



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 07:55 PM UTC

PDB ID : 7KO5 / pdb_00007ko5
EMDB ID : EMD-22965
Title : Structure of cardiac native thin filament at pCa=5.8 having upper and lower troponins in Ca²⁺ bound state
Authors : Galkin, V.E.; Risi, C.M.
Deposited on : 2020-11-06
Resolution : 7.80 Å(reported)
Based on initial model : 6KN8

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

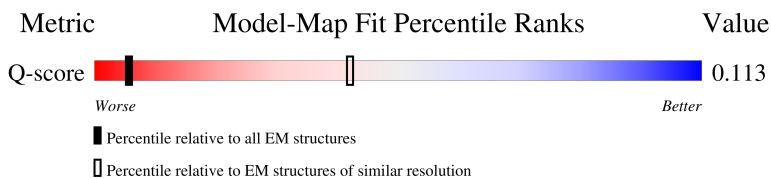
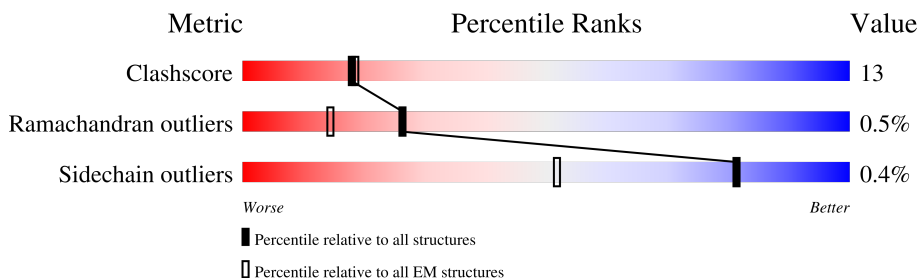
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.80 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.



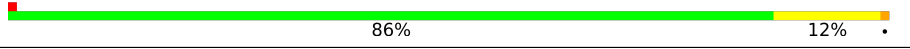
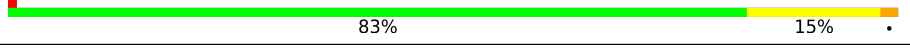
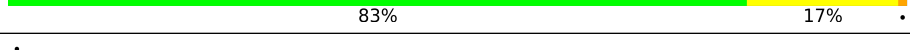
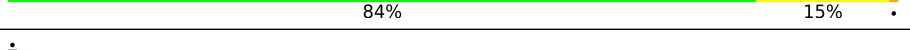
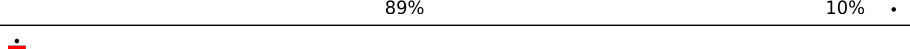
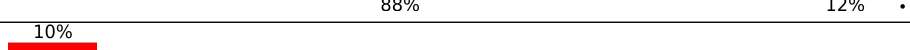
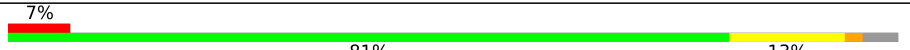
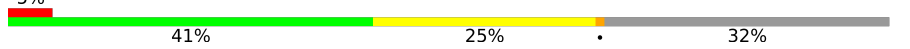
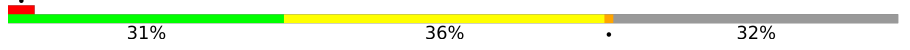
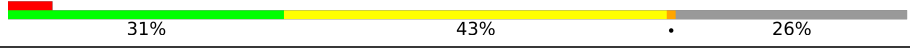
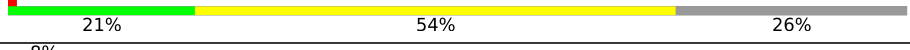
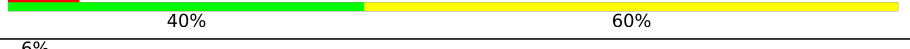
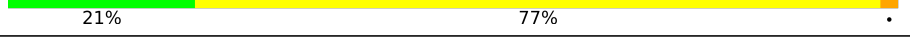
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	370 (7.30 - 8.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

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

Continued on next page...

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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 60511 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Actin, alpha skeletal muscle.

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	T	126	Total	C	N	O	0	0
			1101	673	219	209		
3	a	126	Total	C	N	O	0	0
			1101	673	219	209		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	126	Total	C	N	O	S	0	0
			1008	624	193	187	4		
4	b	126	Total	C	N	O	S	0	0
			1008	624	193	187	4		

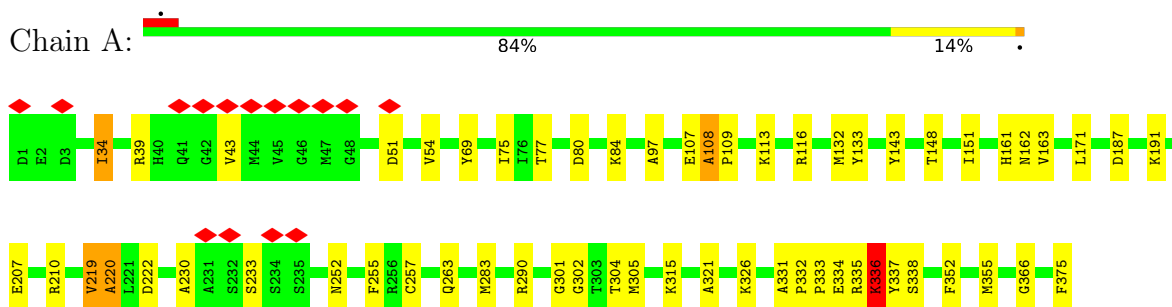
- Molecule 5 is a protein called Troponin C.

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

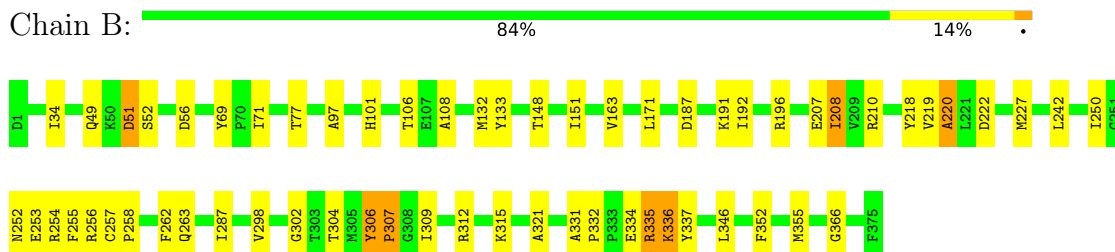
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

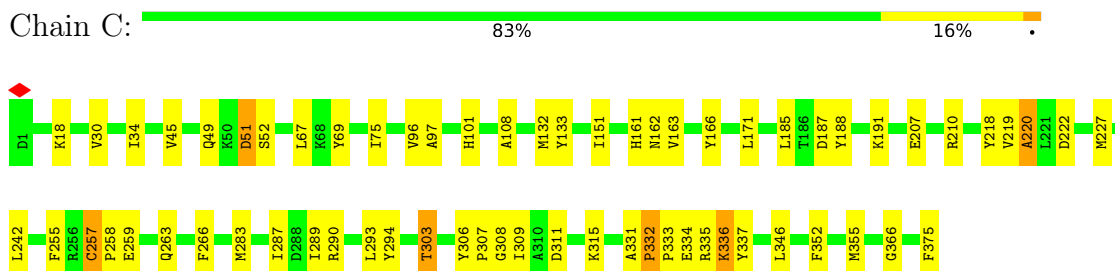
- Molecule 1: Actin, alpha skeletal muscle



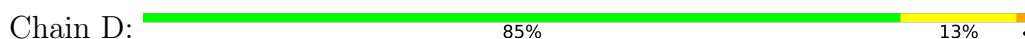
- Molecule 1: Actin, alpha skeletal muscle

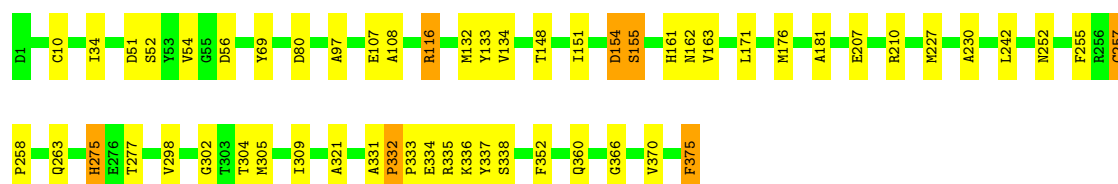


- Molecule 1: Actin, alpha skeletal muscle

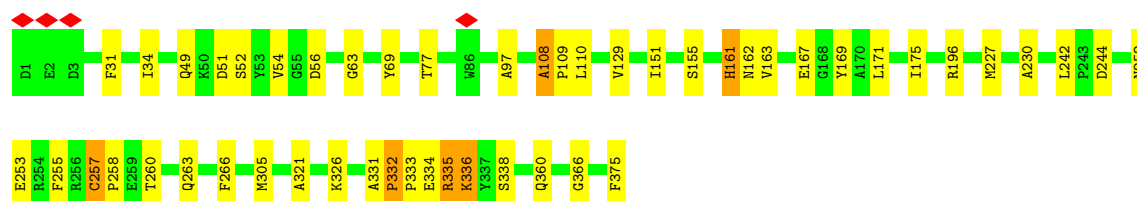
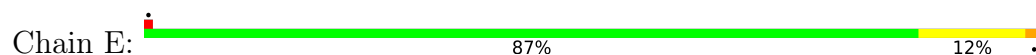


- Molecule 1: Actin, alpha skeletal muscle

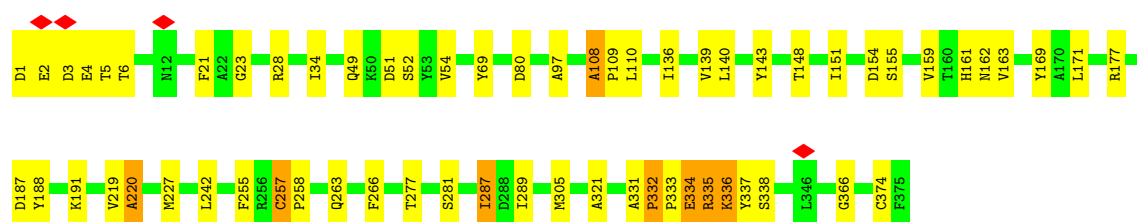
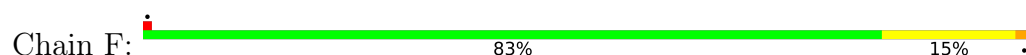




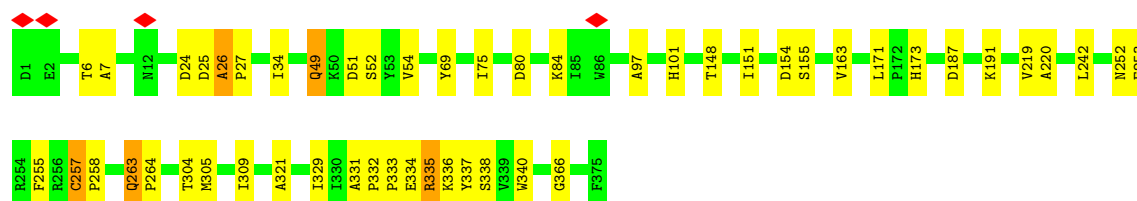
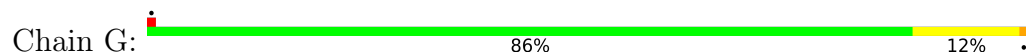
- Molecule 1: Actin, alpha skeletal muscle



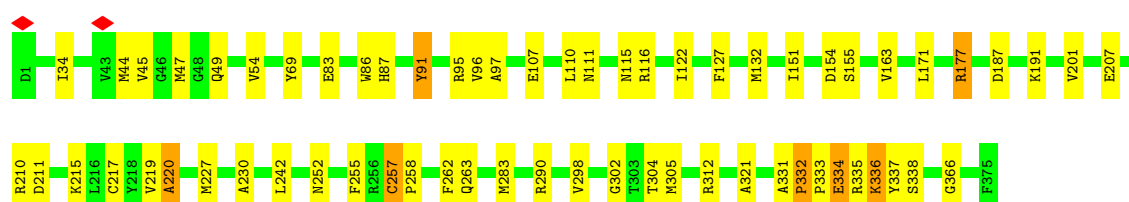
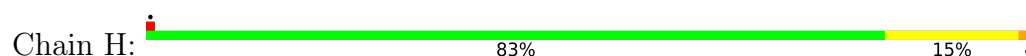
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle

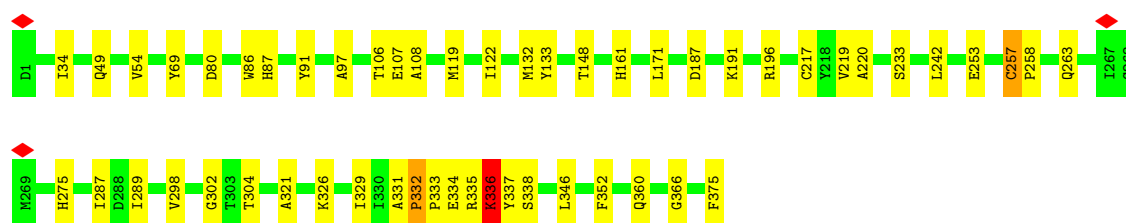


- Molecule 1: Actin, alpha skeletal muscle



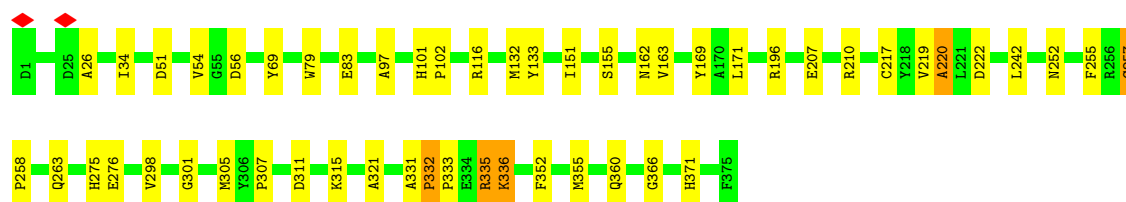
- Molecule 1: Actin, alpha skeletal muscle

Chain I:  86% 13%



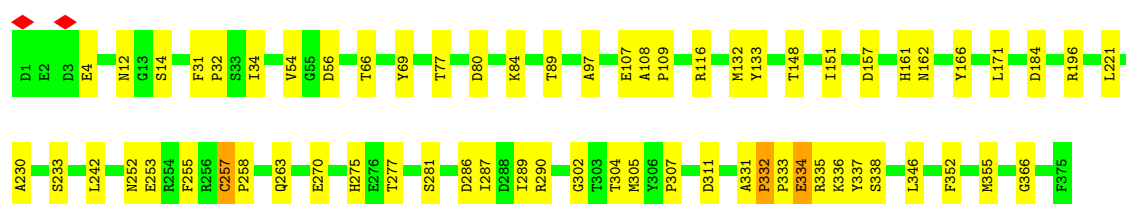
- Molecule 1: Actin, alpha skeletal muscle

Chain J:  86% 13%



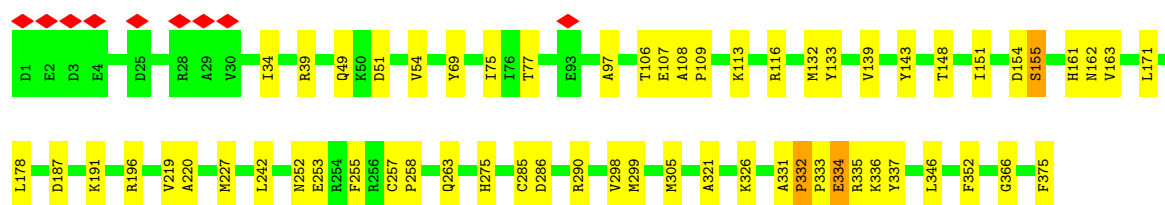
- Molecule 1: Actin, alpha skeletal muscle

Chain K:  83% 17%

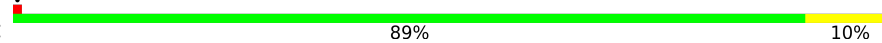


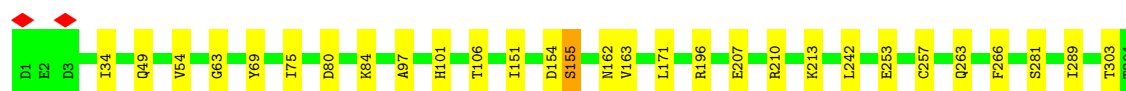
- Molecule 1: Actin, alpha skeletal muscle

Chain L:  84% 15%



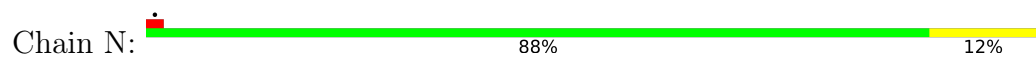
- Molecule 1: Actin, alpha skeletal muscle

Chain M:  89% 10%

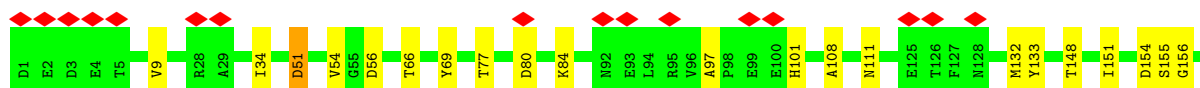
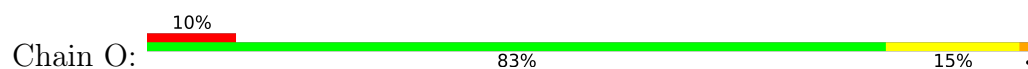




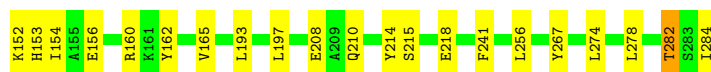
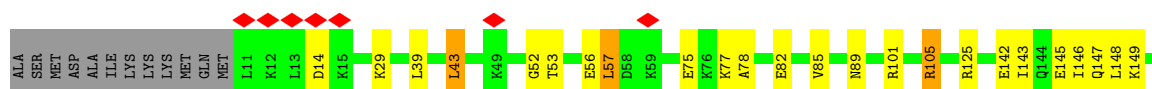
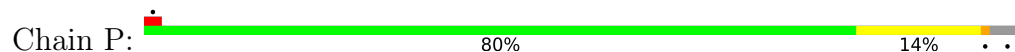
- Molecule 1: Actin, alpha skeletal muscle



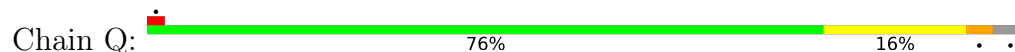
- Molecule 1: Actin, alpha skeletal muscle



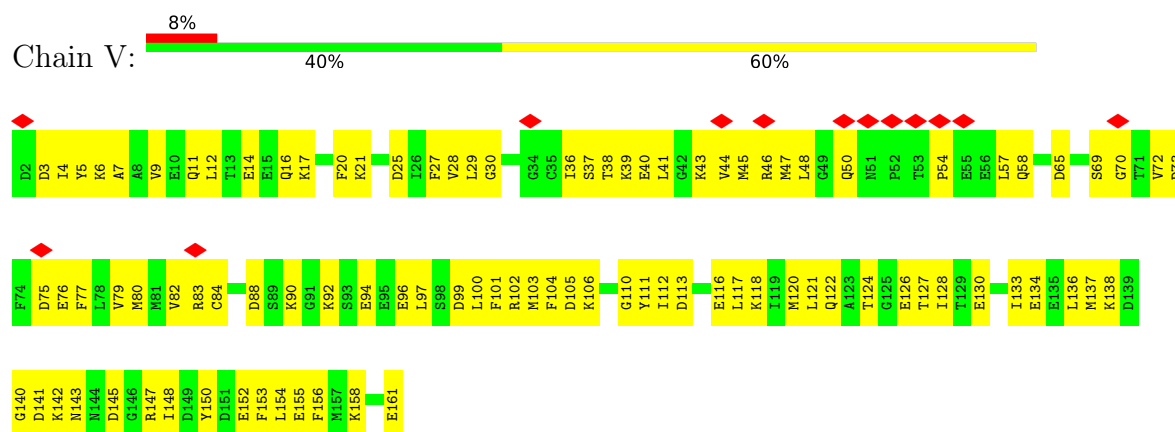
- Molecule 2: Tropomyosin alpha-1 chain



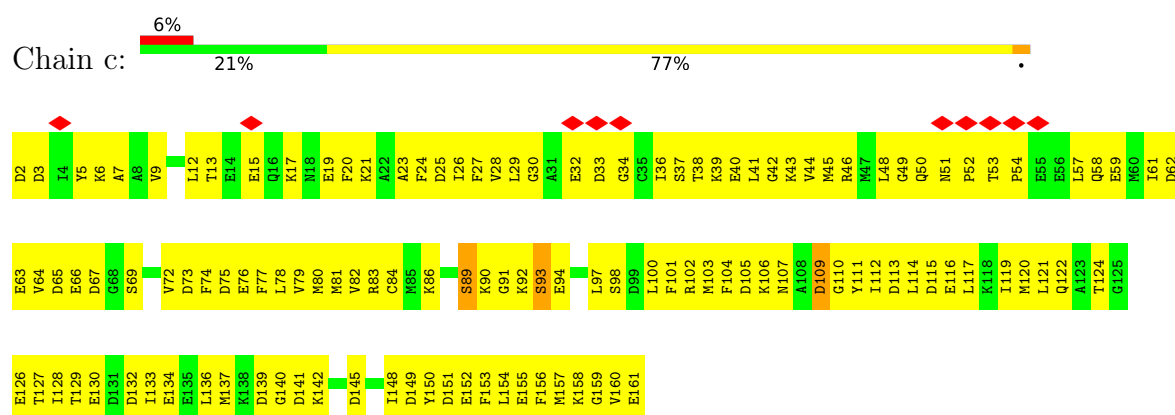
- Molecule 2: Tropomyosin alpha-1 chain



● Molecule 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	15569	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	0.120	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.032	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	0.91	0/2996	1.31	35/4058 (0.9%)
1	B	0.89	0/2996	1.27	35/4058 (0.9%)
1	C	0.95	1/2996 (0.0%)	1.29	37/4058 (0.9%)
1	D	0.92	1/2996 (0.0%)	1.32	43/4058 (1.1%)
1	E	0.90	0/2996	1.30	40/4058 (1.0%)
1	F	0.91	0/2996	1.31	33/4058 (0.8%)
1	G	0.92	0/2996	1.31	35/4058 (0.9%)
1	H	0.90	0/2996	1.33	37/4058 (0.9%)
1	I	0.93	1/2996 (0.0%)	1.31	33/4058 (0.8%)
1	J	0.91	1/2996 (0.0%)	1.32	35/4058 (0.9%)
1	K	0.92	0/2996	1.31	32/4058 (0.8%)
1	L	0.93	1/2996 (0.0%)	1.30	37/4058 (0.9%)
1	M	0.92	0/2996	1.30	35/4058 (0.9%)
1	N	0.91	0/2996	1.32	34/4058 (0.8%)
1	O	0.94	0/2996	1.35	40/4058 (1.0%)
2	P	1.37	0/2215	1.32	14/2954 (0.5%)
2	Q	1.37	2/2215 (0.1%)	1.38	23/2954 (0.8%)
2	R	1.39	1/230 (0.4%)	1.28	2/301 (0.7%)
2	S	1.35	1/230 (0.4%)	1.22	0/301
2	W	1.37	0/2215	1.32	16/2954 (0.5%)
2	X	1.37	2/2215 (0.1%)	1.38	22/2954 (0.7%)
2	Y	1.40	1/230 (0.4%)	1.28	2/301 (0.7%)
2	Z	1.35	1/230 (0.4%)	1.22	0/301
3	T	0.69	0/1108	0.84	2/1466 (0.1%)
3	a	0.72	0/1108	0.88	2/1466 (0.1%)
4	U	0.19	0/1014	0.50	1/1352 (0.1%)
4	b	0.33	0/1014	0.56	0/1352
5	V	0.18	0/1286	0.46	0/1719
5	c	0.33	0/1286	0.61	0/1719
All	All	0.97	13/61536 (0.0%)	1.26	625/82964 (0.8%)

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	c	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	8	MET	SD-CE	-6.28	1.63	1.79
1	D	161	HIS	CB-CG	-6.25	1.41	1.50
2	Z	8	MET	SD-CE	-6.24	1.64	1.79
2	R	4	ILE	CA-CB	-6.16	1.47	1.54
2	Y	4	ILE	CA-CB	-6.12	1.47	1.54
2	Q	241	PHE	CA-C	-5.54	1.45	1.52
2	X	241	PHE	CA-C	-5.46	1.45	1.52
1	I	161	HIS	CB-CG	-5.24	1.42	1.50
2	X	281	MET	CA-C	-5.10	1.46	1.52
1	J	196	ARG	NE-CZ	5.09	1.38	1.33
1	C	67	LEU	CB-CG	5.08	1.63	1.53
2	Q	281	MET	CA-C	-5.07	1.46	1.52
1	L	39	ARG	NE-CZ	5.04	1.38	1.33

All (625) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	163	VAL	N-CA-C	10.98	117.55	107.56
1	N	331	ALA	CA-C-N	10.11	126.94	119.66
1	N	331	ALA	C-N-CA	10.11	126.94	119.66
1	L	163	VAL	N-CA-C	8.88	117.58	107.89
1	C	263	GLN	CA-C-N	8.54	128.19	119.82
1	C	263	GLN	C-N-CA	8.54	128.19	119.82
1	N	263	GLN	CA-C-N	8.47	128.20	119.56
1	N	263	GLN	C-N-CA	8.47	128.20	119.56
1	J	69	TYR	CA-C-N	8.40	128.12	119.56
1	J	69	TYR	C-N-CA	8.40	128.12	119.56
1	A	263	GLN	CA-C-N	8.40	128.12	119.56
1	A	263	GLN	C-N-CA	8.40	128.12	119.56
1	I	263	GLN	CA-C-N	8.38	128.03	119.82
1	I	263	GLN	C-N-CA	8.38	128.03	119.82
2	P	282	THR	N-CA-C	-8.36	102.25	111.36
2	W	282	THR	N-CA-C	-8.33	102.28	111.36
1	K	34	ILE	N-CA-C	8.28	120.70	108.45
1	F	69	TYR	CA-C-N	8.25	127.97	119.56
1	F	69	TYR	C-N-CA	8.25	127.97	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	163	VAL	N-CA-C	8.24	116.87	107.89
2	X	250	GLU	N-CA-C	-8.18	102.44	111.36
1	N	332	PRO	O-C-N	8.15	124.98	121.15
2	Q	250	GLU	N-CA-C	-8.14	102.49	111.36
1	I	69	TYR	CA-C-N	8.09	127.81	119.56
1	I	69	TYR	C-N-CA	8.09	127.81	119.56
1	L	263	GLN	CA-C-N	8.09	127.81	119.56
1	L	263	GLN	C-N-CA	8.09	127.81	119.56
1	K	69	TYR	CA-C-N	8.08	128.27	119.87
1	K	69	TYR	C-N-CA	8.08	128.27	119.87
1	G	69	TYR	CA-C-N	8.06	127.78	119.56
1	G	69	TYR	C-N-CA	8.06	127.78	119.56
1	B	263	GLN	CA-C-N	8.02	127.74	119.56
1	B	263	GLN	C-N-CA	8.02	127.74	119.56
1	A	219	VAL	N-CA-C	7.99	118.04	110.53
1	C	69	TYR	CA-C-N	7.98	127.70	119.56
1	C	69	TYR	C-N-CA	7.98	127.70	119.56
1	M	75	ILE	N-CA-C	7.93	119.90	108.48
1	H	163	VAL	N-CA-C	7.90	116.74	107.73
1	O	263	GLN	CA-C-N	7.90	127.62	119.56
1	O	263	GLN	C-N-CA	7.90	127.62	119.56
1	D	366	GLY	CA-C-N	7.85	127.56	119.56
1	D	366	GLY	C-N-CA	7.85	127.56	119.56
1	J	263	GLN	CA-C-N	7.79	127.51	119.56
1	J	263	GLN	C-N-CA	7.79	127.51	119.56
1	E	69	TYR	CA-C-N	7.74	127.45	119.56
1	E	69	TYR	C-N-CA	7.74	127.45	119.56
1	C	171	LEU	CA-C-N	7.73	127.37	119.56
1	C	171	LEU	C-N-CA	7.73	127.37	119.56
1	F	257	CYS	CA-C-N	7.72	127.77	119.28
1	F	257	CYS	C-N-CA	7.72	127.77	119.28
1	E	366	GLY	CA-C-N	7.71	127.42	119.56
1	E	366	GLY	C-N-CA	7.71	127.42	119.56
1	F	263	GLN	CA-C-N	7.68	127.32	119.56
1	F	263	GLN	C-N-CA	7.68	127.32	119.56
2	P	241	PHE	CA-CB-CG	-7.61	106.19	113.80
2	W	241	PHE	CA-CB-CG	-7.59	106.21	113.80
1	A	366	GLY	CA-C-N	7.54	127.25	119.56
1	A	366	GLY	C-N-CA	7.54	127.25	119.56
1	D	263	GLN	CA-C-N	7.41	127.04	119.56
1	D	263	GLN	C-N-CA	7.41	127.04	119.56
1	A	97	ALA	CA-C-N	7.40	127.11	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ALA	C-N-CA	7.40	127.11	119.56
2	P	43	LEU	N-CA-C	-7.40	102.91	112.23
1	O	208	ILE	CB-CA-C	-7.39	102.34	112.02
1	L	366	GLY	CA-C-N	7.37	127.08	119.56
1	L	366	GLY	C-N-CA	7.37	127.08	119.56
2	W	43	LEU	N-CA-C	-7.36	102.95	112.23
1	J	163	VAL	N-CA-C	7.36	115.91	107.89
1	M	163	VAL	N-CA-C	7.33	114.81	107.55
1	N	171	LEU	CA-C-N	7.32	127.96	119.47
1	N	171	LEU	C-N-CA	7.32	127.96	119.47
1	M	69	TYR	CA-C-N	7.28	126.98	119.56
1	M	69	TYR	C-N-CA	7.28	126.98	119.56
1	C	366	GLY	CA-C-N	7.23	126.94	119.56
1	C	366	GLY	C-N-CA	7.23	126.94	119.56
1	F	97	ALA	CA-C-N	7.22	126.93	119.56
1	F	97	ALA	C-N-CA	7.22	126.93	119.56
1	K	331	ALA	CA-C-N	7.22	127.81	120.38
1	K	331	ALA	C-N-CA	7.22	127.81	120.38
1	G	263	GLN	CA-C-N	7.21	126.92	119.56
1	G	263	GLN	C-N-CA	7.21	126.92	119.56
1	H	263	GLN	CA-C-N	7.19	126.82	119.56
1	H	263	GLN	C-N-CA	7.19	126.82	119.56
1	M	263	GLN	CA-C-N	7.18	126.88	119.56
1	M	263	GLN	C-N-CA	7.18	126.88	119.56
1	N	366	GLY	CA-C-N	7.17	126.87	119.56
1	N	366	GLY	C-N-CA	7.17	126.87	119.56
1	B	366	GLY	CA-C-N	7.15	126.86	119.56
1	B	366	GLY	C-N-CA	7.15	126.86	119.56
1	G	97	ALA	CA-C-N	7.14	126.84	119.56
1	G	97	ALA	C-N-CA	7.14	126.84	119.56
1	O	321	ALA	CA-C-N	7.11	127.06	120.03
1	O	321	ALA	C-N-CA	7.11	127.06	120.03
1	C	163	VAL	N-CA-C	7.10	116.06	107.61
2	Q	268	LYS	N-CA-C	-7.10	102.96	111.69
1	K	171	LEU	CA-C-N	7.05	126.75	119.56
1	K	171	LEU	C-N-CA	7.05	126.75	119.56
2	X	268	LYS	N-CA-C	-7.04	103.03	111.69
1	I	257	CYS	CA-C-N	7.04	127.64	119.47
1	I	257	CYS	C-N-CA	7.04	127.64	119.47
1	A	171	LEU	CA-C-N	7.04	126.74	119.56
1	A	171	LEU	C-N-CA	7.04	126.74	119.56
1	O	108	ALA	CA-C-N	7.03	127.34	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	108	ALA	C-N-CA	7.03	127.34	119.32
2	W	154	ILE	N-CA-C	-7.03	103.62	110.72
1	O	171	LEU	CA-C-N	7.02	126.72	119.56
1	O	171	LEU	C-N-CA	7.02	126.72	119.56
1	E	263	GLN	CA-C-N	7.00	126.69	119.56
1	E	263	GLN	C-N-CA	7.00	126.69	119.56
1	F	332	PRO	CA-C-N	6.97	126.67	119.56
1	F	332	PRO	C-N-CA	6.97	126.67	119.56
2	W	208	GLU	N-CA-C	-6.94	103.79	111.36
1	N	75	ILE	N-CA-C	6.92	118.45	108.48
1	B	148	THR	N-CA-C	-6.91	105.40	114.31
1	D	375	PHE	CA-CB-CG	6.90	120.70	113.80
1	O	366	GLY	CA-C-N	6.89	126.59	119.56
1	O	366	GLY	C-N-CA	6.89	126.59	119.56
1	H	151	ILE	CA-C-N	-6.89	114.08	122.90
1	H	151	ILE	C-N-CA	-6.89	114.08	122.90
1	O	163	VAL	N-CA-C	6.87	118.57	107.71
1	E	171	LEU	CA-C-N	6.87	126.56	119.56
1	E	171	LEU	C-N-CA	6.87	126.56	119.56
2	P	208	GLU	N-CA-C	-6.86	103.88	111.36
2	P	154	ILE	N-CA-C	-6.86	103.79	110.72
1	H	69	TYR	CA-C-N	6.86	127.44	120.04
1	H	69	TYR	C-N-CA	6.86	127.44	120.04
1	L	171	LEU	CA-C-N	6.86	126.55	119.56
1	L	171	LEU	C-N-CA	6.86	126.55	119.56
1	O	69	TYR	CA-C-N	6.85	127.00	119.87
1	O	69	TYR	C-N-CA	6.85	127.00	119.87
1	J	97	ALA	CA-C-N	6.85	127.42	119.47
1	J	97	ALA	C-N-CA	6.85	127.42	119.47
1	J	366	GLY	CA-C-N	6.85	127.41	119.47
1	J	366	GLY	C-N-CA	6.85	127.41	119.47
1	O	97	ALA	CA-C-N	6.84	126.54	119.56
1	O	97	ALA	C-N-CA	6.84	126.54	119.56
2	X	283	SER	N-CA-C	-6.84	101.71	110.53
2	Q	283	SER	N-CA-C	-6.83	101.72	110.53
1	N	332	PRO	CA-C-N	6.83	127.70	120.12
1	N	332	PRO	C-N-CA	6.83	127.70	120.12
1	M	34	ILE	N-CA-C	6.83	117.96	108.12
1	I	148	THR	N-CA-C	-6.82	105.51	114.31
1	G	366	GLY	CA-C-N	6.82	126.51	119.56
1	G	366	GLY	C-N-CA	6.82	126.51	119.56
1	A	148	THR	N-CA-C	-6.81	105.52	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	151	ILE	CA-C-N	-6.81	114.01	122.93
1	D	151	ILE	C-N-CA	-6.81	114.01	122.93
1	D	34	ILE	N-CA-C	6.80	117.64	108.11
1	F	366	GLY	CA-C-N	6.80	126.49	119.56
1	F	366	GLY	C-N-CA	6.80	126.49	119.56
2	P	52	GLY	N-CA-C	-6.79	104.63	112.50
1	J	257	CYS	CA-C-N	6.78	127.33	119.47
1	J	257	CYS	C-N-CA	6.78	127.33	119.47
3	a	110	PHE	N-CA-C	6.78	118.32	111.07
2	W	52	GLY	N-CA-C	-6.76	104.66	112.50
1	E	163	VAL	N-CA-C	6.75	116.01	108.05
3	T	110	PHE	N-CA-C	6.74	118.28	111.07
2	X	121	ASP	CA-CB-CG	6.74	119.34	112.60
1	D	132	MET	N-CA-C	6.72	119.64	109.23
1	D	148	THR	N-CA-C	-6.70	105.67	114.31
1	G	332	PRO	CA-C-N	6.70	126.32	119.56
1	G	332	PRO	C-N-CA	6.70	126.32	119.56
1	G	257	CYS	CA-C-N	6.66	127.20	119.47
1	G	257	CYS	C-N-CA	6.66	127.20	119.47
2	Q	121	ASP	CA-CB-CG	6.66	119.26	112.60
1	O	111	ASN	CA-C-N	6.65	126.69	119.90
1	O	111	ASN	C-N-CA	6.65	126.69	119.90
1	L	34	ILE	N-CA-C	6.64	118.35	108.46
1	K	263	GLN	CA-C-N	6.63	126.77	119.87
1	K	263	GLN	C-N-CA	6.63	126.77	119.87
1	M	289	ILE	N-CA-C	-6.62	105.38	111.67
1	M	151	ILE	CA-C-N	-6.61	114.27	122.93
1	M	151	ILE	C-N-CA	-6.61	114.27	122.93
1	D	69	TYR	CA-C-N	6.61	127.18	120.04
1	D	69	TYR	C-N-CA	6.61	127.18	120.04
1	H	132	MET	N-CA-C	6.58	119.43	109.23
1	J	26	ALA	CA-C-N	6.58	126.27	119.82
1	J	26	ALA	C-N-CA	6.58	126.27	119.82
1	J	332	PRO	CA-C-N	6.56	126.25	119.56
1	J	332	PRO	C-N-CA	6.56	126.25	119.56
1	G	329	ILE	N-CA-C	6.56	117.29	108.11
1	H	366	GLY	CA-C-N	6.56	126.25	119.56
1	H	366	GLY	C-N-CA	6.56	126.25	119.56
1	F	151	ILE	CA-C-N	-6.54	114.19	122.37
1	F	151	ILE	C-N-CA	-6.54	114.19	122.37
1	L	298	VAL	N-CA-C	6.54	117.54	107.99
1	N	321	ALA	CA-C-N	6.51	126.48	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	321	ALA	C-N-CA	6.51	126.48	120.03
1	B	171	LEU	CA-C-N	6.51	126.20	119.56
1	B	171	LEU	C-N-CA	6.51	126.20	119.56
1	H	171	LEU	CA-C-N	6.48	126.17	119.56
1	H	171	LEU	C-N-CA	6.48	126.17	119.56
1	I	366	GLY	CA-C-N	6.48	126.41	119.28
1	I	366	GLY	C-N-CA	6.48	126.41	119.28
1	E	54	VAL	N-CA-C	6.48	117.18	108.11
1	G	75	ILE	N-CA-C	6.47	117.80	108.48
1	E	34	ILE	N-CA-C	6.46	117.16	108.11
1	D	163	VAL	N-CA-C	6.46	115.29	107.61
1	I	97	ALA	CA-C-N	6.46	126.15	119.56
1	I	97	ALA	C-N-CA	6.46	126.15	119.56
1	D	97	ALA	CA-C-N	6.45	126.14	119.56
1	D	97	ALA	C-N-CA	6.45	126.14	119.56
2	Q	126	GLY	N-CA-C	-6.44	105.03	112.50
1	B	151	ILE	CA-C-N	-6.44	114.66	122.90
1	B	151	ILE	C-N-CA	-6.44	114.66	122.90
2	X	126	GLY	N-CA-C	-6.43	105.03	112.50
1	F	374	CYS	N-CA-C	6.43	119.24	111.40
1	H	91	TYR	N-CA-C	6.43	117.95	111.07
1	I	108	ALA	CA-C-N	6.43	126.12	119.56
1	I	108	ALA	C-N-CA	6.43	126.12	119.56
1	M	266	PHE	CA-CB-CG	6.42	120.22	113.80
1	G	171	LEU	CA-C-N	6.42	126.11	119.56
1	G	171	LEU	C-N-CA	6.42	126.11	119.56
1	C	257	CYS	CA-C-N	6.41	126.10	119.56
1	C	257	CYS	C-N-CA	6.41	126.10	119.56
1	J	171	LEU	CA-C-N	6.40	126.09	119.56
1	J	171	LEU	C-N-CA	6.40	126.09	119.56
1	M	366	GLY	CA-C-N	6.40	126.32	119.28
1	M	366	GLY	C-N-CA	6.40	126.32	119.28
1	E	331	ALA	CA-C-N	6.39	126.97	120.38
1	E	331	ALA	C-N-CA	6.39	126.97	120.38
1	C	34	ILE	N-CA-C	6.39	117.98	108.46
1	C	332	PRO	CA-C-N	6.38	126.30	119.28
1	C	332	PRO	C-N-CA	6.38	126.30	119.28
1	C	151	ILE	CA-C-N	-6.37	114.59	122.93
1	C	151	ILE	C-N-CA	-6.37	114.59	122.93
2	Y	20	ASP	N-CA-C	-6.37	104.26	111.07
2	W	125	ARG	N-CA-C	-6.36	104.27	111.14
2	R	20	ASP	N-CA-C	-6.34	104.29	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	125	ARG	N-CA-C	-6.33	104.30	111.14
1	E	151	ILE	CA-C-N	-6.33	114.79	122.90
1	E	151	ILE	C-N-CA	-6.33	114.79	122.90
1	J	34	ILE	N-CA-C	6.32	117.22	108.12
1	I	132	MET	N-CA-C	6.31	119.00	109.23
1	H	97	ALA	CA-C-N	6.30	127.72	119.84
1	H	97	ALA	C-N-CA	6.30	127.72	119.84
1	D	309	ILE	N-CA-C	6.30	117.08	110.72
1	M	331	ALA	CA-C-N	6.29	126.86	120.38
1	M	331	ALA	C-N-CA	6.29	126.86	120.38
1	L	69	TYR	CA-C-N	6.28	126.83	120.04
1	L	69	TYR	C-N-CA	6.28	126.83	120.04
1	K	257	CYS	CA-C-N	6.28	126.76	119.47
1	K	257	CYS	C-N-CA	6.28	126.76	119.47
1	E	31	PHE	CA-C-N	6.26	126.23	119.78
1	E	31	PHE	C-N-CA	6.26	126.23	119.78
1	A	43	VAL	N-CA-C	6.25	116.96	111.90
1	G	34	ILE	N-CA-C	6.24	117.10	108.12
1	M	329	ILE	N-CA-C	6.24	116.90	108.17
1	K	151	ILE	CA-C-N	-6.24	114.76	122.93
1	K	151	ILE	C-N-CA	-6.24	114.76	122.93
1	B	71	ILE	N-CA-C	6.21	116.87	108.17
1	F	148	THR	N-CA-C	-6.20	106.31	114.31
1	B	257	CYS	CA-C-N	6.20	125.88	119.56
1	B	257	CYS	C-N-CA	6.20	125.88	119.56
1	H	54	VAL	N-CA-C	6.19	117.39	108.48
1	M	171	LEU	CA-C-N	6.18	125.87	119.56
1	M	171	LEU	C-N-CA	6.18	125.87	119.56
1	B	331	ALA	CA-C-N	6.18	126.75	120.38
1	B	331	ALA	C-N-CA	6.18	126.75	120.38
1	J	331	ALA	CA-C-N	6.18	126.75	120.38
1	J	331	ALA	C-N-CA	6.18	126.75	120.38
1	K	366	GLY	CA-C-N	6.16	126.06	119.28
1	K	366	GLY	C-N-CA	6.16	126.06	119.28
1	L	331	ALA	CA-C-N	6.16	126.72	120.38
1	L	331	ALA	C-N-CA	6.16	126.72	120.38
1	I	331	ALA	CA-C-N	6.16	126.72	120.38
1	I	331	ALA	C-N-CA	6.16	126.72	120.38
1	F	108	ALA	CA-C-N	6.15	126.33	119.32
1	F	108	ALA	C-N-CA	6.15	126.33	119.32
1	M	332	PRO	CA-C-N	6.14	125.82	119.56
1	M	332	PRO	C-N-CA	6.14	125.82	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	375	PHE	CA-CB-CG	6.13	119.93	113.80
1	I	54	VAL	N-CA-C	6.12	117.30	108.48
1	A	331	ALA	CA-C-N	6.10	126.67	120.38
1	A	331	ALA	C-N-CA	6.10	126.67	120.38
1	O	148	THR	N-CA-C	-6.08	106.46	114.31
1	F	163	VAL	CA-C-N	6.08	125.84	119.76
1	F	163	VAL	C-N-CA	6.08	125.84	119.76
1	K	148	THR	N-CA-C	-6.07	105.68	114.12
1	N	34	ILE	N-CA-C	6.07	117.51	108.46
1	I	332	PRO	CA-C-N	6.06	125.74	119.56
1	I	332	PRO	C-N-CA	6.06	125.74	119.56
1	O	331	ALA	CA-C-N	6.06	126.62	120.38
1	O	331	ALA	C-N-CA	6.06	126.62	120.38
1	I	80	ASP	N-CA-C	-6.04	104.06	112.45
1	L	54	VAL	N-CA-C	6.03	117.45	108.46
2	R	5	LYS	N-CA-C	-6.03	104.70	111.28
2	W	57	LEU	CB-CA-C	-6.03	100.78	110.79
1	O	332	PRO	CA-C-N	6.03	125.71	119.56
1	O	332	PRO	C-N-CA	6.03	125.71	119.56
1	D	331	ALA	CA-C-N	6.02	126.58	120.38
1	D	331	ALA	C-N-CA	6.02	126.58	120.38
1	N	69	TYR	CA-C-N	6.02	125.70	119.56
1	N	69	TYR	C-N-CA	6.02	125.70	119.56
2	P	57	LEU	CB-CA-C	-6.01	100.81	110.79
1	A	34	ILE	N-CA-C	6.01	116.52	108.11
1	H	332	PRO	CA-C-N	6.00	125.69	119.56
1	H	332	PRO	C-N-CA	6.00	125.69	119.56
2	Y	5	LYS	N-CA-C	-5.99	104.75	111.28
1	O	132	MET	N-CA-C	5.98	118.50	109.23
1	H	321	ALA	CA-C-N	5.98	126.32	119.92
1	H	321	ALA	C-N-CA	5.98	126.32	119.92
1	B	242	LEU	CA-C-N	5.97	126.39	119.47
1	B	242	LEU	C-N-CA	5.97	126.39	119.47
1	G	151	ILE	CA-C-N	-5.97	115.26	122.90
1	G	151	ILE	C-N-CA	-5.97	115.26	122.90
1	A	321	ALA	CA-C-N	5.95	126.29	119.92
1	A	321	ALA	C-N-CA	5.95	126.29	119.92
1	K	132	MET	N-CA-C	5.95	118.44	109.23
1	N	163	VAL	CB-CA-C	-5.93	104.07	110.95
1	A	332	PRO	CA-C-N	5.93	125.61	119.56
1	A	332	PRO	C-N-CA	5.93	125.61	119.56
1	B	34	ILE	N-CA-C	5.93	118.73	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	PHE	CA-CB-CG	5.91	119.71	113.80
1	L	148	THR	N-CA-C	-5.91	105.90	114.12
2	Q	52	GLY	N-CA-C	-5.90	105.65	112.50
1	N	97	ALA	CA-C-N	5.90	126.31	119.47
1	N	97	ALA	C-N-CA	5.90	126.31	119.47
1	A	54	VAL	N-CA-C	5.89	116.96	108.48
1	E	257	CYS	CA-C-N	5.87	126.28	119.47
1	E	257	CYS	C-N-CA	5.87	126.28	119.47
1	L	332	PRO	CA-C-N	5.87	126.28	119.47
1	L	332	PRO	C-N-CA	5.87	126.28	119.47
1	I	171	LEU	CA-C-N	5.87	125.55	119.56
1	I	171	LEU	C-N-CA	5.87	125.55	119.56
1	J	217	CYS	N-CA-C	5.85	119.14	110.48
1	J	242	LEU	CA-C-N	5.84	126.24	119.47
1	J	242	LEU	C-N-CA	5.84	126.24	119.47
1	G	331	ALA	CA-C-N	5.83	126.39	120.38
1	G	331	ALA	C-N-CA	5.83	126.39	120.38
2	P	14	ASP	N-CA-C	-5.83	105.26	112.90
1	D	332	PRO	CA-C-N	5.83	125.50	119.56
1	D	332	PRO	C-N-CA	5.83	125.50	119.56
1	G	54	VAL	N-CA-C	5.83	116.87	108.48
1	J	151	ILE	CA-C-N	-5.83	115.44	122.90
1	J	151	ILE	C-N-CA	-5.83	115.44	122.90
2	X	52	GLY	N-CA-C	-5.83	105.74	112.50
1	L	299	MET	N-CA-C	5.82	119.31	109.76
2	W	14	ASP	N-CA-C	-5.82	105.28	112.90
2	X	171	ILE	CA-C-N	5.81	128.42	120.46
2	X	171	ILE	C-N-CA	5.81	128.42	120.46
1	K	332	PRO	CA-C-N	5.80	125.48	119.56
1	K	332	PRO	C-N-CA	5.80	125.48	119.56
2	X	225	ILE	N-CA-C	-5.80	105.08	110.53
2	Q	225	ILE	N-CA-C	-5.80	105.08	110.53
1	A	162	ASN	CA-C-N	-5.80	118.29	123.33
1	A	162	ASN	C-N-CA	-5.80	118.29	123.33
1	H	331	ALA	CA-C-N	5.79	126.35	120.38
1	H	331	ALA	C-N-CA	5.79	126.35	120.38
1	A	132	MET	N-CA-C	5.78	117.97	109.24
1	H	163	VAL	CA-C-N	5.78	126.66	120.13
1	H	163	VAL	C-N-CA	5.78	126.66	120.13
1	B	69	TYR	CA-C-N	5.78	125.88	119.87
1	B	69	TYR	C-N-CA	5.78	125.88	119.87
1	D	80	ASP	N-CA-C	-5.78	104.58	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	375	PHE	CA-CB-CG	5.77	119.57	113.80
1	M	242	LEU	N-CA-C	-5.77	101.82	110.24
2	Q	171	ILE	CA-C-N	5.77	128.36	120.46
2	Q	171	ILE	C-N-CA	5.77	128.36	120.46
1	D	171	LEU	CA-C-N	5.77	125.44	119.56
1	D	171	LEU	C-N-CA	5.77	125.44	119.56
1	E	108	ALA	CA-C-N	5.77	126.16	119.47
1	E	108	ALA	C-N-CA	5.77	126.16	119.47
1	E	175	ILE	CB-CA-C	-5.77	105.69	111.80
1	G	321	ALA	CA-C-N	5.76	125.72	119.78
1	G	321	ALA	C-N-CA	5.76	125.72	119.78
1	J	162	ASN	N-CA-C	5.76	118.23	111.02
1	F	331	ALA	CA-C-N	5.76	126.32	120.38
1	F	331	ALA	C-N-CA	5.76	126.32	120.38
1	E	162	ASN	CA-C-N	-5.76	117.74	123.04
1	E	162	ASN	C-N-CA	-5.76	117.74	123.04
2	P	105	ARG	N-CA-C	-5.75	105.10	111.36
1	B	101	HIS	CA-C-N	5.74	125.69	119.78
1	B	101	HIS	C-N-CA	5.74	125.69	119.78
1	N	51	ASP	CA-CB-CG	-5.74	106.86	112.60
1	I	329	ILE	N-CA-C	5.74	116.20	108.17
1	J	54	VAL	N-CA-C	5.72	116.72	108.48
1	I	34	ILE	N-CA-C	5.72	116.98	108.46
2	W	105	ARG	N-CA-C	-5.72	105.13	111.36
1	I	242	LEU	CA-C-N	5.71	126.09	119.47
1	I	242	LEU	C-N-CA	5.71	126.09	119.47
1	B	298	VAL	N-CA-C	5.70	116.15	108.17
1	C	375	PHE	CA-CB-CG	5.70	119.50	113.80
1	D	257	CYS	CA-C-N	5.69	126.08	119.47
1	D	257	CYS	C-N-CA	5.69	126.08	119.47
2	Q	75	GLU	N-CA-C	-5.69	105.16	111.36
1	L	132	MET	N-CA-C	5.69	118.05	109.23
1	D	321	ALA	CA-C-N	5.68	125.66	120.03
1	D	321	ALA	C-N-CA	5.68	125.66	120.03
1	D	10	CYS	N-CA-C	5.68	116.72	107.23
1	H	257	CYS	CA-C-N	5.68	126.05	119.47
1	H	257	CYS	C-N-CA	5.68	126.05	119.47
1	A	108	ALA	CA-C-N	5.67	126.05	119.47
1	A	108	ALA	C-N-CA	5.67	126.05	119.47
2	X	75	GLU	N-CA-C	-5.67	105.18	111.36
1	N	54	VAL	N-CA-C	5.67	116.65	108.48
1	H	201	VAL	N-CA-C	5.67	116.10	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	321	ALA	CA-C-N	5.66	125.61	119.78
1	F	321	ALA	C-N-CA	5.66	125.61	119.78
1	G	148	THR	N-CA-C	-5.66	106.25	114.12
1	C	75	ILE	N-CA-C	5.65	116.08	108.17
1	G	309	ILE	N-CA-C	5.64	116.42	110.72
1	M	101	HIS	CA-C-N	5.64	125.59	119.78
1	M	101	HIS	C-N-CA	5.64	125.59	119.78
1	K	54	VAL	N-CA-C	5.64	116.60	108.48
1	E	266	PHE	CA-CB-CG	5.63	119.43	113.80
1	C	161	HIS	CA-CB-CG	5.63	119.43	113.80
1	E	242	LEU	CA-C-N	5.63	125.30	119.56
1	E	242	LEU	C-N-CA	5.63	125.30	119.56
2	W	215	SER	N-CA-C	-5.62	105.30	111.82
1	K	184	ASP	N-CA-C	-5.61	105.55	112.90
1	K	242	LEU	CA-C-N	5.61	125.98	119.47
1	K	242	LEU	C-N-CA	5.61	125.98	119.47
1	M	306	TYR	N-CA-C	-5.61	102.71	109.72
1	D	154	ASP	N-CA-C	5.61	119.75	113.02
1	F	171	LEU	CA-C-N	5.60	125.27	119.56
1	F	171	LEU	C-N-CA	5.60	125.27	119.56
2	Q	132	SER	N-CA-C	-5.60	105.25	111.36
1	F	242	LEU	CA-C-N	5.60	125.96	119.47
1	F	242	LEU	C-N-CA	5.60	125.96	119.47
1	B	321	ALA	CA-C-N	5.58	125.53	119.78
1	B	321	ALA	C-N-CA	5.58	125.53	119.78
1	K	108	ALA	CA-C-N	5.58	125.94	119.47
1	K	108	ALA	C-N-CA	5.58	125.94	119.47
1	A	39	ARG	N-CA-C	-5.57	105.83	113.30
1	C	101	HIS	CA-C-N	5.57	125.52	119.78
1	C	101	HIS	C-N-CA	5.57	125.52	119.78
2	P	215	SER	N-CA-C	-5.57	105.36	111.82
2	X	132	SER	N-CA-C	-5.57	105.29	111.36
1	N	132	MET	N-CA-C	5.56	117.85	109.23
1	D	298	VAL	N-CA-C	5.56	115.87	107.80
1	L	75	ILE	N-CA-C	5.56	115.95	108.17
1	L	321	ALA	CA-C-N	5.55	125.53	120.03
1	L	321	ALA	C-N-CA	5.55	125.53	120.03
1	O	77	THR	N-CA-C	-5.55	106.86	113.97
1	A	75	ILE	N-CA-C	5.55	117.91	108.86
1	B	163	VAL	CA-C-N	5.55	125.98	119.99
1	B	163	VAL	C-N-CA	5.55	125.98	119.99
2	P	29	LYS	N-CA-C	-5.55	105.31	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	34	ILE	N-CA-C	5.55	116.11	108.12
1	H	298	VAL	N-CA-C	5.54	115.93	108.17
1	L	151	ILE	CA-C-N	-5.54	115.81	122.90
1	L	151	ILE	C-N-CA	-5.54	115.81	122.90
2	W	29	LYS	N-CA-C	-5.54	105.32	111.36
1	M	257	CYS	CA-C-N	5.54	125.21	119.56
1	M	257	CYS	C-N-CA	5.54	125.21	119.56
1	L	108	ALA	CA-C-N	5.53	125.20	119.56
1	L	108	ALA	C-N-CA	5.53	125.20	119.56
1	J	321	ALA	CA-C-N	5.52	125.83	119.92
1	J	321	ALA	C-N-CA	5.52	125.83	119.92
1	E	260	THR	N-CA-C	-5.52	105.36	111.71
1	M	163	VAL	CA-C-N	5.51	125.68	119.90
1	M	163	VAL	C-N-CA	5.51	125.68	119.90
1	O	54	VAL	N-CA-C	5.50	116.40	108.48
1	O	34	ILE	N-CA-C	5.50	116.66	108.46
1	C	132	MET	N-CA-C	5.50	117.75	109.23
1	L	275	HIS	CA-CB-CG	-5.49	108.31	113.80
2	P	77	LYS	N-CA-C	-5.49	105.30	111.28
1	G	173	HIS	CA-CB-CG	-5.49	108.31	113.80
1	J	132	MET	N-CA-C	5.47	117.72	109.23
2	W	77	LYS	N-CA-C	-5.47	105.32	111.28
1	D	54	VAL	N-CA-C	5.47	116.35	108.48
1	L	162	ASN	N-CA-C	5.47	118.78	111.24
2	X	34	ASP	N-CA-C	-5.46	105.41	111.36
1	D	275	HIS	CA-CB-CG	-5.46	108.34	113.80
1	E	97	ALA	CA-C-N	5.46	126.66	119.84
1	E	97	ALA	C-N-CA	5.46	126.66	119.84
1	M	106	THR	N-CA-C	5.45	118.44	109.72
1	H	217	CYS	N-CA-C	5.43	118.55	110.52
1	O	163	VAL	CA-C-N	5.42	125.18	119.76
1	O	163	VAL	C-N-CA	5.42	125.18	119.76
1	E	162	ASN	N-CA-C	5.42	118.72	111.24
1	G	304	THR	N-CA-C	-5.42	106.25	112.92
1	C	162	ASN	CA-C-N	-5.42	118.62	123.33
1	C	162	ASN	C-N-CA	-5.42	118.62	123.33
1	H	34	ILE	N-CA-C	5.42	115.92	108.12
4	U	144	LEU	CB-CA-C	5.42	119.46	109.71
1	O	101	HIS	CA-C-N	5.41	125.35	119.78
1	O	101	HIS	C-N-CA	5.41	125.35	119.78
1	B	108	ALA	CA-C-N	5.41	125.23	119.28
1	B	108	ALA	C-N-CA	5.41	125.23	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	233	SER	N-CA-C	5.40	117.98	108.75
1	H	96	VAL	N-CA-C	5.40	116.25	108.48
1	D	107	GLU	N-CA-C	5.40	116.72	108.52
2	Q	34	ASP	N-CA-C	-5.39	105.48	111.36
1	E	161	HIS	N-CA-C	5.38	116.95	111.14
1	E	332	PRO	CA-C-N	5.38	125.20	119.28
1	E	332	PRO	C-N-CA	5.38	125.20	119.28
1	I	217	CYS	N-CA-C	5.38	118.44	110.48
1	D	163	VAL	CA-C-N	5.38	125.54	119.90
1	D	163	VAL	C-N-CA	5.38	125.54	119.90
1	L	242	LEU	CA-C-N	5.37	125.03	119.56
1	L	242	LEU	C-N-CA	5.37	125.03	119.56
1	C	97	ALA	CA-C-N	5.35	125.68	119.47
1	C	97	ALA	C-N-CA	5.35	125.68	119.47
1	C	303	THR	CA-C-N	5.35	130.78	122.49
1	C	303	THR	C-N-CA	5.35	130.78	122.49
1	O	9	VAL	N-CA-C	5.34	115.81	108.12
1	A	151	ILE	CA-C-N	-5.33	115.72	122.43
1	A	151	ILE	C-N-CA	-5.33	115.72	122.43
1	I	375	PHE	CA-CB-CG	5.32	119.12	113.80
1	E	77	THR	N-CA-C	-5.32	107.16	113.97
1	H	242	LEU	N-CA-C	-5.32	102.48	110.24
1	C	331	ALA	CA-C-N	5.31	125.85	120.38
1	C	331	ALA	C-N-CA	5.31	125.85	120.38
1	G	101	HIS	CA-C-N	5.31	125.31	119.90
1	G	101	HIS	C-N-CA	5.31	125.31	119.90
1	J	102	PRO	N-CA-C	-5.29	102.79	111.21
2	Q	169	LEU	N-CA-C	-5.29	105.41	111.07
1	D	108	ALA	CA-C-N	5.28	125.59	119.47
1	D	108	ALA	C-N-CA	5.28	125.59	119.47
2	Q	276	HIS	N-CA-C	-5.27	105.45	111.14
2	X	276	HIS	N-CA-C	-5.27	105.45	111.14
1	M	373	LYS	N-CA-C	5.26	119.83	113.41
1	N	162	ASN	CA-C-N	-5.26	119.02	122.60
1	N	162	ASN	C-N-CA	-5.26	119.02	122.60
2	P	75	GLU	N-CA-C	-5.26	105.63	111.36
1	A	77	THR	N-CA-C	-5.26	107.24	113.97
1	H	111	ASN	CA-C-N	5.26	125.26	119.90
1	H	111	ASN	C-N-CA	5.26	125.26	119.90
2	X	29	LYS	N-CA-C	-5.25	105.73	111.82
2	Q	29	LYS	N-CA-C	-5.25	105.73	111.82
1	N	174	ALA	CA-C-N	-5.24	115.83	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	174	ALA	C-N-CA	-5.24	115.83	122.43
1	O	247	VAL	N-CA-C	5.24	116.03	108.48
1	E	129	VAL	CA-C-N	5.24	124.85	119.56
1	E	129	VAL	C-N-CA	5.24	124.85	119.56
1	O	257	CYS	CA-C-N	5.24	124.85	119.56
1	O	257	CYS	C-N-CA	5.24	124.85	119.56
1	E	321	ALA	CA-C-N	5.24	125.14	119.85
1	E	321	ALA	C-N-CA	5.24	125.14	119.85
1	I	289	ILE	N-CA-C	-5.24	107.31	111.81
1	K	32	PRO	N-CA-CB	-5.23	99.34	102.79
1	B	106	THR	N-CA-C	5.22	117.62	109.52
1	M	54	VAL	N-CA-C	5.22	115.42	108.11
1	J	101	HIS	CB-CA-C	-5.22	102.43	110.62
1	N	151	ILE	CA-C-N	-5.22	115.85	122.43
1	N	151	ILE	C-N-CA	-5.22	115.85	122.43
2	X	169	LEU	N-CA-C	-5.22	105.48	111.07
2	W	75	GLU	N-CA-C	-5.22	105.67	111.36
2	X	85	VAL	CB-CA-C	-5.21	105.30	111.97
1	K	12	ASN	N-CA-C	5.21	117.21	107.99
1	H	151	ILE	CB-CA-C	-5.20	103.85	110.98
1	G	242	LEU	CA-C-N	5.20	125.50	119.47
1	G	242	LEU	C-N-CA	5.20	125.50	119.47
1	M	97	ALA	CA-C-N	5.20	126.34	119.84
1	M	97	ALA	C-N-CA	5.20	126.34	119.84
1	H	242	LEU	CA-C-N	5.20	124.86	119.56
1	H	242	LEU	C-N-CA	5.20	124.86	119.56
2	Q	229	SER	N-CA-C	-5.20	105.70	111.36
1	B	77	THR	N-CA-C	-5.19	107.50	113.88
1	N	257	CYS	CA-C-N	5.18	125.48	119.47
1	N	257	CYS	C-N-CA	5.18	125.48	119.47
2	X	229	SER	N-CA-C	-5.18	105.71	111.36
3	T	102	LEU	N-CA-C	-5.17	105.82	111.82
1	A	233	SER	N-CA-C	5.17	117.59	108.75
1	F	80	ASP	N-CA-C	-5.17	105.33	111.69
1	J	298	VAL	N-CA-C	5.17	115.34	108.11
1	K	233	SER	N-CA-C	5.17	117.11	108.99
1	D	162	ASN	CA-C-N	-5.17	118.84	123.33
1	D	162	ASN	C-N-CA	-5.17	118.84	123.33
1	B	97	ALA	CA-C-N	5.16	126.29	119.84
1	B	97	ALA	C-N-CA	5.16	126.29	119.84
1	A	257	CYS	CA-C-N	5.15	124.81	119.56
1	A	257	CYS	C-N-CA	5.15	124.81	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	151	ILE	CB-CA-C	-5.14	103.94	110.98
1	M	309	ILE	N-CA-C	5.14	115.91	110.72
1	F	289	ILE	N-CA-C	-5.14	107.39	111.81
1	O	151	ILE	CA-C-N	-5.14	115.95	122.43
1	O	151	ILE	C-N-CA	-5.14	115.95	122.43
1	L	106	THR	N-CA-C	5.14	117.48	109.52
2	Q	85	VAL	CB-CA-C	-5.14	105.39	111.97
1	L	77	THR	N-CA-C	-5.14	106.96	113.43
2	Q	159	ASP	CA-CB-CG	5.14	117.74	112.60
1	I	321	ALA	CA-C-N	5.13	125.07	119.78
1	I	321	ALA	C-N-CA	5.13	125.07	119.78
3	a	102	LEU	N-CA-C	-5.13	105.87	111.82
1	O	212	ILE	CB-CA-C	-5.13	105.41	111.97
1	L	151	ILE	CB-CA-C	-5.12	103.96	110.98
2	X	159	ASP	CA-CB-CG	5.12	117.72	112.60
1	J	151	ILE	CB-CA-C	-5.12	103.96	110.98
1	L	97	ALA	CA-C-N	5.12	125.41	119.47
1	L	97	ALA	C-N-CA	5.12	125.41	119.47
1	A	163	VAL	N-CA-C	5.10	113.68	107.61
2	W	180	GLU	N-CA-C	-5.10	105.80	111.36
1	C	51	ASP	CA-CB-CG	-5.10	107.50	112.60
1	K	77	THR	N-CA-C	-5.10	107.01	113.43
1	M	151	ILE	CB-CA-C	-5.10	104.00	110.98
2	Q	272	GLU	N-CA-C	-5.09	105.92	111.82
1	O	51	ASP	CA-CB-CG	-5.09	107.51	112.60
1	C	242	LEU	CA-C-N	5.08	126.19	119.84
1	C	242	LEU	C-N-CA	5.08	126.19	119.84
1	F	54	VAL	N-CA-C	5.08	117.14	108.86
1	B	51	ASP	CA-CB-CG	-5.07	107.53	112.60
1	K	97	ALA	CA-C-N	5.07	125.35	119.47
1	K	97	ALA	C-N-CA	5.07	125.35	119.47
1	J	51	ASP	CA-CB-CG	-5.07	107.53	112.60
2	X	92	ILE	N-CA-C	-5.07	105.60	110.72
1	D	242	LEU	CA-C-N	5.06	126.17	119.84
1	D	242	LEU	C-N-CA	5.06	126.17	119.84
1	C	108	ALA	CA-C-N	5.06	125.34	119.47
1	C	108	ALA	C-N-CA	5.06	125.34	119.47
2	X	272	GLU	N-CA-C	-5.06	105.95	111.82
1	I	298	VAL	N-CA-C	5.05	115.13	107.80
2	X	240	GLU	N-CA-C	-5.05	105.47	111.69
1	C	96	VAL	N-CA-C	5.05	115.40	108.12
2	Q	240	GLU	N-CA-C	-5.05	105.47	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	233	SER	N-CA-C	5.05	117.39	108.75
2	Q	92	ILE	N-CA-C	-5.05	105.62	110.72
2	Q	273	GLU	N-CA-C	-5.05	105.86	111.36
1	C	151	ILE	CB-CA-C	-5.04	104.86	110.96
1	L	178	LEU	N-CA-C	5.04	117.61	108.69
2	W	92	ILE	N-CA-C	-5.03	105.51	111.00
1	G	253	GLU	CA-C-N	5.03	127.53	120.28
1	G	253	GLU	C-N-CA	5.03	127.53	120.28
2	Q	253	ILE	N-CA-C	-5.03	105.64	110.72
2	X	253	ILE	N-CA-C	-5.03	105.64	110.72
1	N	112	PRO	CA-C-N	5.02	127.26	120.38
1	N	112	PRO	C-N-CA	5.02	127.26	120.38
1	A	51	ASP	CA-CB-CG	-5.02	107.58	112.60
1	B	132	MET	N-CA-C	5.01	117.00	109.23
1	K	66	THR	N-CA-C	-5.01	101.54	109.96
1	B	151	ILE	CB-CA-C	-5.01	104.12	110.98
1	D	181	ALA	N-CA-C	5.01	116.42	108.96
1	F	151	ILE	CB-CA-C	-5.00	104.13	110.98

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	c	109	ASP	Peptide
5	c	89	SER	Peptide
5	c	93	SER	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	56	0
1	B	2933	0	2894	50	0
1	C	2933	0	2894	88	0
1	D	2933	0	2894	45	0
1	E	2933	0	2894	52	0
1	F	2933	0	2894	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2933	0	2894	45	0
1	H	2933	0	2894	67	0
1	I	2933	0	2894	47	0
1	J	2933	0	2894	60	0
1	K	2933	0	2894	69	0
1	L	2933	0	2894	69	0
1	M	2933	0	2894	31	0
1	N	2933	0	2894	41	0
1	O	2933	0	2894	66	0
2	P	2207	0	2200	59	0
2	Q	2207	0	2200	56	0
2	R	231	0	245	0	0
2	S	231	0	245	2	0
2	W	2207	0	2200	73	0
2	X	2207	0	2200	60	0
2	Y	231	0	245	1	0
2	Z	231	0	245	2	0
3	T	1101	0	1120	77	0
3	a	1101	0	1120	139	0
4	U	1008	0	1064	122	0
4	b	1008	0	1064	187	0
5	V	1273	0	1201	133	0
5	c	1273	0	1201	188	0
All	All	60511	0	59960	1596	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 13.

All (1596) 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:F:1:ASP:HB3	4:U:149:ILE:CD1	1.25	1.57
1:F:305:MET:CE	1:F:335:ARG:HB2	1.35	1.55
1:M:305:MET:CE	1:M:335:ARG:HG3	1.33	1.53
5:V:38:THR:CB	2:W:149:LYS:HE2	1.53	1.37
1:F:305:MET:HE2	1:F:335:ARG:CB	1.52	1.37
1:J:311:ASP:OD1	2:X:248:LYS:HD2	1.24	1.37
1:B:252:ASN:HA	1:B:255:PHE:CE2	1.59	1.36
5:V:38:THR:HB	2:W:149:LYS:CE	1.56	1.36
1:F:1:ASP:CB	4:U:149:ILE:CD1	2.08	1.32
1:O:252:ASN:HA	1:O:255:PHE:CE2	1.65	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:39:LYS:HG2	2:W:149:LYS:NZ	1.46	1.29
1:G:24:ASP:OD1	4:b:146:ARG:HB3	1.30	1.27
1:H:87:HIS:HD2	1:H:127:PHE:CE2	1.50	1.27
1:F:143:TYR:CE1	1:H:44:MET:HE2	1.71	1.25
1:L:133:TYR:CD2	1:L:352:PHE:HZ	1.54	1.25
5:V:39:LYS:H	2:W:149:LYS:NZ	1.31	1.25
1:D:252:ASN:HA	1:D:255:PHE:CE2	1.70	1.24
1:L:143:TYR:CE2	1:N:44:MET:HE2	1.71	1.24
1:I:332:PRO:O	1:I:335:ARG:HG3	1.38	1.24
1:A:252:ASN:HA	1:A:255:PHE:CE2	1.73	1.23
1:G:24:ASP:CG	4:b:146:ARG:HB3	1.62	1.21
1:I:133:TYR:CD2	1:I:352:PHE:HZ	1.58	1.21
1:K:252:ASN:HA	1:K:255:PHE:CE2	1.75	1.19
1:L:133:TYR:CE2	1:L:352:PHE:CE1	2.30	1.19
1:G:25:ASP:OD2	4:b:147:VAL:HG11	1.39	1.19
1:J:311:ASP:CG	2:X:248:LYS:CD	2.16	1.18
1:C:133:TYR:CD2	1:C:352:PHE:HZ	1.62	1.17
1:K:332:PRO:O	1:K:335:ARG:HG3	1.45	1.17
1:J:311:ASP:CG	2:X:248:LYS:HD2	1.69	1.17
1:F:332:PRO:O	1:F:335:ARG:HG2	1.44	1.16
1:L:133:TYR:CD2	1:L:352:PHE:CZ	2.33	1.16
1:L:143:TYR:CZ	1:N:44:MET:HE2	1.81	1.16
1:A:133:TYR:CD2	1:A:352:PHE:HZ	1.63	1.15
1:E:109:PRO:HD2	1:E:161:HIS:NE2	1.59	1.15
1:D:332:PRO:O	1:D:335:ARG:HG3	1.45	1.15
1:H:87:HIS:CD2	1:H:127:PHE:CE2	2.33	1.15
1:J:311:ASP:OD2	2:X:248:LYS:HD3	1.47	1.15
1:O:217:CYS:HB2	1:O:306:TYR:CE2	1.82	1.15
1:F:136:ILE:O	1:F:139:VAL:HG22	1.45	1.15
1:H:87:HIS:CD2	1:H:127:PHE:CZ	2.35	1.14
1:C:18:LYS:HD2	1:C:337:TYR:CD1	1.84	1.12
1:C:332:PRO:O	1:C:335:ARG:HG3	1.49	1.12
1:J:252:ASN:HA	1:J:255:PHE:CE2	1.84	1.12
1:L:332:PRO:O	1:L:335:ARG:HG3	1.50	1.11
1:N:252:ASN:HA	1:N:255:PHE:CE2	1.83	1.11
1:C:290:ARG:HD3	1:E:244:ASP:CB	1.79	1.11
1:K:133:TYR:CD2	1:K:352:PHE:HZ	1.66	1.11
1:I:133:TYR:CD2	1:I:352:PHE:CZ	2.38	1.11
1:M:213:LYS:HG2	1:M:306:TYR:OH	1.48	1.10
1:M:305:MET:CE	1:M:335:ARG:CG	2.29	1.10
1:C:18:LYS:HD2	1:C:337:TYR:HD1	1.04	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:289:ILE:HD11	1:M:63:GLY:O	1.52	1.09
1:I:107:GLU:HG2	1:I:119:MET:HE1	1.30	1.09
1:I:133:TYR:CE2	1:I:352:PHE:CE1	2.39	1.09
1:C:133:TYR:CE2	1:C:352:PHE:CE1	2.41	1.09
1:F:1:ASP:HB3	4:U:149:ILE:HD12	1.13	1.09
5:V:58:GLN:HG2	2:W:156:GLU:OE2	1.53	1.09
1:H:83:GLU:HG2	1:H:122:ILE:HD11	1.23	1.09
1:H:332:PRO:O	1:H:335:ARG:HG3	1.51	1.09
1:J:332:PRO:O	1:J:335:ARG:HG2	1.51	1.09
1:L:143:TYR:OH	1:N:44:MET:HB3	1.51	1.09
1:L:133:TYR:CZ	1:L:352:PHE:HE1	1.71	1.08
1:M:305:MET:HE2	1:M:335:ARG:HG3	1.14	1.07
1:F:1:ASP:HB3	4:U:149:ILE:HD11	1.07	1.07
1:C:133:TYR:CD2	1:C:352:PHE:CZ	2.43	1.06
1:J:311:ASP:OD2	2:X:248:LYS:CD	2.04	1.06
1:C:133:TYR:CZ	1:C:352:PHE:HE1	1.72	1.06
1:H:252:ASN:HA	1:H:255:PHE:CE2	1.91	1.06
1:N:252:ASN:HA	1:N:255:PHE:CZ	1.91	1.05
1:M:305:MET:HE1	1:M:335:ARG:HG3	1.15	1.05
1:I:86:TRP:CE3	1:I:122:ILE:HD13	1.92	1.04
5:V:39:LYS:N	2:W:149:LYS:NZ	2.05	1.04
1:C:18:LYS:CD	1:C:337:TYR:HD1	1.70	1.04
1:G:26:ALA:HB1	1:G:27:PRO:HD2	1.07	1.04
1:F:1:ASP:H1	4:U:149:ILE:HD13	1.16	1.03
5:V:39:LYS:N	2:W:149:LYS:HZ3	1.55	1.03
1:I:133:TYR:CZ	1:I:352:PHE:HE1	1.76	1.03
1:I:87:HIS:CD2	1:I:91:TYR:CE2	2.47	1.02
1:E:252:ASN:HA	1:E:255:PHE:CZ	1.94	1.02
1:F:1:ASP:CB	4:U:149:ILE:HD12	1.76	1.01
1:G:26:ALA:HB1	1:G:27:PRO:CD	1.90	1.01
1:C:290:ARG:HD3	1:E:244:ASP:HB3	1.40	1.01
1:O:217:CYS:CB	1:O:306:TYR:CE2	2.44	1.01
1:O:252:ASN:HB2	1:O:255:PHE:CZ	1.95	1.01
2:W:142:GLU:HG2	2:W:145:GLU:OE2	1.60	1.01
2:P:142:GLU:HG2	2:P:145:GLU:OE2	1.61	1.00
5:V:39:LYS:CG	2:W:149:LYS:NZ	2.24	1.00
1:J:305:MET:SD	1:J:335:ARG:HB2	2.00	1.00
5:V:39:LYS:CB	2:W:149:LYS:HZ1	1.75	1.00
5:V:39:LYS:CG	2:W:149:LYS:HZ1	1.73	1.00
1:C:18:LYS:CD	1:C:337:TYR:CD1	2.42	0.99
1:K:133:TYR:CZ	1:K:352:PHE:HE1	1.81	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:252:ASN:HB2	1:K:255:PHE:CZ	1.97	0.99
1:A:326:LYS:HE3	2:Q:47:GLN:HE21	1.22	0.99
1:E:252:ASN:HA	1:E:255:PHE:CE2	1.96	0.99
1:G:25:ASP:CB	4:b:147:VAL:HG13	1.93	0.99
1:A:326:LYS:HE3	2:Q:47:GLN:NE2	1.76	0.98
1:E:109:PRO:CD	1:E:161:HIS:NE2	2.25	0.98
1:O:217:CYS:CB	1:O:306:TYR:HE2	1.75	0.98
1:M:305:MET:HE1	1:M:335:ARG:CG	1.90	0.97
1:A:133:TYR:CD2	1:A:352:PHE:CZ	2.52	0.97
1:F:143:TYR:CE1	1:H:44:MET:CE	2.47	0.97
1:L:133:TYR:CE2	1:L:352:PHE:HE1	1.70	0.97
1:H:87:HIS:HD2	1:H:127:PHE:HE2	1.10	0.96
1:M:213:LYS:HG2	1:M:306:TYR:HH	1.30	0.96
1:K:166:TYR:CD1	1:K:289:ILE:HG23	2.01	0.96
1:K:133:TYR:CD2	1:K:352:PHE:CZ	2.52	0.96
1:F:1:ASP:N	4:U:149:ILE:HD13	1.78	0.96
1:K:31:PHE:CZ	1:K:89:THR:HA	2.01	0.96
1:G:25:ASP:OD2	4:b:147:VAL:CG1	2.12	0.95
1:C:188:TYR:CE1	1:C:266:PHE:HB3	2.02	0.95
1:B:252:ASN:CA	1:B:255:PHE:CE2	2.48	0.95
1:J:311:ASP:OD1	2:X:248:LYS:CD	2.08	0.95
1:H:87:HIS:HD2	1:H:127:PHE:CZ	1.79	0.95
1:D:252:ASN:HA	1:D:255:PHE:CZ	2.02	0.94
1:D:305:MET:CE	1:D:335:ARG:HB2	1.97	0.94
1:F:2:GLU:OE1	1:F:21:PHE:CE2	2.20	0.94
1:L:133:TYR:CE2	1:L:352:PHE:CZ	2.55	0.94
1:O:217:CYS:HB2	1:O:306:TYR:HE2	1.22	0.94
1:I:133:TYR:CE2	1:I:352:PHE:HE1	1.81	0.94
1:K:133:TYR:CE2	1:K:352:PHE:CE1	2.56	0.93
1:M:305:MET:SD	1:M:335:ARG:NE	2.41	0.93
1:G:26:ALA:CB	1:G:27:PRO:HD2	1.99	0.93
1:C:290:ARG:CD	1:E:244:ASP:CB	2.47	0.93
1:A:252:ASN:HA	1:A:255:PHE:CZ	2.03	0.92
1:B:252:ASN:HA	1:B:255:PHE:HE2	1.31	0.92
1:A:133:TYR:CE2	1:A:352:PHE:CZ	2.57	0.92
5:V:58:GLN:CG	2:W:156:GLU:OE2	2.15	0.92
1:B:252:ASN:HA	1:B:255:PHE:CZ	2.05	0.92
1:C:218:TYR:HA	1:C:307:PRO:HD2	1.52	0.92
1:A:133:TYR:CE2	1:A:352:PHE:CE1	2.57	0.91
1:O:186:THR:OG1	1:O:213:LYS:HE2	1.70	0.91
1:L:143:TYR:CE2	1:N:44:MET:CE	2.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:142:GLU:HA	2:W:145:GLU:HG2	1.51	0.91
1:L:143:TYR:HE2	1:N:47:MET:CE	1.83	0.91
1:C:133:TYR:CZ	1:C:352:PHE:CE1	2.58	0.91
1:G:24:ASP:OD1	4:b:146:ARG:CB	2.19	0.90
1:O:252:ASN:CA	1:O:255:PHE:CE2	2.53	0.90
1:C:133:TYR:CE2	1:C:352:PHE:CZ	2.59	0.90
1:H:83:GLU:HG2	1:H:122:ILE:CD1	2.02	0.90
2:X:161:LYS:O	2:X:165:VAL:HG22	1.72	0.89
1:E:109:PRO:HD2	1:E:161:HIS:CD2	2.06	0.89
1:F:109:PRO:HD2	1:F:161:HIS:CD2	2.06	0.89
1:C:133:TYR:CE2	1:C:352:PHE:HE1	1.82	0.89
1:G:305:MET:SD	1:G:335:ARG:HG3	2.12	0.89
1:C:290:ARG:CD	1:E:244:ASP:HB2	2.03	0.89
1:O:252:ASN:HA	1:O:255:PHE:HE2	1.38	0.89
1:I:107:GLU:CG	1:I:119:MET:HE1	2.03	0.88
1:O:186:THR:HA	1:O:213:LYS:HD3	1.54	0.88
2:P:142:GLU:HA	2:P:145:GLU:HG2	1.51	0.88
1:D:133:TYR:CD2	1:D:352:PHE:HZ	1.91	0.88
1:B:252:ASN:CB	1:B:255:PHE:CZ	2.56	0.88
1:M:213:LYS:CG	1:M:306:TYR:OH	2.22	0.88
2:Q:161:LYS:O	2:Q:165:VAL:HG22	1.72	0.87
5:c:136:LEU:HB3	5:c:156:PHE:HE1	1.38	0.87
1:K:252:ASN:CB	1:K:255:PHE:CZ	2.56	0.87
1:J:252:ASN:HB2	1:J:255:PHE:CZ	2.09	0.87
1:D:305:MET:HE2	1:D:335:ARG:HB2	1.54	0.87
1:B:252:ASN:HB2	1:B:255:PHE:CZ	2.09	0.87
3:a:252:GLU:HG3	4:b:69:ARG:HH22	1.38	0.87
5:V:39:LYS:HG2	2:W:149:LYS:HZ2	1.32	0.86
1:K:133:TYR:CZ	1:K:352:PHE:CE1	2.63	0.86
1:D:133:TYR:CD2	1:D:352:PHE:CZ	2.63	0.86
1:D:133:TYR:CE2	1:D:352:PHE:HE1	1.94	0.86
1:I:133:TYR:CE2	1:I:352:PHE:CZ	2.59	0.85
1:K:133:TYR:CE2	1:K:352:PHE:CZ	2.63	0.85
3:a:219:LEU:HD13	3:a:236:LEU:HD11	1.56	0.85
5:c:112:ILE:HB	5:c:148:ILE:HB	1.58	0.85
1:A:252:ASN:CB	1:A:255:PHE:CZ	2.60	0.85
1:D:133:TYR:CE2	1:D:352:PHE:CE1	2.65	0.85
1:O:252:ASN:CB	1:O:255:PHE:CZ	2.59	0.85
5:V:39:LYS:HG2	2:W:149:LYS:HZ1	1.25	0.85
1:B:250:ILE:O	1:B:254:ARG:HD2	1.77	0.85
1:F:332:PRO:O	1:F:335:ARG:CG	2.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:196:ARG:HD2	1:I:253:GLU:CD	2.02	0.84
1:L:143:TYR:CE2	1:N:47:MET:HE3	2.12	0.84
1:K:196:ARG:HD2	1:K:253:GLU:CD	2.03	0.84
1:L:143:TYR:HE2	1:N:47:MET:HE1	1.41	0.84
1:O:189:LEU:CD2	1:O:213:LYS:HG2	2.06	0.84
5:c:102:ARG:O	5:c:102:ARG:NH1	2.09	0.83
1:B:133:TYR:CE2	1:B:352:PHE:HE1	1.96	0.83
1:J:305:MET:SD	1:J:335:ARG:CB	2.66	0.83
5:c:130:GLU:O	5:c:134:GLU:HB3	1.77	0.83
1:A:252:ASN:HB2	1:A:255:PHE:CZ	2.13	0.83
5:V:111:TYR:HB3	5:V:147:ARG:HB2	1.60	0.83
1:D:230:ALA:HB3	1:D:255:PHE:HZ	1.44	0.83
1:L:143:TYR:OH	1:N:47:MET:HE3	1.78	0.83
2:X:253:ILE:O	2:X:257:GLU:HG2	1.79	0.83
5:c:91:GLY:HA2	5:c:159:GLY:HA2	1.60	0.83
1:N:252:ASN:CA	1:N:255:PHE:CZ	2.62	0.82
1:I:196:ARG:HD2	1:I:253:GLU:OE2	1.78	0.82
1:K:252:ASN:CA	1:K:255:PHE:CE2	2.62	0.82
3:T:212:LEU:HD22	4:U:109:GLU:HG2	1.61	0.82
1:D:116:ARG:HG3	1:D:134:VAL:HG11	1.60	0.82
1:B:252:ASN:CA	1:B:255:PHE:CZ	2.61	0.82
1:J:252:ASN:CB	1:J:255:PHE:CZ	2.63	0.82
2:W:142:GLU:HA	2:W:145:GLU:CG	2.09	0.82
1:B:133:TYR:CD2	1:B:352:PHE:CZ	2.68	0.82
2:P:142:GLU:HA	2:P:145:GLU:CG	2.09	0.82
1:I:133:TYR:CZ	1:I:352:PHE:CE1	2.63	0.82
1:L:133:TYR:CZ	1:L:352:PHE:CE1	2.58	0.82
1:J:311:ASP:CG	2:X:248:LYS:HD3	1.92	0.81
2:W:53:THR:HA	2:X:57:LEU:HD11	1.62	0.81
1:M:305:MET:HE2	1:M:335:ARG:CG	2.01	0.81
5:c:151:ASP:HA	5:c:154:LEU:HG	1.62	0.81
2:W:148:LEU:HG	2:W:152:LYS:HE2	1.62	0.81
1:B:133:TYR:CD2	1:B:352:PHE:HZ	1.98	0.81
1:L:196:ARG:HD2	1:L:253:GLU:CD	2.06	0.81
2:P:148:LEU:HG	2:P:152:LYS:HE2	1.62	0.81
1:J:133:TYR:CE2	1:J:352:PHE:HE1	1.99	0.81
2:W:142:GLU:HA	2:W:145:GLU:OE2	1.81	0.80
1:N:305:MET:HG2	1:N:335:ARG:HD2	1.62	0.80
2:P:142:GLU:HA	2:P:145:GLU:OE2	1.81	0.80
4:b:129:THR:O	4:b:133:PHE:HB3	1.80	0.80
2:P:53:THR:HA	2:Q:57:LEU:HD11	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:305:MET:CE	1:K:335:ARG:HB2	2.11	0.80
1:L:143:TYR:CE2	1:N:47:MET:CE	2.64	0.80
1:K:305:MET:HE1	1:K:335:ARG:HB2	1.64	0.80
2:Q:253:ILE:O	2:Q:257:GLU:HG2	1.79	0.80
3:a:213:ALA:O	3:a:216:ARG:NE	2.15	0.80
3:a:264:LEU:HA	3:a:267:ARG:HD3	1.64	0.80
1:F:1:ASP:CA	4:U:149:ILE:CD1	2.60	0.80
1:A:109:PRO:HD2	1:A:161:HIS:NE2	1.97	0.79
5:V:38:THR:HB	2:W:149:LYS:CD	2.13	0.79
1:E:109:PRO:CG	1:E:161:HIS:NE2	2.46	0.79
1:A:326:LYS:CE	2:Q:47:GLN:NE2	2.44	0.79
2:P:142:GLU:HA	2:P:145:GLU:CD	2.07	0.79
1:B:133:TYR:CE2	1:B:352:PHE:CE1	2.70	0.79
1:C:290:ARG:NE	1:E:244:ASP:HB2	1.98	0.79
1:I:86:TRP:CZ3	1:I:122:ILE:HD13	2.17	0.79
1:K:31:PHE:CE1	1:K:89:THR:HG23	2.17	0.79
1:E:109:PRO:HD2	1:E:161:HIS:CE1	2.15	0.79
2:W:148:LEU:CG	2:W:152:LYS:HE2	2.12	0.79
4:b:132:ILE:O	4:b:136:ARG:N	2.14	0.79
5:c:58:GLN:HA	5:c:61:ILE:HD12	1.65	0.79
1:K:196:ARG:HD2	1:K:253:GLU:OE2	1.83	0.79
1:J:332:PRO:O	1:J:335:ARG:CG	2.31	0.78
5:c:94:GLU:HA	5:c:154:LEU:HD22	1.64	0.78
3:a:219:LEU:HD22	4:b:101:HIS:HB2	1.64	0.78
2:P:148:LEU:CG	2:P:152:LYS:HE2	2.12	0.78
2:W:142:GLU:HA	2:W:145:GLU:CD	2.07	0.78
1:G:24:ASP:CG	4:b:146:ARG:CB	2.52	0.78
1:O:217:CYS:HB2	1:O:306:TYR:CZ	2.19	0.78
1:N:252:ASN:CB	1:N:255:PHE:CZ	2.67	0.78
4:b:159:LEU:HD23	4:b:162:ARG:HG3	1.64	0.78
1:G:305:MET:SD	1:G:335:ARG:CG	2.72	0.78
5:V:40:GLU:HA	5:V:43:LYS:HE2	1.66	0.78
1:F:143:TYR:HE1	1:H:44:MET:HE2	1.47	0.78
1:A:133:TYR:CZ	1:A:352:PHE:HE1	2.01	0.77
1:A:334:GLU:O	1:A:338:SER:HB3	1.84	0.77
1:D:116:ARG:HG2	1:D:370:VAL:HG21	1.65	0.77
1:L:133:TYR:CG	1:L:352:PHE:HZ	2.02	0.77
4:b:133:PHE:HA	4:b:136:ARG:HH11	1.47	0.77
1:C:283:MET:HE1	1:C:290:ARG:HH22	1.49	0.77
1:H:252:ASN:HB2	1:H:255:PHE:CZ	2.19	0.77
1:F:1:ASP:CA	4:U:149:ILE:HD13	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:227:MET:HB3	1:N:255:PHE:HE1	1.48	0.77
1:D:305:MET:HE2	1:D:335:ARG:CB	2.14	0.77
1:H:207:GLU:HA	1:H:210:ARG:HG2	1.67	0.77
1:J:311:ASP:OD2	2:X:248:LYS:NZ	2.18	0.77
1:L:252:ASN:HB2	1:L:255:PHE:CE2	2.20	0.77
1:F:1:ASP:CG	4:U:149:ILE:HD12	2.08	0.77
5:V:130:GLU:HA	5:V:133:ILE:HD12	1.65	0.77
3:a:257:GLN:HB3	4:b:121:ASN:HD22	1.50	0.77
3:T:244:GLU:HB3	4:U:79:ARG:HD3	1.67	0.77
3:a:224:LEU:HD23	3:a:228:GLN:HG3	1.67	0.77
1:A:207:GLU:HA	1:A:210:ARG:HG2	1.66	0.77
1:B:250:ILE:HG22	1:B:254:ARG:HG3	1.67	0.76
1:K:311:ASP:OD2	2:Q:248:LYS:HD3	1.84	0.76
1:C:18:LYS:HD3	1:C:337:TYR:CD1	2.19	0.76
1:G:25:ASP:HB3	4:b:147:VAL:HG13	1.67	0.76
4:b:45:ARG:NH2	5:c:132:ASP:OD2	2.18	0.76
1:F:1:ASP:CB	4:U:149:ILE:HD11	1.96	0.76
3:a:262:ASN:OD1	3:a:265:ARG:NH1	2.18	0.76
1:E:230:ALA:HB3	1:E:255:PHE:HZ	1.50	0.76
1:L:252:ASN:HB2	1:L:255:PHE:CZ	2.21	0.76
1:O:189:LEU:HD22	1:O:213:LYS:HG2	1.67	0.76
4:U:159:LEU:HB3	4:U:163:ALA:HB2	1.67	0.76
1:D:252:ASN:CB	1:D:255:PHE:CZ	2.69	0.75
1:H:95:ARG:HH22	3:T:265:ARG:HD3	1.50	0.75
2:P:142:GLU:CA	2:P:145:GLU:HG2	2.16	0.75
1:A:252:ASN:CA	1:A:255:PHE:CZ	2.69	0.75
1:D:252:ASN:CA	1:D:255:PHE:CZ	2.69	0.75
1:C:289:ILE:HD11	1:E:63:GLY:O	1.85	0.75
1:E:252:ASN:CA	1:E:255:PHE:CZ	2.69	0.75
1:J:133:TYR:CE2	1:J:352:PHE:CE1	2.74	0.75
4:b:159:LEU:HB2	4:b:163:ALA:HB2	1.69	0.75
1:J:252:ASN:HA	1:J:255:PHE:CZ	2.22	0.75
4:b:58:LYS:HE2	5:c:100:LEU:HD21	1.69	0.75
1:F:6:THR:HG21	4:U:146:ARG:HH12	1.52	0.74
3:T:224:LEU:HB3	3:T:228:GLN:HB2	1.67	0.74
2:W:142:GLU:CA	2:W:145:GLU:HG2	2.16	0.74
1:C:207:GLU:HA	1:C:210:ARG:HG2	1.68	0.74
5:V:38:THR:HB	2:W:149:LYS:HE2	0.77	0.74
1:F:169:TYR:OH	1:H:49:GLN:HB3	1.88	0.74
1:O:252:ASN:HA	1:O:255:PHE:CZ	2.20	0.74
4:b:117:LYS:HA	4:b:120:LYS:HD2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ASN:HB2	1:D:255:PHE:CZ	2.23	0.74
5:V:36:ILE:HB	5:V:72:VAL:HB	1.67	0.74
4:b:108:ASP:OD1	4:b:111:ARG:NH2	2.20	0.74
3:a:252:GLU:HA	3:a:255:LYS:HE2	1.70	0.74
1:F:139:VAL:HG23	1:F:140:LEU:N	2.01	0.74
1:C:227:MET:HB3	1:C:255:PHE:CZ	2.23	0.74
1:F:21:PHE:HD1	1:F:28:ARG:HE	1.35	0.74
1:G:25:ASP:HB2	4:b:147:VAL:HG13	1.68	0.74
3:a:257:GLN:NE2	4:b:118:VAL:O	2.19	0.74
1:H:87:HIS:CD2	1:H:127:PHE:HZ	2.01	0.73
3:a:267:ARG:HE	4:b:132:ILE:HG21	1.53	0.73
1:I:334:GLU:O	1:I:338:SER:HB3	1.88	0.73
1:B:219:VAL:HG23	1:B:306:TYR:HB3	1.70	0.73
1:D:252:ASN:CA	1:D:255:PHE:CE2	2.64	0.73
1:K:289:ILE:HD11	1:M:63:GLY:C	2.13	0.73
1:K:133:TYR:CE2	1:K:352:PHE:HE1	2.02	0.73
3:T:237:TRP:NE1	4:U:81:GLN:O	2.21	0.73
1:F:305:MET:CE	1:F:335:ARG:CB	2.31	0.73
5:V:38:THR:HA	5:V:57:LEU:HD21	1.71	0.73
1:C:290:ARG:CD	1:E:244:ASP:HB3	2.14	0.73
1:I:107:GLU:HG2	1:I:119:MET:CE	2.15	0.73
3:a:230:ARG:HB3	4:b:85:LEU:HD13	1.71	0.73
1:H:87:HIS:O	1:H:91:TYR:HD2	1.71	0.73
5:c:41:LEU:HB3	5:c:57:LEU:HD22	1.71	0.73
5:c:121:LEU:HD11	5:c:136:LEU:HD12	1.71	0.73
5:c:136:LEU:HB3	5:c:156:PHE:CE1	2.23	0.72
2:P:148:LEU:CD2	2:P:152:LYS:HE2	2.19	0.72
3:T:263:VAL:HG22	5:V:110:GLY:HA2	1.69	0.72
1:J:133:TYR:CZ	1:J:352:PHE:HE1	2.06	0.72
2:W:148:LEU:CD2	2:W:152:LYS:HE2	2.19	0.72
1:D:230:ALA:HB3	1:D:255:PHE:CZ	2.24	0.72
2:P:152:LYS:HE3	5:c:54:PRO:CB	2.19	0.72
3:a:249:ASP:OD1	4:b:69:ARG:NH1	2.23	0.72
5:V:38:THR:CG2	2:W:149:LYS:HE2	2.17	0.72
1:O:217:CYS:O	1:O:306:TYR:CD2	2.42	0.72
3:a:247:LYS:HG3	4:b:114:ILE:HG13	1.71	0.72
4:b:68:ARG:HB3	4:b:69:ARG:HH21	1.54	0.72
3:a:200:LYS:HB3	3:a:201:ARG:HH21	1.54	0.72
1:B:252:ASN:CB	1:B:255:PHE:HZ	2.03	0.71
1:C:227:MET:HB3	1:C:255:PHE:HZ	1.54	0.71
1:E:169:TYR:OH	1:G:49:GLN:HG3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:326:LYS:NZ	2:Q:219:ASP:OD1	2.22	0.71
1:F:305:MET:HE1	1:F:335:ARG:HB2	1.62	0.71
1:L:143:TYR:CZ	1:N:47:MET:HE3	2.24	0.71
1:C:188:TYR:CZ	1:C:266:PHE:HB3	2.25	0.71
1:O:217:CYS:C	1:O:306:TYR:CE2	2.69	0.71
4:b:50:LYS:NZ	5:c:156:PHE:O	2.19	0.71
1:A:133:TYR:CZ	1:A:352:PHE:CE1	2.76	0.71
1:B:258:PRO:HB3	1:B:306:TYR:CE1	2.26	0.71
1:I:107:GLU:CG	1:I:119:MET:CE	2.68	0.71
1:N:290:ARG:HE	1:N:325:MET:HE1	1.54	0.71
2:P:152:LYS:HE3	5:c:54:PRO:HB2	1.72	0.71
1:G:25:ASP:CB	4:b:147:VAL:CG1	2.68	0.70
1:L:143:TYR:CZ	1:N:44:MET:CE	2.70	0.70
1:N:230:ALA:HB3	1:N:255:PHE:HZ	1.56	0.70
1:C:188:TYR:CE2	1:C:266:PHE:CD2	2.79	0.70
1:H:305:MET:SD	1:H:335:ARG:NE	2.63	0.70
1:J:169:TYR:OH	1:L:49:GLN:HB3	1.90	0.70
5:V:14:GLU:HA	5:V:17:LYS:HD2	1.71	0.70
1:J:133:TYR:CD2	1:J:352:PHE:CZ	2.79	0.70
1:L:252:ASN:HA	1:L:255:PHE:CE2	2.27	0.70
5:V:102:ARG:O	5:V:102:ARG:NH1	2.24	0.70
1:C:18:LYS:CD	1:C:337:TYR:CE1	2.75	0.70
1:L:252:ASN:CB	1:L:255:PHE:CE2	2.73	0.70
2:P:149:LYS:HE3	2:P:153:HIS:NE2	2.06	0.70
5:c:73:ASP:O	5:c:77:PHE:N	2.25	0.70
1:C:258:PRO:HG3	1:C:306:TYR:CE2	2.27	0.70
1:O:290:ARG:HE	1:O:325:MET:HE1	1.57	0.70
4:U:47:LEU:HD22	5:V:4:ILE:HA	1.72	0.70
4:U:56:ILE:HG13	5:V:124:THR:HA	1.72	0.70
1:F:139:VAL:CG2	1:F:140:LEU:N	2.54	0.70
2:W:57:LEU:HA	2:X:57:LEU:HD23	1.74	0.70
1:O:207:GLU:HA	1:O:210:ARG:HG2	1.72	0.70
2:P:57:LEU:HA	2:Q:57:LEU:HD23	1.74	0.70
4:b:162:ARG:NE	4:b:162:ARG:O	2.25	0.70
1:C:133:TYR:CG	1:C:352:PHE:HZ	2.09	0.70
1:C:283:MET:HE1	1:C:290:ARG:NH2	2.07	0.69
1:O:252:ASN:CA	1:O:255:PHE:CZ	2.75	0.69
5:c:139:ASP:O	5:c:142:LYS:NZ	2.24	0.69
1:I:87:HIS:CD2	1:I:91:TYR:CD2	2.79	0.69
5:V:102:ARG:NH1	5:V:105:ASP:O	2.25	0.69
1:O:189:LEU:HD23	1:O:213:LYS:CG	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:57:LEU:N	2:Q:57:LEU:HD21	2.08	0.69
1:O:252:ASN:HB2	1:O:255:PHE:HZ	1.56	0.69
4:b:133:PHE:O	4:b:137:GLY:N	2.25	0.69
3:a:222:ASP:HA	4:b:94:GLN:HE21	1.58	0.69
5:c:114:LEU:HD11	5:c:133:ILE:HG22	1.75	0.69
1:H:333:PRO:C	1:H:335:ARG:H	2.01	0.68
1:A:109:PRO:HD2	1:A:161:HIS:CE1	2.28	0.68
5:V:37:SER:OG	5:V:40:GLU:OE1	2.10	0.68
1:N:252:ASN:HB2	1:N:255:PHE:CZ	2.28	0.68
1:F:333:PRO:C	1:F:335:ARG:H	2.02	0.68
1:K:252:ASN:HA	1:K:255:PHE:CZ	2.27	0.68
1:K:333:PRO:C	1:K:335:ARG:H	2.02	0.68
5:c:89:SER:N	5:c:161:GLU:OE1	2.26	0.68
5:c:40:GLU:O	5:c:44:VAL:HG23	1.94	0.68
1:B:133:TYR:CZ	1:B:352:PHE:HE1	2.11	0.68
3:T:244:GLU:O	4:U:79:ARG:NH1	2.26	0.68
1:D:305:MET:HE1	1:D:335:ARG:HB2	1.76	0.68
1:F:188:TYR:CE1	1:F:266:PHE:HB3	2.28	0.68
3:a:224:LEU:HB2	3:a:229:LEU:HG	1.77	0.68
2:W:57:LEU:N	2:X:57:LEU:HD21	2.08	0.67
1:F:143:TYR:OH	1:H:45:VAL:N	2.27	0.67
1:J:307:PRO:HG2	2:X:244:ARG:HH12	1.59	0.67
4:b:45:ARG:NH2	5:c:127:THR:O	2.27	0.67
4:b:145:ARG:H	4:b:148:ARG:HH12	1.41	0.67
1:A:109:PRO:HD2	1:A:161:HIS:CD2	2.30	0.67
1:K:133:TYR:CG	1:K:352:PHE:HZ	2.11	0.67
1:E:169:TYR:OH	1:G:49:GLN:HB3	1.95	0.67
5:V:39:LYS:H	2:W:149:LYS:HZ3	0.70	0.67
1:H:207:GLU:O	1:H:210:ARG:HG3	1.94	0.67
3:T:268:ILE:HG12	4:U:131:LYS:HZ2	1.59	0.67
5:c:32:GLU:OE1	5:c:37:SER:OG	2.13	0.67
3:a:240:ILE:HA	3:a:243:LEU:HD12	1.75	0.67
1:O:352:PHE:CE1	1:O:355:MET:CB	2.78	0.66
4:U:78:THR:O	4:U:81:GLN:NE2	2.28	0.66
1:O:209:VAL:O	1:O:213:LYS:HG3	1.94	0.66
4:b:68:ARG:HB3	4:b:69:ARG:NH2	2.10	0.66
1:C:333:PRO:C	1:C:335:ARG:H	2.03	0.66
1:L:109:PRO:HD2	1:L:161:HIS:NE2	2.11	0.66
1:O:334:GLU:O	1:O:338:SER:HB3	1.96	0.66
3:a:221:ILE:HG21	4:b:98:ARG:HG2	1.78	0.66
1:D:133:TYR:CZ	1:D:352:PHE:HE1	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:TYR:OH	1:H:44:MET:HB3	1.96	0.66
5:V:21:LYS:NZ	5:V:25:ASP:OD1	2.27	0.66
1:E:252:ASN:CB	1:E:255:PHE:CZ	2.79	0.66
1:D:116:ARG:HG2	1:D:370:VAL:CG2	2.25	0.66
1:O:352:PHE:CD1	1:O:355:MET:HG3	2.30	0.66
2:P:142:GLU:CG	2:P:145:GLU:OE2	2.42	0.66
2:W:148:LEU:HD21	2:W:152:LYS:HE2	1.77	0.66
1:E:169:TYR:OH	1:G:49:GLN:CG	2.43	0.66
4:U:165:GLU:OE1	5:V:16:GLN:NE2	2.28	0.66
5:c:76:GLU:O	5:c:80:MET:HG3	1.96	0.66
1:C:218:TYR:CA	1:C:307:PRO:HD2	2.24	0.65
1:H:252:ASN:CB	1:H:255:PHE:CZ	2.79	0.65
1:L:133:TYR:HE2	1:L:346:LEU:HD21	1.59	0.65
1:L:333:PRO:C	1:L:335:ARG:H	2.04	0.65
1:I:133:TYR:CG	1:I:352:PHE:HZ	2.10	0.65
1:O:217:CYS:O	1:O:306:TYR:HD2	1.79	0.65
1:A:133:TYR:CE2	1:A:352:PHE:HE1	2.05	0.65
2:P:148:LEU:HD21	2:P:152:LYS:HE2	1.77	0.65
3:T:267:ARG:HD2	5:V:150:TYR:HB3	1.78	0.65
5:c:114:LEU:HD13	5:c:137:MET:HB2	1.79	0.65
1:M:207:GLU:HA	1:M:210:ARG:HG2	1.78	0.65
2:P:156:GLU:HG2	2:P:160:ARG:NH2	2.10	0.65
4:b:154:MET:HG2	4:b:155:MET:HE2	1.79	0.65
5:c:101:PHE:CE1	5:c:112:ILE:HG13	2.32	0.65
1:K:252:ASN:CA	1:K:255:PHE:CZ	2.80	0.65
4:b:149:ILE:HD12	5:c:45:MET:HE1	1.77	0.65
1:J:307:PRO:CG	2:X:244:ARG:HH12	2.10	0.65
3:a:267:ARG:O	3:a:271:ASN:N	2.30	0.65
3:a:271:ASN:HB3	4:b:135:LEU:HD13	1.79	0.65
1:I:87:HIS:CG	1:I:91:TYR:CD2	2.85	0.65
2:W:142:GLU:CG	2:W:145:GLU:OE2	2.41	0.65
4:b:103:ARG:HA	4:b:106:LYS:HD2	1.79	0.65
3:T:267:ARG:O	3:T:271:ASN:N	2.30	0.65
4:b:152:ASP:OD2	5:c:86:LYS:NZ	2.29	0.65
1:C:30:VAL:HG21	1:C:337:TYR:OH	1.95	0.64
1:O:189:LEU:HD23	1:O:213:LYS:HG2	1.78	0.64
1:A:305:MET:SD	1:A:336:LYS:HB3	2.37	0.64
1:N:335:ARG:C	1:N:337:TYR:H	2.05	0.64
1:O:217:CYS:CA	1:O:306:TYR:HE2	2.09	0.64
4:b:63:ARG:NH2	5:c:103:MET:SD	2.70	0.64
4:U:108:ASP:OD1	4:U:111:ARG:NH2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:234:LYS:HD2	4:b:83:LEU:HD12	1.79	0.64
3:a:239:SER:O	3:a:243:LEU:HG	1.97	0.64
2:P:149:LYS:NZ	5:c:37:SER:HB2	2.11	0.64
5:V:39:LYS:CB	2:W:149:LYS:NZ	2.57	0.64
1:C:188:TYR:CZ	1:C:266:PHE:CD2	2.84	0.64
1:E:305:MET:SD	1:E:336:LYS:HD2	2.38	0.64
1:O:352:PHE:CE1	1:O:355:MET:HB2	2.33	0.64
3:a:268:ILE:HD11	4:b:128:LEU:HD22	1.79	0.64
5:c:65:ASP:OD1	5:c:69:SER:N	2.30	0.64
3:a:213:ALA:HA	3:a:216:ARG:HB3	1.80	0.64
3:a:261:ILE:HA	3:a:264:LEU:HD12	1.80	0.64
1:F:1:ASP:N	4:U:149:ILE:CD1	2.57	0.63
1:I:86:TRP:CE3	1:I:122:ILE:CD1	2.77	0.63
1:K:252:ASN:HA	1:K:255:PHE:HE2	1.55	0.63
4:b:155:MET:HE3	5:c:20:PHE:HE2	1.64	0.63
1:L:143:TYR:CZ	1:N:44:MET:HB3	2.33	0.63
2:P:142:GLU:C	2:P:145:GLU:HG2	2.24	0.63
3:T:244:GLU:OE1	3:T:247:LYS:NZ	2.31	0.63
5:V:48:LEU:HB3	5:V:50:GLN:HE22	1.64	0.63
3:a:237:TRP:HA	3:a:240:ILE:HD12	1.79	0.63
1:F:139:VAL:CG2	1:F:140:LEU:HG	2.29	0.63
3:a:229:LEU:HB3	4:b:93:LEU:HB3	1.81	0.62
1:I:87:HIS:O	1:I:91:TYR:HD2	1.82	0.62
4:U:165:GLU:HB3	5:V:16:GLN:HE21	1.63	0.62
2:X:272:GLU:OE1	2:X:272:GLU:HA	1.99	0.62
1:C:18:LYS:HD3	1:C:337:TYR:CE1	2.33	0.62
4:b:140:LYS:HE3	4:b:141:ARG:NH2	2.14	0.62
4:b:151:ALA:HA	4:b:154:MET:HB3	1.81	0.62
5:c:2:ASP:HA	5:c:64:VAL:HG23	1.82	0.62
1:M:207:GLU:O	1:M:210:ARG:CG	2.48	0.62
2:W:142:GLU:C	2:W:145:GLU:HG2	2.24	0.62
1:J:169:TYR:OH	1:L:49:GLN:CG	2.47	0.61
1:A:333:PRO:C	1:A:335:ARG:H	2.07	0.61
1:J:333:PRO:C	1:J:335:ARG:H	2.08	0.61
1:C:289:ILE:HD11	1:E:63:GLY:C	2.25	0.61
1:G:24:ASP:OD2	4:b:146:ARG:HB3	1.98	0.61
5:c:24:PHE:HB2	5:c:77:PHE:CE2	2.36	0.61
5:c:59:GLU:O	5:c:63:GLU:N	2.33	0.61
1:J:252:ASN:CA	1:J:255:PHE:CZ	2.82	0.61
4:U:75:ALA:O	4:U:79:ARG:HB2	2.01	0.61
4:b:133:PHE:HA	4:b:136:ARG:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:287:ILE:HA	1:K:290:ARG:HD2	1.82	0.61
1:K:307:PRO:HB3	2:Q:244:ARG:HH12	1.64	0.61
1:E:169:TYR:OH	1:G:49:GLN:CB	2.48	0.61
3:a:237:TRP:NE1	4:b:81:GLN:O	2.33	0.61
1:L:252:ASN:CA	1:L:255:PHE:CE2	2.82	0.61
1:I:106:THR:O	1:I:107:GLU:HG2	2.00	0.61
3:a:217:LYS:HB2	4:b:101:HIS:HE1	1.66	0.61
3:a:247:LYS:NZ	4:b:110:GLU:OE1	2.34	0.61
3:a:271:ASN:HD21	4:b:132:ILE:HG23	1.64	0.61
1:G:334:GLU:O	1:G:338:SER:HB3	2.00	0.61
5:c:30:GLY:O	5:c:39:LYS:NZ	2.31	0.61
2:Q:272:GLU:OE1	2:Q:272:GLU:HA	1.99	0.61
5:c:37:SER:OG	5:c:40:GLU:OE1	2.18	0.61
1:C:335:ARG:C	1:C:337:TYR:H	2.09	0.60
1:E:230:ALA:CB	1:E:255:PHE:HZ	2.13	0.60
1:F:143:TYR:CD1	1:H:44:MET:CE	2.84	0.60
4:b:52:LEU:O	4:b:56:ILE:HG12	2.01	0.60
5:c:21:LYS:HD2	5:c:74:PHE:CZ	2.36	0.60
5:c:121:LEU:HA	5:c:124:THR:HG23	1.82	0.60
1:C:290:ARG:O	1:C:294:TYR:CD1	2.54	0.60
1:F:159:VAL:HG21	1:F:177:ARG:HE	1.67	0.60
1:K:335:ARG:C	1:K:337:TYR:H	2.08	0.60
4:U:45:ARG:NH1	5:V:127:THR:OG1	2.34	0.60
5:V:121:LEU:HD11	5:V:136:LEU:HD12	1.82	0.60
3:a:251:GLN:O	3:a:255:LYS:HG3	2.00	0.60
4:b:151:ALA:N	5:c:84:CYS:HB3	2.16	0.60
5:V:76:GLU:O	5:V:80:MET:HG2	2.01	0.60
2:X:269:ALA:O	2:X:273:GLU:HB2	2.01	0.60
5:c:112:ILE:N	5:c:148:ILE:O	2.33	0.60
1:G:25:ASP:CG	4:b:147:VAL:CG1	2.74	0.60
1:J:207:GLU:HA	1:J:210:ARG:HG2	1.82	0.60
1:K:286:ASP:O	1:K:290:ARG:HG3	2.01	0.60
5:c:89:SER:O	5:c:90:LYS:HG2	2.01	0.60
1:H:87:HIS:NE2	1:H:127:PHE:CZ	2.70	0.60
3:T:250:LEU:HD22	4:U:115:GLU:HA	1.83	0.60
5:c:94:GLU:O	5:c:150:TYR:OH	2.19	0.60
1:I:332:PRO:O	1:I:335:ARG:CG	2.31	0.60
1:K:31:PHE:CE2	1:K:89:THR:HA	2.35	0.60
1:M:207:GLU:O	1:M:210:ARG:HG2	2.02	0.60
2:Q:269:ALA:O	2:Q:273:GLU:HB2	2.01	0.60
3:a:216:ARG:NH1	3:a:217:LYS:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:C	1:A:337:TYR:H	2.10	0.60
1:E:334:GLU:O	1:E:338:SER:HB3	2.02	0.60
3:T:208:LYS:O	3:T:212:LEU:HG	2.02	0.60
4:U:134:ASP:O	4:U:138:LYS:NZ	2.32	0.60
5:V:39:LYS:N	2:W:149:LYS:CE	2.65	0.60
5:V:154:LEU:O	5:V:158:LYS:N	2.35	0.60
1:C:290:ARG:O	1:C:294:TYR:HD1	1.85	0.59
1:H:335:ARG:C	1:H:337:TYR:H	2.09	0.59
5:V:44:VAL:HA	5:V:47:MET:HE3	1.84	0.59
1:N:252:ASN:HB2	1:N:255:PHE:CE1	2.37	0.59
3:T:263:VAL:HG11	5:V:150:TYR:HB2	1.83	0.59
4:U:159:LEU:HD11	4:U:162:ARG:HE	1.66	0.59
1:G:26:ALA:CB	1:G:27:PRO:CD	2.65	0.59
5:V:54:PRO:HB2	2:W:152:LYS:HZ2	1.66	0.59
3:a:216:ARG:HG2	4:b:101:HIS:HE2	1.68	0.59
4:b:134:ASP:O	4:b:138:LYS:NZ	2.34	0.59
1:H:252:ASN:HA	1:H:255:PHE:CZ	2.36	0.59
4:b:114:ILE:HA	4:b:117:LYS:HD2	1.83	0.59
1:E:109:PRO:HG2	1:E:161:HIS:NE2	2.17	0.59
3:T:237:TRP:HA	3:T:240:ILE:HD12	1.85	0.59
4:b:136:ARG:O	4:b:140:LYS:HB2	2.02	0.59
5:c:132:ASP:O	5:c:136:LEU:HG	2.03	0.59
1:D:207:GLU:HA	1:D:210:ARG:HG2	1.85	0.59
1:J:257:CYS:HB3	1:J:258:PRO:HD3	1.85	0.59
4:U:137:GLY:HA3	4:U:141:ARG:HH22	1.67	0.59
1:J:133:TYR:CD2	1:J:352:PHE:HZ	2.17	0.59
5:c:92:LYS:HZ1	5:c:161:GLU:HA	1.67	0.59
1:D:230:ALA:CB	1:D:255:PHE:CZ	2.85	0.59
1:O:217:CYS:C	1:O:306:TYR:HE2	2.09	0.59
3:T:256:GLN:HE22	5:V:102:ARG:HB2	1.68	0.59
5:V:39:LYS:HB3	2:W:149:LYS:HZ1	1.60	0.59
3:a:210:LYS:HA	3:a:213:ALA:HB3	1.85	0.59
1:B:332:PRO:C	1:B:334:GLU:H	2.10	0.59
4:U:103:ARG:O	4:U:107:VAL:HG12	2.02	0.59
1:F:143:TYR:HH	1:H:45:VAL:N	2.01	0.59
1:H:252:ASN:CA	1:H:255:PHE:CE2	2.79	0.59
4:b:45:ARG:NH2	5:c:129:THR:HG23	2.17	0.59
3:a:243:LEU:HD22	4:b:111:ARG:HE	1.68	0.58
3:a:230:ARG:NE	4:b:85:LEU:O	2.32	0.58
4:b:72:LYS:O	4:b:76:LEU:HG	2.03	0.58
1:J:311:ASP:OD2	2:X:248:LYS:CE	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:217:CYS:C	1:O:306:TYR:CD2	2.81	0.58
2:P:142:GLU:O	2:P:145:GLU:HG2	2.03	0.58
1:I:333:PRO:C	1:I:335:ARG:H	2.11	0.58
1:L:305:MET:SD	1:L:335:ARG:CB	2.92	0.58
4:U:140:LYS:NZ	5:V:155:GLU:OE2	2.36	0.58
1:E:108:ALA:HB1	1:E:161:HIS:ND1	2.19	0.58
1:O:217:CYS:HB2	1:O:306:TYR:OH	2.03	0.58
3:a:254:PHE:HD2	3:a:258:LYS:HZ2	1.51	0.58
1:A:305:MET:SD	1:A:336:LYS:HD2	2.44	0.58
1:J:169:TYR:OH	1:L:49:GLN:CB	2.51	0.58
3:a:248:PHE:O	3:a:252:GLU:HG2	2.03	0.58
1:F:305:MET:HE2	1:F:335:ARG:HB2	0.63	0.58
1:G:26:ALA:HA	1:G:340:TRP:CZ3	2.39	0.58
1:J:169:TYR:OH	1:L:49:GLN:HG3	2.03	0.58
2:W:142:GLU:O	2:W:145:GLU:HG2	2.03	0.58
3:a:219:LEU:O	4:b:98:ARG:NH2	2.37	0.58
4:b:45:ARG:HH21	5:c:129:THR:HG23	1.68	0.58
5:c:46:ARG:NH1	5:c:51:ASN:OD1	2.36	0.58
1:C:218:TYR:CB	1:C:307:PRO:HD2	2.34	0.58
1:E:109:PRO:CD	1:E:161:HIS:CE1	2.84	0.58
4:b:45:ARG:NH1	5:c:127:THR:OG1	2.36	0.58
5:c:150:TYR:CZ	5:c:154:LEU:HD21	2.39	0.58
5:c:154:LEU:HB3	5:c:158:LYS:NZ	2.19	0.58
1:C:306:TYR:HB2	1:C:309:ILE:HB	1.84	0.57
1:L:305:MET:SD	1:L:335:ARG:HB2	2.43	0.57
5:V:7:ALA:O	5:V:11:GLN:N	2.37	0.57
5:V:112:ILE:HD12	5:V:148:ILE:HB	1.85	0.57
4:b:137:GLY:C	4:b:139:PHE:H	2.11	0.57
1:E:252:ASN:HB2	1:E:255:PHE:CZ	2.39	0.57
1:I:335:ARG:C	1:I:337:TYR:H	2.12	0.57
1:K:166:TYR:CG	1:K:289:ILE:HG23	2.38	0.57
3:T:243:LEU:HB2	4:U:107:VAL:HG13	1.86	0.57
5:c:149:ASP:O	5:c:153:PHE:N	2.37	0.57
1:A:222:ASP:OD1	1:A:315:LYS:NZ	2.38	0.57
1:I:257:CYS:HB3	1:I:258:PRO:HD3	1.85	0.57
4:b:60:GLU:HA	4:b:63:ARG:HG3	1.85	0.57
5:c:26:ILE:HG23	5:c:29:LEU:HD22	1.86	0.57
5:c:117:LEU:HG	5:c:133:ILE:HG23	1.86	0.57
2:Q:157:ASP:OD2	2:Q:161:LYS:NZ	2.37	0.57
5:V:20:PHE:HB3	5:V:77:PHE:HE2	1.70	0.57
1:L:139:VAL:CG1	1:L:143:TYR:CE1	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:56:GLU:C	2:X:57:LEU:HD21	2.30	0.57
2:X:157:ASP:OD2	2:X:161:LYS:NZ	2.37	0.57
2:P:162:TYR:CE1	2:Q:165:VAL:HG11	2.40	0.57
2:W:162:TYR:CE1	2:X:165:VAL:HG11	2.40	0.57
3:a:271:ASN:HD21	4:b:132:ILE:HG12	1.69	0.57
3:a:250:LEU:HD22	4:b:115:GLU:HA	1.86	0.57
4:U:132:ILE:O	4:U:136:ARG:N	2.21	0.57
1:E:230:ALA:CB	1:E:255:PHE:CZ	2.87	0.57
1:J:133:TYR:CD2	1:J:352:PHE:CE1	2.93	0.57
1:K:157:ASP:OD1	1:K:157:ASP:N	2.38	0.57
1:K:289:ILE:CD1	1:M:63:GLY:O	2.38	0.57
5:V:154:LEU:HB3	5:V:158:LYS:HE3	1.87	0.57
1:C:207:GLU:O	1:C:210:ARG:HG3	2.05	0.57
1:K:305:MET:HE2	1:K:335:ARG:HB2	1.86	0.57
3:a:219:LEU:HB2	4:b:101:HIS:CE1	2.40	0.57
4:b:43:ALA:HB2	5:c:6:LYS:HE3	1.86	0.57
5:c:38:THR:O	5:c:57:LEU:HD13	2.04	0.57
1:C:257:CYS:HB3	1:C:258:PRO:HD3	1.87	0.56
1:M:196:ARG:HD2	1:M:253:GLU:CD	2.30	0.56
2:P:56:GLU:C	2:Q:57:LEU:HD21	2.30	0.56
4:U:64:GLU:OE2	4:U:68:ARG:NH2	2.38	0.56
4:b:133:PHE:HA	4:b:136:ARG:HB2	1.87	0.56
1:B:133:TYR:CD2	1:B:352:PHE:CE1	2.93	0.56
1:C:283:MET:CE	1:C:290:ARG:NH2	2.68	0.56
1:E:326:LYS:HE3	2:Q:131:GLU:OE2	2.05	0.56
1:K:270:GLU:O	1:K:270:GLU:HG2	2.04	0.56
1:K:133:TYR:HE2	1:K:346:LEU:HD21	1.71	0.56
1:L:196:ARG:HD2	1:L:253:GLU:OE2	2.04	0.56
2:P:278:LEU:O	2:P:282:THR:N	2.38	0.56
3:T:225:ASN:HA	4:U:90:PHE:HE1	1.69	0.56
4:U:165:GLU:HB3	5:V:16:GLN:HG2	1.88	0.56
4:b:111:ARG:HD2	4:b:112:TYR:N	2.20	0.56
5:c:101:PHE:HB2	5:c:153:PHE:CD2	2.40	0.56
3:T:247:LYS:HG3	4:U:114:ILE:HG13	1.87	0.56
1:A:207:GLU:O	1:A:210:ARG:HG2	2.06	0.56
1:B:250:ILE:O	1:B:254:ARG:CD	2.52	0.56
4:U:88:LEU:HD23	4:U:93:LEU:HD23	1.85	0.56
2:W:278:LEU:O	2:W:282:THR:N	2.38	0.56
1:A:187:ASP:OD2	1:A:191:LYS:NZ	2.39	0.56
1:J:252:ASN:CA	1:J:255:PHE:CE2	2.75	0.56
1:I:107:GLU:HG3	1:I:119:MET:CE	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:332:PRO:O	1:L:335:ARG:CG	2.40	0.56
5:V:29:LEU:HD23	5:V:43:LYS:HE3	1.86	0.56
1:K:252:ASN:CB	1:K:255:PHE:HZ	2.17	0.56
4:U:117:LYS:HA	4:U:120:LYS:HD2	1.87	0.56
5:V:96:GLU:O	5:V:100:LEU:HG	2.06	0.56
3:a:264:LEU:HD13	4:b:128:LEU:HB2	1.88	0.56
4:b:140:LYS:HB3	4:b:141:ARG:HH21	1.70	0.56
5:c:106:LYS:H	5:c:116:GLU:HG2	1.70	0.56
1:B:187:ASP:OD2	1:B:191:LYS:NZ	2.39	0.56
1:C:188:TYR:CE2	1:C:266:PHE:HD2	2.22	0.56
5:V:83:ARG:NH1	5:V:84:CYS:SG	2.77	0.56
3:a:234:LYS:HD3	4:b:85:LEU:HD11	1.88	0.55
1:F:2:GLU:HG3	1:F:2:GLU:O	2.06	0.55
1:O:217:CYS:HB3	1:O:306:TYR:CE2	2.39	0.55
3:T:259:TYR:O	3:T:263:VAL:HG23	2.06	0.55
3:a:244:GLU:HG3	4:b:80:CYS:HB2	1.87	0.55
1:A:207:GLU:O	1:A:210:ARG:CG	2.54	0.55
1:C:207:GLU:O	1:C:210:ARG:CG	2.55	0.55
1:C:332:PRO:O	1:C:335:ARG:CG	2.38	0.55
1:G:187:ASP:OD2	1:G:191:LYS:NZ	2.40	0.55
1:J:307:PRO:CB	2:X:244:ARG:NH1	2.70	0.55
5:V:72:VAL:HG13	5:V:76:GLU:HB2	1.88	0.55
5:V:105:ASP:OD2	5:V:110:GLY:N	2.29	0.55
3:a:226:GLU:O	3:a:230:ARG:HG3	2.06	0.55
1:C:283:MET:CE	1:C:290:ARG:HH22	2.19	0.55
1:L:51:ASP:N	1:L:51:ASP:OD1	2.39	0.55
1:L:143:TYR:HH	1:N:47:MET:HE3	1.71	0.55
2:P:214:TYR:CD2	2:Q:211:ALA:HB1	2.42	0.55
5:V:54:PRO:CB	2:W:152:LYS:NZ	2.69	0.55
3:a:254:PHE:HA	3:a:257:GLN:HB2	1.87	0.55
1:H:211:ASP:OD1	1:H:215:LYS:NZ	2.39	0.55
2:W:214:TYR:CD2	2:X:211:ALA:HB1	2.42	0.55
3:a:244:GLU:O	4:b:79:ARG:NH1	2.39	0.55
4:b:54:LEU:HG	5:c:157:MET:HE3	1.88	0.55
1:A:109:PRO:CD	1:A:161:HIS:NE2	2.67	0.55
1:E:252:ASN:HB2	1:E:255:PHE:CE1	2.42	0.55
1:K:221:LEU:HD21	1:K:311:ASP:OD2	2.06	0.55
1:D:333:PRO:C	1:D:335:ARG:H	2.13	0.55
1:F:108:ALA:HB1	1:F:161:HIS:CE1	2.42	0.55
1:O:186:THR:HG1	1:O:213:LYS:HE2	1.67	0.55
1:B:335:ARG:C	1:B:337:TYR:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:GLU:O	1:D:338:SER:HB3	2.06	0.55
5:V:54:PRO:HB3	2:W:152:LYS:HE3	1.87	0.55
5:V:104:PHE:O	5:V:116:GLU:HB3	2.07	0.55
3:a:203:THR:HG22	3:a:207:LYS:HD2	1.89	0.55
1:O:189:LEU:HD23	1:O:213:LYS:HG3	1.87	0.55
4:b:45:ARG:HH22	5:c:127:THR:C	2.15	0.55
5:c:5:TYR:CE2	5:c:83:ARG:HG2	2.41	0.55
5:c:142:LYS:HG2	5:c:155:GLU:OE1	2.06	0.55
1:C:289:ILE:O	1:C:289:ILE:HG22	2.07	0.55
1:H:83:GLU:CG	1:H:122:ILE:CD1	2.82	0.55
1:K:289:ILE:HG22	1:K:289:ILE:O	2.06	0.55
5:c:30:GLY:C	5:c:39:LYS:HZ1	2.14	0.55
3:a:243:LEU:HB3	4:b:111:ARG:HG2	1.89	0.54
5:c:36:ILE:HG21	5:c:41:LEU:HD13	1.89	0.54
1:B:51:ASP:N	1:B:51:ASP:OD1	2.40	0.54
1:C:51:ASP:OD1	1:C:51:ASP:N	2.38	0.54
1:O:133:TYR:CG	1:O:352:PHE:HZ	2.24	0.54
3:T:216:ARG:HA	4:U:105:ASP:OD1	2.07	0.54
1:C:283:MET:SD	1:C:290:ARG:NH2	2.80	0.54
1:D:133:TYR:CD2	1:D:352:PHE:CE1	2.92	0.54
1:H:257:CYS:HB3	1:H:258:PRO:HD3	1.89	0.54
1:I:133:TYR:HE2	1:I:346:LEU:HD21	1.72	0.54
1:O:287:ILE:HA	1:O:290:ARG:CD	2.37	0.54
3:T:262:ASN:OD1	3:T:265:ARG:NH1	2.36	0.54
4:U:137:GLY:C	4:U:139:PHE:H	2.15	0.54
1:G:305:MET:SD	1:G:335:ARG:HB2	2.47	0.54
5:V:118:LYS:HA	5:V:133:ILE:HG12	1.88	0.54
1:A:252:ASN:CA	1:A:255:PHE:CE2	2.67	0.54
1:C:187:ASP:OD2	1:C:191:LYS:NZ	2.41	0.54
1:I:107:GLU:HG3	1:I:119:MET:HE2	1.89	0.54
1:K:311:ASP:HB3	2:Q:248:LYS:HZ3	1.72	0.54
5:c:33:ASP:OD1	5:c:37:SER:HB3	2.06	0.54
1:F:108:ALA:HB1	1:F:161:HIS:ND1	2.21	0.54
4:b:152:ASP:OD1	4:b:153:ALA:N	2.37	0.54
1:A:113:LYS:O	1:A:116:ARG:HG2	2.07	0.54
1:L:143:TYR:CD2	1:N:44:MET:CE	2.91	0.54
1:O:133:TYR:CD2	1:O:352:PHE:HZ	2.25	0.54
4:U:50:LYS:NZ	5:V:156:PHE:O	2.36	0.54
5:V:75:ASP:O	5:V:79:VAL:HG23	2.08	0.54
2:X:268:LYS:O	2:X:272:GLU:HB2	2.08	0.54
1:B:222:ASP:OD1	1:B:315:LYS:NZ	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:HIS:O	1:H:91:TYR:CD2	2.58	0.54
5:c:139:ASP:OD2	5:c:140:GLY:N	2.41	0.54
1:B:196:ARG:HD2	1:B:253:GLU:CD	2.33	0.54
1:I:187:ASP:OD2	1:I:191:LYS:NZ	2.41	0.54
5:V:43:LYS:HA	5:V:46:ARG:HG3	1.88	0.54
5:c:40:GLU:OE1	5:c:40:GLU:N	2.40	0.54
1:K:257:CYS:HB3	1:K:258:PRO:HD3	1.90	0.54
1:L:227:MET:HB3	1:L:255:PHE:CZ	2.43	0.54
3:T:251:GLN:HG3	4:U:114:ILE:HG21	1.90	0.54
5:V:58:GLN:HG3	2:W:156:GLU:OE2	2.01	0.54
1:G:257:CYS:HB2	1:G:258:PRO:HD3	1.90	0.53
3:a:240:ILE:HG23	4:b:107:VAL:HG21	1.90	0.53
3:a:257:GLN:NE2	4:b:122:ILE:HG13	2.23	0.53
5:c:64:VAL:HG21	5:c:79:VAL:HG11	1.89	0.53
1:L:133:TYR:CG	1:L:352:PHE:CZ	2.86	0.53
3:a:212:LEU:O	3:a:216:ARG:N	2.39	0.53
3:a:220:ALA:HB1	3:a:224:LEU:HD11	1.89	0.53
3:a:271:ASN:ND2	4:b:132:ILE:HG12	2.22	0.53
5:c:130:GLU:O	5:c:134:GLU:CB	2.51	0.53
1:E:227:MET:HA	1:E:255:PHE:CE1	2.43	0.53
3:T:200:LYS:HZ2	3:T:203:THR:HG21	1.74	0.53
3:a:222:ASP:OD1	4:b:94:GLN:NE2	2.40	0.53
5:c:74:PHE:HA	5:c:77:PHE:HB3	1.90	0.53
1:C:166:TYR:CD1	1:C:289:ILE:HG23	2.43	0.53
1:G:51:ASP:OD1	1:G:51:ASP:N	2.40	0.53
5:V:137:MET:O	5:V:141:ASP:N	2.41	0.53
3:a:259:TYR:HA	3:a:262:ASN:HD22	1.74	0.53
5:c:9:VAL:HA	5:c:12:LEU:HB2	1.90	0.53
1:C:133:TYR:CG	1:C:352:PHE:CZ	2.92	0.53
1:H:187:ASP:OD2	1:H:191:LYS:NZ	2.42	0.53
1:F:169:TYR:HH	1:H:49:GLN:HB3	1.72	0.53
2:P:146:ILE:HG23	2:P:147:GLN:N	2.24	0.53
1:A:252:ASN:HB2	1:A:255:PHE:CE1	2.43	0.53
3:T:236:LEU:HD22	4:U:101:HIS:HA	1.91	0.53
3:a:216:ARG:HH12	3:a:218:VAL:HA	1.73	0.53
1:F:110:LEU:H	1:F:161:HIS:CE1	2.26	0.53
1:G:25:ASP:HB3	4:b:147:VAL:CG1	2.36	0.53
1:I:86:TRP:HE3	1:I:122:ILE:HD13	1.68	0.53
1:N:287:ILE:HA	1:N:290:ARG:HD3	1.90	0.53
1:O:252:ASN:CB	1:O:255:PHE:HZ	2.14	0.53
3:a:200:LYS:O	3:a:203:THR:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:124:THR:OG1	5:c:128:ILE:HD11	2.08	0.53
2:P:149:LYS:HG2	2:P:153:HIS:CD2	2.43	0.53
2:P:256:LEU:HD11	2:Q:257:GLU:OE2	2.09	0.53
2:Q:165:VAL:O	2:Q:169:LEU:N	2.42	0.53
2:Q:268:LYS:O	2:Q:272:GLU:HB2	2.08	0.53
5:c:21:LYS:NZ	5:c:25:ASP:OD1	2.35	0.53
1:C:133:TYR:HE2	1:C:346:LEU:HD21	1.73	0.53
3:a:215:ARG:HD3	4:b:108:ASP:OD1	2.09	0.53
1:B:253:GLU:HA	1:B:256:ARG:HB2	1.91	0.52
1:O:51:ASP:OD1	1:O:51:ASP:N	2.38	0.52
4:U:60:GLU:O	4:U:63:ARG:HG3	2.08	0.52
4:b:136:ARG:NH2	5:c:94:GLU:OE1	2.42	0.52
5:c:9:VAL:HG12	5:c:82:VAL:HG21	1.91	0.52
1:F:335:ARG:C	1:F:337:TYR:H	2.17	0.52
1:H:87:HIS:CD2	1:H:127:PHE:HE2	1.97	0.52
5:c:79:VAL:O	5:c:83:ARG:HG3	2.09	0.52
1:F:227:MET:HB3	1:F:255:PHE:HZ	1.75	0.52
1:L:334:GLU:N	1:L:334:GLU:OE1	2.40	0.52
5:c:105:ASP:OD2	5:c:111:TYR:N	2.42	0.52
1:A:252:ASN:CB	1:A:255:PHE:HZ	2.22	0.52
1:E:51:ASP:OD1	1:E:51:ASP:N	2.42	0.52
3:T:247:LYS:HB3	4:U:79:ARG:HH12	1.73	0.52
5:V:140:GLY:HA2	5:V:156:PHE:HB2	1.91	0.52
2:W:256:LEU:HD11	2:X:257:GLU:OE2	2.09	0.52
5:c:92:LYS:HG3	5:c:157:MET:O	2.10	0.52
1:C:133:TYR:CE1	1:C:355:MET:HB3	2.44	0.52
1:G:335:ARG:C	1:G:337:TYR:H	2.17	0.52
3:T:225:ASN:N	3:T:228:GLN:OE1	2.43	0.52
3:T:268:ILE:HD11	4:U:128:LEU:HD22	1.91	0.52
1:D:51:ASP:OD1	1:D:51:ASP:N	2.43	0.52
1:D:207:GLU:O	1:D:210:ARG:CG	2.58	0.52
1:G:333:PRO:C	1:G:335:ARG:H	2.18	0.52
1:K:230:ALA:HB3	1:K:255:PHE:CZ	2.45	0.52
3:T:243:LEU:HA	3:T:246:GLU:OE1	2.10	0.52
1:B:250:ILE:HB	1:B:254:ARG:HG2	1.92	0.52
5:c:61:ILE:HG12	5:c:72:VAL:CG2	2.40	0.52
5:c:106:LYS:N	5:c:116:GLU:HG2	2.24	0.52
1:H:110:LEU:HB3	1:H:177:ARG:HG3	1.92	0.52
1:L:139:VAL:HG13	1:L:143:TYR:CE1	2.44	0.52
3:T:268:ILE:O	3:T:272:GLN:N	2.42	0.52
3:a:256:GLN:HE22	5:c:102:ARG:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:261:ILE:HG21	4:b:124:GLU:CD	2.35	0.52
5:c:121:LEU:O	5:c:124:THR:OG1	2.21	0.52
5:c:156:PHE:CE2	5:c:157:MET:HE2	2.45	0.52
1:D:257:CYS:HB3	1:D:258:PRO:HD3	1.91	0.52
1:F:51:ASP:OD1	1:F:51:ASP:N	2.42	0.52
1:J:169:TYR:HH	1:L:49:GLN:HB3	1.71	0.52
1:K:305:MET:HE2	1:K:335:ARG:CB	2.40	0.52
4:b:48:GLN:HB3	5:c:126:GLU:OE1	2.10	0.52
1:J:257:CYS:CB	1:J:258:PRO:HD3	2.40	0.52
1:N:227:MET:CB	1:N:255:PHE:HE1	2.19	0.52
2:P:149:LYS:HZ2	5:c:37:SER:HB2	1.74	0.52
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.91	0.51
1:M:335:ARG:C	1:M:337:TYR:H	2.17	0.51
4:b:59:GLN:HA	4:b:62:GLU:CD	2.34	0.51
5:c:57:LEU:O	5:c:61:ILE:HG13	2.10	0.51
5:c:61:ILE:HA	5:c:80:MET:HE1	1.92	0.51
5:c:104:PHE:HD2	5:c:153:PHE:CE1	2.28	0.51
1:E:257:CYS:HB3	1:E:258:PRO:HD3	1.93	0.51
1:O:217:CYS:O	1:O:306:TYR:CE2	2.61	0.51
2:X:165:VAL:O	2:X:169:LEU:N	2.42	0.51
3:T:217:LYS:O	4:U:101:HIS:NE2	2.43	0.51
2:X:240:GLU:O	2:X:244:ARG:HG3	2.11	0.51
3:a:252:GLU:HG3	4:b:69:ARG:NH2	2.18	0.51
1:L:286:ASP:O	1:L:290:ARG:HG3	2.11	0.51
2:Q:240:GLU:O	2:Q:244:ARG:HG3	2.11	0.51
3:T:257:GLN:NE2	4:U:122:ILE:HG13	2.25	0.51
5:V:73:ASP:HB3	5:V:75:ASP:OD1	2.11	0.51
3:a:262:ASN:HA	3:a:265:ARG:HD2	1.91	0.51
1:O:352:PHE:CD1	1:O:355:MET:CG	2.93	0.51
4:b:91:ALA:HA	4:b:94:GLN:HG3	1.92	0.51
1:D:335:ARG:C	1:D:337:TYR:H	2.17	0.51
5:V:94:GLU:HA	5:V:154:LEU:HD22	1.91	0.51
3:a:212:LEU:HA	3:a:215:ARG:HB2	1.92	0.51
5:c:91:GLY:CA	5:c:159:GLY:HA2	2.36	0.51
5:c:62:ASP:HA	5:c:65:ASP:HB2	1.93	0.51
1:H:252:ASN:CA	1:H:255:PHE:CZ	2.94	0.51
1:J:222:ASP:OD1	1:J:315:LYS:NZ	2.43	0.51
1:K:166:TYR:CE1	1:K:289:ILE:HG23	2.45	0.51
1:M:207:GLU:O	1:M:210:ARG:HG3	2.10	0.51
3:a:263:VAL:HG22	5:c:110:GLY:HA2	1.91	0.51
5:c:109:ASP:HB2	5:c:111:TYR:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:LEU:H	1:E:161:HIS:HE1	1.57	0.51
1:J:79:TRP:HZ3	1:J:83:GLU:OE1	1.94	0.51
1:K:311:ASP:OD2	2:Q:248:LYS:CD	2.58	0.51
1:K:311:ASP:HB3	2:Q:248:LYS:NZ	2.25	0.51
5:V:150:TYR:CZ	5:V:154:LEU:HD21	2.46	0.51
2:W:53:THR:CA	2:X:57:LEU:HD11	2.39	0.51
3:a:219:LEU:HD22	4:b:101:HIS:CB	2.39	0.51
3:a:253:LYS:HE3	4:b:118:VAL:HG13	1.92	0.51
1:C:222:ASP:OD1	1:C:315:LYS:NZ	2.43	0.51
2:P:57:LEU:N	2:Q:57:LEU:CD2	2.74	0.51
2:X:221:TYR:O	2:X:225:ILE:N	2.38	0.51
3:a:247:LYS:HZ2	4:b:110:GLU:HB2	1.74	0.51
4:b:110:GLU:O	4:b:114:ILE:HG12	2.11	0.51
1:L:305:MET:SD	1:L:335:ARG:HB3	2.51	0.50
4:U:41:ILE:HD12	4:U:45:ARG:HE	1.76	0.50
5:V:12:LEU:HD13	5:V:20:PHE:HE1	1.76	0.50
5:V:94:GLU:O	5:V:150:TYR:OH	2.28	0.50
2:W:57:LEU:N	2:X:57:LEU:CD2	2.74	0.50
5:c:101:PHE:HE1	5:c:112:ILE:HG13	1.76	0.50
1:F:136:ILE:HB	1:F:139:VAL:HG13	1.93	0.50
1:O:210:ARG:HA	1:O:213:LYS:HE3	1.92	0.50
2:Q:221:TYR:O	2:Q:225:ILE:N	2.38	0.50
5:V:117:LEU:HD23	5:V:137:MET:HE2	1.93	0.50
1:H:154:ASP:O	1:H:155:SER:C	2.54	0.50
5:V:104:PHE:HB3	5:V:112:ILE:HG12	1.93	0.50
3:a:202:GLN:OE1	3:a:205:ARG:HB3	2.11	0.50
1:F:109:PRO:HD2	1:F:161:HIS:NE2	2.27	0.50
1:K:107:GLU:OE2	1:K:116:ARG:NE	2.45	0.50
1:L:227:MET:HB3	1:L:255:PHE:HZ	1.76	0.50
3:T:261:ILE:HA	3:T:264:LEU:HD12	1.93	0.50
1:A:207:GLU:CA	1:A:210:ARG:HG2	2.36	0.50
1:J:307:PRO:HB3	2:X:244:ARG:NH1	2.27	0.50
4:b:46:LYS:HA	4:b:49:LEU:HD12	1.92	0.50
4:b:154:MET:HG3	5:c:48:LEU:HD11	1.92	0.50
1:F:333:PRO:C	1:F:335:ARG:N	2.69	0.50
1:N:335:ARG:C	1:N:337:TYR:N	2.70	0.50
2:X:246:VAL:O	2:X:250:GLU:N	2.45	0.50
1:I:106:THR:O	1:I:107:GLU:CG	2.59	0.50
3:T:243:LEU:HD22	4:U:111:ARG:HE	1.77	0.50
5:V:134:GLU:OE2	5:V:138:LYS:NZ	2.34	0.50
3:a:221:ILE:O	3:a:229:LEU:HD21	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:OD2	1:A:84:LYS:NZ	2.45	0.50
1:A:109:PRO:CG	1:A:161:HIS:NE2	2.75	0.50
1:I:257:CYS:CB	1:I:258:PRO:HD3	2.42	0.50
1:K:230:ALA:HB3	1:K:255:PHE:HZ	1.76	0.50
3:T:265:ARG:HA	3:T:268:ILE:HD12	1.93	0.50
4:U:103:ARG:CZ	4:U:107:VAL:HB	2.42	0.50
5:c:2:ASP:OD2	5:c:66:GLU:HG2	2.12	0.50
5:c:38:THR:HB	5:c:54:PRO:HB3	1.93	0.50
1:C:188:TYR:CZ	1:C:266:PHE:CG	3.00	0.50
1:D:252:ASN:HA	1:D:255:PHE:HE2	1.61	0.50
1:K:221:LEU:HD11	2:Q:248:LYS:HZ3	1.77	0.50
3:a:267:ARG:HH21	4:b:132:ILE:HB	1.77	0.50
1:C:207:GLU:CA	1:C:210:ARG:HG2	2.41	0.49
1:C:333:PRO:C	1:C:335:ARG:N	2.70	0.49
1:E:332:PRO:O	1:E:335:ARG:HB3	2.12	0.49
3:T:263:VAL:HG11	5:V:101:PHE:CE2	2.47	0.49
3:a:219:LEU:HD11	4:b:97:CYS:HB3	1.93	0.49
3:a:247:LYS:HD3	4:b:111:ARG:N	2.26	0.49
1:D:332:PRO:O	1:D:335:ARG:CG	2.38	0.49
1:H:207:GLU:O	1:H:210:ARG:CG	2.60	0.49
1:O:333:PRO:C	1:O:335:ARG:H	2.19	0.49
3:T:230:ARG:HG2	4:U:85:LEU:HB3	1.94	0.49
5:V:54:PRO:CB	2:W:152:LYS:HZ2	2.25	0.49
1:D:207:GLU:O	1:D:210:ARG:HG3	2.11	0.49
1:F:187:ASP:OD2	1:F:191:LYS:NZ	2.44	0.49
1:N:230:ALA:HB3	1:N:255:PHE:CZ	2.41	0.49
3:a:247:LYS:NZ	4:b:110:GLU:HB2	2.27	0.49
5:c:20:PHE:CZ	5:c:81:MET:HB3	2.47	0.49
1:C:257:CYS:CB	1:C:258:PRO:HD3	2.42	0.49
1:J:301:GLY:C	1:J:336:LYS:HA	2.37	0.49
1:K:335:ARG:C	1:K:337:TYR:N	2.71	0.49
1:L:187:ASP:OD2	1:L:191:LYS:NZ	2.46	0.49
3:T:263:VAL:CG1	5:V:150:TYR:HB2	2.43	0.49
1:L:333:PRO:C	1:L:335:ARG:N	2.70	0.49
5:c:48:LEU:HB3	5:c:50:GLN:OE1	2.13	0.49
4:U:61:LEU:N	5:V:103:MET:HG3	2.26	0.49
4:b:154:MET:HG3	5:c:48:LEU:HD21	1.94	0.49
3:T:243:LEU:HD22	4:U:108:ASP:HA	1.95	0.49
4:U:155:MET:HG3	4:U:163:ALA:HB1	1.94	0.49
5:c:46:ARG:NH2	5:c:49:GLY:HA2	2.27	0.49
2:P:162:TYR:HE1	2:Q:165:VAL:HG11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:101:PHE:HZ	5:c:110:GLY:C	2.20	0.49
5:c:137:MET:HA	5:c:148:ILE:HD11	1.94	0.49
1:E:167:GLU:O	1:E:169:TYR:CD1	2.65	0.49
1:G:305:MET:SD	1:G:335:ARG:CD	3.01	0.49
1:K:14:SER:N	1:K:157:ASP:OD2	2.46	0.49
1:O:352:PHE:CD1	1:O:355:MET:HB2	2.48	0.49
5:V:39:LYS:CA	2:W:149:LYS:HZ1	2.26	0.49
3:a:247:LYS:HB2	4:b:111:ARG:HB3	1.95	0.49
1:N:230:ALA:CB	1:N:255:PHE:CZ	2.96	0.49
1:O:207:GLU:O	1:O:210:ARG:HG2	2.12	0.49
4:b:129:THR:O	4:b:133:PHE:CB	2.56	0.49
5:c:153:PHE:HA	5:c:156:PHE:HB3	1.95	0.49
1:F:188:TYR:CZ	1:F:266:PHE:CD2	3.00	0.48
1:I:133:TYR:CG	1:I:352:PHE:CZ	2.92	0.48
1:J:252:ASN:HB2	1:J:255:PHE:CE1	2.46	0.48
1:K:80:ASP:OD2	1:K:84:LYS:NZ	2.45	0.48
4:U:110:GLU:O	4:U:114:ILE:HG12	2.13	0.48
4:b:155:MET:HE1	5:c:27:PHE:HZ	1.78	0.48
1:C:30:VAL:HG21	1:C:337:TYR:CZ	2.48	0.48
2:W:39:LEU:O	2:W:43:LEU:N	2.46	0.48
5:c:45:MET:HA	5:c:48:LEU:HD12	1.95	0.48
1:A:335:ARG:O	1:A:337:TYR:N	2.44	0.48
1:H:335:ARG:C	1:H:337:TYR:N	2.72	0.48
1:L:139:VAL:CG1	1:L:143:TYR:HE1	2.26	0.48
4:b:64:GLU:HA	4:b:67:GLU:OE1	2.12	0.48
5:c:40:GLU:O	5:c:43:LYS:HG2	2.13	0.48
1:J:207:GLU:O	1:J:210:ARG:CG	2.62	0.48
2:Q:246:VAL:O	2:Q:250:GLU:N	2.45	0.48
3:T:254:PHE:CE1	4:U:117:LYS:HB3	2.48	0.48
5:V:137:MET:SD	5:V:148:ILE:HG13	2.54	0.48
5:V:143:ASN:ND2	5:V:152:GLU:OE2	2.47	0.48
3:a:240:ILE:O	3:a:244:GLU:HG2	2.13	0.48
3:a:265:ARG:O	3:a:269:ASN:ND2	2.46	0.48
4:b:145:ARG:O	4:b:148:ARG:NH2	2.47	0.48
1:H:87:HIS:C	1:H:91:TYR:HD2	2.21	0.48
1:L:109:PRO:HD2	1:L:161:HIS:CE1	2.48	0.48
2:P:39:LEU:O	2:P:43:LEU:N	2.46	0.48
5:c:42:GLY:HA2	5:c:52:PRO:CG	2.43	0.48
1:F:6:THR:CG2	4:U:146:ARG:HH12	2.22	0.48
2:Q:11:LEU:N	2:Q:14:ASP:OD2	2.47	0.48
4:U:61:LEU:HD22	5:V:99:ASP:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:11:LEU:N	2:X:14:ASP:OD2	2.47	0.48
4:b:135:LEU:HA	4:b:138:LYS:HZ1	1.78	0.48
5:c:36:ILE:HA	5:c:40:GLU:HB2	1.96	0.48
5:c:97:LEU:HD12	5:c:154:LEU:HA	1.95	0.48
1:B:133:TYR:CE1	1:B:355:MET:HB3	2.49	0.48
5:V:9:VAL:HA	5:V:12:LEU:HG	1.96	0.48
5:V:39:LYS:N	2:W:149:LYS:HZ1	2.02	0.48
5:V:142:LYS:HG2	5:V:152:GLU:HG2	1.95	0.48
5:c:17:LYS:HD3	5:c:17:LYS:C	2.39	0.48
5:c:97:LEU:CD1	5:c:154:LEU:HA	2.43	0.48
1:B:302:GLY:C	1:B:304:THR:H	2.21	0.48
1:E:333:PRO:C	1:E:335:ARG:H	2.20	0.48
1:H:333:PRO:C	1:H:335:ARG:N	2.69	0.48
1:J:305:MET:SD	1:J:335:ARG:HB3	2.52	0.48
1:O:80:ASP:OD2	1:O:84:LYS:NZ	2.47	0.48
3:a:217:LYS:O	4:b:101:HIS:NE2	2.46	0.48
5:c:54:PRO:HA	5:c:57:LEU:HB2	1.95	0.48
5:c:63:GLU:HB3	5:c:83:ARG:NH2	2.28	0.48
5:c:141:ASP:HA	5:c:152:GLU:CD	2.39	0.48
1:B:133:TYR:CG	1:B:352:PHE:HZ	2.31	0.48
1:H:207:GLU:HA	1:H:210:ARG:CG	2.42	0.48
1:N:287:ILE:HA	1:N:290:ARG:CD	2.44	0.48
3:T:243:LEU:HD13	4:U:108:ASP:HB2	1.95	0.48
5:V:27:PHE:CG	5:V:44:VAL:HG21	2.48	0.48
3:a:220:ALA:CB	3:a:224:LEU:HD11	2.44	0.48
3:a:252:GLU:OE1	3:a:255:LYS:NZ	2.41	0.48
4:b:114:ILE:HD13	4:b:117:LYS:NZ	2.29	0.48
1:B:250:ILE:CG2	1:B:254:ARG:HG3	2.40	0.48
1:K:289:ILE:HG12	1:M:63:GLY:HA3	1.96	0.48
3:a:243:LEU:HA	3:a:246:GLU:OE1	2.14	0.48
1:C:290:ARG:CG	1:E:244:ASP:HB3	2.43	0.47
1:H:262:PHE:CZ	1:H:312:ARG:HG2	2.48	0.47
1:H:305:MET:SD	1:H:335:ARG:HB2	2.54	0.47
3:a:216:ARG:HB2	4:b:105:ASP:OD1	2.14	0.47
3:a:221:ILE:O	4:b:94:GLN:HG2	2.14	0.47
5:c:28:VAL:C	5:c:43:LYS:HZ1	2.22	0.47
1:L:257:CYS:HB3	1:L:258:PRO:HD3	1.96	0.47
3:T:268:ILE:HG13	4:U:132:ILE:HD11	1.96	0.47
3:a:254:PHE:C	3:a:258:LYS:HZ3	2.22	0.47
1:B:335:ARG:H	1:B:335:ARG:HG2	1.44	0.47
1:G:252:ASN:HB2	1:G:255:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:257:CYS:CB	1:H:258:PRO:HD3	2.44	0.47
1:J:133:TYR:CG	1:J:352:PHE:HZ	2.32	0.47
1:K:334:GLU:O	1:K:338:SER:HB3	2.14	0.47
3:a:226:GLU:HB3	3:a:230:ARG:NH1	2.29	0.47
4:b:136:ARG:NH1	4:b:140:LYS:HE2	2.29	0.47
5:c:149:ASP:HB3	5:c:152:GLU:HB2	1.97	0.47
1:O:335:ARG:C	1:O:337:TYR:H	2.22	0.47
5:V:28:VAL:HG12	5:V:40:GLU:HG2	1.96	0.47
2:X:127:MET:O	2:X:131:GLU:N	2.45	0.47
4:b:44:SER:OG	5:c:7:ALA:HA	2.14	0.47
5:c:5:TYR:O	5:c:9:VAL:HG13	2.14	0.47
1:A:133:TYR:CG	1:A:352:PHE:HZ	2.25	0.47
1:A:326:LYS:CE	2:Q:47:GLN:HE22	2.24	0.47
1:F:139:VAL:HG23	1:F:140:LEU:HG	1.95	0.47
1:H:207:GLU:CA	1:H:210:ARG:HG2	2.42	0.47
1:M:333:PRO:C	1:M:335:ARG:H	2.21	0.47
3:T:227:ASP:OD1	3:T:227:ASP:N	2.47	0.47
1:C:219:VAL:HG23	1:C:306:TYR:HB3	1.96	0.47
1:C:255:PHE:CD1	1:C:255:PHE:C	2.92	0.47
1:I:87:HIS:CE1	1:I:91:TYR:CD2	3.02	0.47
2:P:152:LYS:CE	5:c:54:PRO:HB2	2.42	0.47
3:T:241:TYR:CD1	4:U:80:CYS:HB3	2.49	0.47
3:T:244:GLU:HG2	4:U:107:VAL:HG21	1.95	0.47
1:A:109:PRO:HG2	1:A:161:HIS:NE2	2.29	0.47
1:D:116:ARG:NH1	1:D:375:PHE:CE1	2.82	0.47
1:E:108:ALA:HB1	1:E:161:HIS:CE1	2.49	0.47
1:J:133:TYR:CE1	1:J:355:MET:HB3	2.50	0.47
3:a:234:LYS:HZ3	4:b:83:LEU:H	1.63	0.47
3:a:237:TRP:NE1	4:b:80:CYS:SG	2.88	0.47
3:a:266:ASN:ND2	5:c:110:GLY:HA3	2.30	0.47
4:b:151:ALA:H	5:c:84:CYS:HB3	1.79	0.47
5:c:61:ILE:HG12	5:c:72:VAL:HG23	1.97	0.47
5:c:93:SER:O	5:c:97:LEU:HG	2.14	0.47
1:B:56:ASP:OD1	1:B:56:ASP:N	2.46	0.47
1:G:80:ASP:OD2	1:G:84:LYS:NZ	2.48	0.47
4:U:60:GLU:HA	4:U:63:ARG:HG3	1.97	0.47
5:V:30:GLY:O	5:V:39:LYS:NZ	2.37	0.47
2:W:78:ALA:O	2:W:82:GLU:N	2.47	0.47
3:a:200:LYS:O	3:a:204:GLU:HG2	2.15	0.47
4:b:137:GLY:HA2	4:b:141:ARG:HH21	1.79	0.47
5:c:52:PRO:HG2	5:c:57:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:80:MET:O	5:c:83:ARG:HB2	2.15	0.47
1:E:196:ARG:HD2	1:E:253:GLU:CD	2.39	0.47
1:F:4:GLU:O	1:F:6:THR:N	2.46	0.47
1:F:336:LYS:HG2	1:F:337:TYR:CD1	2.49	0.47
1:B:133:TYR:HE2	1:B:346:LEU:HD21	1.80	0.47
1:F:305:MET:HE2	1:F:335:ARG:CA	2.37	0.47
5:c:53:THR:O	5:c:57:LEU:HG	2.15	0.47
1:C:303:THR:O	1:C:306:TYR:CD1	2.68	0.46
2:W:56:GLU:C	2:X:57:LEU:CD2	2.89	0.46
3:a:227:ASP:HA	3:a:230:ARG:HD2	1.97	0.46
4:b:49:LEU:N	5:c:126:GLU:OE1	2.48	0.46
4:b:131:LYS:HZ3	4:b:135:LEU:HD12	1.79	0.46
1:C:18:LYS:HG2	1:C:337:TYR:HE1	1.80	0.46
1:E:305:MET:SD	1:E:336:LYS:CD	3.03	0.46
1:J:252:ASN:CB	1:J:255:PHE:HZ	2.27	0.46
1:K:133:TYR:CG	1:K:352:PHE:CZ	2.95	0.46
1:M:154:ASP:O	1:M:155:SER:C	2.58	0.46
1:M:196:ARG:HD2	1:M:253:GLU:OE2	2.15	0.46
1:N:302:GLY:C	1:N:304:THR:H	2.23	0.46
1:J:307:PRO:CG	2:X:244:ARG:NH1	2.77	0.46
1:K:333:PRO:C	1:K:335:ARG:N	2.69	0.46
4:b:151:ALA:H	5:c:84:CYS:C	2.22	0.46
1:H:305:MET:SD	1:H:335:ARG:CB	3.03	0.46
1:O:352:PHE:HD1	1:O:355:MET:HG3	1.80	0.46
2:P:78:ALA:O	2:P:82:GLU:N	2.47	0.46
2:P:85:VAL:O	2:P:89:ASN:N	2.45	0.46
5:V:116:GLU:N	5:V:116:GLU:OE1	2.49	0.46
5:V:137:MET:HA	5:V:148:ILE:HD11	1.97	0.46
1:K:302:GLY:C	1:K:304:THR:H	2.23	0.46
1:O:352:PHE:CE1	1:O:355:MET:HG3	2.50	0.46
2:P:53:THR:CA	2:Q:57:LEU:HD11	2.39	0.46
2:P:56:GLU:C	2:Q:57:LEU:CD2	2.89	0.46
3:T:200:LYS:O	3:T:204:GLU:HG2	2.15	0.46
3:T:232:LYS:O	3:T:235:GLU:HG3	2.15	0.46
3:a:225:ASN:ND2	3:a:227:ASP:H	2.13	0.46
3:a:230:ARG:HH21	4:b:88:LEU:N	2.13	0.46
1:A:230:ALA:HB3	1:A:255:PHE:HZ	1.81	0.46
1:C:219:VAL:HG23	1:C:306:TYR:CB	2.45	0.46
1:K:230:ALA:CB	1:K:255:PHE:CE2	2.98	0.46
2:P:284:ILE:HD12	2:S:11:LEU:HB2	1.98	0.46
2:Q:265:LEU:O	2:Q:269:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:154:ILE:O	2:W:158:ALA:N	2.42	0.46
3:a:216:ARG:HG2	4:b:101:HIS:NE2	2.29	0.46
3:a:238:GLN:NE2	3:a:242:ASN:OD1	2.46	0.46
4:b:47:LEU:HD13	5:c:7:ALA:HB1	1.98	0.46
4:b:111:ARG:HD2	4:b:111:ARG:C	2.41	0.46
5:c:80:MET:HA	5:c:83:ARG:CD	2.46	0.46
1:A:143:TYR:OH	1:C:45:VAL:N	2.47	0.46
1:F:108:ALA:HB1	1:F:161:HIS:CG	2.51	0.46
1:L:252:ASN:CB	1:L:255:PHE:HE2	2.27	0.46
2:P:149:LYS:HG2	2:P:153:HIS:NE2	2.30	0.46
2:X:265:LEU:O	2:X:269:ALA:HB3	2.16	0.46
3:a:208:LYS:O	3:a:212:LEU:HG	2.16	0.46
4:b:52:LEU:HD23	4:b:55:GLN:OE1	2.16	0.46
1:J:332:PRO:O	1:J:335:ARG:CD	2.63	0.46
3:a:236:LEU:O	3:a:239:SER:OG	2.26	0.46
3:a:243:LEU:HD22	4:b:108:ASP:HA	1.97	0.46
4:b:108:ASP:O	4:b:112:TYR:HB3	2.16	0.46
1:C:219:VAL:O	1:C:220:ALA:HB3	2.16	0.46
1:H:334:GLU:O	1:H:338:SER:HB3	2.16	0.46
1:O:286:ASP:O	1:O:290:ARG:HG2	2.15	0.46
4:U:41:ILE:HD12	4:U:45:ARG:NE	2.30	0.46
2:W:274:LEU:HD13	2:X:274:LEU:HB3	1.98	0.46
3:a:267:ARG:HB2	4:b:132:ILE:HD13	1.98	0.46
4:b:41:ILE:HG13	4:b:46:LYS:HD3	1.97	0.46
5:c:24:PHE:O	5:c:28:VAL:HG22	2.15	0.46
1:F:257:CYS:CB	1:F:258:PRO:HD3	2.46	0.46
1:M:207:GLU:C	1:M:210:ARG:HG2	2.41	0.46
4:U:138:LYS:H	4:U:141:ARG:HH12	1.64	0.46
5:V:4:ILE:HG13	5:V:5:TYR:H	1.80	0.46
3:a:230:ARG:HG2	4:b:85:LEU:HB3	1.97	0.46
1:C:255:PHE:CE1	1:C:259:GLU:OE1	2.70	0.45
1:F:143:TYR:OH	1:H:44:MET:CB	2.64	0.45
1:F:169:TYR:OH	1:H:49:GLN:CB	2.62	0.45
2:Q:214:TYR:O	2:Q:218:GLU:HG3	2.16	0.45
2:W:162:TYR:HE1	2:X:165:VAL:HG11	1.77	0.45
2:W:193:LEU:O	2:W:197:LEU:N	2.45	0.45
5:c:5:TYR:CD2	5:c:83:ARG:HG2	2.51	0.45
1:H:230:ALA:HB3	1:H:255:PHE:CZ	2.51	0.45
2:P:148:LEU:HD21	2:P:152:LYS:CE	2.46	0.45
5:c:13:THR:OG1	5:c:15:GLU:OE2	2.31	0.45
5:c:75:ASP:O	5:c:79:VAL:HG23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:283:MET:O	1:H:290:ARG:NH2	2.47	0.45
2:P:193:LEU:O	2:P:197:LEU:N	2.45	0.45
5:c:58:GLN:O	5:c:61:ILE:HB	2.16	0.45
1:G:305:MET:SD	1:G:335:ARG:CB	3.05	0.45
2:Q:40:GLU:OE1	2:Q:40:GLU:HA	2.16	0.45
4:U:54:LEU:HD13	5:V:92:LYS:HD3	1.99	0.45
3:a:237:TRP:NE1	4:b:80:CYS:HG	2.14	0.45
3:a:244:GLU:OE1	4:b:79:ARG:HD3	2.16	0.45
3:a:270:ASP:OD2	5:c:111:TYR:OH	2.26	0.45
4:b:146:ARG:NH2	4:b:148:ARG:O	2.30	0.45
1:D:302:GLY:C	1:D:304:THR:H	2.24	0.45
1:H:230:ALA:HB3	1:H:255:PHE:HZ	1.82	0.45
1:O:230:ALA:HB3	1:O:255:PHE:CZ	2.52	0.45
2:P:142:GLU:CA	2:P:145:GLU:OE2	2.58	0.45
3:T:226:GLU:HB3	3:T:230:ARG:NH1	2.32	0.45
4:U:148:ARG:HG2	5:V:83:ARG:NH2	2.32	0.45
5:c:117:LEU:HD21	5:c:136:LEU:HB2	1.97	0.45
1:A:230:ALA:HB3	1:A:255:PHE:CZ	2.52	0.45
1:H:110:LEU:CB	1:H:177:ARG:HG3	2.47	0.45
1:M:213:LYS:CD	1:M:306:TYR:OH	2.64	0.45
2:Q:127:MET:O	2:Q:131:GLU:N	2.45	0.45
5:V:27:PHE:CE2	5:V:40:GLU:HB3	2.52	0.45
5:V:38:THR:CA	2:W:149:LYS:HE2	2.37	0.45
2:W:284:ILE:HD12	2:Z:11:LEU:HB2	1.97	0.45
3:a:230:ARG:CG	4:b:85:LEU:HB3	2.46	0.45
3:a:266:ASN:HD22	5:c:110:GLY:HA3	1.81	0.45
4:b:41:ILE:HD12	4:b:46:LYS:HG2	1.98	0.45
4:b:150:SER:OG	5:c:86:LYS:NZ	2.49	0.45
1:E:169:TYR:CZ	1:G:49:GLN:HG3	2.52	0.45
3:T:204:GLU:HA	3:T:207:LYS:HB2	1.99	0.45
3:T:262:ASN:HA	3:T:265:ARG:NH1	2.32	0.45
5:V:9:VAL:HG13	5:V:82:VAL:HG21	1.99	0.45
2:W:85:VAL:O	2:W:89:ASN:N	2.45	0.45
2:W:142:GLU:CA	2:W:145:GLU:OE2	2.58	0.45
4:b:146:ARG:NH2	4:b:148:ARG:HG3	2.32	0.45
1:C:218:TYR:HB3	1:C:307:PRO:HG2	1.98	0.45
1:J:219:VAL:O	1:J:220:ALA:HB3	2.17	0.45
2:P:101:ARG:O	2:P:105:ARG:HG3	2.16	0.45
2:X:40:GLU:OE1	2:X:40:GLU:HA	2.16	0.45
3:a:208:LYS:HA	3:a:211:ILE:HB	1.99	0.45
3:a:238:GLN:NE2	3:a:241:TYR:HB3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:51:THR:HA	4:b:54:LEU:HD12	1.98	0.45
4:b:132:ILE:HG22	4:b:136:ARG:HD2	1.97	0.45
5:c:112:ILE:O	5:c:148:ILE:N	2.45	0.45
1:J:207:GLU:O	1:J:210:ARG:HG2	2.17	0.45
1:K:221:LEU:HD21	1:K:311:ASP:CG	2.41	0.45
1:N:257:CYS:HB3	1:N:258:PRO:HD3	1.99	0.45
2:P:162:TYR:HE1	2:Q:165:VAL:CG1	2.30	0.45
5:V:65:ASP:OD2	5:V:70:GLY:N	2.27	0.45
2:X:214:TYR:O	2:X:218:GLU:HG3	2.16	0.45
2:X:246:VAL:O	2:X:250:GLU:HG3	2.16	0.45
4:b:90:PHE:O	4:b:94:GLN:HG3	2.16	0.45
5:c:27:PHE:CD2	5:c:77:PHE:HE1	2.34	0.45
5:c:33:ASP:OD2	5:c:33:ASP:N	2.49	0.45
1:B:227:MET:HB2	1:B:255:PHE:HE1	1.82	0.45
1:D:154:ASP:O	1:D:155:SER:C	2.60	0.45
5:V:54:PRO:HB3	2:W:152:LYS:CE	2.46	0.45
5:V:141:ASP:N	5:V:148:ILE:HG12	2.32	0.45
5:V:153:PHE:HA	5:V:156:PHE:HB3	1.99	0.45
5:c:158:LYS:HA	5:c:158:LYS:HD3	1.72	0.45
1:C:290:ARG:NH1	1:E:244:ASP:OD2	2.50	0.44
1:D:257:CYS:CB	1:D:258:PRO:HD3	2.47	0.44
1:H:262:PHE:CE2	1:H:312:ARG:HG2	2.52	0.44
3:T:252:GLU:HA	3:T:255:LYS:HE3	1.98	0.44
4:b:61:LEU:N	5:c:103:MET:HG3	2.32	0.44
1:C:188:TYR:CZ	1:C:266:PHE:CB	2.99	0.44
1:C:308:GLY:HA2	1:C:311:ASP:OD2	2.18	0.44
1:K:4:GLU:OE2	1:K:4:GLU:HA	2.17	0.44
1:O:207:GLU:CA	1:O:210:ARG:HG2	2.43	0.44
2:Q:143:ILE:O	2:Q:147:GLN:HG3	2.18	0.44
2:Q:246:VAL:O	2:Q:250:GLU:HG3	2.16	0.44
2:W:101:ARG:O	2:W:105:ARG:HG3	2.16	0.44
2:W:162:TYR:HE1	2:X:165:VAL:CG1	2.30	0.44
3:a:243:LEU:HB2	4:b:107:VAL:HG12	1.99	0.44
5:c:98:SER:HB3	5:c:150:TYR:OH	2.17	0.44
1:A:207:GLU:C	1:A:210:ARG:HG2	2.43	0.44
1:D:207:GLU:O	1:D:210:ARG:HG2	2.18	0.44
1:D:227:MET:HA	1:D:255:PHE:CE1	2.53	0.44
1:N:154:ASP:O	1:N:155:SER:C	2.60	0.44
4:U:61:LEU:HD12	5:V:103:MET:HE3	1.98	0.44
4:U:152:ASP:OD1	4:U:153:ALA:N	2.51	0.44
5:V:88:ASP:HA	5:V:161:GLU:CD	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:210:GLN:O	2:W:214:TYR:CG	2.71	0.44
3:a:202:GLN:O	3:a:206:GLU:HG3	2.17	0.44
5:c:92:LYS:NZ	5:c:161:GLU:HA	2.32	0.44
1:C:188:TYR:CD1	1:C:266:PHE:HB3	2.51	0.44
1:K:56:ASP:OD1	1:K:56:ASP:N	2.50	0.44
2:P:143:ILE:O	2:P:146:ILE:HG22	2.17	0.44
2:P:210:GLN:O	2:P:214:TYR:CG	2.70	0.44
4:U:106:LYS:NZ	4:U:110:GLU:HG3	2.32	0.44
4:U:113:ASP:O	4:U:117:LYS:HG3	2.16	0.44
1:M:207:GLU:CA	1:M:210:ARG:HG2	2.45	0.44
4:U:132:ILE:HG22	4:U:136:ARG:HH11	1.82	0.44
4:U:147:VAL:HG23	5:V:83:ARG:HH22	1.81	0.44
5:V:21:LYS:HD2	5:V:21:LYS:HA	1.80	0.44
2:W:214:TYR:HB3	2:X:214:TYR:CB	2.47	0.44
3:a:232:LYS:HA	3:a:235:GLU:CD	2.42	0.44
5:c:24:PHE:HB2	5:c:77:PHE:CZ	2.53	0.44
1:B:192:ILE:CD1	1:B:256:ARG:HD3	2.47	0.44
2:Q:237:THR:O	2:Q:241:PHE:N	2.46	0.44
2:Q:257:GLU:HA	2:Q:257:GLU:OE1	2.18	0.44
5:V:90:LYS:NZ	5:V:92:LYS:HB3	2.33	0.44
3:a:110:PHE:CD1	3:a:110:PHE:C	2.94	0.44
4:b:112:TYR:HA	4:b:115:GLU:HB3	1.99	0.44
1:O:352:PHE:CG	1:O:352:PHE:O	2.71	0.44
3:a:221:ILE:HB	4:b:94:GLN:HA	2.00	0.44
4:b:59:GLN:HA	4:b:62:GLU:OE1	2.18	0.44
4:b:60:GLU:HA	4:b:63:ARG:CG	2.47	0.44
5:c:119:ILE:HA	5:c:122:GLN:OE1	2.18	0.44
1:F:227:MET:CB	1:F:255:PHE:HZ	2.30	0.44
2:P:218:GLU:OE1	2:Q:214:TYR:CE1	2.71	0.44
2:P:274:LEU:HD13	2:Q:274:LEU:HB3	1.98	0.44
4:b:98:ARG:HA	4:b:98:ARG:HD3	1.77	0.44
5:c:61:ILE:HG23	5:c:72:VAL:HG23	1.99	0.44
1:B:133:TYR:CG	1:B:352:PHE:CZ	3.06	0.44
1:C:287:ILE:O	1:C:290:ARG:HG2	2.18	0.44
1:H:227:MET:HA	1:H:255:PHE:CE1	2.53	0.44
1:M:80:ASP:OD2	1:M:84:LYS:NZ	2.51	0.44
4:U:54:LEU:HD22	5:V:92:LYS:HE2	2.00	0.44
2:W:218:GLU:OE1	2:X:214:TYR:CE1	2.71	0.44
3:a:219:LEU:HD23	4:b:98:ARG:CZ	2.47	0.44
4:b:162:ARG:HA	4:b:164:LYS:HZ3	1.83	0.44
4:b:162:ARG:HA	4:b:164:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:121:LEU:C	5:c:128:ILE:HG13	2.43	0.44
1:A:133:TYR:CE1	1:A:355:MET:HB3	2.53	0.43
1:A:207:GLU:O	1:A:210:ARG:HG3	2.17	0.43
1:B:335:ARG:C	1:B:337:TYR:N	2.76	0.43
1:J:332:PRO:O	1:J:335:ARG:HD3	2.17	0.43
3:a:268:ILE:HG13	4:b:132:ILE:HD11	1.99	0.43
4:b:161:ALA:O	4:b:164:LYS:HG3	2.18	0.43
5:c:73:ASP:OD1	5:c:74:PHE:N	2.51	0.43
1:B:207:GLU:O	1:B:210:ARG:HB3	2.18	0.43
1:B:332:PRO:C	1:B:334:GLU:N	2.76	0.43
1:F:139:VAL:HG23	1:F:140:LEU:HD23	2.00	0.43
2:P:214:TYR:HB3	2:Q:214:TYR:CB	2.48	0.43
3:T:257:GLN:HE22	4:U:122:ILE:HG13	1.83	0.43
5:V:40:GLU:HG3	5:V:43:LYS:HE2	2.00	0.43
5:V:150:TYR:O	5:V:154:LEU:HG	2.19	0.43
2:W:53:THR:HG22	2:X:57:LEU:HD12	2.01	0.43
5:c:45:MET:O	5:c:48:LEU:HB2	2.18	0.43
1:C:258:PRO:CG	1:C:306:TYR:CE2	2.98	0.43
1:G:154:ASP:O	1:G:155:SER:C	2.61	0.43
1:O:305:MET:SD	1:O:336:LYS:HD2	2.57	0.43
3:T:212:LEU:HD23	3:T:215:ARG:HH21	1.83	0.43
4:U:108:ASP:O	4:U:111:ARG:HG3	2.18	0.43
4:U:151:ALA:O	4:U:155:MET:HB2	2.18	0.43
1:A:302:GLY:C	1:A:304:THR:H	2.26	0.43
1:B:208:ILE:HD13	1:B:208:ILE:HA	1.79	0.43
1:J:311:ASP:CG	2:X:248:LYS:NZ	2.76	0.43
1:N:80:ASP:OD2	1:N:84:LYS:NZ	2.51	0.43
2:P:214:TYR:HB3	2:Q:214:TYR:HB2	2.00	0.43
3:T:241:TYR:CE2	4:U:76:LEU:HB3	2.53	0.43
4:U:66:GLU:HA	4:U:69:ARG:HG3	2.00	0.43
5:V:136:LEU:HD22	5:V:156:PHE:HE1	1.83	0.43
3:a:267:ARG:HB3	4:b:132:ILE:HG21	2.00	0.43
4:b:70:GLY:O	4:b:74:ARG:HG3	2.18	0.43
5:c:20:PHE:HA	5:c:23:ALA:HB3	2.00	0.43
1:G:335:ARG:O	1:G:337:TYR:N	2.47	0.43
1:I:302:GLY:C	1:I:304:THR:H	2.25	0.43
1:K:162:ASN:ND2	1:K:281:SER:OG	2.51	0.43
1:K:257:CYS:CB	1:K:258:PRO:HD3	2.48	0.43
3:T:229:LEU:HB3	4:U:93:LEU:HB3	2.01	0.43
4:U:63:ARG:HA	4:U:66:GLU:OE1	2.18	0.43
1:C:290:ARG:CG	1:E:244:ASP:CB	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:GLU:CD	1:H:115:ASN:HD22	2.27	0.43
1:J:169:TYR:HE1	1:L:49:GLN:CD	2.26	0.43
4:U:145:ARG:H	4:U:148:ARG:NH2	2.17	0.43
5:V:126:GLU:HG2	5:V:127:THR:H	1.82	0.43
2:X:257:GLU:HA	2:X:257:GLU:OE1	2.18	0.43
5:c:26:ILE:HA	5:c:29:LEU:HB2	2.00	0.43
1:H:83:GLU:O	1:H:87:HIS:CG	2.72	0.43
1:I:336:LYS:HG2	1:I:337:TYR:CD1	2.53	0.43
1:K:230:ALA:CB	1:K:255:PHE:CZ	3.02	0.43
1:N:31:PHE:CZ	1:N:93:GLU:HG2	2.54	0.43
3:T:247:LYS:HB2	4:U:111:ARG:HB3	2.01	0.43
4:U:165:GLU:HB3	5:V:16:GLN:NE2	2.31	0.43
2:W:214:TYR:HB3	2:X:214:TYR:HB2	2.00	0.43
3:a:265:ARG:HA	3:a:268:ILE:HD12	1.99	0.43
1:A:335:ARG:C	1:A:337:TYR:N	2.73	0.43
1:B:262:PHE:CE2	1:B:312:ARG:HG2	2.54	0.43
1:K:109:PRO:HD2	1:K:161:HIS:CD2	2.54	0.43
3:T:100:ASN:OD1	3:T:100:ASN:N	2.52	0.43
3:T:264:LEU:HD22	4:U:128:LEU:HB2	2.00	0.43
2:Z:13:LEU:O	2:Z:14:ASP:C	2.59	0.43
5:c:23:ALA:HB1	5:c:27:PHE:CZ	2.53	0.43
5:c:74:PHE:CZ	5:c:78:LEU:HD11	2.54	0.43
1:H:219:VAL:O	1:H:220:ALA:HB3	2.17	0.43
1:I:87:HIS:O	1:I:91:TYR:CD2	2.69	0.43
1:L:219:VAL:O	1:L:220:ALA:HB3	2.18	0.43
2:P:53:THR:HG22	2:Q:57:LEU:HD12	2.00	0.43
3:T:240:ILE:O	3:T:244:GLU:HG2	2.19	0.43
5:V:72:VAL:HA	5:V:76:GLU:OE1	2.18	0.43
2:X:232:LEU:O	2:X:236:GLU:N	2.47	0.43
3:a:254:PHE:HE1	4:b:117:LYS:O	2.00	0.43
5:c:111:TYR:HA	5:c:149:ASP:HA	2.00	0.43
1:D:56:ASP:OD1	1:D:56:ASP:N	2.50	0.43
1:N:334:GLU:O	1:N:338:SER:HB3	2.18	0.43
4:U:152:ASP:O	4:U:156:GLN:HG2	2.19	0.43
3:a:221:ILE:HG22	4:b:97:CYS:CB	2.49	0.43
4:b:135:LEU:HA	4:b:135:LEU:HD23	1.78	0.43
1:F:305:MET:HE2	1:F:335:ARG:C	2.44	0.42
1:F:334:GLU:OE1	1:F:334:GLU:N	2.49	0.42
1:J:133:TYR:CG	1:J:352:PHE:CZ	3.06	0.42
1:N:270:GLU:OE2	1:O:66:THR:HA	2.19	0.42
2:P:156:GLU:CD	2:P:160:ARG:NH2	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:237:THR:O	2:X:241:PHE:N	2.46	0.42
2:X:263:GLN:O	2:X:267:TYR:N	2.45	0.42
5:c:24:PHE:HA	5:c:27:PHE:HB2	2.00	0.42
5:c:141:ASP:OD2	5:c:145:ASP:N	2.52	0.42
1:F:334:GLU:O	1:F:338:SER:HB3	2.19	0.42
3:T:219:LEU:HB2	4:U:101:HIS:ND1	2.34	0.42
4:b:138:LYS:HE2	4:b:139:PHE:CE1	2.54	0.42
5:c:67:ASP:OD1	5:c:67:ASP:N	2.52	0.42
5:c:104:PHE:CD2	5:c:153:PHE:CE1	3.07	0.42
1:H:86:TRP:CZ3	1:H:122:ILE:HD13	2.53	0.42
1:H:302:GLY:C	1:H:304:THR:H	2.27	0.42
1:O:275:HIS:ND1	1:O:275:HIS:N	2.66	0.42
2:P:146:ILE:CG2	2:P:147:GLN:N	2.82	0.42
3:T:221:ILE:HG22	3:T:224:LEU:HD12	2.01	0.42
3:T:256:GLN:HB2	4:U:68:ARG:HH12	1.83	0.42
4:U:74:ARG:O	4:U:78:THR:HG23	2.20	0.42
4:b:130:GLN:NE2	4:b:134:ASP:OD1	2.53	0.42
5:c:101:PHE:CE2	5:c:150:TYR:HB2	2.55	0.42
1:L:285:CYS:O	1:L:290:ARG:NE	2.52	0.42
1:O:219:VAL:O	1:O:220:ALA:HB3	2.20	0.42
5:V:41:LEU:O	5:V:45:MET:HG2	2.19	0.42
5:V:65:ASP:OD2	5:V:69:SER:N	2.52	0.42
2:X:54:GLU:O	2:X:57:LEU:HB2	2.20	0.42
3:a:100:ASN:N	3:a:100:ASN:OD1	2.52	0.42
1:G:26:ALA:CA	1:G:340:TRP:CZ3	3.02	0.42
3:T:219:LEU:HD23	4:U:98:ARG:CZ	2.49	0.42
3:T:219:LEU:HD23	4:U:98:ARG:NE	2.34	0.42
5:V:121:LEU:O	5:V:128:ILE:HG13	2.19	0.42
3:a:250:LEU:HB3	4:b:114:ILE:HG22	2.02	0.42
1:F:23:GLY:O	4:U:144:LEU:O	2.38	0.42
3:T:110:PHE:CD1	3:T:110:PHE:C	2.94	0.42
4:U:138:LYS:H	4:U:141:ARG:HH22	1.67	0.42
2:W:144:GLN:O	2:W:148:LEU:N	2.53	0.42
2:X:162:TYR:O	2:X:166:ALA:N	2.52	0.42
3:a:200:LYS:HD2	3:a:201:ARG:HH21	1.84	0.42
3:a:261:ILE:HD13	4:b:124:GLU:OE1	2.19	0.42
4:b:63:ARG:HD2	4:b:64:GLU:N	2.34	0.42
1:F:3:ASP:OD1	1:F:3:ASP:N	2.41	0.42
1:F:154:ASP:O	1:F:155:SER:C	2.60	0.42
1:L:227:MET:CB	1:L:255:PHE:HZ	2.33	0.42
2:Q:50:LEU:O	2:Q:54:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:225:ASN:O	3:T:229:LEU:HG	2.20	0.42
3:T:234:LYS:HE2	4:U:83:LEU:HB2	2.01	0.42
5:V:104:PHE:CE1	5:V:120:MET:HE2	2.54	0.42
2:W:241:PHE:CD2	2:W:241:PHE:C	2.95	0.42
4:b:166:SER:OG	5:c:19:GLU:OE1	2.18	0.42
5:c:42:GLY:HA2	5:c:52:PRO:HG2	2.01	0.42
1:A:108:ALA:HB1	1:A:161:HIS:ND1	2.35	0.42
1:B:258:PRO:HB3	1:B:306:TYR:CZ	2.54	0.42
1:B:306:TYR:HB2	1:B:309:ILE:HB	2.02	0.42
1:F:6:THR:HG21	4:U:146:ARG:NH1	2.28	0.42
1:I:333:PRO:C	1:I:335:ARG:N	2.77	0.42
2:P:156:GLU:CG	2:P:160:ARG:NH2	2.81	0.42
4:U:43:ALA:HB3	5:V:6:LYS:CG	2.49	0.42
4:U:159:LEU:HG	4:U:162:ARG:HB2	2.02	0.42
5:V:126:GLU:O	5:V:128:ILE:HG12	2.20	0.42
1:E:169:TYR:HH	1:G:49:GLN:HB3	1.81	0.42
1:F:51:ASP:CG	1:F:52:SER:N	2.78	0.42
1:L:154:ASP:O	1:L:155:SER:C	2.63	0.42
2:Q:277:ALA:O	2:Q:281:MET:N	2.40	0.42
2:S:13:LEU:O	2:S:14:ASP:C	2.59	0.42
3:a:248:PHE:HA	3:a:251:GLN:OE1	2.20	0.42
4:b:137:GLY:HA2	4:b:140:LYS:CB	2.50	0.42
5:c:80:MET:HA	5:c:83:ARG:HD3	2.02	0.42
5:c:101:PHE:O	5:c:105:ASP:N	2.37	0.42
5:c:107:ASN:ND2	5:c:113:ASP:HB2	2.35	0.42
5:c:121:LEU:HD23	5:c:124:THR:HG21	2.02	0.42
1:A:335:ARG:H	1:A:335:ARG:HG2	1.60	0.42
1:J:169:TYR:CZ	1:L:49:GLN:HG3	2.55	0.42
1:L:107:GLU:OE1	1:L:116:ARG:HB3	2.20	0.42
2:Q:162:TYR:O	2:Q:166:ALA:N	2.52	0.42
3:T:216:ARG:HA	4:U:105:ASP:CG	2.45	0.42
3:a:225:ASN:O	3:a:229:LEU:HB2	2.20	0.42
1:B:219:VAL:O	1:B:220:ALA:HB3	2.19	0.41
1:F:139:VAL:CG2	1:F:140:LEU:H	2.29	0.41
1:F:219:VAL:O	1:F:220:ALA:HB3	2.19	0.41
1:G:51:ASP:CG	1:G:52:SER:N	2.78	0.41
1:O:154:ASP:O	1:O:156:GLY:N	2.51	0.41
1:O:212:ILE:HG12	1:O:240:TYR:CD2	2.55	0.41
2:P:156:GLU:CD	2:P:160:ARG:HH22	2.28	0.41
2:Q:54:GLU:O	2:Q:57:LEU:HB2	2.20	0.41
3:T:237:TRP:NE1	4:U:80:CYS:SG	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:56:ILE:HA	4:U:56:ILE:HD13	1.86	0.41
5:V:113:ASP:HB3	5:V:116:GLU:OE1	2.20	0.41
3:a:204:GLU:HA	3:a:207:LYS:HB2	2.02	0.41
3:a:268:ILE:HA	3:a:271:ASN:HD22	1.84	0.41
4:b:43:ALA:HB2	5:c:3:ASP:HB3	2.02	0.41
5:c:92:LYS:NZ	5:c:160:VAL:O	2.48	0.41
5:c:97:LEU:O	5:c:153:PHE:HE2	2.03	0.41
1:D:51:ASP:CG	1:D:52:SER:N	2.78	0.41
1:D:207:GLU:OE1	1:D:210:ARG:HD3	2.20	0.41
1:L:143:TYR:OH	1:N:44:MET:CB	2.43	0.41
1:M:305:MET:SD	1:M:335:ARG:CD	3.07	0.41
1:N:56:ASP:OD1	1:N:56:ASP:N	2.51	0.41
4:U:43:ALA:HB3	5:V:6:LYS:HG3	2.01	0.41
4:U:53:LEU:HD22	5:V:104:PHE:HZ	1.85	0.41
5:V:122:GLN:HA	5:V:128:ILE:HG21	2.02	0.41
3:a:215:ARG:HD3	4:b:108:ASP:CG	2.45	0.41
3:a:261:ILE:HG12	3:a:264:LEU:HD12	2.01	0.41
4:b:57:ALA:C	5:c:100:LEU:HD22	2.45	0.41
4:b:144:LEU:HB3	4:b:148:ARG:HH22	1.85	0.41
1:A:34:ILE:HD11	1:A:69:TYR:OH	2.20	0.41
1:G:335:ARG:C	1:G:337:TYR:N	2.79	0.41
1:J:207:GLU:O	1:J:210:ARG:HG3	2.20	0.41
1:O:287:ILE:HA	1:O:290:ARG:HD3	2.02	0.41
3:T:234:LYS:NZ	4:U:83:LEU:H	2.19	0.41
4:U:63:ARG:HD2	4:U:64:GLU:N	2.36	0.41
5:c:20:PHE:CE1	5:c:81:MET:HB3	2.55	0.41
5:c:97:LEU:HD11	5:c:157:MET:O	2.20	0.41
1:B:250:ILE:CG2	1:B:254:ARG:CG	2.98	0.41
1:C:227:MET:HB3	1:C:255:PHE:CE2	2.55	0.41
1:E:51:ASP:CG	1:E:52:SER:N	2.78	0.41
1:E:56:ASP:OD1	1:E:56:ASP:N	2.53	0.41
1:F:143:TYR:OH	1:H:44:MET:CA	2.68	0.41
1:M:162:ASN:ND2	1:M:281:SER:OG	2.53	0.41
2:P:142:GLU:O	2:P:146:ILE:HG22	2.19	0.41
2:P:267:TYR:HB2	2:Q:267:TYR:HB3	2.02	0.41
4:U:57:ALA:HB3	5:V:100:LEU:HD22	2.02	0.41
4:U:137:GLY:HA3	4:U:141:ARG:NH2	2.33	0.41
5:V:106:LYS:HB2	5:V:116:GLU:HG3	2.02	0.41
2:W:148:LEU:HD21	2:W:152:LYS:CE	2.46	0.41
2:X:50:LEU:O	2:X:54:GLU:N	2.52	0.41
3:a:247:LYS:HB2	3:a:247:LYS:HE2	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ARG:HD3	1:E:244:ASP:CG	2.38	0.41
1:F:143:TYR:HE1	1:H:47:MET:HE3	1.85	0.41
1:F:162:ASN:ND2	1:F:277:THR:OG1	2.54	0.41
1:I:275:HIS:ND1	1:I:275:HIS:N	2.67	0.41
1:J:116:ARG:HD2	1:J:371:HIS:CE1	2.56	0.41
1:L:113:LYS:O	1:L:116:ARG:HG2	2.20	0.41
1:L:326:LYS:HE2	2:Y:23:GLU:OE2	2.21	0.41
4:b:48:GLN:HA	4:b:51:THR:HG22	2.02	0.41
1:B:51:ASP:CG	1:B:52:SER:N	2.79	0.41
1:B:192:ILE:HD11	1:B:256:ARG:HD3	2.01	0.41
1:C:51:ASP:CG	1:C:52:SER:N	2.79	0.41
1:D:275:HIS:ND1	1:D:275:HIS:N	2.63	0.41
1:H:107:GLU:OE1	1:H:116:ARG:HB3	2.20	0.41
1:L:109:PRO:CD	1:L:161:HIS:NE2	2.80	0.41
4:U:95:ASP:OD1	4:U:99:GLN:NE2	2.54	0.41
5:V:121:LEU:HB3	5:V:128:ILE:HD12	2.03	0.41
4:b:58:LYS:HG3	4:b:62:GLU:OE2	2.20	0.41
4:b:84:GLU:OE1	4:b:84:GLU:N	2.53	0.41
1:A:301:GLY:C	1:A:336:LYS:HA	2.45	0.41
1:F:2:GLU:OE1	1:F:21:PHE:CD2	2.71	0.41
1:I:87:HIS:NE2	1:I:91:TYR:CE2	2.85	0.41
1:I:219:VAL:O	1:I:220:ALA:HB3	2.21	0.41
1:J:275:HIS:CG	1:J:276:GLU:N	2.88	0.41
1:O:207:GLU:OE1	1:O:210:ARG:HD3	2.21	0.41
5:V:97:LEU:HD23	5:V:100:LEU:HD12	2.01	0.41
2:X:277:ALA:O	2:X:281:MET:N	2.40	0.41
3:a:221:ILE:HG22	4:b:97:CYS:HB3	2.01	0.41
4:b:133:PHE:CA	4:b:136:ARG:HD3	2.49	0.41
5:c:72:VAL:HG22	5:c:80:MET:CE	2.51	0.41
5:c:107:ASN:ND2	5:c:113:ASP:OD2	2.49	0.41
5:c:142:LYS:HD3	5:c:142:LYS:HA	1.84	0.41
1:F:159:VAL:HG21	1:F:177:ARG:NE	2.34	0.41
1:M:335:ARG:C	1:M:337:TYR:N	2.78	0.41
1:O:56:ASP:OD1	1:O:56:ASP:N	2.48	0.41
1:O:302:GLY:C	1:O:304:THR:H	2.29	0.41
2:Q:263:GLN:O	2:Q:267:TYR:HB2	2.21	0.41
2:Q:263:GLN:O	2:Q:267:TYR:N	2.45	0.41
3:T:240:ILE:HG12	4:U:103:ARG:HG3	2.03	0.41
3:T:241:TYR:CZ	4:U:76:LEU:HB3	2.55	0.41
4:U:58:LYS:NZ	5:V:96:GLU:OE1	2.48	0.41
5:V:3:ASP:OD1	5:V:4:ILE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:128:ILE:HA	5:V:128:ILE:HD13	1.85	0.41
1:A:333:PRO:C	1:A:335:ARG:N	2.74	0.41
1:C:207:GLU:O	1:C:210:ARG:HG2	2.19	0.41
1:F:227:MET:HB3	1:F:255:PHE:CZ	2.56	0.41
1:G:219:VAL:O	1:G:220:ALA:HB3	2.20	0.41
1:I:86:TRP:HE3	1:I:122:ILE:CD1	2.28	0.41
1:K:275:HIS:ND1	1:K:275:HIS:N	2.64	0.41
1:N:51:ASP:OD1	1:N:51:ASP:N	2.49	0.41
3:T:240:ILE:HA	4:U:107:VAL:HG11	2.03	0.41
3:T:264:LEU:HA	3:T:267:ARG:HD3	2.01	0.41
4:U:50:LYS:O	4:U:54:LEU:HG	2.21	0.41
5:V:141:ASP:OD2	5:V:145:ASP:N	2.54	0.41
3:a:200:LYS:HD2	3:a:201:ARG:NH2	2.35	0.41
3:a:202:GLN:OE1	3:a:205:ARG:NE	2.50	0.41
4:b:50:LYS:HB2	5:c:160:VAL:HG21	2.02	0.41
4:b:52:LEU:HA	4:b:55:GLN:CD	2.45	0.41
5:c:74:PHE:CE2	5:c:78:LEU:HD11	2.56	0.41
1:B:250:ILE:HG22	1:B:254:ARG:CG	2.44	0.41
1:J:56:ASP:OD1	1:J:56:ASP:N	2.52	0.41
2:P:152:LYS:HE3	5:c:54:PRO:CG	2.50	0.41
3:T:203:THR:HG22	3:T:207:LYS:HD2	2.02	0.41
2:X:175:ASP:O	2:X:179:ALA:N	2.47	0.41
2:X:263:GLN:O	2:X:267:TYR:HB2	2.21	0.41
3:a:221:ILE:HD13	4:b:98:ARG:HG2	2.02	0.41
5:c:46:ARG:HA	5:c:50:GLN:O	2.21	0.41
1:A:283:MET:O	1:A:290:ARG:NE	2.54	0.40
1:G:263:GLN:N	1:G:264:PRO:HD3	2.36	0.40
1:O:335:ARG:H	1:O:335:ARG:HG2	1.69	0.40
3:T:215:ARG:HH12	4:U:112:TYR:HB2	1.86	0.40
3:T:237:TRP:NE1	4:U:80:CYS:HG	2.19	0.40
4:U:53:LEU:HD21	5:V:121:LEU:HG	2.02	0.40
1:A:107:GLU:OE2	1:A:116:ARG:NE	2.48	0.40
1:F:287:ILE:H	1:F:287:ILE:HD13	1.85	0.40
1:L:335:ARG:C	1:L:337:TYR:H	2.29	0.40
1:M:155:SER:OG	1:M:303:THR:OG1	2.34	0.40
4:U:70:GLY:O	4:U:74:ARG:HG3	2.21	0.40
2:W:165:VAL:HG13	2:X:165:VAL:HG23	2.03	0.40
3:a:224:LEU:HD12	3:a:224:LEU:H	1.86	0.40
4:b:60:GLU:HB2	5:c:103:MET:HB3	2.02	0.40
5:c:120:MET:O	5:c:124:THR:HG23	2.21	0.40
1:B:218:TYR:HB2	1:B:307:PRO:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ILE:O	1:C:293:LEU:HG	2.21	0.40
1:D:176:MET:HB2	1:D:277:THR:OG1	2.21	0.40
1:D:335:ARG:C	1:D:337:TYR:N	2.80	0.40
1:E:109:PRO:CB	1:E:161:HIS:NE2	2.84	0.40
1:E:257:CYS:CB	1:E:258:PRO:HD3	2.49	0.40
1:G:6:THR:OG1	1:G:7:ALA:N	2.54	0.40
1:K:133:TYR:CE1	1:K:355:MET:HB3	2.57	0.40
1:L:107:GLU:OE2	1:L:116:ARG:NE	2.46	0.40
4:U:56:ILE:O	4:U:60:GLU:HG2	2.21	0.40
3:a:229:LEU:HD13	4:b:93:LEU:HB2	2.03	0.40
4:b:58:LYS:HD3	4:b:58:LYS:HA	1.73	0.40
1:C:185:LEU:HD13	1:C:306:TYR:OH	2.21	0.40
1:C:303:THR:O	1:C:306:TYR:HD1	2.04	0.40
1:F:162:ASN:ND2	1:F:281:SER:OG	2.54	0.40
1:F:335:ARG:C	1:F:337:TYR:N	2.80	0.40
2:P:165:VAL:HG13	2:Q:165:VAL:HG23	2.03	0.40
2:X:134:ALA:O	2:X:138:GLU:N	2.49	0.40
3:a:267:ARG:HG2	5:c:151:ASP:OD2	2.21	0.40
5:c:28:VAL:HG11	5:c:34:GLY:O	2.22	0.40
5:c:45:MET:HA	5:c:48:LEU:HB2	2.04	0.40
5:c:103:MET:O	5:c:106:LYS:HG2	2.21	0.40
5:c:149:ASP:OD1	5:c:150:TYR:N	2.52	0.40
1:A:219:VAL:O	1:A:220:ALA:HB3	2.22	0.40
1:F:21:PHE:CE1	1:F:28:ARG:NE	2.86	0.40
1:I:87:HIS:NE2	1:I:91:TYR:CD2	2.89	0.40
4:U:53:LEU:HD22	5:V:104:PHE:CZ	2.56	0.40
5:V:152:GLU:O	5:V:156:PHE:HB2	2.22	0.40
3:a:261:ILE:HD13	4:b:124:GLU:CD	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	373/375 (100%)	361 (97%)	10 (3%)	2 (0%)	24	63
1	B	373/375 (100%)	360 (96%)	9 (2%)	4 (1%)	11	46
1	C	373/375 (100%)	362 (97%)	7 (2%)	4 (1%)	11	46
1	D	373/375 (100%)	361 (97%)	10 (3%)	2 (0%)	24	63
1	E	373/375 (100%)	363 (97%)	7 (2%)	3 (1%)	16	54
1	F	373/375 (100%)	361 (97%)	7 (2%)	5 (1%)	9	42
1	G	373/375 (100%)	358 (96%)	13 (4%)	2 (0%)	24	63
1	H	373/375 (100%)	362 (97%)	8 (2%)	3 (1%)	16	54
1	I	373/375 (100%)	361 (97%)	9 (2%)	3 (1%)	16	54
1	J	373/375 (100%)	357 (96%)	13 (4%)	3 (1%)	16	54
1	K	373/375 (100%)	358 (96%)	13 (4%)	2 (0%)	24	63
1	L	373/375 (100%)	360 (96%)	11 (3%)	2 (0%)	24	63
1	M	373/375 (100%)	362 (97%)	9 (2%)	2 (0%)	24	63
1	N	373/375 (100%)	363 (97%)	8 (2%)	2 (0%)	24	63
1	O	373/375 (100%)	359 (96%)	12 (3%)	2 (0%)	24	63
2	P	272/286 (95%)	272 (100%)	0	0	100	100
2	Q	272/286 (95%)	272 (100%)	0	0	100	100
2	R	27/286 (9%)	27 (100%)	0	0	100	100
2	S	27/286 (9%)	27 (100%)	0	0	100	100
2	W	272/286 (95%)	272 (100%)	0	0	100	100
2	X	272/286 (95%)	272 (100%)	0	0	100	100
2	Y	27/286 (9%)	27 (100%)	0	0	100	100
2	Z	27/286 (9%)	27 (100%)	0	0	100	100
3	T	122/186 (66%)	121 (99%)	1 (1%)	0	100	100
3	a	122/186 (66%)	120 (98%)	2 (2%)	0	100	100
4	U	124/170 (73%)	120 (97%)	4 (3%)	0	100	100
4	b	124/170 (73%)	115 (93%)	9 (7%)	0	100	100
5	V	158/160 (99%)	149 (94%)	9 (6%)	0	100	100
5	c	158/160 (99%)	139 (88%)	19 (12%)	0	100	100
All	All	7599/8945 (85%)	7368 (97%)	190 (2%)	41 (0%)	26	63

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	155	SER
1	J	155	SER
1	L	155	SER
1	M	155	SER
1	O	155	SER
1	D	360	GLN
1	E	360	GLN
1	I	360	GLN
1	J	360	GLN
1	D	155	SER
1	L	334	GLU
1	A	220	ALA
1	A	336	LYS
1	B	49	GLN
1	C	334	GLU
1	C	336	LYS
1	F	220	ALA
1	F	334	GLU
1	F	336	LYS
1	H	220	ALA
1	H	334	GLU
1	H	336	LYS
1	K	336	LYS
1	N	336	LYS
1	B	336	LYS
1	C	220	ALA
1	F	5	THR
1	I	49	GLN
1	I	336	LYS
1	J	220	ALA
1	K	334	GLU
1	O	220	ALA
1	B	220	ALA
1	B	307	PRO
1	C	49	GLN
1	E	49	GLN
1	F	49	GLN
1	G	49	GLN
1	M	49	GLN
1	N	49	GLN
1	G	26	ALA

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%)	317 (100%)	1 (0%)	86	86
1	B	318/318 (100%)	313 (98%)	5 (2%)	55	70
1	C	318/318 (100%)	317 (100%)	1 (0%)	86	86
1	D	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	E	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	F	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	G	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	H	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	I	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	J	318/318 (100%)	316 (99%)	2 (1%)	78	83
1	K	318/318 (100%)	317 (100%)	1 (0%)	86	86
1	L	318/318 (100%)	317 (100%)	1 (0%)	86	86
1	M	318/318 (100%)	317 (100%)	1 (0%)	86	86
1	N	318/318 (100%)	318 (100%)	0	100	100
1	O	318/318 (100%)	315 (99%)	3 (1%)	70	79
2	P	236/246 (96%)	236 (100%)	0	100	100
2	Q	236/246 (96%)	236 (100%)	0	100	100
2	R	24/246 (10%)	24 (100%)	0	100	100
2	S	24/246 (10%)	24 (100%)	0	100	100
2	W	236/246 (96%)	236 (100%)	0	100	100
2	X	236/246 (96%)	236 (100%)	0	100	100
2	Y	24/246 (10%)	24 (100%)	0	100	100
2	Z	24/246 (10%)	24 (100%)	0	100	100
3	T	117/169 (69%)	116 (99%)	1 (1%)	70	79
3	a	117/169 (69%)	117 (100%)	0	100	100
4	U	106/145 (73%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	b	106/145 (73%)	106 (100%)	0	100	100
5	V	141/141 (100%)	141 (100%)	0	100	100
5	c	141/141 (100%)	140 (99%)	1 (1%)	76	81
All	All	6538/7648 (86%)	6509 (100%)	29 (0%)	81	84

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	LYS
1	B	208	ILE
1	B	287	ILE
1	B	306	TYR
1	B	335	ARG
1	B	336	LYS
1	C	336	LYS
1	D	116	ARG
1	D	336	LYS
1	E	335	ARG
1	E	336	LYS
1	F	287	ILE
1	F	335	ARG
1	G	335	ARG
1	G	336	LYS
1	H	177	ARG
1	H	336	LYS
1	I	287	ILE
1	I	336	LYS
1	J	335	ARG
1	J	336	LYS
1	K	277	THR
1	L	336	LYS
1	M	336	LYS
1	O	163	VAL
1	O	213	LYS
1	O	336	LYS
3	T	263	VAL
5	c	115	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	B	49	GLN
1	B	263	GLN
1	C	111	ASN
1	D	353	GLN
1	D	371	HIS
1	E	40	HIS
1	E	246	GLN
1	E	371	HIS
1	F	162	ASN
1	F	371	HIS
1	H	87	HIS
1	H	115	ASN
1	H	296	ASN
1	I	87	HIS
1	I	111	ASN
1	J	121	GLN
1	K	111	ASN
1	L	87	HIS
1	L	88	HIS
1	L	92	ASN
1	L	111	ASN
1	M	161	HIS
1	N	162	ASN
1	O	49	GLN
1	O	128	ASN
1	O	162	ASN
1	O	371	HIS
2	Q	47	GLN
3	T	202	GLN
3	T	238	GLN
3	T	242	ASN
3	T	269	ASN
3	T	272	GLN
4	U	99	GLN
4	U	130	GLN
5	V	107	ASN
5	V	143	ASN
2	X	47	GLN
3	a	225	ASN
3	a	228	GLN
3	a	266	ASN
3	a	269	ASN

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Mol	Chain	Res	Type
3	a	271	ASN
4	b	94	GLN
4	b	121	ASN
4	b	130	GLN
4	b	156	GLN
5	c	107	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

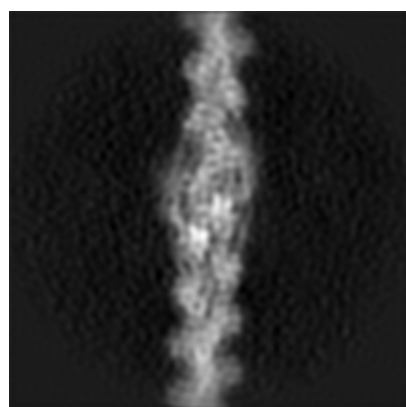
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22965. These allow visual inspection of the internal detail of the map and identification of artifacts.

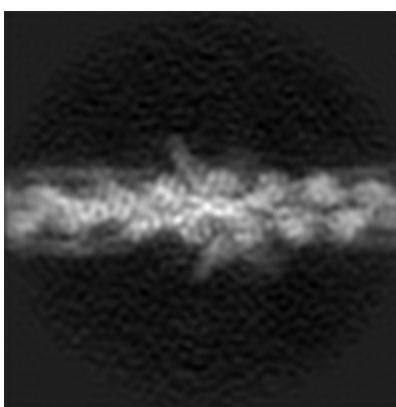
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

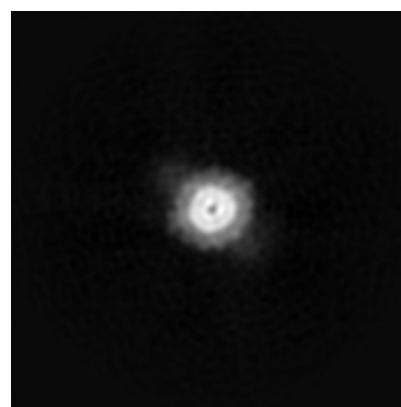
6.1.1 Primary map



X



Y



Z

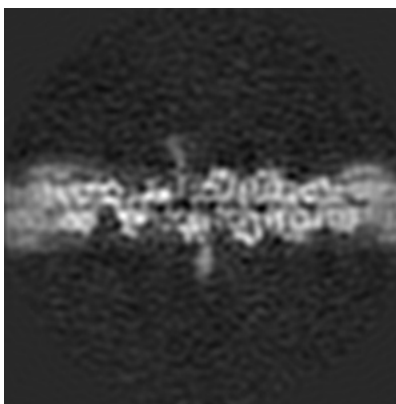
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

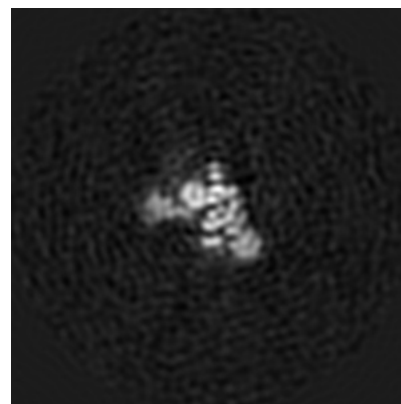
6.2.1 Primary map



X Index: 81



Y Index: 81

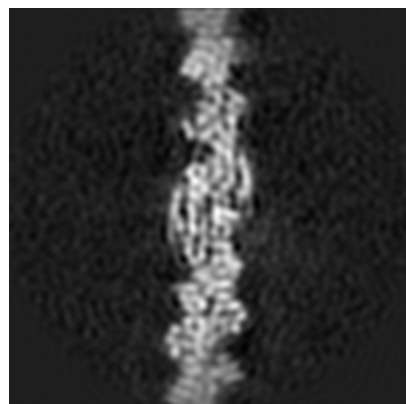


Z Index: 81

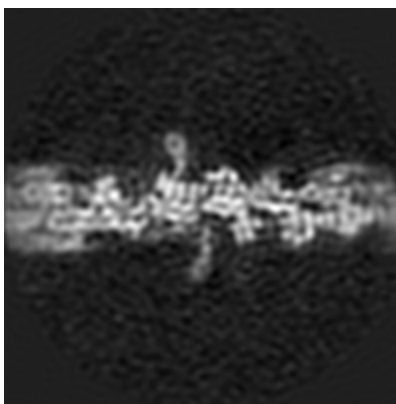
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

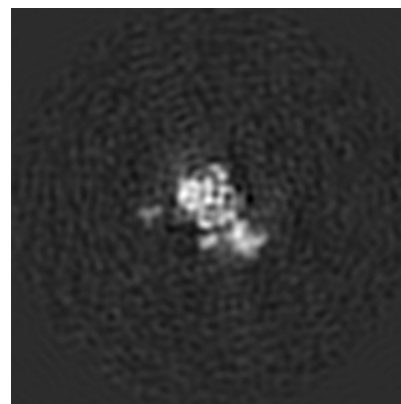
6.3.1 Primary map



X Index: 79



Y Index: 78

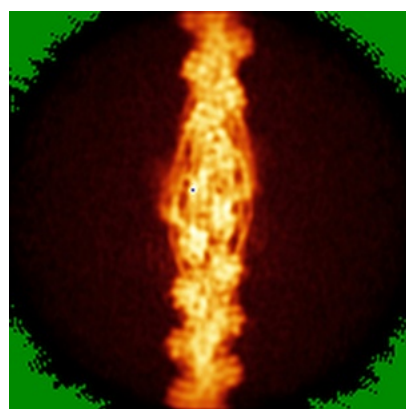


Z Index: 77

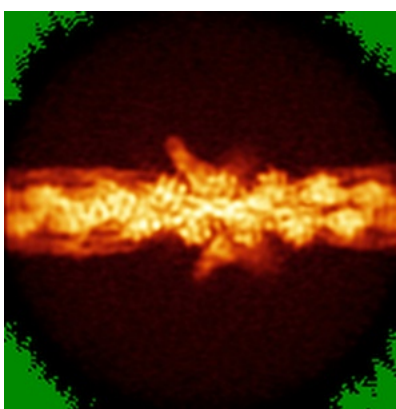
The images above show the largest variance slices of the map in three orthogonal directions.

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

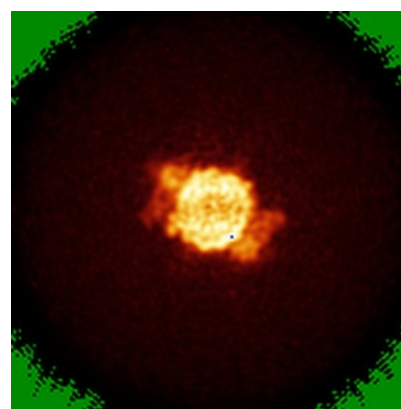
6.4.1 Primary map



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

This section was not generated.

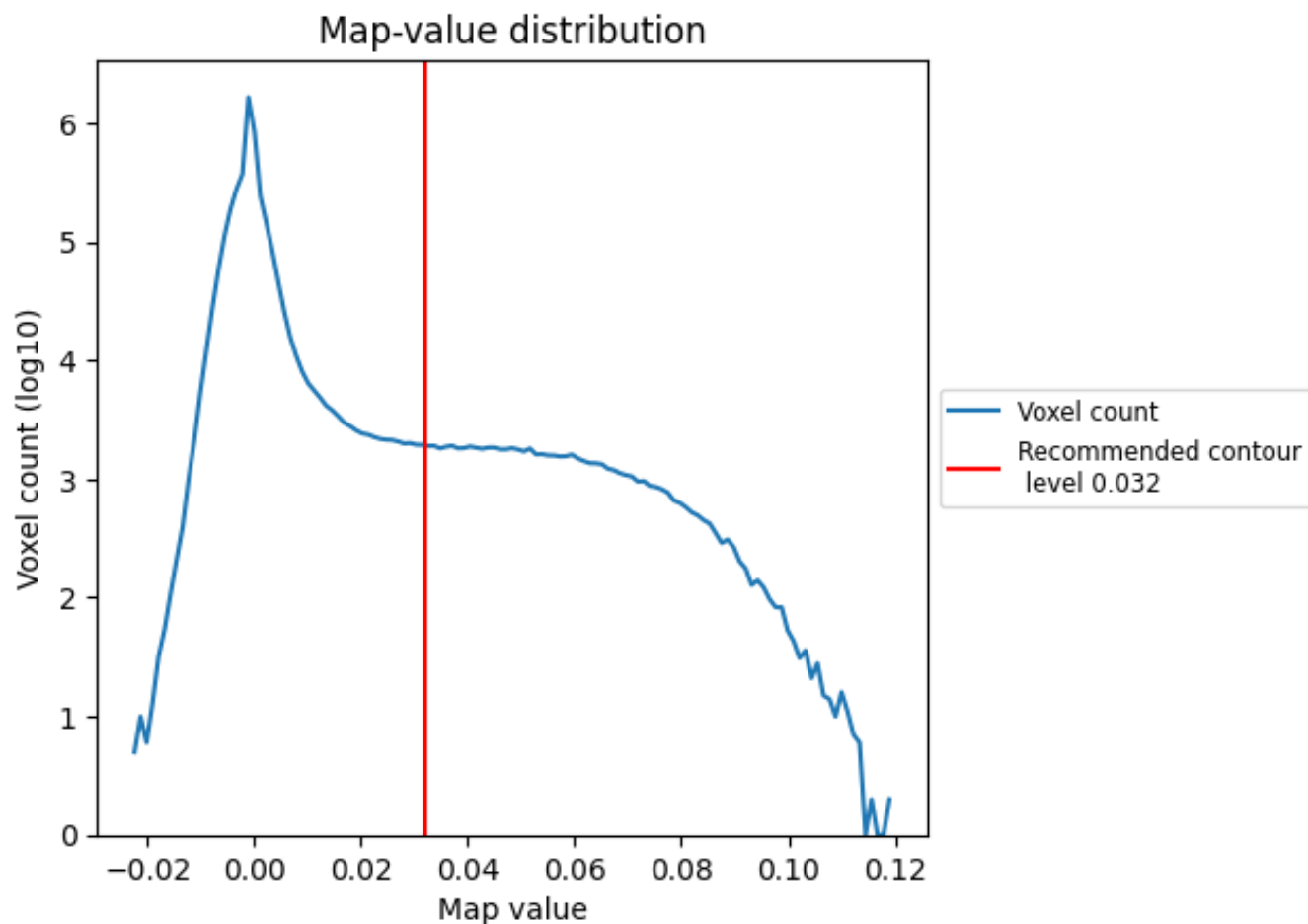
6.6 Mask visualisation

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

7 Map analysis [i](#)

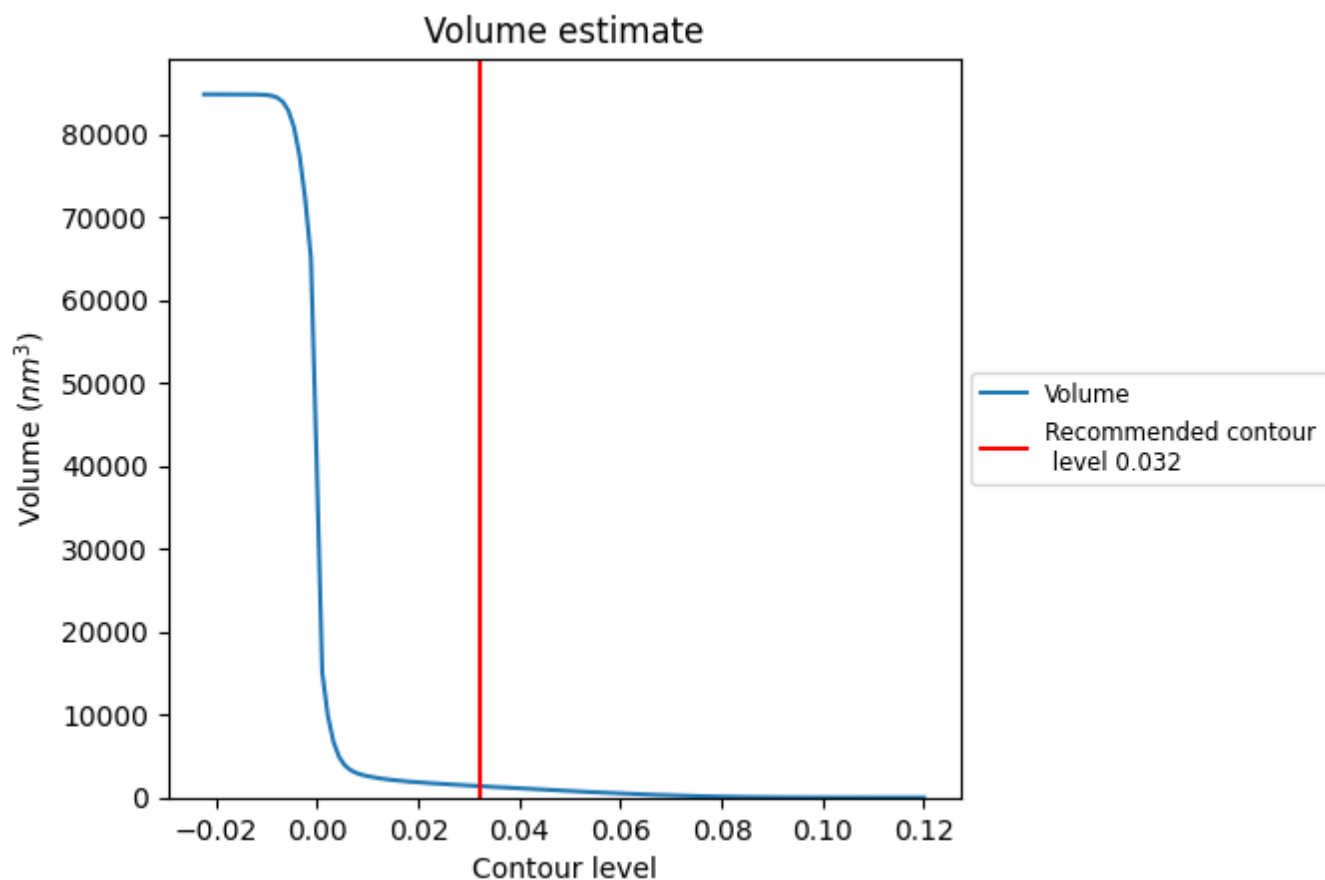
This section contains the results of statistical analysis of the map.

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.

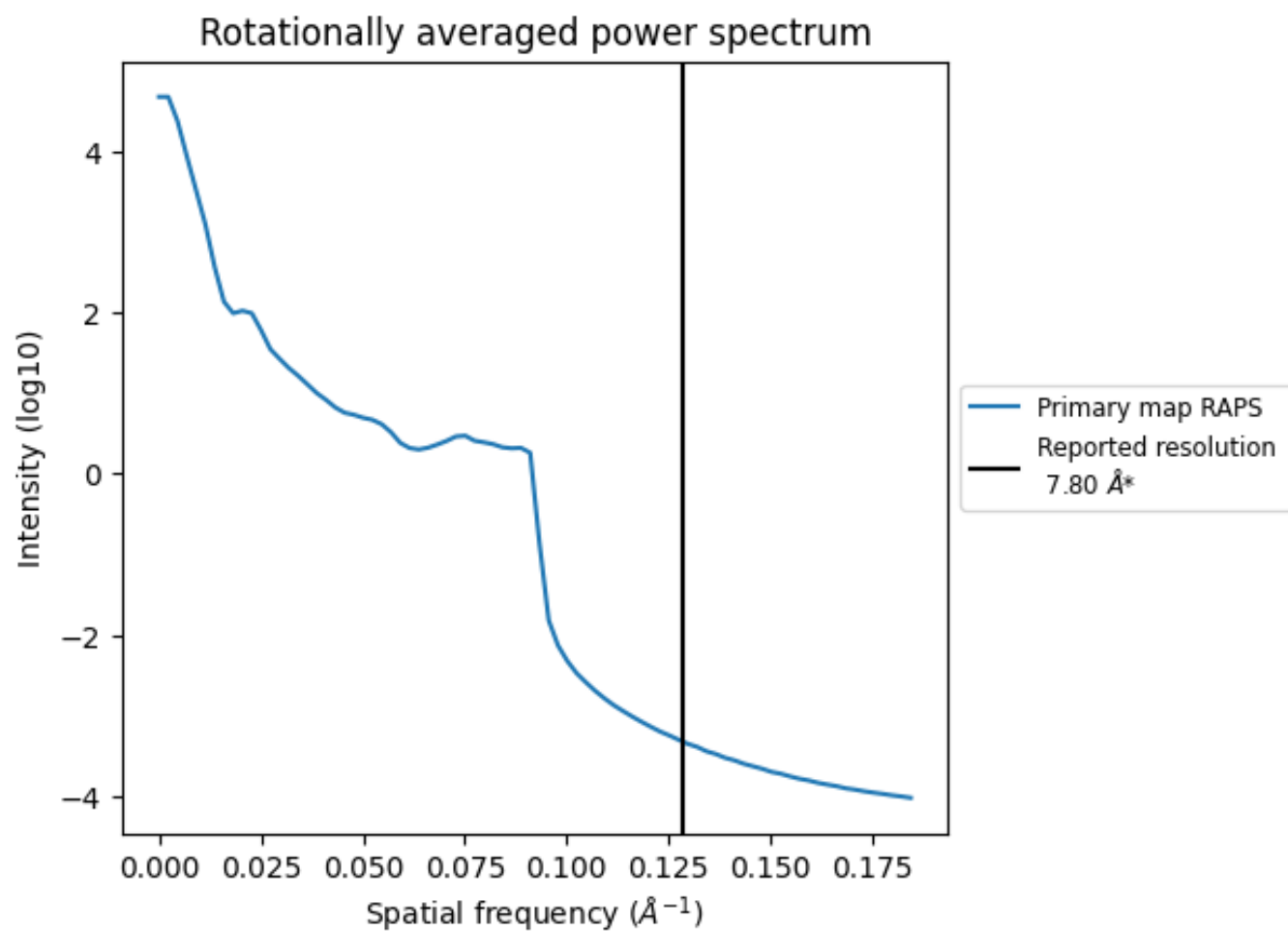
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1379 nm³; this corresponds to an approximate mass of 1246 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 ⓘ

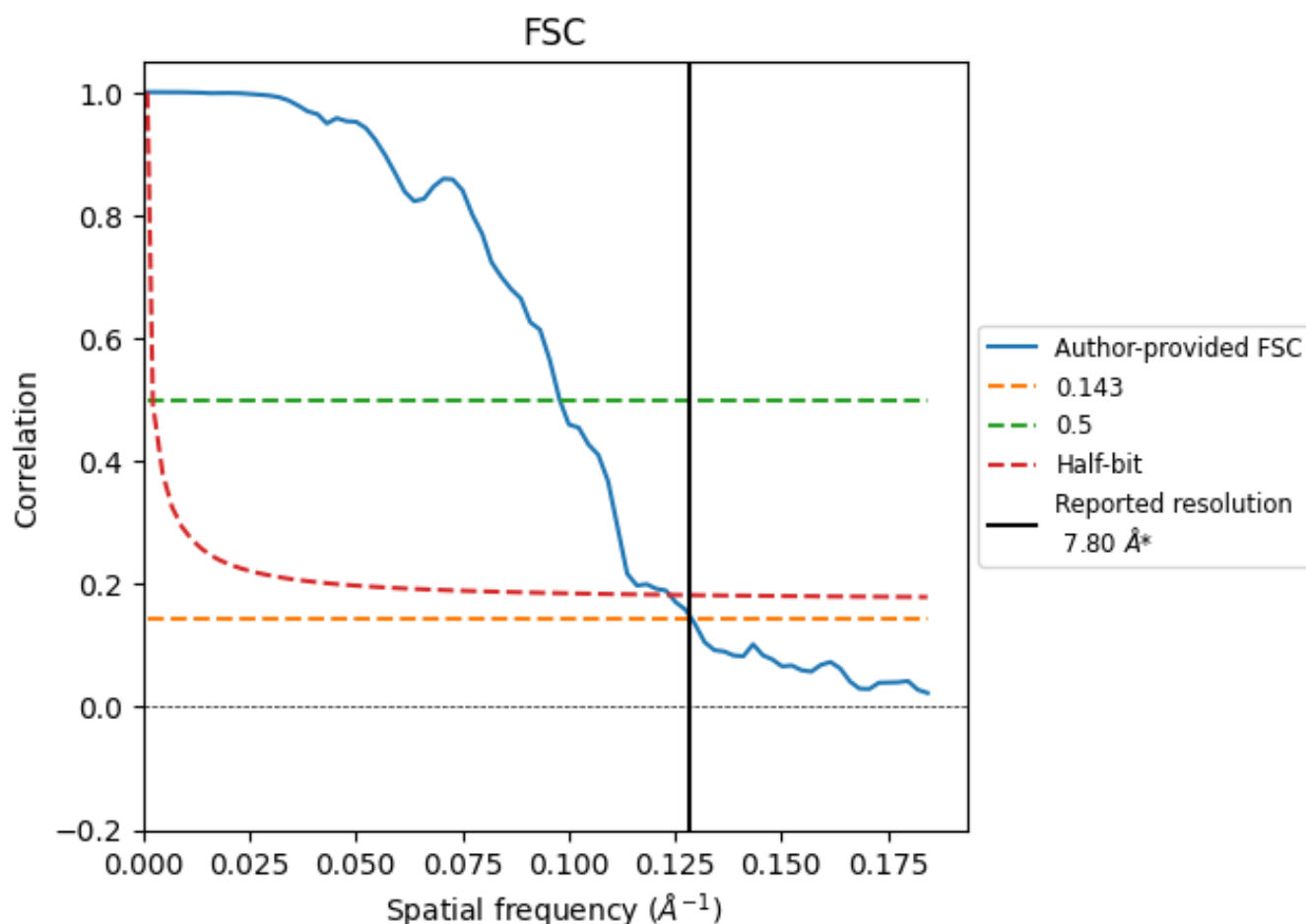


*Reported resolution corresponds to spatial frequency of 0.128 Å⁻¹

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 0.128 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.80	-	-
Author-provided FSC curve	7.75	10.21	8.08
Unmasked-calculated*	-	-	-

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

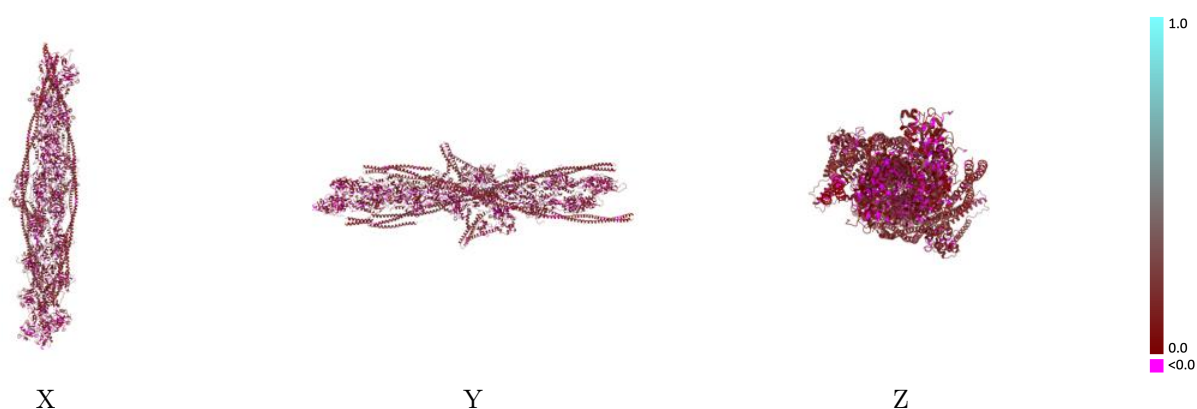
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22965 and PDB model 7KO5. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

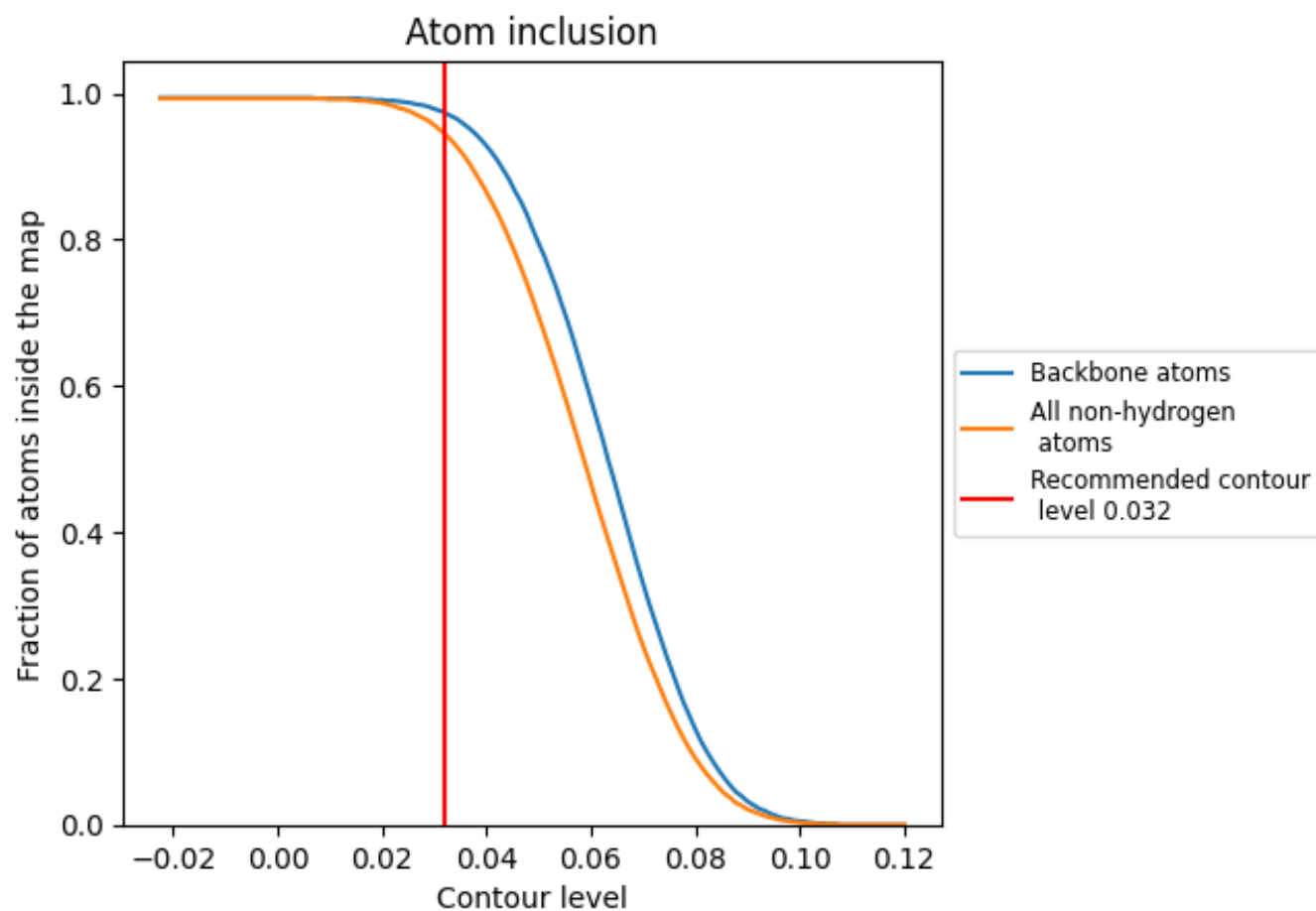


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9450	 0.1130
A	 0.9470	 0.0870
B	 0.9910	 0.1020
C	 0.9890	 0.1040
D	 0.9790	 0.1010
E	 0.9710	 0.1040
F	 0.9650	 0.1080
G	 0.9670	 0.1140
H	 0.9760	 0.1020
I	 0.9750	 0.1030
J	 0.9800	 0.1010
K	 0.9810	 0.1070
L	 0.9620	 0.1030
M	 0.9840	 0.0950
N	 0.9680	 0.0930
O	 0.8800	 0.0600
P	 0.8970	 0.1560
Q	 0.9020	 0.1530
R	 0.9870	 0.1600
S	 0.8650	 0.1060
T	 0.8370	 0.1640
U	 0.8780	 0.1490
V	 0.9040	 0.1260
W	 0.8610	 0.1530
X	 0.8210	 0.1250
Y	 0.9390	 0.1790
Z	 0.9610	 0.1660
a	 0.8480	 0.1560
b	 0.9870	 0.1780
c	 0.9120	 0.1470

