
3:a:234:LYS:HD2	3:a:234:LYS:N	2.12	0.64
1:E:108:ALA:HB1	1:E:161:HIS:CE1	2.31	0.64
1:G:252:ASN:CB	1:G:255:PHE:CZ	2.81	0.64
1:G:333:PRO:C	1:G:335:ARG:H	2.05	0.64
3:T:217:LYS:HB2	3:T:236:LEU:HD21	1.80	0.64
3:a:200:LYS:HD3	3:a:200:LYS:C	2.22	0.64
3:a:256:GLN:NE2	3:a:259:TYR:CE2	2.65	0.64
1:F:227:MET:HE3	1:F:255:PHE:HE1	1.60	0.64
1:O:207:GLU:HA	1:O:210:ARG:HG2	1.80	0.64
2:P:91:ARG:CZ	2:Q:92:ILE:HG13	2.26	0.64
4:U:42:SER:O	4:U:46:LYS:NZ	2.30	0.64
3:a:101:GLU:HG3	3:a:105:LEU:HD11	1.78	0.64
1:D:25:ASP:HB3	4:U:181:THR:HA	1.80	0.64
2:X:273:GLU:HA	3:a:113:ARG:NH1	2.12	0.64
3:a:101:GLU:OE2	3:a:105:LEU:HD21	1.98	0.64
2:X:261:TYR:HE1	2:X:265:LEU:HD22	1.61	0.64
1:N:262:PHE:CE2	1:N:312:ARG:HG2	2.33	0.63
4:b:44:SER:N	5:c:4:ILE:CB	2.43	0.63
2:X:279:ASN:HD22	3:a:109:HIS:HB2	1.63	0.63
1:B:207:GLU:CA	1:B:210:ARG:HG2	2.26	0.63
1:B:252:ASN:CB	1:B:255:PHE:CZ	2.81	0.63
1:L:207:GLU:CA	1:L:210:ARG:HG2	2.28	0.63
3:a:210:LYS:HE3	3:a:210:LYS:CA	2.21	0.63
4:b:44:SER:CB	5:c:4:ILE:N	2.58	0.63
1:B:227:MET:HA	1:B:255:PHE:CE1	2.33	0.63
1:D:146:GLY:H	4:U:177:LYS:CE	2.12	0.63
1:K:352:PHE:CD1	1:K:355:MET:CG	2.80	0.63
3:a:267:ARG:NH1	5:c:150:TYR:CE2	2.67	0.63
1:A:330:ILE:CD1	2:Q:37:LYS:HZ3	2.10	0.63
1:C:192:ILE:CD1	1:C:256:ARG:CD	2.61	0.63
1:H:163:VAL:CG2	1:H:175:ILE:HG21	2.27	0.63
1:K:257:CYS:HB2	1:K:258:PRO:CD	2.27	0.63
1:M:336:LYS:C	1:M:338:SER:H	2.06	0.63
2:P:256:LEU:HG	2:Q:260:LEU:CD1	2.29	0.63
2:Q:272:GLU:HG3	3:T:113:ARG:NH1	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:248:PHE:CE2	4:b:72:LYS:HB2	2.33	0.63
4:b:177:LYS:O	4:b:180:ASP:OD1	2.17	0.63
1:A:328:LYS:HZ2	2:Q:40:GLU:CD	2.06	0.63
1:D:133:TYR:CD2	1:D:352:PHE:CZ	2.87	0.63
1:I:169:TYR:OH	1:K:49:GLN:CG	2.47	0.63
1:L:109:PRO:HD2	1:L:161:HIS:CD2	2.34	0.63
2:P:162:TYR:CD1	2:Q:165:VAL:HG11	2.34	0.63
4:U:204:ARG:HD3	2:W:76:LYS:HZ3	1.64	0.63
4:b:84:GLU:O	4:b:96:LEU:HD11	1.99	0.63
2:X:272:GLU:OE2	3:a:113:ARG:CB	2.47	0.63
5:V:121:LEU:O	5:V:124:THR:OG1	2.14	0.63
2:X:272:GLU:OE2	3:a:113:ARG:C	2.42	0.63
1:F:24:ASP:C	4:U:147:VAL:HG21	2.24	0.63
1:M:262:PHE:CZ	1:M:312:ARG:HG2	2.33	0.63
2:W:256:LEU:HG	2:X:260:LEU:CD1	2.29	0.63
2:X:252:SER:O	2:X:256:LEU:HG	1.99	0.63
1:D:23:GLY:O	4:U:180:ASP:HB2	1.98	0.62
1:D:147:ARG:CA	4:U:173:LEU:CD1	2.77	0.62
1:F:334:GLU:O	1:F:338:SER:HB3	1.99	0.62
2:W:162:TYR:CD1	2:X:165:VAL:HG11	2.34	0.62
1:E:133:TYR:CE2	1:E:352:PHE:CE1	2.86	0.62
2:Q:252:SER:O	2:Q:256:LEU:HG	1.99	0.62
4:b:53:LEU:HD21	5:c:157:MET:HE3	1.80	0.62
4:b:54:LEU:CD2	5:c:160:VAL:O	2.46	0.62
4:b:174:LYS:NZ	4:b:178:LYS:HE2	2.08	0.62
1:F:23:GLY:O	4:U:147:VAL:HG12	1.99	0.62
1:J:303:THR:O	1:J:306:TYR:CD1	2.53	0.62
5:V:113:ASP:HA	5:V:147:ARG:HB2	1.81	0.62
4:b:137:GLY:HA2	4:b:140:LYS:HG2	1.81	0.62
1:E:305:MET:HE3	1:E:336:LYS:CD	2.26	0.62
1:O:109:PRO:CB	1:O:163:VAL:HG21	2.29	0.62
2:P:88:LEU:HD13	2:P:91:ARG:NH2	2.14	0.62
5:V:101:PHE:CE1	5:V:112:ILE:HG13	2.34	0.62
3:a:203:THR:O	3:a:207:LYS:HG3	1.99	0.62
3:a:256:GLN:NE2	3:a:259:TYR:HE2	1.97	0.62
4:b:102:ALA:O	4:b:106:LYS:HG2	1.99	0.62
4:b:131:LYS:HD2	4:b:131:LYS:C	2.24	0.62
4:b:151:ALA:HA	4:b:154:MET:HE2	1.82	0.62
4:b:170:ARG:NH1	4:b:174:LYS:HE3	2.14	0.62
5:V:73:ASP:OD1	5:V:74:PHE:N	2.33	0.62
2:W:256:LEU:HD11	2:X:257:GLU:HG2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:273:GLU:HA	3:a:113:ARG:CZ	2.29	0.62
5:V:37:SER:OG	5:V:40:GLU:OE2	2.14	0.62
4:b:54:LEU:HD23	5:c:161:GLU:CA	2.28	0.62
1:G:332:PRO:O	1:G:335:ARG:HG2	1.99	0.62
1:H:163:VAL:CG2	1:H:175:ILE:HG23	2.25	0.62
1:L:305:MET:HE1	1:L:335:ARG:CB	2.28	0.62
1:B:169:TYR:OH	1:D:49:GLN:HB3	2.00	0.62
1:N:333:PRO:C	1:N:335:ARG:H	2.08	0.62
4:U:204:ARG:HD3	2:W:76:LYS:NZ	2.15	0.62
5:c:44:VAL:HA	5:c:47:MET:CG	2.29	0.62
5:c:46:ARG:HH21	5:c:57:LEU:CD1	2.13	0.62
1:N:334:GLU:O	1:N:338:SER:HB3	1.99	0.62
4:b:47:LEU:HD21	5:c:7:ALA:N	2.15	0.62
4:b:53:LEU:HD23	5:c:157:MET:HE2	1.80	0.62
1:A:326:LYS:HB2	2:Q:48:LYS:HE2	1.76	0.61
1:I:262:PHE:CZ	1:I:312:ARG:HG2	2.35	0.61
3:T:248:PHE:HE2	4:U:68:ARG:HA	1.64	0.61
2:X:253:ILE:HA	2:X:256:LEU:HB2	1.82	0.61
1:D:146:GLY:CA	4:U:177:LYS:NZ	2.45	0.61
2:P:88:LEU:CD1	2:P:91:ARG:NH2	2.63	0.61
1:H:227:MET:HB3	1:H:255:PHE:CE1	2.35	0.61
1:N:252:ASN:HB2	1:N:255:PHE:HZ	1.62	0.61
4:U:125:ILE:O	4:U:129:THR:OG1	2.14	0.61
5:V:64:VAL:HG22	5:V:80:MET:HE2	1.82	0.61
1:O:196:ARG:HD2	1:O:253:GLU:CD	2.25	0.61
1:A:326:LYS:HG2	2:Q:44:VAL:HG11	1.83	0.61
2:P:91:ARG:HH21	2:Q:92:ILE:CG1	1.97	0.61
4:b:135:LEU:HA	4:b:138:LYS:CD	2.30	0.61
1:E:334:GLU:O	1:E:338:SER:HB3	2.01	0.61
5:V:131:ASP:OD1	5:V:132:ASP:N	2.34	0.61
1:E:133:TYR:HE1	1:E:355:MET:HB3	1.65	0.61
4:b:54:LEU:HD23	5:c:161:GLU:HA	1.81	0.61
1:K:252:ASN:HA	1:K:255:PHE:HE2	1.59	0.61
2:Q:276:HIS:CG	3:T:110:PHE:CE1	2.84	0.61
4:b:151:ALA:O	4:b:155:MET:HE3	2.00	0.61
1:G:25:ASP:HB3	4:b:145:ARG:NH2	2.12	0.61
1:H:133:TYR:CE1	1:H:352:PHE:CZ	2.89	0.61
1:I:301:GLY:O	1:I:336:LYS:CB	2.49	0.61
1:M:109:PRO:CD	1:M:161:HIS:NE2	2.63	0.61
1:N:109:PRO:CD	1:N:161:HIS:CE1	2.81	0.61
5:V:117:LEU:HB3	5:V:133:ILE:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:105:ASP:HB3	5:V:109:ASP:H	1.66	0.60
2:X:272:GLU:CG	3:a:113:ARG:CB	2.79	0.60
1:E:109:PRO:HD2	1:E:161:HIS:CE1	2.36	0.60
1:M:305:MET:SD	1:M:335:ARG:NE	2.74	0.60
1:O:252:ASN:HA	1:O:255:PHE:CZ	2.36	0.60
2:Q:136:LYS:O	2:Q:140:LYS:HG2	2.01	0.60
4:b:180:ASP:HA	4:b:183:LYS:CG	2.30	0.60
1:M:196:ARG:HD2	1:M:253:GLU:CD	2.26	0.60
4:b:170:ARG:HH12	4:b:174:LYS:HE3	1.65	0.60
1:L:305:MET:HE2	1:L:335:ARG:CB	2.19	0.60
2:Q:253:ILE:HA	2:Q:256:LEU:HB2	1.82	0.60
3:T:201:ARG:O	3:T:205:ARG:N	2.32	0.60
3:a:240:ILE:HG12	4:b:104:VAL:HG23	1.83	0.60
4:b:150:SER:O	4:b:154:MET:HG2	2.01	0.60
1:F:25:ASP:CB	4:U:147:VAL:HG21	2.28	0.60
1:H:133:TYR:CE1	1:H:352:PHE:HE1	2.08	0.60
3:a:259:TYR:HB3	5:c:102:ARG:CD	2.20	0.60
4:b:171:ALA:HB1	4:b:175:GLN:HE22	1.65	0.60
4:U:204:ARG:CB	2:W:76:LYS:HZ3	2.13	0.60
2:X:276:HIS:CE1	3:a:110:PHE:CD1	2.90	0.60
5:c:8:ALA:CA	5:c:82:VAL:HG21	2.15	0.60
1:B:207:GLU:O	1:B:210:ARG:HG3	2.02	0.60
3:T:241:TYR:CD2	4:U:76:LEU:HD22	2.37	0.60
2:X:273:GLU:CA	3:a:113:ARG:CZ	2.79	0.60
1:F:23:GLY:O	4:U:147:VAL:CG1	2.50	0.60
2:Q:272:GLU:OE1	3:T:117:GLU:OE1	2.20	0.60
4:U:128:LEU:HA	4:U:131:LYS:HD2	1.84	0.60
5:V:11:GLN:HB3	5:V:88:ASP:HA	1.84	0.60
1:A:227:MET:HA	1:A:255:PHE:CE1	2.37	0.60
1:D:146:GLY:N	4:U:177:LYS:NZ	2.49	0.60
1:H:252:ASN:CA	1:H:255:PHE:CE2	2.78	0.60
1:K:252:ASN:HA	1:K:255:PHE:CZ	2.34	0.60
1:O:163:VAL:HG13	1:O:175:ILE:HG12	1.84	0.60
1:O:230:ALA:HB3	1:O:255:PHE:CZ	2.37	0.60
4:U:114:ILE:HG12	4:U:117:LYS:HZ3	1.67	0.60
1:H:160:THR:HG22	1:H:162:ASN:ND2	2.17	0.59
1:J:113:LYS:O	1:J:116:ARG:HG2	2.01	0.59
1:J:219:VAL:HG11	1:J:312:ARG:HG2	1.83	0.59
1:M:230:ALA:CB	1:M:255:PHE:CZ	2.84	0.59
1:M:252:ASN:CA	1:M:255:PHE:CZ	2.85	0.59
3:T:260:GLU:HG2	5:V:98:SER:OG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:174:LYS:HG2	4:b:178:LYS:HE2	1.81	0.59
1:A:162:ASN:ND2	1:A:281:SER:OG	2.35	0.59
1:B:146:GLY:HA3	4:U:209:GLU:CB	2.31	0.59
1:G:133:TYR:CE2	1:G:352:PHE:HE1	2.20	0.59
1:O:287:ILE:HD12	1:O:290:ARG:HD2	1.83	0.59
4:U:197:ALA:CB	2:W:87:SER:HB3	2.32	0.59
3:a:221:ILE:HD13	4:b:97:CYS:SG	2.41	0.59
1:B:345:ILE:HG23	1:B:346:LEU:N	2.18	0.59
1:D:301:GLY:O	1:D:336:LYS:HA	2.02	0.59
1:L:133:TYR:CD2	1:L:352:PHE:CZ	2.90	0.59
2:P:152:LYS:HE3	2:P:156:GLU:OE2	2.01	0.59
4:b:53:LEU:CD2	5:c:156:PHE:HE2	2.15	0.59
4:b:54:LEU:HD21	5:c:92:LYS:NZ	2.17	0.59
1:H:305:MET:SD	1:H:336:LYS:HD2	2.42	0.59
1:K:352:PHE:CE1	1:K:355:MET:CG	2.85	0.59
4:U:204:ARG:CD	2:W:76:LYS:HZ3	2.15	0.59
4:b:147:VAL:C	4:b:149:ILE:HD12	2.27	0.59
1:A:330:ILE:CD1	2:Q:37:LYS:HE2	2.32	0.59
5:V:141:ASP:OD2	5:V:146:GLY:N	2.36	0.59
2:W:256:LEU:HG	2:X:260:LEU:HD12	1.85	0.59
4:b:47:LEU:HD13	5:c:7:ALA:CB	2.18	0.59
4:b:195:ILE:HG22	4:b:196:ASP:N	2.18	0.59
3:T:204:GLU:OE2	3:T:208:LYS:NZ	2.29	0.59
4:U:204:ARG:HD2	4:U:210:SER:O	2.02	0.59
5:V:52:PRO:HB2	5:V:57:LEU:HD21	1.84	0.59
1:C:252:ASN:CB	1:C:255:PHE:CZ	2.86	0.59
3:T:253:LYS:O	3:T:257:GLN:HG2	2.03	0.59
5:V:12:LEU:HD22	5:V:78:LEU:HG	1.85	0.59
2:X:272:GLU:CG	3:a:113:ARG:HB3	2.33	0.59
3:a:217:LYS:CE	3:a:239:SER:HB3	2.31	0.59
4:b:50:LYS:HG2	5:c:160:VAL:CG1	2.32	0.59
1:D:334:GLU:O	1:D:338:SER:HB3	2.03	0.59
2:Q:272:GLU:C	2:Q:276:HIS:CD2	2.81	0.59
5:V:59:GLU:HG3	2:W:153:HIS:HE1	1.68	0.59
4:b:192:ARG:HG2	4:b:194:ASN:OD1	2.03	0.59
1:C:133:TYR:CE2	1:C:352:PHE:CZ	2.89	0.59
1:L:109:PRO:HD2	1:L:161:HIS:NE2	2.17	0.59
3:a:217:LYS:HE3	3:a:236:LEU:HD23	1.84	0.59
4:b:174:LYS:O	4:b:178:LYS:HE3	2.02	0.59
1:A:133:TYR:CE1	1:A:352:PHE:CZ	2.90	0.58
1:E:333:PRO:C	1:E:335:ARG:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:10:GLU:OE1	5:V:11:GLN:NE2	2.36	0.58
4:b:41:ILE:HG13	4:b:41:ILE:O	2.02	0.58
4:b:152:ASP:HA	4:b:155:MET:HG2	1.85	0.58
1:K:305:MET:SD	1:K:336:LYS:HD3	2.42	0.58
1:L:143:TYR:HB3	1:L:345:ILE:HD13	1.85	0.58
4:U:159:LEU:CD2	2:X:136:LYS:HB3	2.33	0.58
4:b:158:LEU:HD23	4:b:158:LEU:H	1.68	0.58
1:D:146:GLY:C	4:U:173:LEU:CD1	2.76	0.58
1:J:306:TYR:HB2	1:J:309:ILE:HB	1.85	0.58
1:K:352:PHE:CD1	1:M:45:VAL:HG21	2.38	0.58
1:C:304:THR:HB	1:C:335:ARG:HD2	1.86	0.58
1:N:305:MET:SD	1:N:335:ARG:CD	2.91	0.58
1:A:326:LYS:HE2	2:Q:44:VAL:HG13	1.83	0.58
1:G:23:GLY:O	4:b:145:ARG:CA	2.52	0.58
1:K:102:PRO:O	1:K:129:VAL:HG21	2.03	0.58
1:A:133:TYR:HE2	1:A:346:LEU:HD21	1.68	0.58
1:A:326:LYS:HE2	2:Q:44:VAL:HG21	1.82	0.58
1:B:332:PRO:O	1:B:335:ARG:CG	2.30	0.58
1:B:341:ILE:HG22	4:U:208:PHE:HZ	0.59	0.58
1:F:109:PRO:HD2	1:F:161:HIS:NE2	2.19	0.58
4:b:205:LYS:HG2	4:b:207:LYS:HZ3	1.69	0.58
1:L:109:PRO:CG	1:L:161:HIS:NE2	2.67	0.58
4:U:137:GLY:O	4:U:141:ARG:N	2.30	0.58
3:T:212:LEU:HA	3:T:215:ARG:HB2	1.86	0.58
4:U:104:VAL:HA	4:U:107:VAL:HG12	1.84	0.58
4:b:145:ARG:HD2	4:b:147:VAL:HG12	1.86	0.58
1:B:331:ALA:O	1:B:335:ARG:NH1	2.36	0.58
1:C:252:ASN:CA	1:C:255:PHE:CZ	2.87	0.58
1:E:283:MET:O	1:E:290:ARG:CZ	2.51	0.58
1:K:169:TYR:OH	1:M:49:GLN:HB3	2.03	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:91:ARG:HE	2:Q:92:ILE:HG13	1.69	0.58
2:P:256:LEU:HG	2:Q:260:LEU:HD12	1.85	0.58
2:P:256:LEU:HD23	2:Q:256:LEU:HD13	1.86	0.58
2:X:272:GLU:CB	3:a:113:ARG:NE	2.30	0.58
2:X:272:GLU:HG2	3:a:113:ARG:HB3	1.86	0.58
1:E:283:MET:HA	1:E:290:ARG:CD	2.30	0.58
1:K:230:ALA:HB3	1:K:255:PHE:HZ	1.69	0.58
1:L:230:ALA:HB3	1:L:255:PHE:HZ	1.68	0.58
5:V:112:ILE:N	5:V:148:ILE:O	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:50:LYS:C	5:c:160:VAL:HG11	2.28	0.58
4:b:135:LEU:HD23	4:b:138:LYS:NZ	2.18	0.58
4:b:175:GLN:CA	4:b:178:LYS:HG2	2.33	0.58
5:c:118:LYS:HD2	5:c:122:GLN:HE21	1.67	0.58
3:T:254:PHE:CE1	4:U:117:LYS:HB3	2.39	0.57
2:W:91:ARG:HE	2:X:92:ILE:HG13	1.69	0.57
2:X:261:TYR:CE1	2:X:265:LEU:CD2	2.87	0.57
1:K:252:ASN:CA	1:K:255:PHE:CZ	2.85	0.57
1:N:257:CYS:HB3	1:N:258:PRO:HD3	1.86	0.57
1:O:305:MET:CE	1:O:335:ARG:HE	2.16	0.57
3:T:256:GLN:HG2	5:V:102:ARG:CZ	2.33	0.57
1:E:28:ARG:HB2	4:b:187:GLU:HB3	1.86	0.57
1:G:133:TYR:CZ	1:G:352:PHE:HE1	2.22	0.57
1:H:133:TYR:OH	1:H:352:PHE:HE1	1.87	0.57
1:A:133:TYR:CE1	1:A:352:PHE:CE1	2.92	0.57
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.86	0.57
1:G:24:ASP:O	4:b:145:ARG:HD3	2.04	0.57
1:J:305:MET:HE1	1:J:335:ARG:HE	1.69	0.57
2:X:272:GLU:OE2	3:a:117:GLU:CB	2.49	0.57
1:D:252:ASN:HA	1:D:255:PHE:HE2	1.60	0.57
1:F:23:GLY:C	4:U:147:VAL:HG11	2.30	0.57
1:H:133:TYR:CD1	1:H:352:PHE:CZ	2.92	0.57
1:H:253:GLU:HA	1:H:256:ARG:HB2	1.86	0.57
5:V:111:TYR:HA	5:V:149:ASP:HA	1.86	0.57
5:V:142:LYS:HG2	5:V:152:GLU:HG2	1.86	0.57
4:U:60:GLU:HB3	5:V:103:MET:HB3	1.86	0.57
1:L:252:ASN:HB2	1:L:255:PHE:CZ	2.40	0.57
1:B:230:ALA:CB	1:B:255:PHE:CZ	2.87	0.57
1:B:345:ILE:HD12	4:U:208:PHE:CD1	2.39	0.57
1:E:109:PRO:HD2	1:E:161:HIS:CD2	2.39	0.57
2:P:166:ALA:CA	2:Q:165:VAL:HG21	2.35	0.57
2:W:162:TYR:CE1	2:X:165:VAL:HG11	2.39	0.57
2:W:256:LEU:HD23	2:X:256:LEU:HD13	1.86	0.57
3:a:228:GLN:O	3:a:232:LYS:HG3	2.04	0.57
1:A:305:MET:SD	1:A:335:ARG:HB2	2.45	0.57
1:E:21:PHE:CZ	4:b:184:GLU:HB3	2.33	0.57
1:K:189:LEU:HD13	1:K:257:CYS:SG	2.45	0.57
3:T:241:TYR:CZ	4:U:76:LEU:HB3	2.40	0.57
1:A:133:TYR:CD1	1:A:352:PHE:CZ	2.92	0.57
1:A:331:ALA:O	1:A:335:ARG:NH1	2.37	0.57
1:E:305:MET:CE	1:E:336:LYS:CD	2.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:273:GLU:CA	2:Q:276:HIS:HD2	2.16	0.57
4:U:49:LEU:HB3	5:V:136:LEU:HD11	1.87	0.57
4:U:69:ARG:HA	4:U:72:LYS:HE2	1.87	0.57
2:W:91:ARG:NE	2:X:92:ILE:HG13	2.20	0.57
1:A:326:LYS:HB3	2:Q:48:LYS:HZ3	1.69	0.56
2:Q:261:TYR:CE1	2:Q:265:LEU:CD2	2.87	0.56
3:T:271:ASN:OD1	4:U:136:ARG:NE	2.38	0.56
2:X:132:SER:O	2:X:136:LYS:HG2	2.04	0.56
5:c:126:GLU:OE1	5:c:128:ILE:HD13	2.05	0.56
1:J:219:VAL:CG1	1:J:312:ARG:HG2	2.35	0.56
1:L:342:GLY:HA2	1:L:345:ILE:HG22	1.87	0.56
2:P:91:ARG:NE	2:Q:92:ILE:HG13	2.20	0.56
5:V:60:MET:HA	5:V:63:GLU:HB2	1.86	0.56
1:E:207:GLU:O	1:E:210:ARG:HG3	2.06	0.56
1:I:109:PRO:HD2	1:I:161:HIS:CE1	2.40	0.56
2:P:256:LEU:HD12	2:Q:260:LEU:HD13	1.84	0.56
2:Q:132:SER:O	2:Q:136:LYS:HG2	2.04	0.56
3:T:268:ILE:O	3:T:272:GLN:N	2.39	0.56
3:a:208:LYS:O	3:a:211:ILE:HG22	2.05	0.56
4:b:167:LEU:HD12	4:b:167:LEU:O	2.04	0.56
1:J:51:ASP:OD1	1:J:51:ASP:N	2.38	0.56
2:P:162:TYR:CE1	2:Q:165:VAL:HG11	2.40	0.56
3:a:205:ARG:NH1	3:a:209:LYS:HG3	2.17	0.56
4:b:81:GLN:HE21	4:b:82:PRO:CD	2.17	0.56
1:M:109:PRO:HG2	1:M:161:HIS:NE2	2.20	0.56
4:U:172:HIS:O	4:U:176:VAL:HG23	2.05	0.56
1:G:25:ASP:CG	4:b:145:ARG:HH12	2.13	0.56
1:L:342:GLY:CA	1:L:345:ILE:HG22	2.36	0.56
4:U:83:LEU:HD21	4:U:100:LEU:HD21	1.88	0.56
2:X:265:LEU:HD11	3:a:121:VAL:CG1	2.35	0.56
1:M:109:PRO:HD2	1:M:161:HIS:CE1	2.41	0.56
1:N:196:ARG:HD2	1:N:253:GLU:OE2	2.06	0.56
2:Q:279:ASN:HD22	3:T:110:PHE:HB2	1.71	0.56
2:W:166:ALA:CA	2:X:165:VAL:HG21	2.35	0.56
1:J:80:ASP:OD2	1:J:84:LYS:NZ	2.39	0.56
4:b:205:LYS:HD2	4:b:206:LYS:H	1.71	0.56
1:F:333:PRO:C	1:F:335:ARG:H	2.14	0.56
1:I:189:LEU:CA	1:I:257:CYS:SG	2.93	0.56
4:U:182:GLU:OE1	4:U:183:LYS:NZ	2.39	0.56
2:W:256:LEU:HD13	2:X:257:GLU:HG2	1.88	0.56
4:b:174:LYS:NZ	4:b:178:LYS:HZ3	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:ASP:OD1	1:F:51:ASP:N	2.39	0.56
2:P:256:LEU:CD1	2:Q:260:LEU:CD1	2.77	0.56
5:V:36:ILE:HD11	5:V:71:THR:HA	1.88	0.56
4:b:53:LEU:CD2	5:c:157:MET:HE3	2.31	0.56
1:K:257:CYS:HB2	1:K:258:PRO:HD3	1.87	0.55
3:T:230:ARG:HG2	4:U:85:LEU:HD22	1.88	0.55
1:A:51:ASP:OD1	1:A:51:ASP:N	2.39	0.55
1:J:334:GLU:O	1:J:338:SER:HB3	2.06	0.55
1:J:222:ASP:OD1	1:J:315:LYS:NZ	2.40	0.55
1:K:230:ALA:HB3	1:K:255:PHE:CZ	2.41	0.55
3:a:259:TYR:CB	5:c:102:ARG:CD	2.72	0.55
4:b:174:LYS:HE3	4:b:178:LYS:HZ3	1.71	0.55
4:U:53:LEU:HG	5:V:104:PHE:CE2	2.41	0.55
1:B:187:ASP:OD2	1:B:191:LYS:NZ	2.39	0.55
2:Q:279:ASN:ND2	3:T:110:PHE:HB2	2.21	0.55
5:V:76:GLU:HA	5:V:79:VAL:HG12	1.87	0.55
5:V:79:VAL:HA	5:V:82:VAL:HG22	1.89	0.55
3:a:101:GLU:O	3:a:105:LEU:HG	2.07	0.55
1:D:257:CYS:HB3	1:D:258:PRO:HD3	1.89	0.55
4:U:150:SER:HB3	4:U:154:MET:HG2	1.89	0.55
1:I:301:GLY:O	1:I:336:LYS:HB3	2.07	0.55
2:X:257:GLU:OE1	3:a:131:ARG:HD2	2.07	0.55
3:a:105:LEU:HD22	3:a:109:HIS:NE2	2.20	0.55
1:A:80:ASP:OD2	1:A:84:LYS:NZ	2.40	0.55
3:T:213:ALA:HA	3:T:216:ARG:HG2	1.89	0.55
4:U:197:ALA:HB2	2:W:87:SER:CB	2.34	0.55
4:U:136:ARG:HD3	4:U:139:PHE:HD2	1.72	0.55
5:V:38:THR:HA	5:V:41:LEU:HG	1.88	0.55
5:V:93:SER:HG	5:V:97:LEU:H	1.55	0.55
5:V:96:GLU:O	5:V:100:LEU:HG	2.07	0.55
2:W:256:LEU:CD1	2:X:260:LEU:CD1	2.77	0.55
4:b:134:ASP:O	4:b:138:LYS:HG3	2.06	0.55
1:E:313:MET:CG	1:E:329:ILE:HD13	2.36	0.55
1:L:333:PRO:C	1:L:335:ARG:H	2.15	0.55
3:a:259:TYR:HB2	5:c:102:ARG:CD	2.37	0.55
4:b:198:LEU:O	4:b:201:MET:HG2	2.06	0.55
3:T:238:GLN:HE22	3:T:241:TYR:HD2	1.55	0.54
4:U:53:LEU:HD13	5:V:121:LEU:HG	1.88	0.54
4:b:73:GLY:HA3	4:b:74:ARG:NH2	2.22	0.54
1:H:227:MET:HB3	1:H:255:PHE:HE1	1.73	0.54
2:P:256:LEU:HD13	2:Q:257:GLU:HG2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:197:ALA:O	2:W:84:ASP:CB	2.55	0.54
5:V:5:TYR:HD1	5:V:79:VAL:HG11	1.71	0.54
1:K:51:ASP:N	1:K:51:ASP:OD1	2.40	0.54
4:U:197:ALA:CA	2:W:87:SER:HB3	2.29	0.54
1:D:147:ARG:HA	4:U:173:LEU:CD1	2.37	0.54
1:E:282:ILE:O	1:E:290:ARG:CG	2.53	0.54
1:F:227:MET:HE3	1:F:255:PHE:CE1	2.42	0.54
1:K:305:MET:HG3	1:K:335:ARG:CD	2.28	0.54
3:a:224:LEU:CD1	3:a:232:LYS:HZ3	2.18	0.54
1:A:252:ASN:CB	1:A:255:PHE:CZ	2.90	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:F:169:TYR:OH	1:H:49:GLN:CG	2.55	0.54
1:M:257:CYS:HB3	1:M:258:PRO:HD3	1.89	0.54
2:X:257:GLU:O	2:X:261:TYR:N	2.38	0.54
2:X:272:GLU:OE2	3:a:113:ARG:HA	2.07	0.54
3:T:239:SER:O	3:T:243:LEU:HG	2.07	0.54
5:V:55:GLU:OE1	2:W:153:HIS:NE2	2.40	0.54
5:V:72:VAL:HG13	5:V:76:GLU:HB2	1.90	0.54
5:V:154:LEU:O	5:V:158:LYS:N	2.37	0.54
3:a:105:LEU:O	3:a:109:HIS:CG	2.60	0.54
1:A:301:GLY:C	1:A:336:LYS:HA	2.33	0.54
1:D:51:ASP:OD1	1:D:51:ASP:N	2.39	0.54
1:D:133:TYR:CD2	1:D:352:PHE:HZ	2.25	0.54
1:D:146:GLY:H	4:U:177:LYS:NZ	2.05	0.54
1:D:147:ARG:C	4:U:173:LEU:HD13	2.33	0.54
1:E:207:GLU:CA	1:E:210:ARG:HG2	2.37	0.54
1:H:154:ASP:O	1:H:156:GLY:N	2.41	0.54
4:U:197:ALA:HA	2:W:87:SER:HG	1.69	0.54
2:X:261:TYR:OH	2:X:265:LEU:HD23	2.08	0.54
3:a:200:LYS:HD3	3:a:200:LYS:O	2.07	0.54
1:D:146:GLY:C	4:U:173:LEU:HD13	2.33	0.54
1:F:169:TYR:OH	1:H:49:GLN:CB	2.56	0.54
1:N:335:ARG:C	1:N:337:TYR:H	2.15	0.54
2:Q:257:GLU:O	2:Q:261:TYR:N	2.38	0.54
3:T:203:THR:HG22	3:T:207:LYS:HE3	1.90	0.54
3:a:205:ARG:NH1	3:a:209:LYS:HB2	2.22	0.54
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.90	0.54
1:D:345:ILE:HG23	4:U:176:VAL:HG12	1.90	0.54
1:M:301:GLY:O	1:M:336:LYS:CB	2.54	0.54
2:P:88:LEU:CD1	2:P:91:ARG:HH21	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:153:ALA:HB3	4:U:154:MET:HE2	1.90	0.54
2:X:257:GLU:OE1	3:a:131:ARG:CD	2.57	0.54
1:E:313:MET:O	1:E:317:ILE:HD12	2.08	0.53
1:E:335:ARG:C	1:E:337:TYR:H	2.16	0.53
1:F:169:TYR:OH	1:H:49:GLN:HG3	2.08	0.53
1:G:257:CYS:HB2	1:G:258:PRO:HD3	1.89	0.53
1:L:207:GLU:O	1:L:210:ARG:CG	2.56	0.53
3:T:229:LEU:HG	4:U:93:LEU:HG	1.90	0.53
3:T:241:TYR:O	4:U:76:LEU:HD23	2.08	0.53
5:V:86:LYS:NZ	5:V:88:ASP:OD2	2.38	0.53
5:V:145:ASP:HB2	5:V:147:ARG:HD3	1.91	0.53
1:B:222:ASP:OD1	1:B:315:LYS:NZ	2.42	0.53
1:D:230:ALA:HB3	1:D:255:PHE:HZ	1.72	0.53
1:L:133:TYR:CD2	1:L:352:PHE:HZ	2.25	0.53
4:b:174:LYS:CE	4:b:178:LYS:HZ3	2.21	0.53
4:b:179:GLU:HA	4:b:182:GLU:OE1	2.08	0.53
1:A:326:LYS:HG2	2:Q:44:VAL:HG13	1.90	0.53
1:B:109:PRO:CD	1:B:161:HIS:CD2	2.87	0.53
2:Q:272:GLU:CD	3:T:117:GLU:CB	2.81	0.53
5:V:117:LEU:HD21	5:V:148:ILE:HD12	1.89	0.53
5:V:133:ILE:O	5:V:137:MET:N	2.35	0.53
5:c:126:GLU:HG2	5:c:127:THR:N	2.23	0.53
1:D:146:GLY:N	4:U:177:LYS:HE3	2.22	0.53
3:T:259:TYR:CZ	5:V:102:ARG:HA	2.44	0.53
1:A:133:TYR:CE2	1:A:352:PHE:CE1	2.83	0.53
1:O:257:CYS:HB3	1:O:258:PRO:HD3	1.91	0.53
2:Q:272:GLU:HB2	3:T:113:ARG:NH2	2.20	0.53
2:X:272:GLU:C	3:a:113:ARG:HD2	2.24	0.53
3:a:221:ILE:HG22	4:b:94:GLN:HE22	1.74	0.53
1:H:257:CYS:HB3	1:H:258:PRO:HD3	1.91	0.53
1:H:333:PRO:C	1:H:335:ARG:H	2.15	0.53
1:K:113:LYS:O	1:K:116:ARG:HG2	2.08	0.53
4:b:47:LEU:HB2	5:c:4:ILE:HD12	1.89	0.53
4:b:85:LEU:CD2	4:b:96:LEU:HD13	2.34	0.53
5:c:86:LYS:NZ	5:c:155:GLU:OE2	2.42	0.53
1:A:352:PHE:CD1	1:A:355:MET:HG3	2.44	0.53
2:Q:261:TYR:OH	2:Q:265:LEU:HD23	2.08	0.53
3:T:205:ARG:HA	3:T:205:ARG:NH1	2.23	0.53
4:U:64:GLU:O	4:U:68:ARG:HG3	2.08	0.53
4:b:155:MET:HA	4:b:155:MET:CE	2.28	0.53
1:B:305:MET:HE2	1:B:335:ARG:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:187:ASP:OD2	1:N:191:LYS:NZ	2.42	0.53
1:O:230:ALA:CB	1:O:255:PHE:CE2	2.91	0.53
4:U:41:ILE:HG21	5:V:135:GLU:HG2	1.90	0.53
3:a:224:LEU:HD22	3:a:228:GLN:CD	2.33	0.53
1:B:154:ASP:OD2	1:B:161:HIS:HB2	2.09	0.53
1:E:21:PHE:CZ	4:b:184:GLU:HB2	2.44	0.53
1:L:222:ASP:OD1	1:L:315:LYS:NZ	2.41	0.53
1:L:252:ASN:HA	1:L:255:PHE:CZ	2.43	0.53
3:T:221:ILE:HD13	4:U:98:ARG:HG2	1.90	0.53
2:X:272:GLU:HG3	3:a:113:ARG:CD	2.25	0.53
1:O:164:PRO:HG2	1:O:171:LEU:HB2	1.90	0.53
5:V:5:TYR:HA	5:V:79:VAL:HB	1.90	0.53
1:G:133:TYR:CD2	1:G:352:PHE:CZ	2.97	0.52
1:H:51:ASP:OD1	1:H:51:ASP:N	2.41	0.52
1:L:252:ASN:CB	1:L:255:PHE:CZ	2.92	0.52
1:O:227:MET:HA	1:O:255:PHE:CE1	2.44	0.52
4:U:44:SER:HA	5:V:4:ILE:HB	1.92	0.52
2:W:256:LEU:HD12	2:X:260:LEU:HD13	1.84	0.52
4:b:135:LEU:HA	4:b:138:LYS:HD2	1.91	0.52
4:b:141:ARG:HD3	4:b:144:LEU:HD12	1.91	0.52
1:A:326:LYS:CE	2:Q:44:VAL:CG2	2.84	0.52
1:C:230:ALA:HB3	1:C:255:PHE:HZ	1.75	0.52
1:F:109:PRO:CD	1:F:161:HIS:NE2	2.72	0.52
1:G:133:TYR:CE2	1:G:352:PHE:CE1	2.97	0.52
3:a:224:LEU:HD22	3:a:228:GLN:OE1	2.09	0.52
4:b:156:GLN:H	4:b:156:GLN:CD	2.17	0.52
4:b:180:ASP:CA	4:b:183:LYS:HG2	2.38	0.52
1:A:332:PRO:O	1:A:335:ARG:CG	2.33	0.52
1:I:305:MET:HE1	1:I:335:ARG:HG2	1.90	0.52
1:N:305:MET:HE3	1:N:335:ARG:NH2	2.21	0.52
5:V:104:PHE:HD2	5:V:120:MET:HG3	1.74	0.52
5:c:13:THR:HG23	5:c:16:GLN:OE1	2.09	0.52
5:c:118:LYS:HE2	5:c:133:ILE:HD13	1.90	0.52
1:M:51:ASP:N	1:M:51:ASP:OD1	2.41	0.52
1:M:301:GLY:N	1:M:336:LYS:HB2	2.24	0.52
1:M:333:PRO:HG3	2:R:9:GLN:HG3	1.91	0.52
2:Q:273:GLU:OE2	2:Q:276:HIS:CD2	2.62	0.52
1:B:333:PRO:C	1:B:335:ARG:H	2.17	0.52
5:V:40:GLU:HG3	5:V:43:LYS:HD2	1.92	0.52
3:a:200:LYS:HZ1	3:a:204:GLU:HG3	1.72	0.52
1:B:227:MET:HA	1:B:255:PHE:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:GLY:C	1:B:336:LYS:HA	2.35	0.52
1:E:283:MET:O	1:E:290:ARG:NE	2.43	0.52
1:G:196:ARG:HD2	1:G:253:GLU:CD	2.34	0.52
1:M:252:ASN:CB	1:M:255:PHE:CZ	2.92	0.52
5:V:95:GLU:N	5:V:95:GLU:OE1	2.43	0.52
4:b:74:ARG:NE	4:b:74:ARG:CA	2.73	0.52
4:b:173:LEU:HD12	4:b:177:LYS:HZ2	1.73	0.52
5:c:56:GLU:OE1	5:c:60:MET:HE3	2.10	0.52
1:E:28:ARG:NH2	4:b:191:TRP:CH2	2.75	0.52
1:H:227:MET:HA	1:H:255:PHE:HZ	1.75	0.52
4:U:204:ARG:HB2	2:W:76:LYS:NZ	2.23	0.52
3:a:204:GLU:HA	3:a:207:LYS:HD3	1.92	0.52
4:b:47:LEU:HD23	5:c:6:LYS:HB2	1.91	0.52
4:b:85:LEU:HD22	4:b:93:LEU:HD11	1.92	0.52
1:G:335:ARG:C	1:G:337:TYR:H	2.18	0.52
1:N:257:CYS:CB	1:N:258:PRO:HD3	2.40	0.52
4:U:174:LYS:O	4:U:178:LYS:HG2	2.10	0.52
5:V:113:ASP:OD1	5:V:114:LEU:N	2.43	0.52
4:b:135:LEU:CA	4:b:138:LYS:HZ2	2.22	0.52
4:b:164:LYS:HE3	4:b:168:ASP:OD1	2.10	0.52
1:B:305:MET:CE	1:B:335:ARG:CB	2.76	0.52
1:E:28:ARG:HD3	4:b:187:GLU:HB3	1.92	0.52
4:b:43:ALA:HB3	5:c:4:ILE:CB	2.39	0.52
4:b:85:LEU:HD23	4:b:96:LEU:HD12	1.91	0.52
1:B:207:GLU:HA	1:B:210:ARG:CG	2.32	0.52
2:Q:253:ILE:O	2:Q:257:GLU:N	2.43	0.52
3:T:219:LEU:HD22	3:T:232:LYS:HD2	1.92	0.52
5:V:59:GLU:HG3	2:W:153:HIS:CE1	2.45	0.52
5:V:104:PHE:HB3	5:V:112:ILE:HG12	1.92	0.52
3:a:201:ARG:CZ	3:a:204:GLU:HB2	2.40	0.52
4:b:43:ALA:C	5:c:4:ILE:CG1	2.83	0.52
4:b:175:GLN:HA	4:b:178:LYS:HD2	1.92	0.52
1:H:196:ARG:HD2	1:H:253:GLU:OE2	2.10	0.51
2:P:194:GLU:OE2	2:P:198:LYS:NZ	2.44	0.51
4:U:49:LEU:HB2	5:V:136:LEU:HD21	1.91	0.51
1:B:305:MET:HE2	1:B:335:ARG:O	2.10	0.51
1:E:257:CYS:HB2	1:E:258:PRO:HD3	1.92	0.51
1:K:133:TYR:CD1	1:K:352:PHE:HZ	2.28	0.51
5:V:104:PHE:HA	5:V:120:MET:HG3	1.92	0.51
5:V:111:TYR:CD1	5:V:147:ARG:HG3	2.45	0.51
3:a:88:ASP:OD1	3:a:88:ASP:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:134:GLU:OE2	5:c:137:MET:HE2	2.10	0.51
1:A:295:ALA:HB2	2:Q:48:LYS:NZ	2.26	0.51
1:J:333:PRO:C	1:J:335:ARG:H	2.18	0.51
1:L:305:MET:CE	1:L:335:ARG:CB	2.65	0.51
3:T:200:LYS:NZ	3:T:203:THR:HB	2.22	0.51
5:V:28:VAL:HG22	5:V:30:GLY:H	1.76	0.51
1:D:25:ASP:OD2	4:U:181:THR:HG23	2.10	0.51
1:J:305:MET:HE1	1:J:335:ARG:NE	2.24	0.51
2:W:91:ARG:HG2	2:X:92:ILE:HD12	1.92	0.51
4:b:135:LEU:HA	4:b:138:LYS:HZ2	1.76	0.51
1:D:133:TYR:CD2	1:D:352:PHE:CE1	2.99	0.51
1:G:24:ASP:C	4:b:145:ARG:HD2	2.35	0.51
1:L:207:GLU:HA	1:L:210:ARG:CG	2.32	0.51
1:O:163:VAL:HG22	1:O:175:ILE:HG23	1.91	0.51
2:P:91:ARG:HG2	2:Q:92:ILE:HD12	1.92	0.51
2:Q:235:ALA:O	2:Q:239:ALA:N	2.43	0.51
4:b:51:THR:HG23	5:c:161:GLU:OXT	2.10	0.51
4:b:145:ARG:CD	4:b:147:VAL:HG11	2.40	0.51
1:F:25:ASP:HB3	4:U:148:ARG:HD3	1.92	0.51
1:I:51:ASP:OD1	1:I:51:ASP:N	2.40	0.51
1:I:337:TYR:O	1:I:341:ILE:HD12	2.11	0.51
1:K:305:MET:HG2	1:K:335:ARG:NE	2.26	0.51
2:R:4:ILE:O	2:R:5:LYS:C	2.53	0.51
3:a:217:LYS:HE2	3:a:239:SER:HB3	1.93	0.51
1:A:252:ASN:HB2	1:A:255:PHE:CZ	2.46	0.51
1:C:133:TYR:CG	1:C:352:PHE:CZ	2.96	0.51
1:E:28:ARG:HD3	4:b:187:GLU:CB	2.40	0.51
1:F:154:ASP:OD2	1:F:161:HIS:HB3	2.11	0.51
1:L:109:PRO:CD	1:L:161:HIS:NE2	2.74	0.51
4:U:60:GLU:OE2	4:U:63:ARG:NH2	2.43	0.51
4:U:197:ALA:HB2	2:W:87:SER:HB3	1.92	0.51
2:X:253:ILE:O	2:X:257:GLU:N	2.43	0.51
4:b:47:LEU:CD2	5:c:6:LYS:HB2	2.41	0.51
4:b:206:LYS:HD2	4:b:206:LYS:H	1.75	0.51
1:A:230:ALA:HB3	1:A:255:PHE:CZ	2.42	0.51
1:L:230:ALA:HB3	1:L:255:PHE:CZ	2.46	0.51
1:M:133:TYR:CE1	1:M:352:PHE:HZ	2.29	0.51
1:O:230:ALA:CB	1:O:255:PHE:HE2	2.23	0.51
4:U:42:SER:OG	4:U:43:ALA:N	2.42	0.51
4:U:197:ALA:HB1	2:W:84:ASP:OD1	2.11	0.51
2:W:194:GLU:OE2	2:W:198:LYS:NZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:52:PRO:HB3	5:c:56:GLU:HG3	1.93	0.51
1:B:305:MET:CE	1:B:335:ARG:O	2.59	0.51
1:H:160:THR:HG22	1:H:162:ASN:CG	2.36	0.51
1:H:196:ARG:HD2	1:H:253:GLU:CD	2.36	0.51
1:H:216:LEU:O	1:H:254:ARG:HG2	2.10	0.51
1:I:109:PRO:HG2	1:I:161:HIS:NE2	2.25	0.51
3:T:245:ALA:HA	4:U:72:LYS:HG3	1.92	0.51
5:V:91:GLY:HA3	5:V:159:GLY:H	1.75	0.51
5:V:142:LYS:HE2	5:V:155:GLU:CD	2.36	0.51
4:b:54:LEU:HD23	5:c:161:GLU:C	2.36	0.51
4:b:180:ASP:OD1	4:b:181:THR:N	2.43	0.51
1:E:207:GLU:O	1:E:210:ARG:CG	2.59	0.51
1:H:252:ASN:HB2	1:H:255:PHE:CZ	2.47	0.51
3:T:265:ARG:NH2	4:U:124:GLU:OE2	2.42	0.51
5:V:122:GLN:OE1	5:V:128:ILE:HG12	2.10	0.51
1:B:207:GLU:O	1:B:210:ARG:CG	2.59	0.50
1:H:216:LEU:O	1:H:254:ARG:NE	2.36	0.50
2:P:218:GLU:OE2	2:Q:217:LYS:HB2	2.10	0.50
3:T:237:TRP:NE1	4:U:81:GLN:O	2.43	0.50
3:T:251:GLN:HG3	4:U:114:ILE:HD13	1.93	0.50
4:b:54:LEU:HD23	5:c:161:GLU:O	2.11	0.50
1:B:342:GLY:CA	1:B:345:ILE:HG22	2.41	0.50
1:G:335:ARG:CG	1:G:335:ARG:HH11	2.23	0.50
1:L:133:TYR:CG	1:L:352:PHE:HZ	2.30	0.50
2:P:145:GLU:O	2:P:149:LYS:HG3	2.11	0.50
4:U:136:ARG:HA	4:U:139:PHE:CD2	2.46	0.50
2:X:278:LEU:O	2:X:279:ASN:C	2.54	0.50
3:a:200:LYS:HZ3	3:a:204:GLU:HG3	1.75	0.50
3:a:224:LEU:HD11	3:a:232:LYS:CD	2.39	0.50
5:V:58:GLN:HA	5:V:61:ILE:HD12	1.93	0.50
5:V:78:LEU:O	5:V:81:MET:HB2	2.12	0.50
5:V:150:TYR:CE2	5:V:154:LEU:HD11	2.47	0.50
2:W:84:ASP:OD1	2:W:84:ASP:O	2.30	0.50
3:a:224:LEU:CD1	3:a:232:LYS:HD2	2.40	0.50
1:N:51:ASP:OD1	1:N:51:ASP:N	2.44	0.50
1:O:334:GLU:O	1:O:338:SER:HB3	2.11	0.50
2:Q:265:LEU:O	2:Q:265:LEU:HD12	2.10	0.50
3:T:219:LEU:HD22	3:T:232:LYS:HB3	1.92	0.50
5:V:150:TYR:CE1	5:V:154:LEU:HD21	2.46	0.50
2:X:252:SER:O	2:X:256:LEU:N	2.45	0.50
4:b:44:SER:CA	5:c:4:ILE:CB	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:PHE:CE1	1:A:355:MET:CB	2.95	0.50
1:C:230:ALA:HB3	1:C:255:PHE:CZ	2.46	0.50
1:I:167:GLU:O	1:I:169:TYR:CD1	2.65	0.50
5:V:82:VAL:HA	5:V:85:MET:O	2.12	0.50
2:X:265:LEU:HD12	2:X:265:LEU:O	2.10	0.50
3:a:267:ARG:NH1	5:c:150:TYR:HE2	2.08	0.50
2:Q:252:SER:O	2:Q:256:LEU:N	2.45	0.50
2:X:261:TYR:OH	2:X:265:LEU:CD2	2.60	0.50
1:D:24:ASP:HA	4:U:184:GLU:HB2	1.94	0.50
1:J:335:ARG:C	1:J:337:TYR:N	2.69	0.50
1:K:305:MET:SD	1:K:336:LYS:CD	2.99	0.50
1:O:230:ALA:HB3	1:O:255:PHE:HZ	1.74	0.50
3:T:260:GLU:HA	3:T:263:VAL:HB	1.93	0.50
2:W:218:GLU:OE2	2:X:217:LYS:HB2	2.10	0.50
2:X:272:GLU:HG2	3:a:113:ARG:CB	2.40	0.50
1:C:331:ALA:O	1:C:335:ARG:NH1	2.44	0.50
1:L:109:PRO:HG2	1:L:161:HIS:NE2	2.27	0.50
3:a:250:LEU:HB3	4:b:118:VAL:HG21	1.93	0.50
1:J:306:TYR:C	1:J:308:GLY:H	2.20	0.50
1:K:333:PRO:C	1:K:335:ARG:H	2.19	0.50
1:K:352:PHE:HD1	1:M:45:VAL:HG21	1.74	0.50
1:O:207:GLU:CA	1:O:210:ARG:HG2	2.42	0.50
4:b:204:ARG:NE	4:b:210:SER:O	2.45	0.50
1:L:262:PHE:CE2	1:L:312:ARG:HG3	2.47	0.49
1:M:133:TYR:CD1	1:M:352:PHE:HZ	2.30	0.49
2:Q:272:GLU:HA	3:T:113:ARG:NH2	2.27	0.49
4:U:46:LYS:HD2	5:V:139:ASP:HB2	1.93	0.49
4:b:85:LEU:HD22	4:b:93:LEU:CD1	2.42	0.49
1:C:80:ASP:OD2	1:C:84:LYS:NZ	2.45	0.49
1:G:333:PRO:C	1:G:335:ARG:N	2.70	0.49
1:H:334:GLU:O	1:H:338:SER:HB3	2.12	0.49
1:I:260:THR:HA	1:I:263:GLN:O	2.12	0.49
4:U:175:GLN:HA	4:U:178:LYS:HG2	1.94	0.49
2:W:88:LEU:CD1	2:X:85:VAL:HG13	2.15	0.49
4:b:43:ALA:HB3	5:c:4:ILE:CG2	2.42	0.49
4:b:150:SER:O	4:b:154:MET:HE2	2.12	0.49
5:c:62:ASP:OD1	5:c:63:GLU:N	2.45	0.49
1:D:144:ALA:C	4:U:177:LYS:HE3	2.37	0.49
1:E:80:ASP:OD2	1:E:84:LYS:NZ	2.45	0.49
1:O:222:ASP:OD1	1:O:315:LYS:NZ	2.44	0.49
1:O:227:MET:HA	1:O:255:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:261:TYR:OH	2:Q:265:LEU:CD2	2.60	0.49
2:X:279:ASN:HD22	3:a:109:HIS:HB3	1.75	0.49
5:c:118:LYS:HD2	5:c:122:GLN:NE2	2.26	0.49
1:A:168:GLY:CA	1:C:47:MET:HE2	2.42	0.49
2:W:166:ALA:HA	2:X:165:VAL:CG2	2.42	0.49
1:D:146:GLY:C	4:U:173:LEU:HD12	2.38	0.49
1:M:207:GLU:O	1:M:210:ARG:CG	2.61	0.49
5:V:8:ALA:HA	5:V:11:GLN:HB2	1.93	0.49
5:V:54:PRO:HA	5:V:57:LEU:HD12	1.93	0.49
4:b:176:VAL:HG23	4:b:177:LYS:N	2.27	0.49
1:A:326:LYS:HE2	2:Q:44:VAL:HG11	1.94	0.49
1:D:146:GLY:HA2	4:U:177:LYS:CE	2.34	0.49
1:E:133:TYR:CD2	1:E:352:PHE:CE1	3.01	0.49
1:M:257:CYS:CB	1:M:258:PRO:HD3	2.42	0.49
3:T:243:LEU:HD22	4:U:111:ARG:CZ	2.42	0.49
2:X:279:ASN:HB3	3:a:109:HIS:CG	2.46	0.49
4:b:50:LYS:HD3	5:c:160:VAL:HG23	1.85	0.49
1:J:335:ARG:O	1:J:337:TYR:N	2.46	0.49
1:K:129:VAL:CG2	1:K:130:PRO:HD2	2.41	0.49
1:N:305:MET:HE3	1:N:335:ARG:HH21	1.69	0.49
5:V:137:MET:HA	5:V:148:ILE:HD11	1.95	0.49
2:X:276:HIS:O	2:X:279:ASN:CG	2.55	0.49
3:a:230:ARG:O	3:a:234:LYS:HG2	2.13	0.49
4:b:170:ARG:O	4:b:170:ARG:HD2	2.13	0.49
1:A:330:ILE:HD13	2:Q:37:LYS:HE2	1.94	0.49
1:F:257:CYS:CB	1:F:258:PRO:HD3	2.42	0.49
1:F:335:ARG:C	1:F:337:TYR:H	2.19	0.49
1:J:187:ASP:OD2	1:J:191:LYS:NZ	2.45	0.49
1:L:345:ILE:HG23	1:L:346:LEU:N	2.28	0.49
3:T:267:ARG:O	3:T:271:ASN:ND2	2.46	0.49
1:D:147:ARG:N	4:U:173:LEU:CD1	2.75	0.49
1:D:302:GLY:C	1:D:304:THR:H	2.21	0.49
2:Q:70:LYS:O	2:Q:74:ALA:N	2.42	0.49
2:Q:260:LEU:C	2:Q:260:LEU:CD2	2.85	0.49
3:T:238:GLN:O	3:T:242:ASN:ND2	2.46	0.49
5:V:20:PHE:O	5:V:24:PHE:HB2	2.12	0.49
2:X:272:GLU:CD	3:a:113:ARG:HB3	2.38	0.49
3:a:206:GLU:OE2	3:a:210:LYS:HG2	2.12	0.49
3:a:263:VAL:CG1	5:c:150:TYR:CD1	2.89	0.49
5:c:46:ARG:NE	5:c:57:LEU:HD21	2.22	0.49
5:c:56:GLU:OE2	5:c:59:GLU:OE1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TYR:CZ	1:A:352:PHE:HZ	2.17	0.49
1:C:162:ASN:ND2	1:C:281:SER:OG	2.45	0.49
1:L:109:PRO:HB2	1:L:161:HIS:NE2	2.28	0.49
3:T:200:LYS:NZ	3:T:204:GLU:HG2	2.27	0.49
5:V:59:GLU:CG	2:W:153:HIS:CE1	2.89	0.49
5:V:128:ILE:HD12	5:V:133:ILE:HD11	1.94	0.49
2:X:157:ASP:OD2	2:X:161:LYS:NZ	2.41	0.49
4:b:74:ARG:NE	4:b:74:ARG:HA	2.28	0.49
1:A:143:TYR:CD2	1:C:44:MET:CE	2.96	0.48
1:E:107:GLU:HG3	1:E:134:VAL:HG12	1.94	0.48
5:V:93:SER:OG	5:V:96:GLU:N	2.45	0.48
3:a:252:GLU:OE1	4:b:68:ARG:CD	2.60	0.48
5:c:118:LYS:HZ2	5:c:128:ILE:C	2.21	0.48
1:D:305:MET:SD	1:D:335:ARG:NE	2.86	0.48
1:E:252:ASN:HA	1:E:255:PHE:HE2	1.76	0.48
1:I:300:SER:OG	1:I:338:SER:OG	2.26	0.48
1:L:189:LEU:HB2	1:L:257:CYS:SG	2.52	0.48
1:O:109:PRO:HB2	1:O:163:VAL:HG21	1.94	0.48
2:Q:157:ASP:OD2	2:Q:161:LYS:NZ	2.41	0.48
3:T:217:LYS:HD3	3:T:217:LYS:HA	1.70	0.48
3:T:264:LEU:HD13	4:U:128:LEU:HB2	1.94	0.48
2:X:276:HIS:CE1	3:a:110:PHE:HD1	2.30	0.48
3:a:224:LEU:HD11	3:a:232:LYS:CE	2.43	0.48
4:b:149:ILE:CG1	5:c:51:ASN:ND2	2.74	0.48
5:c:42:GLY:O	5:c:46:ARG:HG3	2.13	0.48
1:F:25:ASP:CA	4:U:147:VAL:HG21	2.43	0.48
1:I:154:ASP:OD2	1:I:161:HIS:HB3	2.13	0.48
2:Q:261:TYR:CE1	2:Q:265:LEU:CB	2.96	0.48
4:U:146:ARG:NH2	4:U:147:VAL:O	2.44	0.48
4:U:180:ASP:HA	4:U:183:LYS:HD2	1.96	0.48
2:X:261:TYR:CE1	2:X:265:LEU:CB	2.96	0.48
4:b:177:LYS:O	4:b:181:THR:CG2	2.43	0.48
1:A:333:PRO:C	1:A:335:ARG:H	2.20	0.48
1:C:187:ASP:OD2	1:C:191:LYS:NZ	2.46	0.48
1:N:230:ALA:HB3	1:N:255:PHE:CZ	2.49	0.48
5:c:14:GLU:O	5:c:14:GLU:OE1	2.30	0.48
1:K:252:ASN:CB	1:K:255:PHE:HZ	2.21	0.48
5:V:11:GLN:HA	5:V:89:SER:HB3	1.96	0.48
5:V:136:LEU:HD22	5:V:156:PHE:HZ	1.79	0.48
2:X:70:LYS:O	2:X:74:ALA:N	2.42	0.48
4:b:106:LYS:CE	4:b:106:LYS:CA	2.85	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:GLY:HA2	1:B:345:ILE:HG22	1.95	0.48
1:F:24:ASP:N	4:U:147:VAL:HG11	2.29	0.48
1:I:169:TYR:OH	1:K:49:GLN:CB	2.61	0.48
5:V:6:LYS:HZ1	5:V:9:VAL:HG11	1.79	0.48
3:a:248:PHE:CE1	4:b:72:LYS:HA	2.48	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:Q:278:LEU:O	2:Q:279:ASN:C	2.54	0.48
4:U:137:GLY:O	4:U:142:PRO:HD2	2.14	0.48
2:X:127:MET:O	2:X:131:GLU:N	2.45	0.48
4:b:173:LEU:HD12	4:b:174:LYS:N	2.28	0.48
1:A:302:GLY:C	1:A:304:THR:H	2.22	0.48
1:E:289:ILE:O	1:E:293:LEU:HG	2.13	0.48
1:M:352:PHE:CD1	1:M:355:MET:HG3	2.48	0.48
3:a:208:LYS:CB	4:b:112:TYR:CD2	2.91	0.48
1:A:326:LYS:HB2	2:Q:48:LYS:HE3	1.78	0.48
1:H:352:PHE:CE1	1:H:355:MET:HB2	2.48	0.48
4:U:57:ALA:HB2	5:V:104:PHE:CZ	2.49	0.48
2:W:256:LEU:CD2	2:X:256:LEU:HB3	2.44	0.48
4:b:90:PHE:CD1	4:b:91:ALA:N	2.82	0.48
4:b:180:ASP:N	4:b:183:LYS:HZ2	2.11	0.48
5:c:130:GLU:OE2	5:c:130:GLU:O	2.32	0.48
1:B:133:TYR:HE2	1:B:346:LEU:HD21	1.78	0.48
1:F:196:ARG:HD2	1:F:253:GLU:CD	2.39	0.48
1:M:109:PRO:HB2	1:M:161:HIS:NE2	2.29	0.48
1:N:252:ASN:CA	1:N:255:PHE:CZ	2.94	0.48
2:Q:276:HIS:CE1	3:T:110:PHE:CE1	3.00	0.48
3:T:233:ALA:O	4:U:100:LEU:HD13	2.13	0.48
4:b:43:ALA:CB	5:c:4:ILE:CB	2.92	0.48
4:b:152:ASP:HA	4:b:155:MET:CG	2.44	0.48
1:B:211:ASP:OD1	1:B:215:LYS:NZ	2.46	0.47
1:B:302:GLY:C	1:B:304:THR:H	2.22	0.47
1:C:335:ARG:C	1:C:337:TYR:H	2.22	0.47
1:F:24:ASP:OD1	4:U:147:VAL:HB	2.14	0.47
1:M:162:ASN:ND2	1:M:281:SER:OG	2.46	0.47
2:Q:266:LYS:O	2:Q:270:ILE:HG13	2.14	0.47
1:A:133:TYR:CE2	1:A:346:LEU:HD21	2.48	0.47
1:E:106:THR:CG2	1:E:140:LEU:CD1	2.92	0.47
1:G:23:GLY:C	4:b:145:ARG:HB2	2.34	0.47
3:T:266:ASN:HD22	5:V:110:GLY:HA3	1.79	0.47
1:E:289:ILE:O	1:E:289:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:169:TYR:OH	1:K:49:GLN:HB3	2.14	0.47
5:V:14:GLU:HG3	5:V:17:LYS:HD2	1.95	0.47
5:c:121:LEU:HB3	5:c:128:ILE:HG13	1.96	0.47
1:O:207:GLU:C	1:O:210:ARG:HG2	2.39	0.47
3:T:210:LYS:O	3:T:210:LYS:NZ	2.47	0.47
3:T:261:ILE:HD13	3:T:264:LEU:HD12	1.96	0.47
4:U:53:LEU:O	4:U:56:ILE:HG22	2.13	0.47
5:V:156:PHE:CE2	5:V:157:MET:HE2	2.49	0.47
2:W:218:GLU:HG2	2:X:221:TYR:CE1	2.49	0.47
2:X:272:GLU:O	3:a:113:ARG:HD3	2.00	0.47
1:K:352:PHE:CE1	1:K:355:MET:HB2	2.50	0.47
1:L:110:LEU:H	1:L:161:HIS:HE1	1.61	0.47
1:L:133:TYR:HE1	1:L:355:MET:HB3	1.78	0.47
4:U:43:ALA:O	4:U:47:LEU:CB	2.63	0.47
5:V:101:PHE:CE2	5:V:150:TYR:HB2	2.49	0.47
2:W:218:GLU:OE2	2:X:214:TYR:HA	2.15	0.47
5:c:134:GLU:OE2	5:c:134:GLU:O	2.32	0.47
1:B:154:ASP:OD2	1:B:161:HIS:CB	2.63	0.47
1:M:333:PRO:CG	2:R:9:GLN:HG3	2.43	0.47
1:O:335:ARG:C	1:O:337:TYR:H	2.22	0.47
2:P:221:TYR:HB3	2:Q:221:TYR:HB3	1.97	0.47
1:E:133:TYR:CG	1:E:352:PHE:CZ	3.02	0.47
1:M:133:TYR:CZ	1:M:352:PHE:HZ	2.33	0.47
2:P:166:ALA:HA	2:Q:165:VAL:CG2	2.42	0.47
2:P:218:GLU:OE2	2:Q:214:TYR:HA	2.15	0.47
2:P:218:GLU:HG2	2:Q:221:TYR:CE1	2.50	0.47
3:T:201:ARG:HG3	3:T:205:ARG:HG2	1.97	0.47
3:T:246:GLU:HB2	4:U:111:ARG:HD2	1.96	0.47
3:T:250:LEU:HA	3:T:253:LYS:HD2	1.97	0.47
4:U:83:LEU:HD22	4:U:96:LEU:HD11	1.96	0.47
2:X:266:LYS:O	2:X:270:ILE:HG13	2.14	0.47
4:b:174:LYS:NZ	4:b:178:LYS:CE	2.77	0.47
4:b:179:GLU:O	4:b:182:GLU:OE1	2.32	0.47
5:c:27:PHE:CZ	5:c:41:LEU:HA	2.50	0.47
1:A:282:ILE:CG2	1:A:294:TYR:CZ	2.98	0.47
1:A:352:PHE:CE1	1:A:355:MET:HB2	2.50	0.47
1:H:282:ILE:O	1:H:290:ARG:HG2	2.15	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:W:221:TYR:HB3	2:X:221:TYR:HB3	1.97	0.47
1:C:107:GLU:OE2	1:C:116:ARG:NE	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:PRO:C	1:C:335:ARG:H	2.23	0.47
1:E:106:THR:CG2	1:E:140:LEU:HD11	2.45	0.47
1:G:133:TYR:CD2	1:G:352:PHE:CE1	3.02	0.47
1:L:133:TYR:CZ	1:L:352:PHE:CE1	2.85	0.47
1:N:109:PRO:CD	1:N:161:HIS:CD2	2.87	0.47
1:N:300:SER:OG	1:N:338:SER:OG	2.31	0.47
5:V:112:ILE:HB	5:V:148:ILE:HB	1.97	0.47
2:W:91:ARG:NE	2:X:92:ILE:CG1	2.77	0.47
3:a:207:LYS:CE	4:b:112:TYR:OH	2.62	0.47
1:A:227:MET:HA	1:A:255:PHE:HE1	1.78	0.47
1:B:308:GLY:O	1:B:312:ARG:HB3	2.15	0.47
1:C:252:ASN:O	1:C:256:ARG:HG2	2.13	0.47
1:D:154:ASP:O	1:D:155:SER:C	2.58	0.47
1:E:301:GLY:C	1:E:336:LYS:HA	2.40	0.47
1:I:257:CYS:HB3	1:I:258:PRO:HD3	1.94	0.47
1:K:80:ASP:OD2	1:K:84:LYS:NZ	2.48	0.47
1:L:133:TYR:HE2	1:L:346:LEU:HD21	1.80	0.47
5:V:7:ALA:O	5:V:11:GLN:HG2	2.15	0.47
5:V:85:MET:O	5:V:87:ASP:N	2.40	0.47
3:a:127:ILE:HG21	3:a:131:ARG:NH1	2.25	0.47
1:D:143:TYR:O	4:U:177:LYS:CE	2.63	0.46
2:P:256:LEU:CD2	2:Q:256:LEU:HB3	2.44	0.46
4:U:136:ARG:NH1	5:V:151:ASP:OD2	2.48	0.46
5:V:143:ASN:N	5:V:152:GLU:OE2	2.39	0.46
4:b:151:ALA:HA	4:b:154:MET:CE	2.46	0.46
4:b:151:ALA:CA	4:b:154:MET:HE2	2.44	0.46
1:A:164:PRO:HD3	1:A:281:SER:HB3	1.96	0.46
1:C:252:ASN:CA	1:C:255:PHE:CE2	2.77	0.46
1:D:146:GLY:HA3	4:U:177:LYS:HE2	1.95	0.46
1:G:188:TYR:CD2	1:G:257:CYS:HA	2.50	0.46
1:K:352:PHE:CE1	1:K:355:MET:HB3	2.48	0.46
5:V:41:LEU:HD12	5:V:61:ILE:HA	1.97	0.46
4:b:50:LYS:C	5:c:160:VAL:CG1	2.89	0.46
1:B:133:TYR:CE1	1:B:355:MET:HB3	2.50	0.46
1:D:144:ALA:O	4:U:177:LYS:HE3	2.16	0.46
1:L:238:LYS:HD3	2:W:276:HIS:NE2	2.30	0.46
2:Q:272:GLU:CD	3:T:117:GLU:HB3	2.41	0.46
2:X:276:HIS:ND1	3:a:110:PHE:HA	2.29	0.46
2:Y:4:ILE:O	2:Y:5:LYS:C	2.53	0.46
3:a:228:GLN:O	3:a:231:GLU:HG3	2.15	0.46
4:b:85:LEU:C	4:b:88:LEU:HD13	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TYR:HE2	1:A:346:LEU:CD2	2.28	0.46
1:E:143:TYR:CE2	1:G:44:MET:HE2	2.51	0.46
1:M:133:TYR:CE1	1:M:352:PHE:CZ	3.03	0.46
2:Q:272:GLU:OE1	3:T:117:GLU:HB3	2.15	0.46
2:X:273:GLU:HB2	3:a:113:ARG:NH2	2.30	0.46
1:D:116:ARG:NH2	1:D:375:PHE:CE1	2.83	0.46
1:L:109:PRO:HD2	1:L:161:HIS:CE1	2.51	0.46
4:U:53:LEU:HD22	5:V:136:LEU:HD13	1.98	0.46
4:U:73:GLY:O	4:U:76:LEU:HB2	2.15	0.46
5:V:4:ILE:HG13	5:V:79:VAL:HG23	1.96	0.46
4:b:164:LYS:HG3	4:b:168:ASP:OD2	2.16	0.46
4:b:164:LYS:O	4:b:168:ASP:OD2	2.33	0.46
1:E:108:ALA:HB1	1:E:161:HIS:ND1	2.30	0.46
1:I:154:ASP:O	1:I:156:GLY:N	2.49	0.46
1:K:129:VAL:HG22	1:K:130:PRO:HD2	1.98	0.46
1:M:133:TYR:CG	1:M:352:PHE:HZ	2.33	0.46
2:P:256:LEU:CG	2:Q:260:LEU:CD1	2.94	0.46
3:T:237:TRP:CD1	4:U:103:ARG:HH22	2.33	0.46
4:U:84:GLU:H	4:U:84:GLU:CD	2.22	0.46
5:V:41:LEU:HA	5:V:44:VAL:HG22	1.98	0.46
4:b:66:GLU:HG3	4:b:69:ARG:NH2	2.31	0.46
1:A:230:ALA:CB	1:A:255:PHE:CZ	2.98	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	3.04	0.46
1:N:56:ASP:OD1	1:N:56:ASP:N	2.48	0.46
1:O:154:ASP:O	1:O:156:GLY:N	2.49	0.46
5:V:53:THR:O	5:V:57:LEU:HG	2.15	0.46
5:V:150:TYR:CZ	5:V:154:LEU:HD21	2.50	0.46
1:A:162:ASN:CG	1:A:281:SER:HG	2.24	0.46
1:E:110:LEU:H	1:E:161:HIS:HE1	1.63	0.46
1:L:335:ARG:C	1:L:337:TYR:H	2.23	0.46
4:U:61:LEU:HD13	5:V:99:ASP:HB3	1.97	0.46
5:V:121:LEU:HA	5:V:124:THR:HG23	1.97	0.46
2:W:84:ASP:OD1	2:W:88:LEU:CG	2.42	0.46
2:X:260:LEU:C	2:X:260:LEU:CD2	2.85	0.46
1:B:80:ASP:OD2	1:B:84:LYS:NZ	2.49	0.46
1:D:345:ILE:CG2	4:U:176:VAL:HG12	2.45	0.46
3:T:205:ARG:HH12	3:T:208:LYS:HB2	1.80	0.46
2:X:261:TYR:HA	2:X:264:LYS:HB3	1.97	0.46
1:N:336:LYS:HG2	1:N:337:TYR:CD1	2.51	0.46
4:b:52:LEU:HD11	5:c:126:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:205:LYS:CE	4:b:206:LYS:NZ	2.77	0.46
5:c:40:GLU:N	5:c:40:GLU:OE2	2.48	0.46
1:C:250:ILE:HG23	1:C:253:GLU:HB2	1.98	0.45
1:D:333:PRO:C	1:D:335:ARG:N	2.70	0.45
1:D:349:LEU:HD21	4:U:176:VAL:HG13	1.97	0.45
1:H:352:PHE:CD1	1:H:355:MET:HG3	2.51	0.45
3:T:88:ASP:OD1	3:T:88:ASP:N	2.42	0.45
5:V:50:GLN:HE22	5:V:81:MET:HE1	1.80	0.45
5:V:93:SER:H	5:V:97:LEU:HD13	1.80	0.45
2:X:276:HIS:HB2	3:a:113:ARG:HD3	1.97	0.45
4:b:67:GLU:O	4:b:71:GLU:HG3	2.15	0.45
4:b:158:LEU:H	4:b:158:LEU:CD2	2.29	0.45
5:c:27:PHE:CD1	5:c:40:GLU:HB2	2.51	0.45
1:B:262:PHE:CE2	1:B:312:ARG:HG2	2.49	0.45
1:H:352:PHE:CE1	1:H:355:MET:CB	2.99	0.45
3:T:255:LYS:HB2	3:T:255:LYS:HE3	1.63	0.45
4:U:43:ALA:O	4:U:47:LEU:HB2	2.15	0.45
4:U:197:ALA:O	2:W:84:ASP:CA	2.64	0.45
3:a:217:LYS:CE	3:a:235:GLU:OE1	2.65	0.45
5:c:35:CYS:O	5:c:71:THR:OG1	2.33	0.45
1:B:341:ILE:HG23	4:U:208:PHE:HE2	1.77	0.45
1:C:230:ALA:CB	1:C:255:PHE:CE2	2.99	0.45
1:D:80:ASP:OD2	1:D:84:LYS:NZ	2.48	0.45
1:F:109:PRO:CD	1:F:161:HIS:CD2	2.95	0.45
1:L:133:TYR:CG	1:L:352:PHE:CZ	3.04	0.45
1:M:109:PRO:CD	1:M:161:HIS:CD2	2.94	0.45
3:T:200:LYS:NZ	3:T:200:LYS:O	2.35	0.45
3:T:243:LEU:HD22	4:U:111:ARG:NE	2.32	0.45
4:U:204:ARG:HB2	2:W:76:LYS:HD3	1.98	0.45
2:W:256:LEU:CG	2:X:260:LEU:CD1	2.94	0.45
2:X:256:LEU:HD23	2:X:256:LEU:HA	1.87	0.45
5:c:36:ILE:O	5:c:71:THR:OG1	2.35	0.45
1:C:51:ASP:OD1	1:C:51:ASP:N	2.49	0.45
1:H:257:CYS:CB	1:H:258:PRO:HD3	2.46	0.45
1:N:333:PRO:C	1:N:335:ARG:N	2.75	0.45
5:V:105:ASP:OD2	5:V:111:TYR:N	2.49	0.45
5:V:121:LEU:HD11	5:V:136:LEU:HD12	1.98	0.45
2:X:235:ALA:O	2:X:239:ALA:N	2.43	0.45
3:a:121:VAL:O	3:a:125:ASP:N	2.47	0.45
4:b:205:LYS:CE	4:b:206:LYS:HZ2	2.19	0.45
1:B:108:ALA:HB1	1:B:161:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:162:ASN:HD21	1:J:278:THR:HA	1.82	0.45
1:L:238:LYS:HD3	2:W:276:HIS:CE1	2.52	0.45
5:V:101:PHE:HE1	5:V:112:ILE:HG13	1.79	0.45
3:a:211:ILE:HG23	3:a:212:LEU:N	2.32	0.45
4:b:130:GLN:O	4:b:134:ASP:OD1	2.34	0.45
1:I:304:THR:OG1	1:I:335:ARG:HD2	2.16	0.45
1:L:336:LYS:HE2	1:L:336:LYS:HB3	1.67	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	2.49	0.45
2:Q:261:TYR:HA	2:Q:264:LYS:HB3	1.98	0.45
5:V:18:ASN:O	5:V:21:LYS:HG2	2.16	0.45
2:X:272:GLU:CD	3:a:117:GLU:CB	2.68	0.45
1:C:192:ILE:HD12	1:C:256:ARG:CG	2.47	0.45
1:E:133:TYR:CG	1:E:352:PHE:HZ	2.33	0.45
1:J:302:GLY:C	1:J:304:THR:H	2.25	0.45
1:K:169:TYR:OH	1:M:49:GLN:CB	2.65	0.45
3:T:251:GLN:O	3:T:255:LYS:HG3	2.17	0.45
4:U:45:ARG:NE	4:U:49:LEU:HD11	2.32	0.45
4:b:141:ARG:HD3	4:b:141:ARG:HA	1.68	0.45
1:A:116:ARG:NH2	1:A:375:PHE:CE1	2.84	0.45
1:E:21:PHE:HZ	4:b:184:GLU:HB2	1.78	0.45
1:E:283:MET:CA	1:E:290:ARG:HD3	2.38	0.45
1:K:56:ASP:OD1	1:K:56:ASP:N	2.50	0.45
3:T:201:ARG:O	3:T:205:ARG:HG2	2.16	0.45
4:U:178:LYS:O	4:U:182:GLU:HG3	2.17	0.45
5:V:58:GLN:O	5:V:61:ILE:HB	2.17	0.45
2:W:204:LEU:O	2:W:208:GLU:N	2.49	0.45
1:E:28:ARG:HD3	4:b:187:GLU:HA	1.99	0.45
1:F:196:ARG:HD2	1:F:253:GLU:OE2	2.17	0.45
1:M:133:TYR:CE2	1:M:352:PHE:HZ	2.35	0.45
2:Q:127:MET:O	2:Q:131:GLU:N	2.45	0.45
3:T:113:ARG:NH2	3:T:117:GLU:OE1	2.49	0.45
5:V:41:LEU:HB3	5:V:45:MET:HE2	1.98	0.45
2:W:91:ARG:NE	2:X:92:ILE:CD1	2.58	0.45
1:B:133:TYR:CG	1:B:352:PHE:CZ	2.96	0.45
1:D:345:ILE:HG23	4:U:176:VAL:CG1	2.47	0.45
1:M:207:GLU:CA	1:M:210:ARG:HG2	2.42	0.45
3:T:236:LEU:HA	3:T:236:LEU:HD23	1.61	0.45
3:T:265:ARG:HG3	4:U:128:LEU:HD13	1.99	0.45
4:U:190:ASP:OD2	4:U:190:ASP:N	2.47	0.45
5:V:4:ILE:HA	5:V:7:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:76:GLU:HA	5:V:79:VAL:CG1	2.47	0.45
5:V:116:GLU:OE1	5:V:116:GLU:N	2.48	0.45
4:b:53:LEU:HG	5:c:157:MET:HE1	1.89	0.45
5:c:118:LYS:HD2	5:c:122:GLN:HG2	1.98	0.45
1:K:230:ALA:CB	1:K:255:PHE:CZ	2.99	0.44
4:U:195:ILE:HG21	2:W:91:ARG:HB2	1.98	0.44
4:b:84:GLU:N	4:b:84:GLU:CD	2.75	0.44
1:I:332:PRO:C	1:I:334:GLU:H	2.24	0.44
3:T:205:ARG:O	3:T:209:LYS:HG2	2.17	0.44
3:T:259:TYR:HA	3:T:262:ASN:HD22	1.81	0.44
4:U:128:LEU:O	4:U:132:ILE:HG13	2.17	0.44
4:U:156:GLN:HE21	4:U:159:LEU:HB2	1.83	0.44
4:U:159:LEU:HD23	2:X:136:LYS:CB	2.47	0.44
1:E:283:MET:O	1:E:290:ARG:NH2	2.50	0.44
1:F:25:ASP:H	4:U:147:VAL:CG2	2.25	0.44
1:J:169:TYR:OH	1:L:49:GLN:CB	2.64	0.44
1:J:252:ASN:CA	1:J:255:PHE:CZ	2.95	0.44
1:N:108:ALA:HB1	1:N:161:HIS:ND1	2.33	0.44
2:P:91:ARG:NE	2:Q:92:ILE:CD1	2.58	0.44
3:T:228:GLN:HE21	3:T:232:LYS:HG2	1.82	0.44
4:b:44:SER:HA	5:c:4:ILE:CB	2.47	0.44
4:b:131:LYS:HD2	4:b:131:LYS:O	2.17	0.44
4:b:169:LEU:HD12	4:b:170:ARG:N	2.32	0.44
5:c:2:ASP:OD1	5:c:2:ASP:O	2.35	0.44
1:B:219:VAL:O	1:B:220:ALA:HB3	2.18	0.44
1:D:147:ARG:C	4:U:173:LEU:CD1	2.90	0.44
1:E:244:ASP:N	1:E:244:ASP:OD1	2.49	0.44
1:H:335:ARG:H	1:H:335:ARG:HG2	1.63	0.44
2:P:88:LEU:HD13	2:P:91:ARG:HH21	1.79	0.44
2:P:204:LEU:O	2:P:208:GLU:N	2.49	0.44
3:T:241:TYR:CE1	4:U:76:LEU:HB3	2.52	0.44
3:a:201:ARG:NH2	3:a:204:GLU:CB	2.80	0.44
3:a:204:GLU:HA	3:a:207:LYS:CD	2.47	0.44
4:b:52:LEU:CD1	5:c:126:GLU:OE2	2.65	0.44
5:c:55:GLU:OE2	5:c:55:GLU:C	2.60	0.44
1:J:113:LYS:O	1:J:116:ARG:CG	2.63	0.44
1:M:238:LYS:NZ	2:P:276:HIS:CE1	2.81	0.44
1:N:252:ASN:CB	1:N:255:PHE:HZ	2.23	0.44
4:U:175:GLN:HA	4:U:178:LYS:CG	2.48	0.44
5:V:5:TYR:HB3	5:V:75:ASP:HB3	1.99	0.44
5:V:93:SER:OG	5:V:95:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:214:GLU:N	3:a:214:GLU:OE2	2.51	0.44
4:b:54:LEU:CD2	5:c:161:GLU:HA	2.47	0.44
4:b:134:ASP:O	4:b:138:LYS:CG	2.66	0.44
4:b:145:ARG:CD	4:b:147:VAL:CG1	2.91	0.44
1:B:345:ILE:CG2	1:B:346:LEU:N	2.79	0.44
1:M:352:PHE:CD2	1:M:352:PHE:O	2.71	0.44
5:V:94:GLU:HA	5:V:154:LEU:HD22	2.00	0.44
3:a:101:GLU:CG	3:a:105:LEU:HD11	2.46	0.44
3:a:210:LYS:O	3:a:214:GLU:OE2	2.35	0.44
4:b:92:GLU:OE1	4:b:92:GLU:HA	2.17	0.44
1:E:282:ILE:O	1:E:290:ARG:CD	2.65	0.44
1:G:23:GLY:CA	4:b:145:ARG:HB3	2.48	0.44
1:H:352:PHE:O	1:H:352:PHE:CG	2.70	0.44
1:K:252:ASN:HB2	1:K:255:PHE:CE1	2.50	0.44
1:K:352:PHE:CG	1:K:352:PHE:O	2.71	0.44
4:U:81:GLN:NE2	4:U:103:ARG:HD2	2.33	0.44
5:V:14:GLU:HA	5:V:17:LYS:HG2	2.00	0.44
4:b:44:SER:HB2	5:c:3:ASP:CA	2.43	0.44
4:b:202:GLU:OE2	4:b:202:GLU:HA	2.16	0.44
1:F:109:PRO:HB2	1:F:161:HIS:CE1	2.53	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
4:b:44:SER:HB3	5:c:3:ASP:N	2.31	0.44
4:b:173:LEU:CD1	4:b:177:LYS:HZ2	2.31	0.44
1:C:192:ILE:CD1	1:C:256:ARG:HG3	2.47	0.44
1:C:334:GLU:HG2	1:C:341:ILE:HD13	2.00	0.44
1:H:352:PHE:CD1	1:H:355:MET:HB2	2.53	0.44
1:O:163:VAL:HG22	1:O:175:ILE:CG2	2.48	0.44
3:T:250:LEU:HD22	4:U:115:GLU:HA	2.00	0.44
3:T:267:ARG:O	3:T:271:ASN:N	2.50	0.44
1:A:326:LYS:CE	2:Q:44:VAL:HG22	2.44	0.43
1:E:227:MET:HB3	1:E:255:PHE:CZ	2.53	0.43
1:M:133:TYR:CD2	1:M:352:PHE:HZ	2.36	0.43
4:b:170:ARG:NH1	4:b:171:ALA:HA	2.33	0.43
5:c:46:ARG:HE	5:c:57:LEU:CD2	2.22	0.43
1:A:143:TYR:CZ	1:C:44:MET:CE	2.83	0.43
1:B:308:GLY:O	1:B:312:ARG:CB	2.66	0.43
1:C:302:GLY:C	1:C:304:THR:H	2.26	0.43
1:D:56:ASP:OD1	1:D:56:ASP:N	2.51	0.43
1:M:227:MET:HB2	1:M:255:PHE:HE1	1.83	0.43
2:Q:261:TYR:CZ	2:Q:265:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:261:TYR:CZ	2:X:265:LEU:HD23	2.53	0.43
4:b:164:LYS:NZ	4:b:168:ASP:OD1	2.51	0.43
4:b:174:LYS:CA	4:b:177:LYS:NZ	2.77	0.43
1:I:304:THR:CB	1:I:335:ARG:HD2	2.48	0.43
4:U:163:ALA:O	4:U:167:LEU:HG	2.18	0.43
4:U:175:GLN:O	4:U:179:GLU:HG2	2.18	0.43
4:U:197:ALA:O	2:W:84:ASP:HA	2.18	0.43
4:b:41:ILE:O	4:b:46:LYS:NZ	2.51	0.43
4:b:165:GLU:O	4:b:165:GLU:OE2	2.36	0.43
1:G:219:VAL:O	1:G:220:ALA:HB3	2.18	0.43
1:I:244:ASP:OD1	1:I:244:ASP:N	2.48	0.43
3:T:89:ASP:OD1	3:T:89:ASP:N	2.51	0.43
4:b:175:GLN:O	4:b:179:GLU:CG	2.66	0.43
1:G:262:PHE:CE2	1:G:312:ARG:HG2	2.53	0.43
1:L:260:THR:HA	1:L:263:GLN:O	2.18	0.43
2:Q:261:TYR:O	2:Q:265:LEU:N	2.41	0.43
5:V:6:LYS:NZ	5:V:75:ASP:OD1	2.37	0.43
5:V:143:ASN:ND2	5:V:149:ASP:OD2	2.52	0.43
4:b:123:THR:O	4:b:127:ASP:OD1	2.36	0.43
4:b:174:LYS:HZ1	4:b:178:LYS:HZ3	1.64	0.43
1:A:305:MET:SD	1:A:335:ARG:CB	3.07	0.43
1:G:302:GLY:C	1:G:304:THR:H	2.26	0.43
5:V:12:LEU:HD23	5:V:17:LYS:HE2	2.00	0.43
5:V:42:GLY:CA	5:V:57:LEU:HD13	2.48	0.43
5:V:92:LYS:NZ	5:V:161:GLU:OXT	2.51	0.43
5:c:131:ASP:OD2	5:c:132:ASP:N	2.52	0.43
1:F:275:HIS:ND1	1:F:275:HIS:N	2.64	0.43
1:G:335:ARG:CG	1:G:335:ARG:NH1	2.80	0.43
1:I:283:MET:O	1:I:290:ARG:NE	2.52	0.43
1:L:51:ASP:OD1	1:L:51:ASP:N	2.44	0.43
1:M:227:MET:HA	1:M:255:PHE:CZ	2.54	0.43
1:O:305:MET:CE	1:O:335:ARG:HH21	2.31	0.43
4:U:83:LEU:HD12	4:U:85:LEU:HD11	1.99	0.43
2:Y:10:MET:SD	3:a:98:ASP:OD2	2.77	0.43
1:A:151:ILE:HG13	1:A:282:ILE:CD1	2.49	0.43
1:J:167:GLU:O	1:J:169:TYR:CD1	2.72	0.43
1:L:133:TYR:CD2	1:L:352:PHE:CE1	3.07	0.43
4:U:64:GLU:HA	4:U:67:GLU:CD	2.44	0.43
5:V:5:TYR:O	5:V:9:VAL:HG23	2.19	0.43
2:W:154:ILE:O	2:W:158:ALA:N	2.42	0.43
4:b:95:ASP:O	4:b:99:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ALA:HB1	1:B:335:ARG:HD3	2.00	0.43
1:B:334:GLU:OE1	1:B:334:GLU:N	2.51	0.43
1:D:252:ASN:CB	1:D:255:PHE:HZ	2.26	0.43
1:L:110:LEU:H	1:L:161:HIS:CE1	2.37	0.43
1:M:110:LEU:H	1:M:161:HIS:HE1	1.66	0.43
1:N:361:GLU:OE2	1:N:373:LYS:NZ	2.52	0.43
3:T:264:LEU:HD23	3:T:267:ARG:NH1	2.34	0.43
4:U:103:ARG:O	4:U:106:LYS:HG3	2.18	0.43
5:V:91:GLY:O	5:V:93:SER:N	2.52	0.43
2:X:154:ILE:O	2:X:155:ALA:C	2.59	0.43
3:a:224:LEU:HD13	3:a:232:LYS:NZ	2.27	0.43
1:E:23:GLY:HA2	4:b:180:ASP:HB3	1.82	0.43
1:E:154:ASP:O	1:E:156:GLY:N	2.52	0.43
1:I:305:MET:HE3	1:I:337:TYR:CE1	2.54	0.43
1:I:337:TYR:O	1:I:341:ILE:CD1	2.67	0.43
3:T:239:SER:HA	3:T:242:ASN:HD21	1.84	0.43
3:a:220:ALA:HB3	3:a:232:LYS:HE2	2.01	0.43
1:D:230:ALA:CB	1:D:255:PHE:CE2	3.02	0.42
1:H:217:CYS:SG	1:H:254:ARG:O	2.77	0.42
1:I:301:GLY:O	1:I:336:LYS:HB2	2.19	0.42
4:U:173:LEU:HB3	4:U:177:LYS:HZ3	1.84	0.42
5:V:13:THR:O	5:V:17:LYS:HE3	2.19	0.42
2:X:279:ASN:OD1	2:X:279:ASN:C	2.61	0.42
3:a:204:GLU:OE1	3:a:207:LYS:NZ	2.52	0.42
4:b:44:SER:HA	5:c:4:ILE:HB	1.97	0.42
1:F:182:GLY:O	1:F:213:LYS:NZ	2.52	0.42
1:J:303:THR:O	1:J:306:TYR:HD1	2.01	0.42
1:K:352:PHE:O	1:K:352:PHE:CD2	2.73	0.42
1:M:109:PRO:CB	1:M:161:HIS:NE2	2.83	0.42
1:M:196:ARG:HD2	1:M:253:GLU:OE2	2.19	0.42
1:N:335:ARG:O	1:N:337:TYR:N	2.46	0.42
2:Q:165:VAL:O	2:Q:169:LEU:N	2.50	0.42
3:T:121:VAL:O	3:T:125:ASP:N	2.47	0.42
3:T:203:THR:HA	3:T:206:GLU:OE1	2.19	0.42
3:T:264:LEU:HD23	3:T:267:ARG:HH12	1.84	0.42
4:U:103:ARG:HA	4:U:106:LYS:HG3	2.00	0.42
2:X:277:ALA:O	2:X:281:MET:HG3	2.19	0.42
1:E:24:ASP:OD1	4:b:188:VAL:HG11	2.20	0.42
1:G:133:TYR:CE1	1:G:355:MET:HB3	2.54	0.42
1:G:188:TYR:CE1	1:G:266:PHE:HB3	2.54	0.42
1:I:301:GLY:C	1:I:336:LYS:HB2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:44:SER:HB2	5:V:3:ASP:CG	2.44	0.42
5:V:73:ASP:O	5:V:77:PHE:N	2.35	0.42
5:V:128:ILE:HG23	5:V:133:ILE:HG12	2.02	0.42
3:a:224:LEU:CD1	3:a:232:LYS:NZ	2.82	0.42
3:a:234:LYS:N	3:a:234:LYS:CD	2.82	0.42
1:A:352:PHE:CG	1:A:352:PHE:O	2.71	0.42
1:E:219:VAL:O	1:E:220:ALA:HB3	2.20	0.42
1:G:133:TYR:CD2	1:G:352:PHE:HZ	2.37	0.42
5:V:139:ASP:O	5:V:142:LYS:HE3	2.18	0.42
1:I:169:TYR:CZ	1:K:49:GLN:HG3	2.54	0.42
1:K:154:ASP:O	1:K:156:GLY:N	2.52	0.42
1:M:154:ASP:O	1:M:156:GLY:N	2.52	0.42
1:O:163:VAL:HA	1:O:164:PRO:HD3	1.94	0.42
2:P:210:GLN:HB3	2:P:214:TYR:CE1	2.55	0.42
2:Q:277:ALA:O	2:Q:281:MET:HG3	2.19	0.42
3:T:244:GLU:HB3	4:U:79:ARG:HD2	2.02	0.42
5:V:79:VAL:HG13	5:V:80:MET:N	2.33	0.42
3:a:219:LEU:HD21	3:a:235:GLU:OE2	2.19	0.42
4:b:195:ILE:CG2	4:b:196:ASP:N	2.82	0.42
1:E:79:TRP:HZ3	1:E:83:GLU:OE1	2.02	0.42
1:H:352:PHE:HB2	1:J:45:VAL:HG21	2.01	0.42
1:K:189:LEU:CB	1:K:257:CYS:SG	3.07	0.42
1:K:230:ALA:CB	1:K:255:PHE:CE2	3.03	0.42
4:U:179:GLU:HG3	4:U:180:ASP:H	1.83	0.42
1:H:302:GLY:C	1:H:304:THR:H	2.27	0.42
1:J:162:ASN:ND2	1:J:277:THR:O	2.52	0.42
1:L:154:ASP:O	1:L:156:GLY:N	2.51	0.42
1:M:352:PHE:O	1:M:352:PHE:CG	2.72	0.42
1:O:333:PRO:C	1:O:335:ARG:N	2.78	0.42
3:T:121:VAL:O	3:T:122:SER:C	2.63	0.42
5:V:67:ASP:OD2	5:V:71:THR:OG1	2.37	0.42
3:a:231:GLU:OE1	3:a:232:LYS:CG	2.68	0.42
1:B:3:ASP:OD1	1:B:3:ASP:N	2.50	0.42
1:E:302:GLY:C	1:E:304:THR:H	2.26	0.42
1:G:133:TYR:CG	1:G:352:PHE:CZ	3.08	0.42
1:I:110:LEU:H	1:I:161:HIS:HE1	1.68	0.42
1:M:219:VAL:O	1:M:220:ALA:HB3	2.19	0.42
1:O:196:ARG:HD2	1:O:253:GLU:OE2	2.19	0.42
2:Q:254:ASP:O	2:Q:258:ASP:HB3	2.19	0.42
3:T:249:ASP:OD1	4:U:72:LYS:NZ	2.35	0.42
4:b:146:ARG:NH2	5:c:51:ASN:OD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:170:ARG:NH1	4:b:174:LYS:HB3	2.35	0.42
1:C:301:GLY:C	1:C:336:LYS:HA	2.45	0.42
1:K:51:ASP:CG	1:K:52:SER:N	2.78	0.42
1:L:342:GLY:HA2	1:L:345:ILE:CG2	2.49	0.42
1:M:230:ALA:CB	1:M:255:PHE:CE2	3.03	0.42
2:P:84:ASP:O	2:P:85:VAL:C	2.60	0.42
2:P:88:LEU:HD11	2:P:91:ARG:NH2	2.34	0.42
2:P:154:ILE:O	2:P:158:ALA:N	2.42	0.42
5:c:62:ASP:OD1	5:c:62:ASP:C	2.63	0.42
1:D:230:ALA:CB	1:D:255:PHE:CZ	3.03	0.41
1:H:133:TYR:HE1	1:H:355:MET:HB3	1.81	0.41
1:L:312:ARG:HA	1:L:312:ARG:HD2	1.91	0.41
1:M:51:ASP:CG	1:M:52:SER:N	2.78	0.41
3:T:210:LYS:HA	3:T:210:LYS:HD2	1.92	0.41
3:T:271:ASN:HB3	4:U:135:LEU:HB3	2.01	0.41
4:U:114:ILE:O	4:U:118:VAL:HG23	2.19	0.41
2:W:84:ASP:O	2:W:85:VAL:C	2.60	0.41
2:X:247:THR:HG21	3:a:142:ASN:HD21	1.85	0.41
2:X:276:HIS:CB	3:a:113:ARG:HH11	2.24	0.41
3:a:201:ARG:HH21	3:a:205:ARG:N	2.18	0.41
4:b:53:LEU:HD23	5:c:157:MET:CE	2.43	0.41
1:A:133:TYR:CE1	1:A:352:PHE:HE1	2.35	0.41
1:A:352:PHE:CD1	1:A:355:MET:HB2	2.54	0.41
1:D:133:TYR:CG	1:D:352:PHE:HZ	2.37	0.41
1:E:207:GLU:HA	1:E:210:ARG:CG	2.45	0.41
1:M:207:GLU:O	1:M:210:ARG:HG2	2.20	0.41
1:M:352:PHE:CE1	1:M:355:MET:CB	3.03	0.41
1:N:279:TYR:CZ	1:N:283:MET:HE2	2.55	0.41
1:O:161:HIS:HB3	1:O:163:VAL:HG23	2.02	0.41
3:T:215:ARG:HH12	4:U:111:ARG:HB3	1.85	0.41
3:T:216:ARG:HD2	4:U:101:HIS:CD2	2.55	0.41
4:U:50:LYS:HG3	5:V:160:VAL:HG11	2.02	0.41
5:V:153:PHE:O	5:V:156:PHE:HB3	2.20	0.41
2:W:210:GLN:HB3	2:W:214:TYR:CE1	2.55	0.41
4:b:170:ARG:HH11	4:b:174:LYS:HB3	1.84	0.41
1:D:335:ARG:C	1:D:337:TYR:H	2.28	0.41
1:E:335:ARG:O	1:E:337:TYR:N	2.44	0.41
1:H:51:ASP:CG	1:H:52:SER:N	2.79	0.41
1:I:109:PRO:HB2	1:I:161:HIS:NE2	2.36	0.41
3:T:264:LEU:O	4:U:132:ILE:HD11	2.20	0.41
3:a:234:LYS:HA	3:a:234:LYS:CE	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:166:SER:HA	4:b:169:LEU:HD21	2.01	0.41
1:M:336:LYS:C	1:M:338:SER:N	2.72	0.41
3:T:247:LYS:HG2	4:U:114:ILE:HD12	2.01	0.41
4:U:65:ALA:HA	4:U:68:ARG:HG3	2.02	0.41
2:X:254:ASP:O	2:X:258:ASP:HB3	2.19	0.41
4:b:195:ILE:HG22	4:b:196:ASP:H	1.85	0.41
5:c:126:GLU:OE1	5:c:128:ILE:CD1	2.68	0.41
1:A:33:SER:O	1:A:70:PRO:HD2	2.21	0.41
1:E:335:ARG:C	1:E:337:TYR:N	2.79	0.41
1:H:219:VAL:O	1:H:220:ALA:HB3	2.20	0.41
1:I:227:MET:HA	1:I:255:PHE:HZ	1.86	0.41
2:Q:266:LYS:O	2:Q:270:ILE:CG1	2.69	0.41
3:T:202:GLN:O	3:T:206:GLU:HG3	2.21	0.41
3:T:261:ILE:HD12	4:U:124:GLU:CD	2.46	0.41
3:T:266:ASN:ND2	5:V:110:GLY:HA3	2.36	0.41
4:U:44:SER:HB3	5:V:4:ILE:H	1.85	0.41
4:b:135:LEU:N	4:b:138:LYS:HZ2	2.18	0.41
4:b:162:ARG:HH21	4:b:166:SER:N	2.19	0.41
5:c:127:THR:O	5:c:127:THR:HG23	2.20	0.41
1:F:167:GLU:O	1:F:169:TYR:CD1	2.74	0.41
1:H:227:MET:HA	1:H:255:PHE:CZ	2.54	0.41
1:J:56:ASP:OD1	1:J:56:ASP:N	2.52	0.41
3:T:199:GLY:C	3:T:201:ARG:H	2.29	0.41
3:T:248:PHE:CZ	4:U:71:GLU:HB2	2.55	0.41
4:U:159:LEU:HD23	2:X:136:LYS:HB3	2.01	0.41
5:V:104:PHE:HE1	5:V:153:PHE:CE1	2.38	0.41
3:a:89:ASP:OD1	3:a:89:ASP:N	2.51	0.41
1:D:3:ASP:OD1	1:D:3:ASP:N	2.49	0.41
1:F:154:ASP:O	1:F:155:SER:C	2.62	0.41
1:L:336:LYS:HG2	1:L:337:TYR:CD1	2.56	0.41
1:N:335:ARG:C	1:N:337:TYR:N	2.79	0.41
2:Q:154:ILE:O	2:Q:155:ALA:C	2.59	0.41
2:Q:252:SER:O	2:Q:256:LEU:CB	2.69	0.41
3:T:220:ALA:HB1	3:T:224:LEU:HD11	2.02	0.41
3:T:245:ALA:HB2	4:U:76:LEU:CD2	2.45	0.41
4:U:41:ILE:HD12	4:U:45:ARG:HG2	2.02	0.41
5:V:9:VAL:HA	5:V:78:LEU:HD23	2.03	0.41
2:W:260:LEU:CD1	2:X:263:GLN:OE1	2.69	0.41
3:a:225:ASN:OD1	3:a:228:GLN:HB2	2.21	0.41
4:b:53:LEU:HD11	5:c:104:PHE:HZ	1.85	0.41
4:b:84:GLU:N	4:b:84:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:164:LYS:CE	4:b:168:ASP:OD1	2.69	0.41
1:A:51:ASP:CG	1:A:52:SER:N	2.79	0.41
1:A:154:ASP:O	1:A:155:SER:C	2.63	0.41
1:C:56:ASP:OD1	1:C:56:ASP:N	2.50	0.41
1:C:192:ILE:CD1	1:C:256:ARG:CG	2.99	0.41
1:E:227:MET:CB	1:E:255:PHE:HZ	2.34	0.41
1:J:182:GLY:O	1:J:213:LYS:NZ	2.53	0.41
2:P:260:LEU:HD11	2:Q:263:GLN:OE1	2.20	0.41
4:U:101:HIS:O	4:U:104:VAL:HG12	2.21	0.41
3:a:201:ARG:NH2	3:a:204:GLU:C	2.79	0.41
4:b:51:THR:HA	5:c:160:VAL:CG1	2.50	0.41
5:c:16:GLN:NE2	5:c:87:ASP:OD1	2.52	0.41
1:A:219:VAL:O	1:A:220:ALA:HB3	2.21	0.41
1:B:56:ASP:OD1	1:B:56:ASP:N	2.53	0.41
1:D:51:ASP:CG	1:D:52:SER:N	2.79	0.41
1:E:335:ARG:H	1:E:335:ARG:HG2	1.56	0.41
1:F:335:ARG:H	1:F:335:ARG:HG2	1.57	0.41
1:H:164:PRO:HG2	1:H:171:LEU:HB2	2.02	0.41
1:J:335:ARG:H	1:J:335:ARG:HG2	1.76	0.41
1:L:332:PRO:HA	1:L:333:PRO:HD3	1.91	0.41
1:M:110:LEU:H	1:M:161:HIS:CE1	2.39	0.41
2:P:260:LEU:CD1	2:Q:263:GLN:OE1	2.69	0.41
2:Q:147:GLN:O	2:Q:151:ALA:N	2.45	0.41
2:Q:253:ILE:CA	2:Q:256:LEU:HB2	2.50	0.41
4:U:44:SER:CA	5:V:4:ILE:HB	2.50	0.41
4:U:46:LYS:HG2	5:V:135:GLU:HB3	2.03	0.41
4:U:59:GLN:HA	4:U:62:GLU:OE1	2.21	0.41
2:W:260:LEU:HD11	2:X:263:GLN:OE1	2.20	0.41
2:X:252:SER:O	2:X:256:LEU:CB	2.69	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: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:265:LEU:HD22	3:T:125:ASP:OD1	2.21	0.41
2:Q:276:HIS:HB3	3:T:110:PHE:CE1	2.56	0.41
3:T:251:GLN:OE1	4:U:79:ARG:NH2	2.49	0.41
2:X:265:LEU:HD11	3:a:121:VAL:HG11	2.03	0.41
1:E:285:CYS:O	1:E:290:ARG:NE	2.49	0.40
1:F:169:TYR:HE1	1:H:49:GLN:CD	2.29	0.40
1:I:196:ARG:HD2	1:I:253:GLU:CD	2.46	0.40
1:N:124:PHE:CD1	1:N:362:TYR:CD1	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:201:ARG:NH2	3:T:204:GLU:HB3	2.35	0.40
2:X:266:LYS:O	2:X:270:ILE:CG1	2.69	0.40
1:D:23:GLY:C	4:U:180:ASP:HB2	2.46	0.40
4:U:127:ASP:O	4:U:131:LYS:HG3	2.22	0.40
2:X:253:ILE:O	2:X:256:LEU:HB2	2.21	0.40
2:X:264:LYS:HE3	3:a:124:LYS:HE3	2.03	0.40
3:a:121:VAL:O	3:a:122:SER:C	2.63	0.40
4:b:84:GLU:C	4:b:96:LEU:HD11	2.46	0.40
1:B:109:PRO:HD2	1:B:161:HIS:NE2	2.35	0.40
1:E:218:TYR:O	1:E:255:PHE:HA	2.22	0.40
1:H:160:THR:HG22	1:H:162:ASN:HD21	1.85	0.40
1:H:163:VAL:HG22	1:H:175:ILE:CB	2.40	0.40
1:O:230:ALA:HB3	1:O:255:PHE:CE2	2.56	0.40
3:a:217:LYS:CE	3:a:239:SER:CB	2.94	0.40
4:b:54:LEU:HD11	5:c:92:LYS:HE2	2.02	0.40
4:b:171:ALA:O	4:b:175:GLN:NE2	2.55	0.40
4:b:174:LYS:CA	4:b:177:LYS:HZ3	2.19	0.40
1:A:143:TYR:CE1	1:C:44:MET:HE2	2.50	0.40
1:I:337:TYR:O	1:I:341:ILE:HG13	2.21	0.40
2:Q:256:LEU:HD23	2:Q:256:LEU:HA	1.87	0.40
3:T:237:TRP:CE2	4:U:82:PRO:HA	2.55	0.40
4:U:148:ARG:HB2	4:U:148:ARG:NH1	2.36	0.40
3:a:205:ARG:NH1	3:a:209:LYS:CB	2.84	0.40
4:b:135:LEU:C	4:b:138:LYS:HG3	2.46	0.40
4:b:162:ARG:NH2	4:b:166:SER:N	2.69	0.40
5:c:69:SER:OG	5:c:71:THR:HG22	2.22	0.40
1:B:342:GLY:HA2	1:B:345:ILE:CG2	2.51	0.40
1:G:230:ALA:HB3	1:G:255:PHE:CZ	2.56	0.40
1:G:336:LYS:HG2	1:G:337:TYR:CD1	2.56	0.40
1:L:230:ALA:CB	1:L:255:PHE:CZ	3.05	0.40
1:L:333:PRO:C	1:L:335:ARG:N	2.79	0.40
1:N:279:TYR:CZ	1:N:283:MET:CE	3.04	0.40
2:Q:253:ILE:O	2:Q:256:LEU:HB2	2.21	0.40
3:T:200:LYS:HD2	3:T:200:LYS:HA	1.85	0.40
4:U:53:LEU:HD21	5:V:117:LEU:HD23	2.03	0.40
2:X:268:LYS:O	2:X:272:GLU:N	2.47	0.40
3:a:247:LYS:HG3	4:b:111:ARG:HG3	2.03	0.40
5:c:56:GLU:OE1	5:c:56:GLU:O	2.39	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%)	360 (96%)	13 (4%)	0	100	100
1	C	373/375 (100%)	362 (97%)	10 (3%)	1 (0%)	36	72
1	D	373/375 (100%)	360 (96%)	11 (3%)	2 (0%)	24	63
1	E	373/375 (100%)	358 (96%)	14 (4%)	1 (0%)	36	72
1	F	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	72
1	G	373/375 (100%)	358 (96%)	13 (4%)	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%)	270 (99%)	2 (1%)	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	134/186 (72%)	129 (96%)	5 (4%)	0	100	100
3	a	134/186 (72%)	133 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	U	168/170 (99%)	157 (94%)	11 (6%)	0	100	100
4	b	168/170 (99%)	166 (99%)	2 (1%)	0	100	100
5	V	158/160 (99%)	140 (89%)	18 (11%)	0	100	100
5	c	158/160 (99%)	153 (97%)	4 (2%)	1 (1%)	21	59
All	All	7711/8945 (86%)	7468 (97%)	217 (3%)	26 (0%)	37	72

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	155	SER
1	H	155	SER
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	c	36	ILE

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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
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%)	235 (100%)	1 (0%)	84	84
2	Q	236/246 (96%)	233 (99%)	3 (1%)	61	74
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	129/169 (76%)	129 (100%)	0	100	100
3	a	129/169 (76%)	129 (100%)	0	100	100
4	U	145/145 (100%)	145 (100%)	0	100	100
4	b	145/145 (100%)	145 (100%)	0	100	100
5	V	141/141 (100%)	140 (99%)	1 (1%)	76	81
5	c	141/141 (100%)	141 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6640/7648 (87%)	6593 (99%)	47 (1%)	73	81

All (47) 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
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

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Mol	Chain	Res	Type
1	O	336	LYS
2	P	274	LEU
2	Q	165	VAL
2	Q	261	TYR
2	Q	264	LYS
5	V	75	ASP
2	W	274	LEU
2	X	165	VAL
2	X	261	TYR
2	X	264	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	111	ASN
1	A	128	ASN
1	A	371	HIS
1	B	92	ASN
1	B	111	ASN
1	C	162	ASN
1	D	40	HIS
1	D	111	ASN
1	D	263	GLN
1	E	137	GLN
1	G	263	GLN
1	H	59	GLN
1	I	111	ASN
1	I	162	ASN
1	J	128	ASN
1	J	162	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	296	ASN
2	P	47	GLN
2	Q	153	HIS
2	Q	210	GLN
2	Q	279	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	R	9	GLN
3	T	228	GLN
3	T	238	GLN
3	T	262	ASN
4	U	121	ASN
4	U	156	GLN
5	V	50	GLN
5	V	143	ASN
2	W	47	GLN
2	W	153	HIS
2	X	153	HIS
2	X	210	GLN
2	X	276	HIS
3	a	202	GLN
3	a	228	GLN
4	b	81	GLN
4	b	94	GLN
4	b	175	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

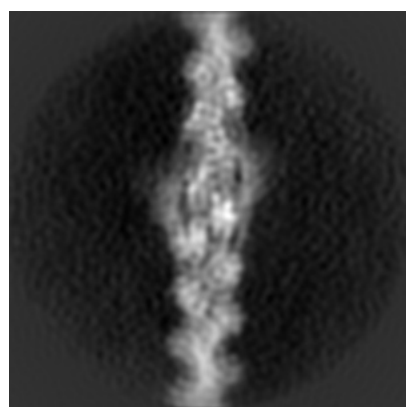
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22964. These allow visual inspection of the internal detail of the map and identification of artifacts.

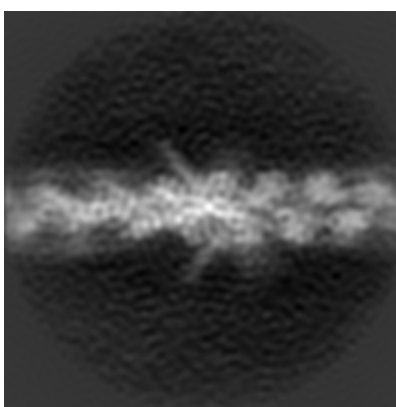
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

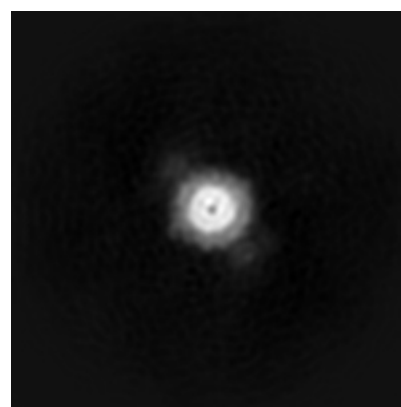
6.1.1 Primary map



X



Y

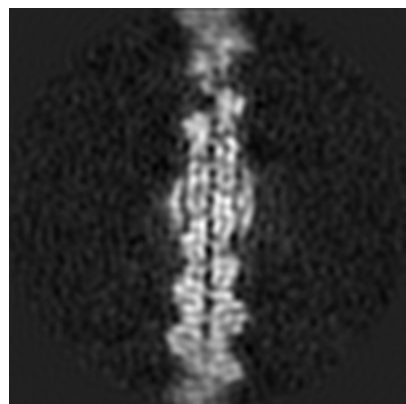


Z

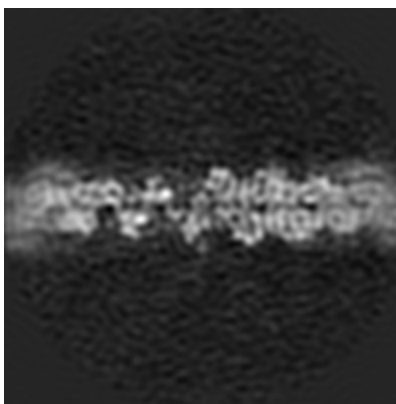
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

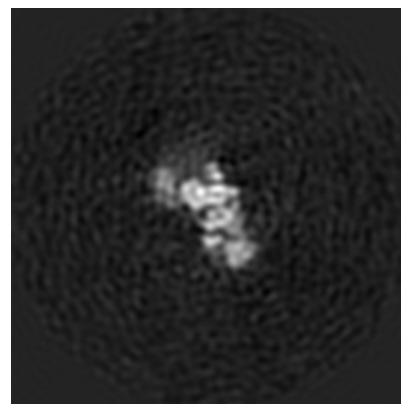
6.2.1 Primary map



X Index: 81



Y Index: 81

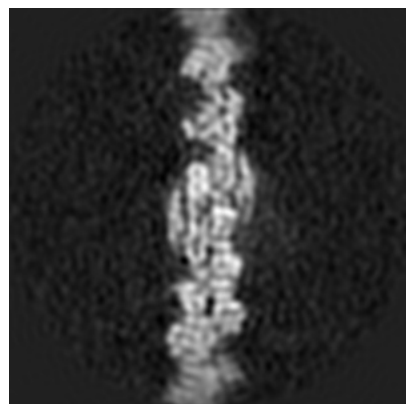


Z Index: 81

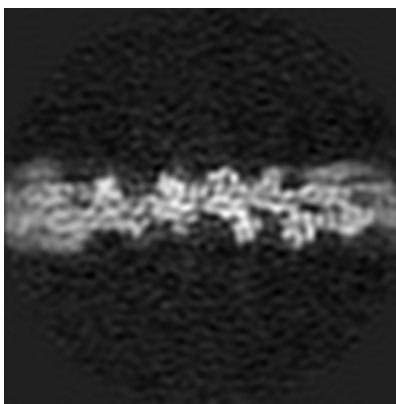
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

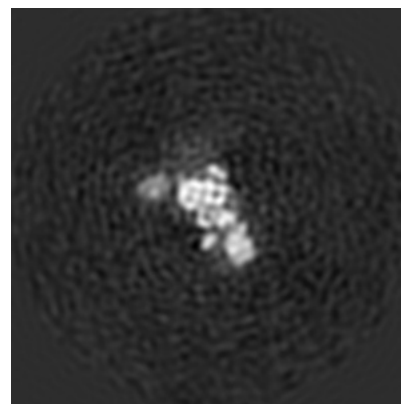
6.3.1 Primary map



X Index: 79



Y Index: 78

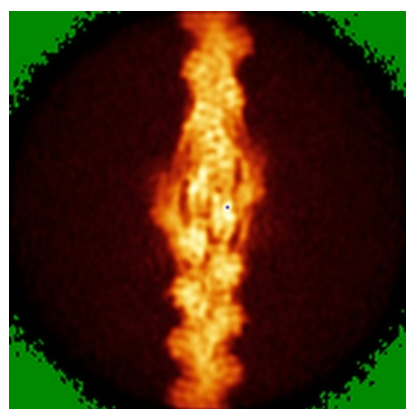


Z Index: 77

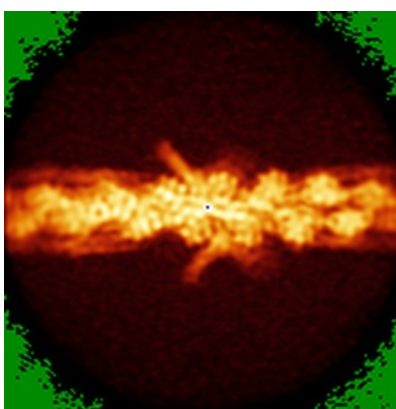
The images above show the largest variance slices of the map in three orthogonal directions.

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

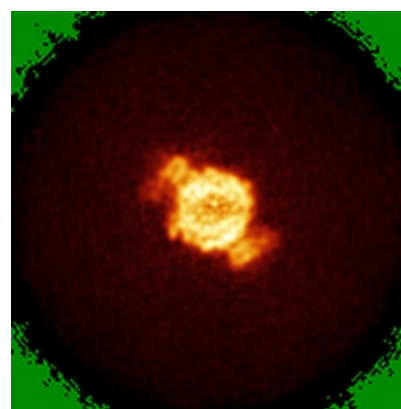
6.4.1 Primary map



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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

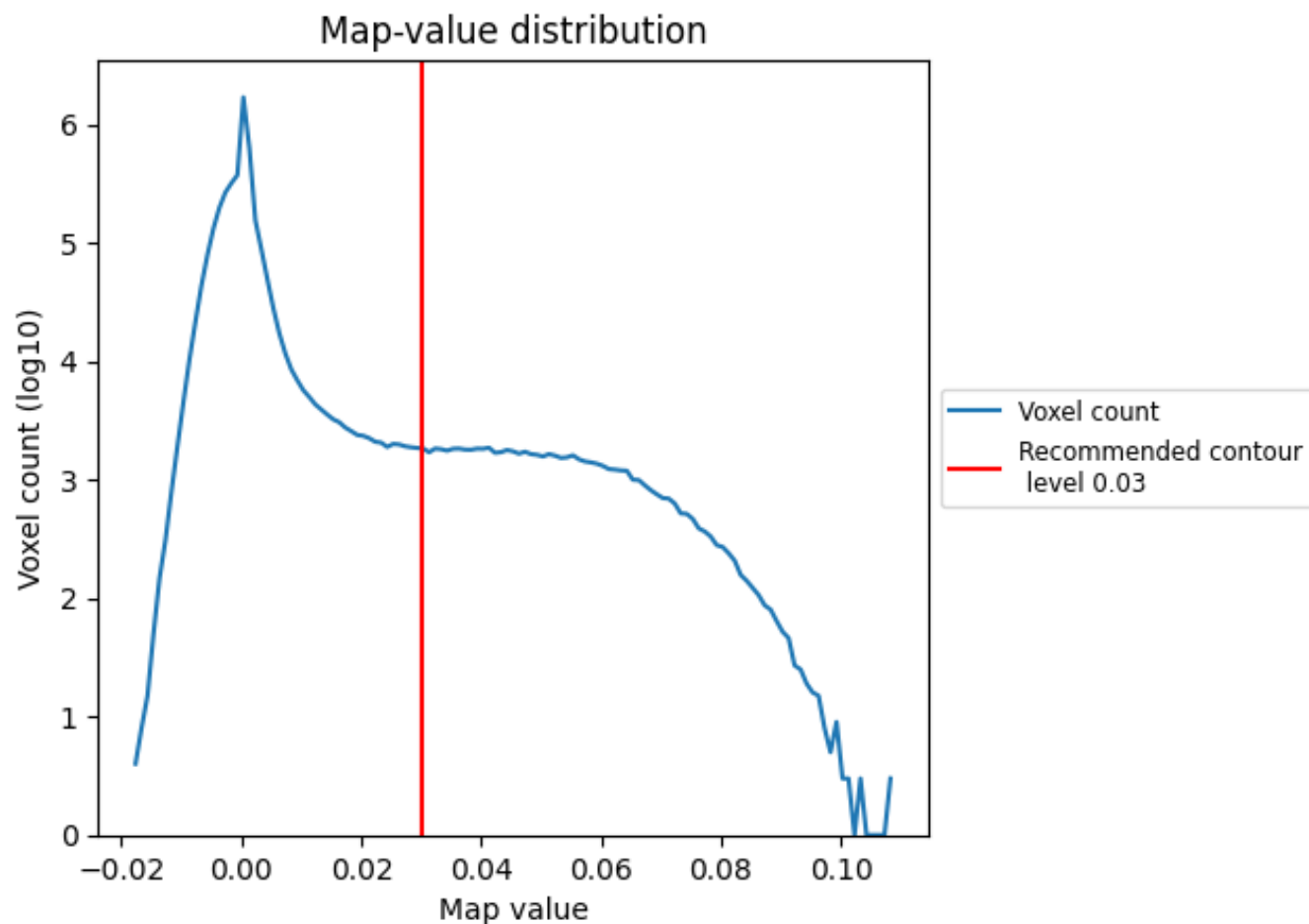
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

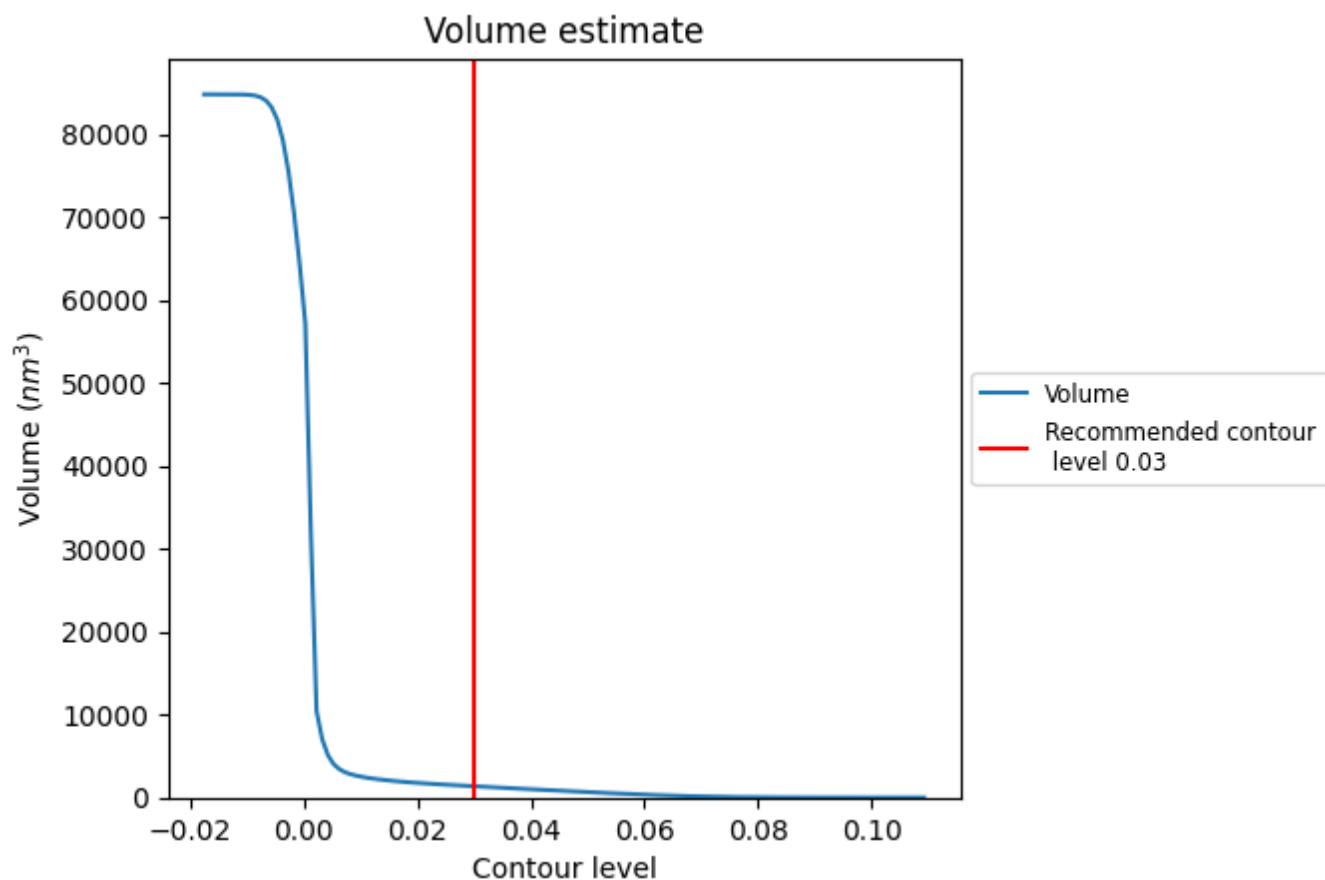
This section contains the results of statistical analysis of the map.

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.

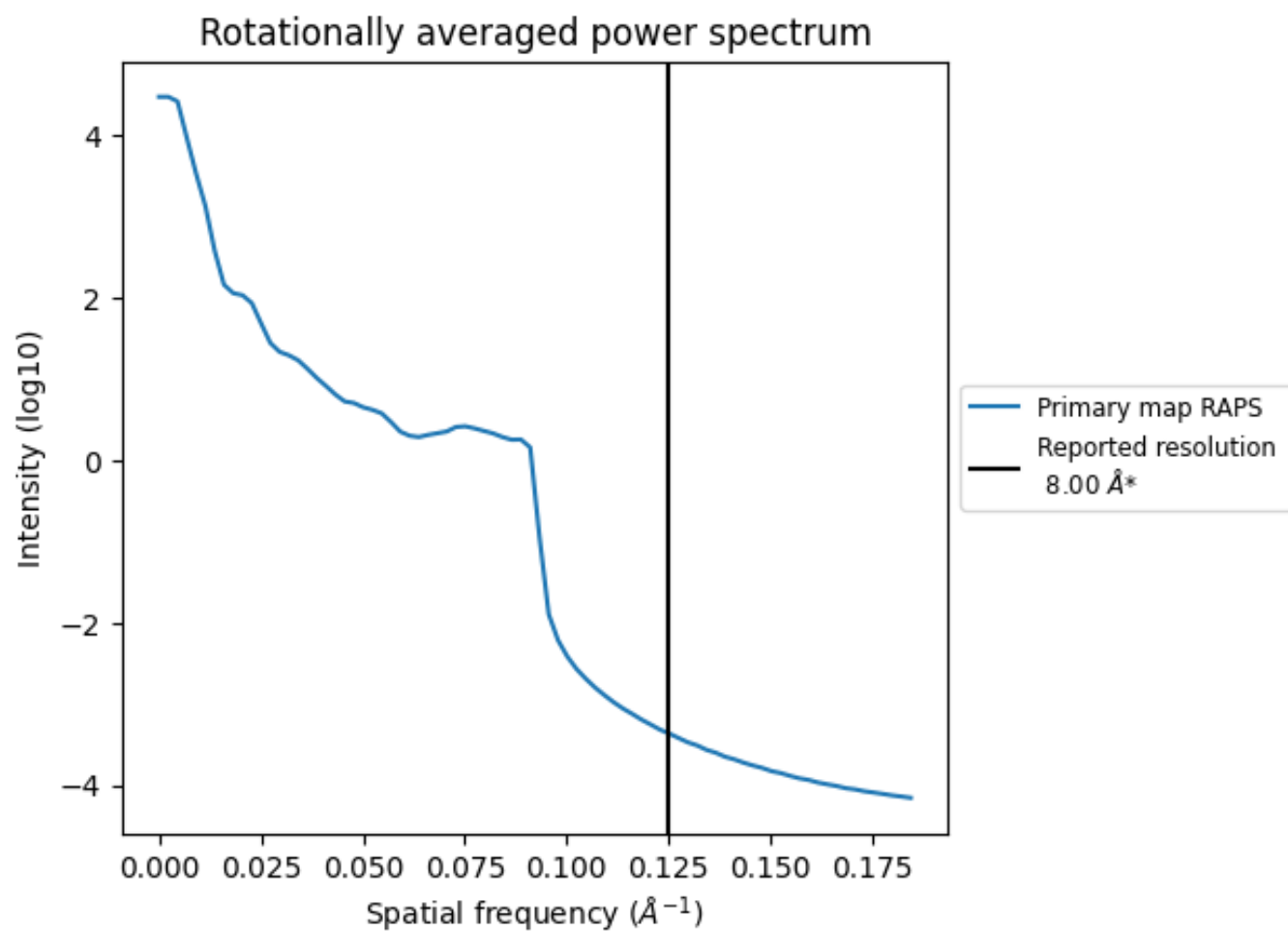
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1358 nm^3 ; this corresponds to an approximate mass of 1227 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 ⓘ

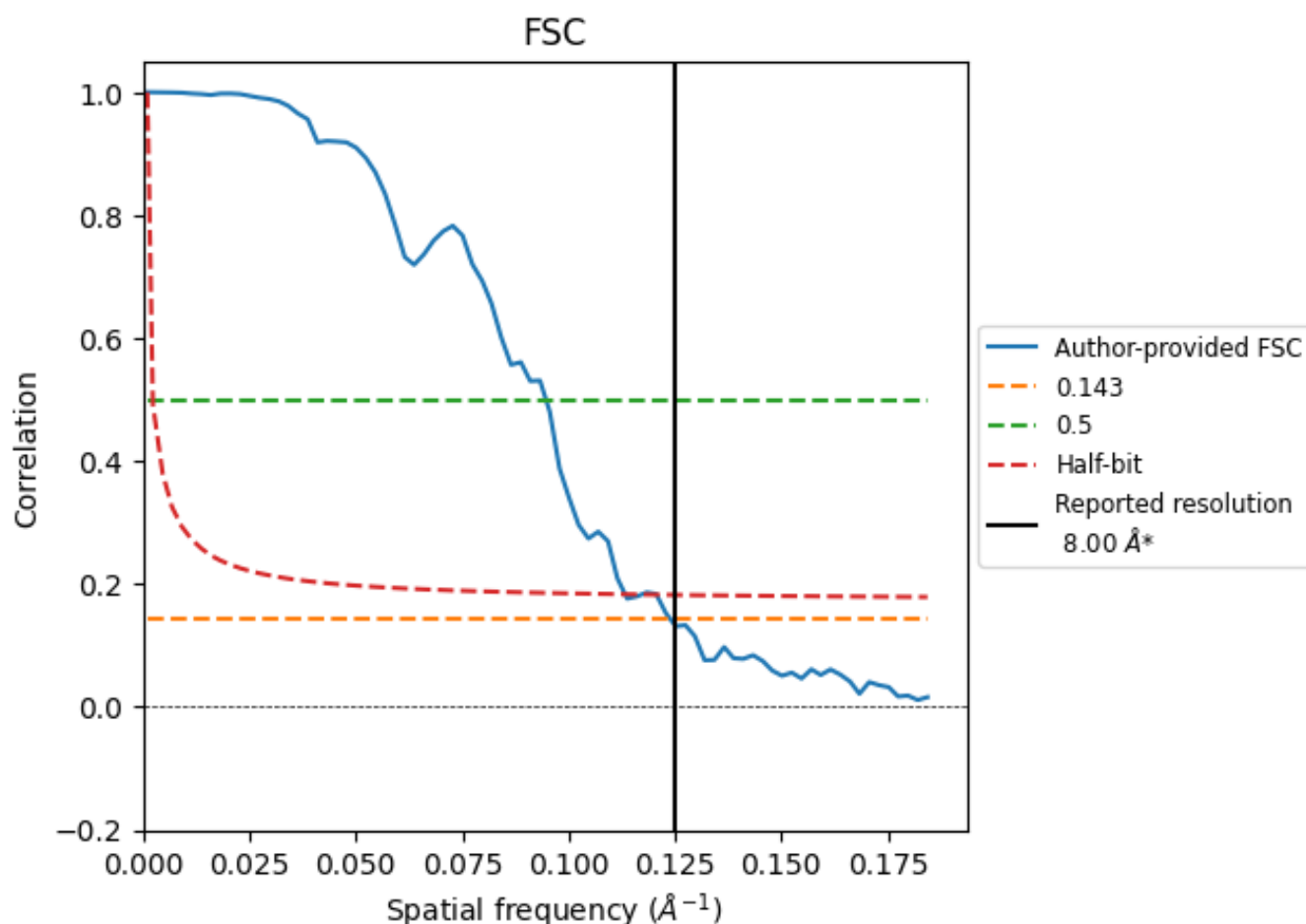


*Reported resolution corresponds to spatial frequency of 0.125 Å⁻¹

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 0.125 Å⁻¹

8.2 Resolution estimates [i](#)

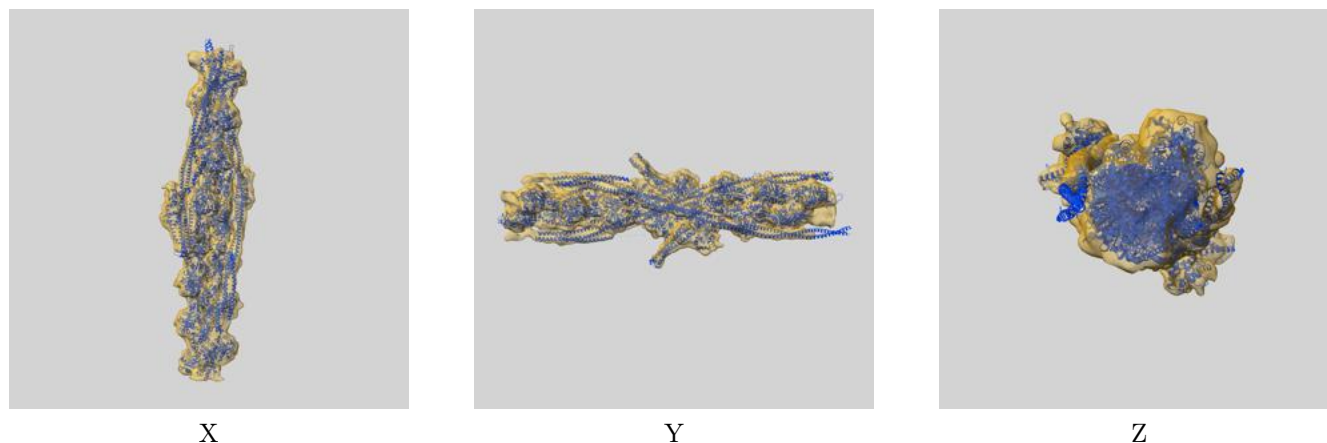
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.00	-	-
Author-provided FSC curve	8.07	10.56	8.83
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

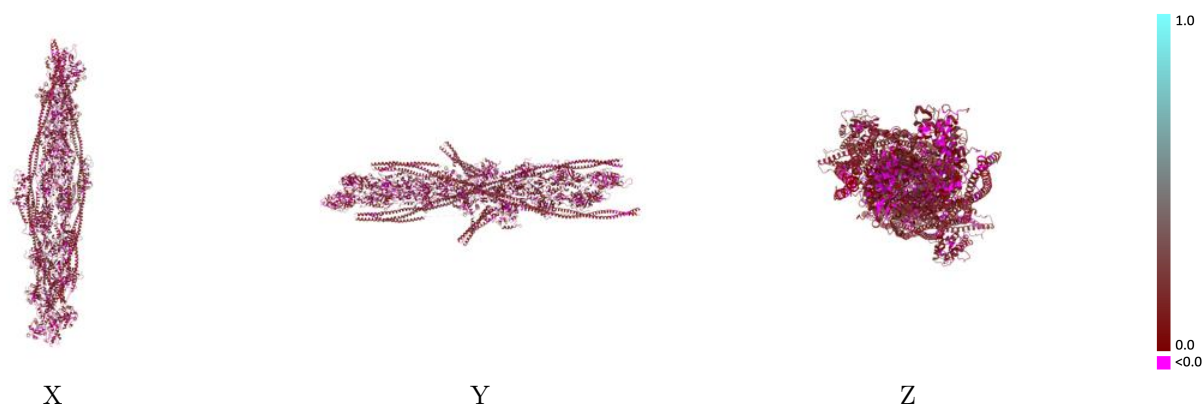
This section contains information regarding the fit between EMDB map EMD-22964 and PDB model 7KO4. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



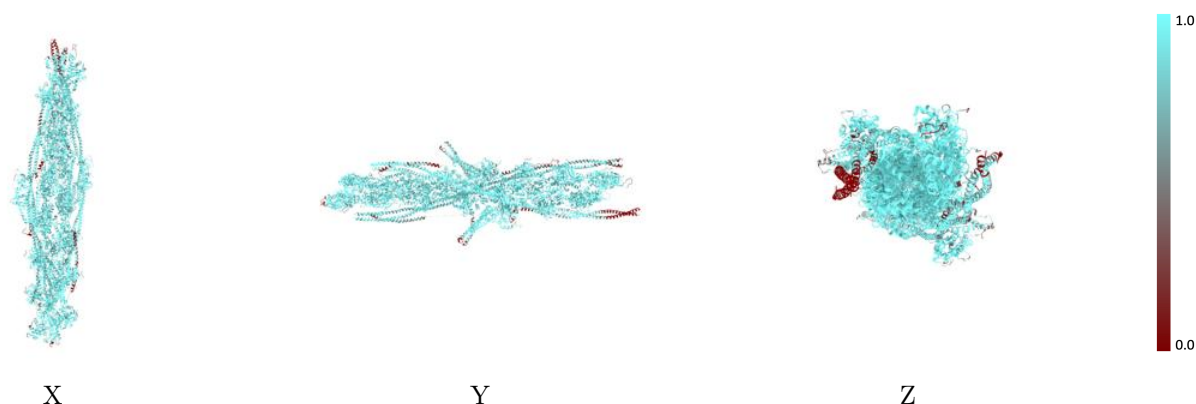
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



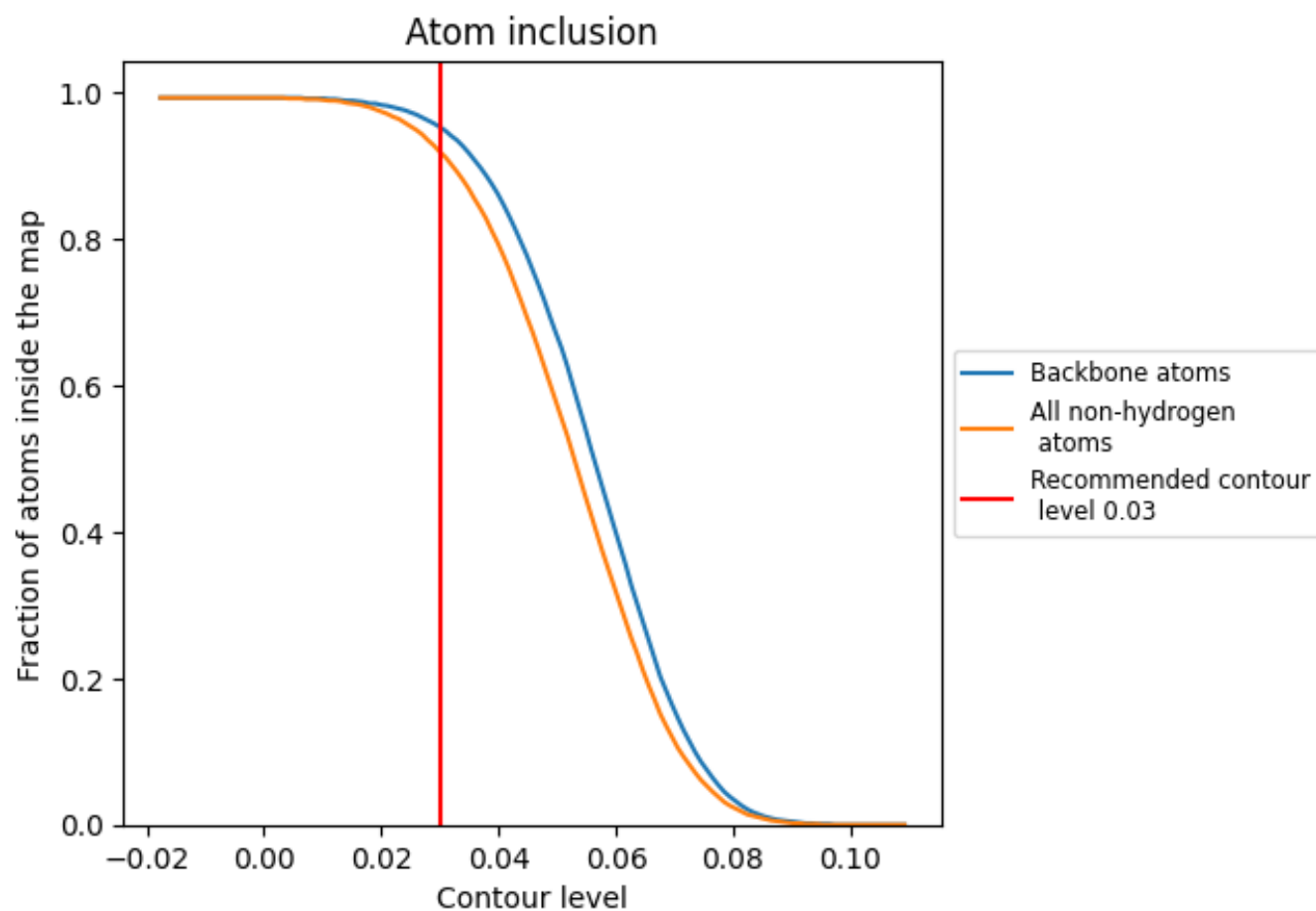
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.1060
A	 0.9340	 0.0810
B	 0.9860	 0.0960
C	 0.9870	 0.1060
D	 0.9810	 0.1040
E	 0.9770	 0.1040
F	 0.9830	 0.1030
G	 0.9770	 0.1010
H	 0.9900	 0.1010
I	 0.9850	 0.1030
J	 0.9830	 0.1040
K	 0.9750	 0.1080
L	 0.9820	 0.1020
M	 0.9710	 0.1010
N	 0.9600	 0.0840
O	 0.8800	 0.0680
P	 0.8490	 0.1370
Q	 0.8440	 0.1500
R	 0.9210	 0.0950
S	 0.8250	 0.1140
T	 0.6720	 0.1380
U	 0.7380	 0.1120
V	 0.9100	 0.1300
W	 0.7470	 0.1290
X	 0.7690	 0.1410
Y	 0.9390	 0.1170
Z	 0.9040	 0.1340
a	 0.6840	 0.1260
b	 0.6990	 0.0940
c	 0.8890	 0.0870

