



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:09 PM UTC

PDB ID : 2C2V / pdb_00002c2v
Title : Crystal structure of the CHIP-UBC13-UEV1a complex
Authors : Zhang, M.; Roe, S.M.; Pearl, L.H.
Deposited on : 2005-09-30
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

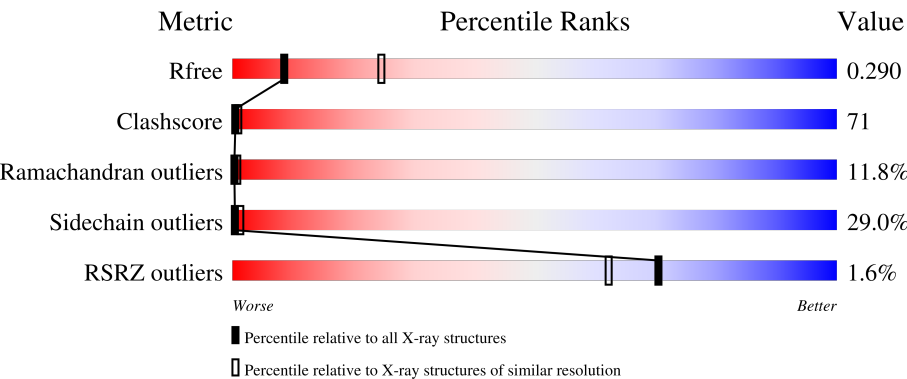
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	154	2% 29%47%21%
1	E	154	3% 8%23%45%20%
1	H	154	% 21%53%19%
1	K	154	3% 25%43%27%
2	C	142	4% 36%45%18%

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Mol	Chain	Length	Quality of chain
2	F	142	%6%30%42%20%.
2	I	142	•31%35%29%.
2	L	142	%7%28%40%23%.
3	S	78	•13%46%33%.
3	T	78	3%•24%44%29%
3	U	78	•19%54%19%6%
3	V	78	•19%31%40%9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11636 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Ubiquitin-conjugating enzyme E2 N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	152	Total	C	N	O	S	0	0	0
			1202	769	208	221	4			
1	E	149	Total	C	N	O	S	0	0	0
			1187	761	205	217	4			
1	H	149	Total	C	N	O	S	0	0	0
			1187	761	205	217	4			
1	K	152	Total	C	N	O	S	0	0	0
			1202	769	208	221	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	ALA	-	expression tag	UNP P61088
B	4	GLY	-	expression tag	UNP P61088
B	5	SER	-	expression tag	UNP P61088
E	3	ALA	-	expression tag	UNP P61088
E	4	GLY	-	expression tag	UNP P61088
E	5	SER	-	expression tag	UNP P61088
H	3	ALA	-	expression tag	UNP P61088
H	4	GLY	-	expression tag	UNP P61088
H	5	SER	-	expression tag	UNP P61088
K	3	ALA	-	expression tag	UNP P61088
K	4	GLY	-	expression tag	UNP P61088
K	5	SER	-	expression tag	UNP P61088

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 variant 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	142	Total	C	N	O	S	0	0	0
			1123	709	195	211	8			
2	F	139	Total	C	N	O	S	0	0	0
			1109	701	192	208	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	139	Total	C	N	O	S	0	0	0
			1109	701	192	208	8			
2	L	139	Total	C	N	O	S	0	0	0
			1109	701	192	208	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	80	LEU	ILE	conflict	UNP Q13404
F	80	LEU	ILE	conflict	UNP Q13404
I	80	LEU	ILE	conflict	UNP Q13404
L	80	LEU	ILE	conflict	UNP Q13404

- Molecule 3 is a protein called STIP1 homology and U box-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	75	Total	C	N	O	S	0	0	1
			598	379	101	114	4			
3	T	78	Total	C	N	O	S	0	0	0
			634	402	104	124	4			
3	U	73	Total	C	N	O	S	0	0	1
			577	365	98	110	4			
3	V	71	Total	C	N	O	S	0	0	1
			564	356	96	108	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	269	ASN	ASP	conflict	UNP Q9WUD1
T	269	ASN	ASP	conflict	UNP Q9WUD1
U	269	ASN	ASP	conflict	UNP Q9WUD1
V	269	ASN	ASP	conflict	UNP Q9WUD1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total	O	0	0
			5	5		
4	C	5	Total	O	0	0
			5	5		
4	E	3	Total	O	0	0
			3	3		

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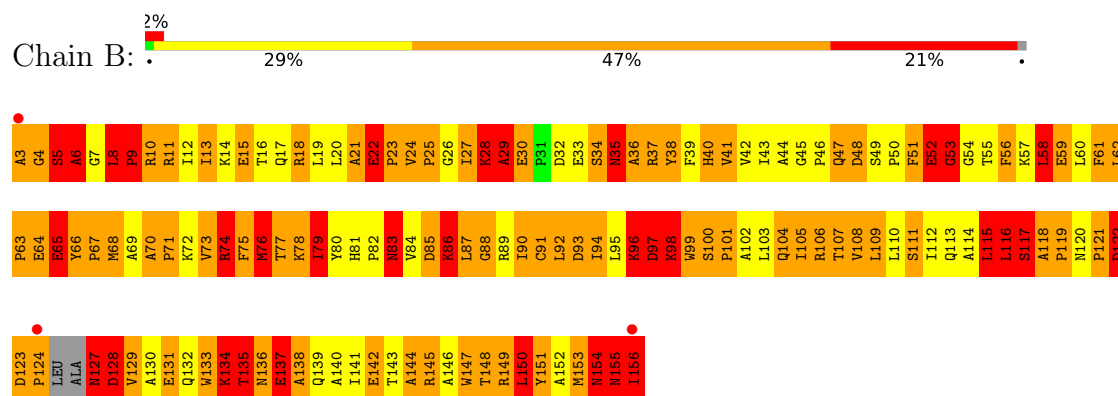
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	7	Total 7	O 7	0	0
4	H	1	Total 1	O 1	0	0
4	I	1	Total 1	O 1	0	0
4	L	1	Total 1	O 1	0	0
4	S	6	Total 6	O 6	0	0
4	T	2	Total 2	O 2	0	0
4	U	1	Total 1	O 1	0	0
4	V	3	Total 3	O 3	0	0

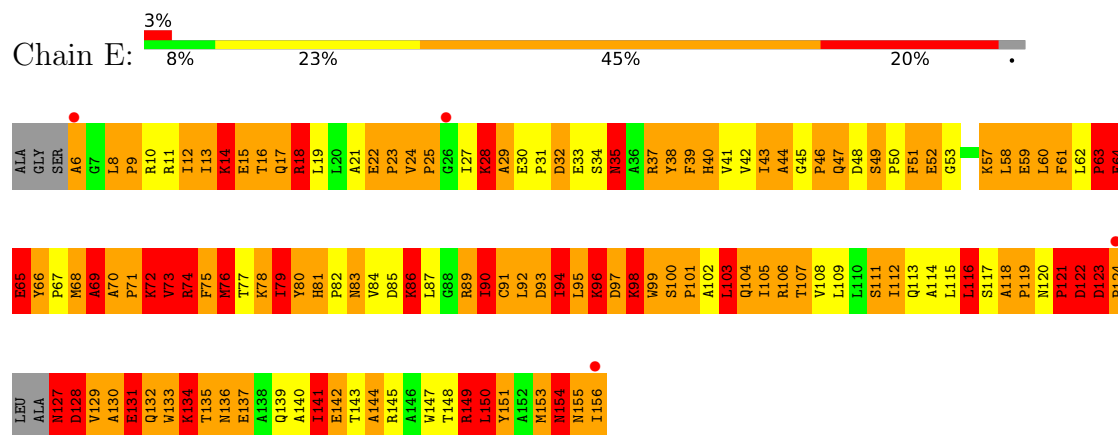
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

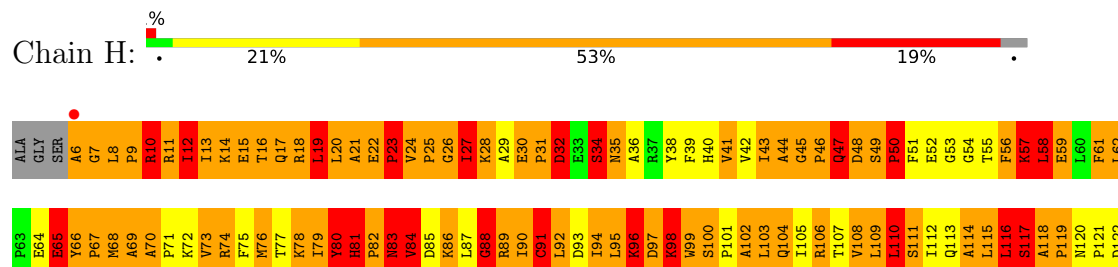
• Molecule 1: Ubiquitin-conjugating enzyme E2 N

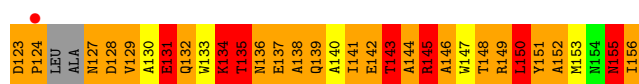


• Molecule 1: Ubiquitin-conjugating enzyme E2 N

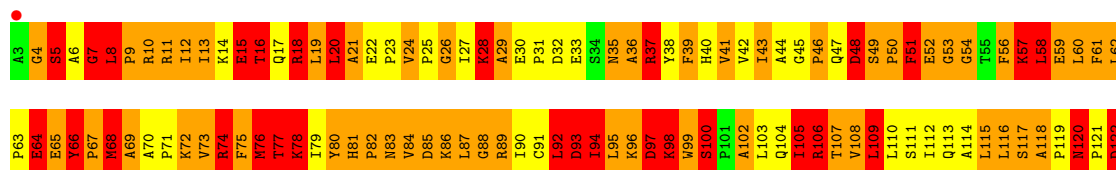


• Molecule 1: Ubiquitin-conjugating enzyme E2 N

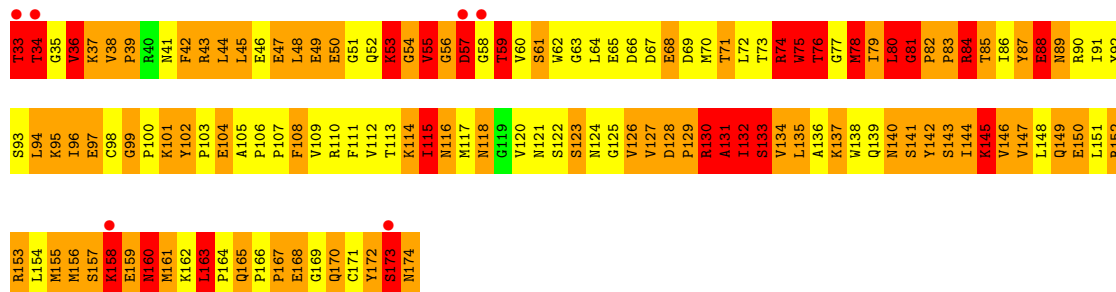




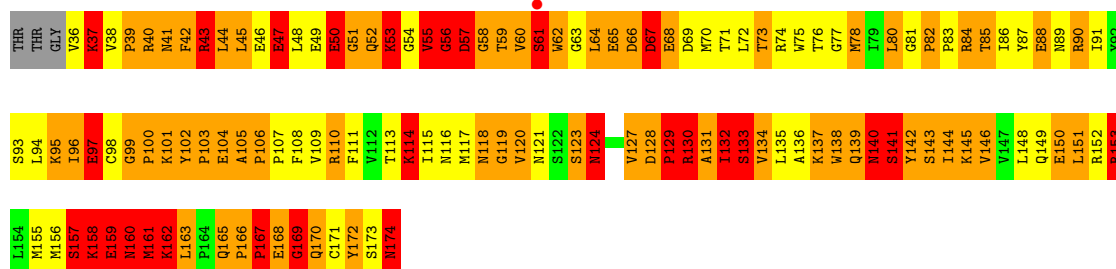
- Molecule 1: Ubiquitin-conjugating enzyme E2 N



- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 1

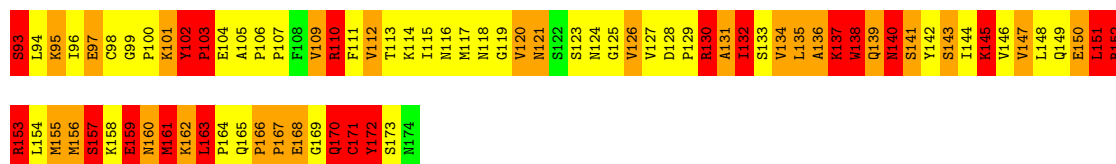


- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 1



- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 1

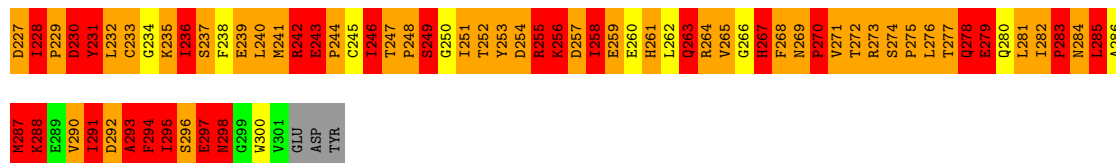
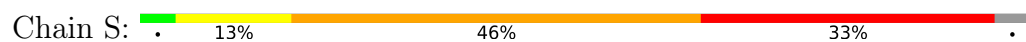




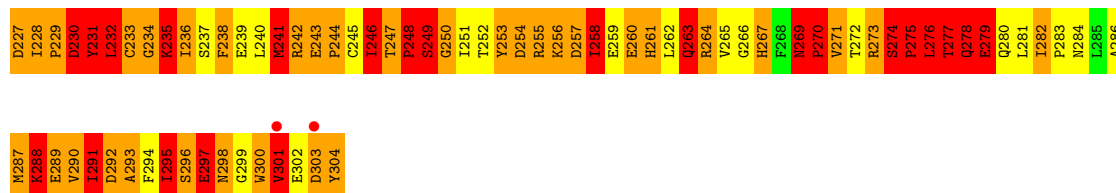
• Molecule 2: Ubiquitin-conjugating enzyme E2 variant 1



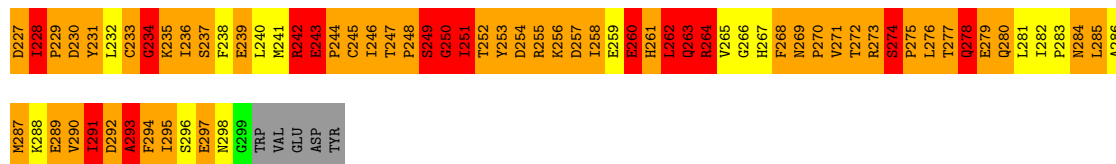
• Molecule 3: STIP1 homology and U box-containing protein 1



• Molecule 3: STIP1 homology and U box-containing protein 1



• Molecule 3: STIP1 homology and U box-containing protein 1



• Molecule 3: STIP1 homology and U box-containing protein 1



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.31Å 69.99Å 204.48Å 90.00° 106.95° 90.00°	Depositor
Resolution (Å)	196.12 – 2.90 195.59 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.3 (196.12-2.90) 95.3 (195.59-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.214 , 0.297 0.214 , 0.290	Depositor DCC
R_{free} test set	2621 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11636	wwPDB-VP
Average B, all atoms (Å ²)	4.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	B	4.01	230/1231 (18.7%)	3.28	179/1673 (10.7%)
1	E	3.64	199/1216 (16.4%)	2.79	122/1653 (7.4%)
1	H	3.36	143/1216 (11.8%)	2.79	122/1653 (7.4%)
1	K	3.54	176/1231 (14.3%)	2.79	114/1673 (6.8%)
2	C	4.15	213/1147 (18.6%)	3.25	187/1551 (12.1%)
2	F	3.76	176/1133 (15.5%)	3.15	168/1532 (11.0%)
2	I	3.12	118/1133 (10.4%)	2.55	81/1532 (5.3%)
2	L	3.26	140/1133 (12.4%)	2.88	124/1532 (8.1%)
3	S	4.01	118/612 (19.3%)	3.61	123/831 (14.8%)
3	T	3.89	108/649 (16.6%)	2.92	74/880 (8.4%)
3	U	3.68	99/589 (16.8%)	3.31	89/799 (11.1%)
3	V	3.77	100/576 (17.4%)	3.21	90/780 (11.5%)
All	All	3.67	1820/11866 (15.3%)	3.01	1473/16089 (9.2%)

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
1	B	0	7
1	E	0	6
1	H	0	7
1	K	0	17
2	C	0	6
2	F	0	4
2	I	0	13
2	L	0	3
3	S	0	4
3	T	0	1
3	U	0	3
3	V	0	2
All	All	0	73

All (1820) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	131	ALA	CA-CB	37.51	2.16	1.53
2	F	55	VAL	CA-CB	27.92	1.85	1.54
2	C	34	THR	CA-CB	23.58	1.93	1.53
3	U	295	ILE	CA-CB	19.12	1.75	1.54
3	S	236	ILE	CA-CB	-18.51	1.29	1.54
1	H	69	ALA	CA-CB	-17.07	1.25	1.53
1	B	72	LYS	CA-C	-17.05	1.31	1.52
2	F	50	GLU	CA-C	16.39	1.74	1.52
3	T	301	VAL	CA-CB	16.12	1.76	1.54
2	I	98	CYS	CA-C	-15.63	1.33	1.52
1	B	142	GLU	CD-OE2	15.55	1.54	1.25
2	F	120	VAL	CA-CB	-15.49	1.34	1.53
1	H	98	LYS	C-O	-15.46	1.04	1.24
2	L	106	PRO	CA-C	-14.99	1.38	1.52
1	B	6	ALA	CA-CB	-14.78	1.31	1.53
2	C	41	ASN	C-O	14.51	1.41	1.24
2	F	106	PRO	CA-C	14.50	1.59	1.51
2	F	55	VAL	N-CA	14.40	1.65	1.46
3	V	235	LYS	CA-C	14.26	1.71	1.52
1	B	144	ALA	CA-CB	-14.23	1.31	1.53
1	E	145	ARG	CZ-NH2	14.18	1.51	1.33
1	K	112	ILE	CA-CB	13.91	1.69	1.54
1	E	45	GLY	C-O	-13.75	1.05	1.24
3	T	248	PRO	C-O	-13.75	1.06	1.24
2	C	78	MET	SD-CE	13.64	2.13	1.79
2	C	38	VAL	N-CA	13.57	1.63	1.46
1	E	97	ASP	CA-C	13.55	1.71	1.52
2	F	105	ALA	CA-CB	-13.52	1.32	1.53
2	L	138	TRP	C-O	-13.46	1.07	1.24
1	K	155	ASN	CA-C	13.37	1.68	1.53
1	B	13	ILE	CA-CB	13.33	1.70	1.54
2	C	126	VAL	CA-C	-13.29	1.36	1.52
1	K	155	ASN	C-O	13.27	1.38	1.23
1	K	142	GLU	CD-OE2	13.24	1.50	1.25
3	V	266	GLY	C-O	12.97	1.41	1.23
3	U	258	ILE	CA-CB	-12.85	1.36	1.54
2	C	131	ALA	CA-C	12.82	1.70	1.52
2	F	139	GLN	N-CA	-12.80	1.29	1.46
3	U	228	ILE	CA-C	12.76	1.66	1.52
1	E	27	ILE	CA-CB	-12.72	1.38	1.54
1	B	123	ASP	N-CA	12.68	1.55	1.46
1	H	58	LEU	CA-C	-12.66	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	105	ILE	N-CA	-12.62	1.32	1.46
1	B	22	GLU	CA-CB	12.56	1.68	1.53
2	C	69	ASP	C-O	12.53	1.40	1.23
2	F	40	ARG	C-O	12.49	1.39	1.24
1	H	55	THR	C-O	12.46	1.38	1.23
1	K	81	HIS	N-CA	12.38	1.58	1.46
1	H	65	GLU	CG-CD	12.37	1.82	1.52
2	F	65	GLU	CA-C	-12.30	1.37	1.52
2	I	76	THR	CA-CB	-12.28	1.34	1.53
3	V	230	ASP	C-O	12.14	1.39	1.24
2	F	74	ARG	CA-C	-12.12	1.38	1.52
1	B	38	TYR	N-CA	-12.11	1.31	1.46
1	H	16	THR	C-O	12.10	1.39	1.24
1	K	134	LYS	CA-C	12.07	1.69	1.52
3	S	279	GLU	C-O	-12.06	1.08	1.24
1	E	144	ALA	CA-CB	-12.06	1.34	1.53
1	B	84	VAL	C-O	-12.02	1.10	1.24
1	B	77	THR	CA-CB	-12.00	1.34	1.53
3	T	286	ALA	C-O	12.00	1.39	1.24
2	C	49	GLU	CA-C	-11.99	1.36	1.52
2	I	152	ARG	CG-CD	11.96	1.88	1.52
3	U	250	GLY	C-O	11.92	1.40	1.23
2	C	82	PRO	C-O	-11.87	1.11	1.24
2	C	127	VAL	CA-CB	-11.85	1.40	1.54
1	E	14	LYS	CA-C	11.82	1.68	1.52
3	U	276	LEU	CA-C	-11.80	1.39	1.52
1	H	109	LEU	C-O	11.79	1.38	1.24
3	T	247	THR	C-O	-11.73	1.12	1.24
2	F	174	ASN	C-O	11.68	1.47	1.23
1	E	78	LYS	CG-CD	11.68	1.87	1.52
3	S	260	GLU	CA-C	-11.67	1.38	1.52
3	V	264	ARG	CA-C	11.66	1.68	1.52
2	C	53	LYS	CE-NZ	11.62	1.84	1.49
1	E	44	ALA	CA-CB	-11.46	1.36	1.53
1	B	92	LEU	N-CA	11.44	1.59	1.46
3	T	286	ALA	CA-CB	-11.43	1.34	1.53
2	F	127	VAL	CA-CB	-11.41	1.40	1.54
2	L	39	PRO	N-CA	11.38	1.57	1.46
1	B	43	ILE	C-O	-11.38	1.11	1.24
1	K	6	ALA	CA-C	11.34	1.68	1.52
2	L	136	ALA	CA-CB	-11.33	1.35	1.53
3	T	303	ASP	C-O	11.33	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	245	CYS	C-O	-11.32	1.09	1.23
1	H	95	LEU	CA-C	-11.32	1.38	1.52
1	B	9	PRO	C-O	11.30	1.37	1.23
3	T	276	LEU	C-O	-11.23	1.09	1.24
1	B	56	PHE	N-CA	-11.22	1.31	1.46
3	S	243	GLU	CD-OE1	11.21	1.46	1.25
2	F	74	ARG	CZ-NH1	11.18	1.48	1.32
3	T	288	LYS	CG-CD	11.15	1.85	1.52
2	C	165	GLN	CA-C	-11.15	1.38	1.52
1	K	81	HIS	CA-C	11.12	1.66	1.52
1	H	84	VAL	CA-CB	-11.10	1.40	1.54
2	I	59	THR	CA-C	11.08	1.67	1.52
3	T	244	PRO	CA-C	11.06	1.65	1.52
1	H	12	ILE	C-O	11.02	1.36	1.24
3	V	282	ILE	CA-CB	10.99	1.69	1.53
1	B	57	LYS	CA-C	-10.98	1.38	1.52
1	B	107	THR	N-CA	-10.96	1.33	1.46
1	K	44	ALA	CA-C	10.95	1.68	1.52
3	T	303	ASP	CA-C	10.94	1.67	1.53
2	C	114	LYS	C-O	-10.94	1.10	1.23
2	C	38	VAL	C-O	10.91	1.38	1.24
1	K	149	ARG	CZ-NH1	10.91	1.48	1.32
1	B	56	PHE	C-O	10.89	1.35	1.23
1	B	155	ASN	CA-C	10.89	1.67	1.52
2	I	105	ALA	CA-CB	-10.89	1.35	1.53
3	V	251	ILE	CA-CB	10.85	1.67	1.54
1	K	21	ALA	CA-CB	10.82	1.71	1.53
1	H	97	ASP	N-CA	10.82	1.53	1.46
1	E	15	GLU	CD-OE1	10.81	1.45	1.25
2	C	92	TYR	C-O	-10.79	1.11	1.23
3	U	253	TYR	CA-C	-10.79	1.39	1.52
2	L	91	ILE	C-O	-10.76	1.10	1.24
2	I	153	ARG	N-CA	10.74	1.59	1.46
3	V	255	ARG	C-O	10.71	1.37	1.24
1	K	70	ALA	CA-CB	-10.70	1.39	1.53
3	V	261	HIS	C-O	10.69	1.36	1.24
1	E	89	ARG	CA-C	-10.65	1.39	1.52
2	I	150	GLU	CA-C	10.65	1.67	1.52
1	E	113	GLN	C-O	-10.63	1.10	1.24
1	E	129	VAL	CA-CB	-10.61	1.39	1.54
3	T	270	PRO	CA-C	-10.61	1.37	1.52
3	T	282	ILE	CA-CB	-10.59	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	113	GLN	C-O	-10.54	1.10	1.24
2	C	96	ILE	CA-CB	-10.53	1.42	1.54
1	E	91	CYS	N-CA	-10.48	1.33	1.45
1	K	6	ALA	N-CA	10.48	1.59	1.46
2	C	63	GLY	N-CA	-10.47	1.34	1.45
1	B	72	LYS	CA-CB	-10.46	1.39	1.53
3	T	270	PRO	C-O	-10.42	1.10	1.24
3	T	277	THR	C-O	-10.41	1.10	1.23
1	B	40	HIS	N-CA	-10.33	1.33	1.46
2	C	34	THR	CA-C	10.33	1.66	1.52
2	C	113	THR	C-O	-10.33	1.11	1.24
1	E	78	LYS	CE-NZ	10.32	1.80	1.49
3	S	234	GLY	N-CA	10.32	1.60	1.45
2	C	109	VAL	CA-CB	-10.31	1.41	1.54
1	B	85	ASP	C-O	-10.29	1.13	1.23
3	S	276	LEU	CA-C	-10.25	1.39	1.52
1	K	123	ASP	N-CA	10.25	1.60	1.46
3	U	235	LYS	CA-C	10.24	1.66	1.52
1	K	11	ARG	C-O	10.20	1.35	1.24
1	B	120	ASN	C-O	10.19	1.37	1.24
1	E	112	ILE	CA-CB	-10.18	1.41	1.54
3	U	252	THR	CA-C	-10.17	1.40	1.52
1	B	33	GLU	N-CA	10.14	1.59	1.46
1	B	6	ALA	CA-C	10.13	1.66	1.53
2	L	85	THR	N-CA	10.13	1.59	1.45
1	B	70	ALA	CA-CB	-10.13	1.37	1.53
3	T	253	TYR	CA-C	-10.12	1.40	1.52
3	T	253	TYR	N-CA	-10.13	1.33	1.45
2	F	57	ASP	N-CA	10.07	1.59	1.46
2	C	38	VAL	CA-CB	10.06	1.67	1.54
1	H	11	ARG	C-O	10.06	1.36	1.24
1	B	95	LEU	CA-CB	-10.04	1.35	1.53
3	S	242	ARG	CG-CD	10.02	1.82	1.52
3	S	257	ASP	CA-C	-10.02	1.39	1.52
1	K	143	THR	CB-OG1	9.99	1.59	1.43
3	S	278	GLN	N-CA	-9.99	1.34	1.46
3	S	252	THR	CA-CB	9.97	1.68	1.53
2	F	158	LYS	CA-C	-9.97	1.39	1.52
1	H	81	HIS	N-CA	9.96	1.60	1.46
1	B	34	SER	C-O	-9.94	1.11	1.24
3	U	275	PRO	C-O	9.93	1.35	1.23
2	C	61	SER	C-O	-9.93	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	81	GLY	C-O	-9.91	1.10	1.24
3	V	251	ILE	CA-C	-9.91	1.39	1.52
1	H	149	ARG	CZ-NH1	9.89	1.46	1.32
1	B	70	ALA	C-N	-9.89	1.21	1.33
1	B	152	ALA	CA-CB	-9.87	1.39	1.53
1	B	6	ALA	C-O	-9.84	1.12	1.23
2	I	132	ILE	CA-CB	-9.84	1.41	1.54
1	B	66	TYR	CA-CB	-9.83	1.39	1.53
2	L	40	ARG	CZ-NH2	9.82	1.46	1.33
3	S	230	ASP	CA-C	-9.80	1.40	1.52
1	E	105	ILE	CA-CB	-9.79	1.43	1.54
1	B	93	ASP	CG-OD1	9.78	1.44	1.25
2	F	111	PHE	CA-C	-9.77	1.41	1.52
1	H	15	GLU	C-O	9.76	1.36	1.24
2	I	38	VAL	N-CA	9.75	1.58	1.46
2	F	63	GLY	N-CA	-9.74	1.35	1.45
3	U	251	ILE	CA-CB	9.74	1.69	1.55
1	H	96	LYS	C-O	-9.74	1.15	1.23
1	H	98	LYS	CE-NZ	9.72	1.78	1.49
1	H	141	ILE	CA-CB	9.72	1.67	1.54
1	H	118	ALA	CA-CB	9.68	1.68	1.53
1	K	18	ARG	C-O	9.68	1.35	1.24
1	K	6	ALA	CA-CB	9.67	1.69	1.53
1	K	154	ASN	CA-C	9.66	1.65	1.52
2	F	38	VAL	C-O	9.66	1.37	1.25
1	K	71	PRO	C-O	9.66	1.35	1.23
1	B	145	ARG	CZ-NH1	9.62	1.46	1.32
3	S	270	PRO	CA-CB	-9.62	1.40	1.53
1	B	59	GLU	CA-C	-9.61	1.41	1.52
1	K	57	LYS	C-O	9.59	1.36	1.24
3	T	290	VAL	CA-CB	-9.59	1.41	1.54
3	T	246	ILE	C-O	-9.58	1.12	1.23
2	C	170	GLN	C-O	9.58	1.37	1.23
2	I	45	LEU	N-CA	9.58	1.58	1.46
1	H	30	GLU	C-O	-9.56	1.12	1.24
3	T	253	TYR	C-O	-9.56	1.12	1.23
1	B	155	ASN	C-O	9.56	1.36	1.24
3	V	241	MET	CA-C	9.55	1.65	1.52
1	B	143	THR	N-CA	-9.54	1.34	1.46
2	F	151	LEU	N-CA	-9.54	1.35	1.46
1	H	100	SER	C-O	-9.52	1.14	1.24
1	B	35	ASN	CA-C	9.52	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	74	ARG	C-O	-9.52	1.12	1.23
1	B	84	VAL	CA-CB	-9.51	1.43	1.54
1	B	69	ALA	CA-CB	-9.50	1.37	1.53
2	C	153	ARG	CB-CG	9.50	1.80	1.52
2	F	95	LYS	CE-NZ	9.50	1.77	1.49
1	E	76	MET	C-O	-9.49	1.11	1.24
1	H	17	GLN	CA-CB	-9.49	1.38	1.53
2	C	106	PRO	C-O	-9.48	1.13	1.24
1	E	77	THR	N-CA	-9.46	1.34	1.45
1	B	63	PRO	C-O	-9.46	1.12	1.23
2	F	91	ILE	CA-C	-9.46	1.41	1.52
1	E	155	ASN	CA-C	9.46	1.64	1.52
1	B	142	GLU	CD-OE1	9.46	1.43	1.25
2	C	94	LEU	CA-C	-9.44	1.41	1.52
1	K	52	GLU	N-CA	9.43	1.58	1.46
1	E	92	LEU	C-O	9.40	1.35	1.23
3	T	260	GLU	C-O	-9.39	1.13	1.24
2	C	146	VAL	CB-CG2	-9.39	1.21	1.52
2	F	48	LEU	N-CA	-9.38	1.35	1.46
3	S	270	PRO	CA-C	-9.38	1.39	1.52
2	F	63	GLY	CA-C	-9.37	1.42	1.52
3	S	256	LYS	N-CA	9.36	1.58	1.46
1	H	36	ALA	CA-CB	-9.36	1.37	1.53
1	E	79	ILE	CA-CB	9.35	1.70	1.54
1	E	78	LYS	C-O	-9.33	1.12	1.24
2	F	131	ALA	CA-C	-9.33	1.40	1.52
2	C	92	TYR	CA-C	-9.32	1.41	1.52
1	B	90	ILE	CA-CB	-9.31	1.42	1.54
2	C	120	VAL	CA-CB	-9.26	1.42	1.54
1	K	84	VAL	CA-CB	9.25	1.65	1.55
3	T	252	THR	N-CA	-9.25	1.34	1.45
2	F	165	GLN	CA-C	-9.24	1.41	1.52
2	C	159	GLU	CB-CG	9.23	1.80	1.52
3	S	300	TRP	N-CA	9.23	1.63	1.46
1	E	43	ILE	CA-CB	-9.22	1.42	1.54
1	H	7	GLY	N-CA	9.20	1.57	1.45
3	S	233	CYS	CA-CB	-9.18	1.37	1.53
3	V	289	GLU	CD-OE2	9.18	1.42	1.25
1	B	70	ALA	C-O	-9.17	1.11	1.23
2	C	43	ARG	CZ-NH1	9.17	1.45	1.32
2	C	41	ASN	CA-CB	-9.17	1.38	1.53
2	F	129	PRO	C-O	-9.16	1.12	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	37	LYS	CD-CE	9.16	1.79	1.52
2	C	164	PRO	C-O	-9.13	1.11	1.23
3	T	245	CYS	CA-C	-9.12	1.41	1.52
3	S	239	GLU	CD-OE1	9.10	1.42	1.25
3	T	236	ILE	CA-CB	-9.10	1.42	1.54
2	F	93	SER	CA-C	-9.10	1.41	1.52
2	L	39	PRO	CA-C	9.10	1.61	1.53
3	V	292	ASP	CG-OD1	9.09	1.42	1.25
1	B	19	LEU	CA-C	-9.08	1.41	1.52
2	C	33	THR	CA-C	9.06	1.72	1.52
2	C	91	ILE	C-O	-9.05	1.14	1.24
1	B	65	GLU	CD-OE1	9.05	1.42	1.25
1	E	42	VAL	C-O	-9.05	1.14	1.24
2	I	63	GLY	N-CA	9.04	1.58	1.45
1	K	99	TRP	C-O	9.03	1.34	1.24
1	B	124	PRO	N-CA	9.03	1.60	1.47
3	U	295	ILE	N-CA	9.03	1.56	1.46
2	L	97	GLU	C-O	-9.02	1.13	1.23
1	K	75	PHE	C-O	9.01	1.34	1.23
3	V	264	ARG	C-O	8.99	1.35	1.24
1	K	89	ARG	C-O	8.99	1.34	1.23
1	K	7	GLY	N-CA	8.98	1.58	1.45
2	C	159	GLU	CG-CD	8.98	1.74	1.52
1	K	156	ILE	CA-CB	8.98	1.78	1.54
1	B	75	PHE	C-O	8.97	1.34	1.23
3	V	268	PHE	N-CA	8.96	1.57	1.45
3	S	279	GLU	N-CA	8.96	1.57	1.46
3	V	255	ARG	CA-C	8.96	1.65	1.52
2	C	48	LEU	N-CA	-8.95	1.35	1.46
2	F	165	GLN	C-O	-8.95	1.12	1.24
1	E	60	LEU	N-CA	8.95	1.57	1.46
1	B	142	GLU	CB-CG	-8.95	1.25	1.52
1	B	74	ARG	CA-C	-8.95	1.41	1.52
3	S	282	ILE	N-CA	8.93	1.54	1.46
1	K	31	PRO	CA-C	-8.93	1.41	1.52
2	I	91	ILE	C-O	8.92	1.35	1.23
2	L	126	VAL	CA-CB	-8.92	1.42	1.54
2	F	61	SER	CA-C	8.92	1.63	1.52
2	C	153	ARG	NE-CZ	8.91	1.42	1.33
1	B	24	VAL	C-O	-8.90	1.12	1.24
1	B	134	LYS	CE-NZ	8.90	1.76	1.49
3	S	248	PRO	C-O	-8.89	1.12	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	ARG	CD-NE	-8.88	1.33	1.46
1	H	10	ARG	N-CA	-8.88	1.35	1.46
3	V	257	ASP	N-CA	8.86	1.56	1.46
1	B	39	PHE	C-O	-8.84	1.12	1.23
1	K	120	ASN	N-CA	8.83	1.58	1.46
3	U	279	GLU	CG-CD	8.82	1.74	1.52
2	C	108	PHE	CB-CG	-8.81	1.30	1.50
1	E	145	ARG	CZ-NH1	8.81	1.45	1.32
1	B	17	GLN	CA-CB	-8.80	1.40	1.53
2	F	55	VAL	CB-CG1	8.80	1.81	1.52
1	H	62	LEU	CA-C	-8.79	1.41	1.52
3	U	251	ILE	C-O	8.79	1.33	1.24
2	I	37	LYS	N-CA	8.78	1.57	1.46
3	S	267	HIS	CA-C	-8.77	1.41	1.52
2	F	153	ARG	N-CA	8.77	1.56	1.46
2	C	49	GLU	CD-OE1	8.76	1.42	1.25
2	I	137	LYS	C-O	-8.76	1.11	1.23
3	S	276	LEU	C-O	-8.75	1.12	1.24
2	C	174	ASN	C-OXT	8.74	1.41	1.23
1	K	95	LEU	C-O	-8.74	1.12	1.24
1	K	42	VAL	C-O	8.74	1.33	1.24
3	S	283	PRO	CA-CB	-8.74	1.41	1.53
3	T	246	ILE	CB-CG2	-8.72	1.23	1.52
3	T	282	ILE	C-O	-8.72	1.13	1.24
1	K	57	LYS	CB-CG	8.71	1.78	1.52
3	S	235	LYS	CB-CG	-8.71	1.26	1.52
2	F	37	LYS	C-N	8.70	1.42	1.33
2	F	111	PHE	N-CA	8.70	1.56	1.46
1	K	46	PRO	N-CA	8.69	1.57	1.47
3	S	263	GLN	CG-CD	8.65	1.73	1.52
1	H	102	ALA	CA-CB	-8.65	1.40	1.53
2	C	45	LEU	CA-CB	-8.64	1.39	1.53
1	E	78	LYS	CB-CG	8.64	1.78	1.52
2	L	144	ILE	C-O	8.64	1.34	1.24
3	S	275	PRO	N-CA	8.64	1.58	1.47
2	C	53	LYS	CG-CD	8.63	1.78	1.52
1	E	70	ALA	N-CA	8.63	1.59	1.45
3	U	230	ASP	CA-C	-8.62	1.41	1.52
3	U	279	GLU	C-O	8.62	1.35	1.24
1	K	42	VAL	CA-CB	-8.62	1.43	1.54
3	S	257	ASP	CG-OD2	8.61	1.41	1.25
1	B	28	LYS	C-O	-8.60	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	126	VAL	CA-CB	-8.60	1.44	1.54
2	C	143	SER	C-O	8.59	1.33	1.23
1	B	25	PRO	CA-C	8.59	1.63	1.52
2	C	132	ILE	CA-CB	8.59	1.66	1.54
1	E	104	GLN	CA-C	8.59	1.63	1.52
2	L	95	LYS	CA-C	-8.59	1.41	1.52
3	U	285	LEU	CA-C	-8.58	1.41	1.52
1	K	106	ARG	CG-CD	8.57	1.78	1.52
2	C	79	ILE	CA-CB	-8.56	1.42	1.54
2	I	41	ASN	C-O	8.56	1.35	1.24
3	T	288	LYS	CD-CE	8.55	1.78	1.52
2	F	124	ASN	N-CA	8.54	1.57	1.45
1	E	92	LEU	CA-C	-8.54	1.42	1.52
1	B	37	ARG	CA-C	8.52	1.64	1.52
1	K	4	GLY	N-CA	8.52	1.57	1.45
2	C	156	MET	SD-CE	8.52	2.00	1.79
2	C	123	SER	N-CA	-8.50	1.37	1.46
1	E	119	PRO	C-O	8.50	1.34	1.23
1	B	43	ILE	CA-CB	-8.48	1.44	1.54
2	L	66	ASP	C-O	8.48	1.33	1.23
2	F	40	ARG	N-CA	8.48	1.57	1.46
1	K	105	ILE	CA-CB	-8.47	1.43	1.54
3	V	279	GLU	C-O	-8.47	1.13	1.24
1	E	29	ALA	N-CA	8.45	1.57	1.46
2	F	74	ARG	NE-CZ	8.45	1.42	1.33
2	L	75	TRP	CA-C	-8.44	1.42	1.52
3	V	248	PRO	CG-CD	8.43	1.79	1.50
3	T	230	ASP	CA-C	-8.43	1.42	1.52
1	H	30	GLU	CA-C	-8.41	1.41	1.52
1	E	96	LYS	CG-CD	8.39	1.77	1.52
1	E	68	MET	CA-C	8.39	1.63	1.52
2	C	55	VAL	CA-CB	8.38	1.65	1.54
1	E	86	LYS	CE-NZ	8.38	1.74	1.49
2	L	132	ILE	N-CA	-8.38	1.35	1.46
1	B	107	THR	CA-CB	-8.37	1.40	1.53
2	I	37	LYS	CA-CB	8.37	1.63	1.52
2	L	153	ARG	CZ-NH1	8.36	1.44	1.32
2	I	168	GLU	N-CA	8.36	1.56	1.46
1	K	110	LEU	C-O	8.35	1.33	1.24
3	T	255	ARG	CZ-NH1	8.35	1.44	1.32
3	U	252	THR	CA-CB	8.35	1.74	1.53
1	K	145	ARG	CZ-NH2	8.35	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	53	LYS	CA-C	8.34	1.63	1.52
2	F	104	GLU	CA-C	-8.33	1.42	1.52
2	F	161	MET	SD-CE	8.32	2.00	1.79
1	E	99	TRP	CA-CB	-8.31	1.40	1.53
2	F	143	SER	C-O	8.30	1.32	1.23
1	K	150	LEU	CG-CD2	8.30	1.79	1.52
3	V	247	THR	CA-CB	-8.30	1.43	1.54
2	F	113	THR	C-O	-8.28	1.13	1.23
3	T	252	THR	C-O	-8.28	1.13	1.23
2	F	56	GLY	N-CA	8.28	1.57	1.45
3	S	236	ILE	N-CA	-8.27	1.36	1.46
2	I	66	ASP	CA-C	8.27	1.61	1.52
1	B	10	ARG	CZ-NH2	8.27	1.44	1.33
2	C	127	VAL	CB-CG2	-8.26	1.25	1.52
1	B	156	ILE	C-OXT	8.26	1.40	1.23
2	C	152	ARG	C-O	-8.26	1.13	1.24
2	F	131	ALA	CA-CB	-8.26	1.40	1.53
2	I	73	THR	CA-CB	-8.26	1.40	1.53
2	F	174	ASN	C-OXT	8.25	1.40	1.23
1	B	47	GLN	C-O	8.24	1.34	1.23
2	C	162	LYS	N-CA	-8.24	1.36	1.46
1	E	156	ILE	CA-C	8.24	1.70	1.52
1	K	48	ASP	CA-C	8.23	1.63	1.52
1	K	25	PRO	CA-C	8.23	1.63	1.52
1	H	15	GLU	CA-C	8.22	1.63	1.52
1	E	129	VAL	N-CA	-8.22	1.35	1.46
1	H	16	THR	CA-CB	8.22	1.67	1.53
3	T	271	VAL	C-O	-8.21	1.13	1.24
2	F	38	VAL	N-CA	8.20	1.57	1.47
1	K	59	GLU	C-O	8.19	1.33	1.23
1	B	151	TYR	N-CA	-8.19	1.35	1.46
2	F	165	GLN	CA-CB	-8.19	1.40	1.53
2	L	145	LYS	CD-CE	8.19	1.77	1.52
2	F	115	ILE	CA-C	-8.18	1.42	1.52
1	B	66	TYR	CA-C	8.18	1.62	1.53
3	T	288	LYS	N-CA	8.17	1.56	1.46
3	S	265	VAL	CA-CB	-8.17	1.45	1.54
1	B	119	PRO	C-O	8.16	1.33	1.23
1	B	98	LYS	N-CA	-8.16	1.35	1.46
1	E	78	LYS	CA-CB	8.16	1.65	1.53
1	E	89	ARG	CZ-NH1	8.16	1.44	1.32
3	V	243	GLU	CD-OE2	8.15	1.40	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	292	ASP	N-CA	8.15	1.56	1.46
2	C	106	PRO	CA-C	-8.14	1.44	1.52
2	C	170	GLN	CA-C	8.13	1.64	1.53
2	I	79	ILE	C-O	8.13	1.33	1.24
2	C	132	ILE	CA-C	8.12	1.63	1.52
2	F	39	PRO	CA-C	8.11	1.62	1.52
1	H	83	ASN	C-O	8.11	1.35	1.24
3	S	248	PRO	CA-C	-8.11	1.40	1.52
1	K	123	ASP	CA-C	8.10	1.63	1.52
1	B	34	SER	CA-CB	8.09	1.67	1.53
2	C	136	ALA	N-CA	-8.09	1.35	1.46
2	C	167	PRO	C-O	-8.09	1.14	1.23
1	E	149	ARG	CG-CD	8.08	1.76	1.52
1	H	7	GLY	CA-C	8.08	1.62	1.51
1	E	81	HIS	CA-CB	8.07	1.66	1.53
2	L	84	ARG	CB-CG	8.07	1.76	1.52
1	H	138	ALA	N-CA	8.06	1.56	1.46
2	I	106	PRO	CA-C	-8.06	1.44	1.52
2	I	131	ALA	CA-CB	-8.05	1.43	1.53
1	B	29	ALA	C-O	-8.04	1.13	1.23
1	B	85	ASP	CG-OD2	8.04	1.40	1.25
2	C	78	MET	C-O	-8.04	1.13	1.23
1	E	35	ASN	C-O	8.02	1.33	1.23
2	I	111	PHE	C-O	-8.02	1.14	1.23
3	S	298	ASN	N-CA	8.01	1.56	1.46
3	U	239	GLU	CB-CG	-8.00	1.28	1.52
1	B	22	GLU	CB-CG	8.00	1.76	1.52
3	U	290	VAL	N-CA	8.00	1.56	1.46
3	V	267	HIS	C-O	8.00	1.34	1.23
2	C	132	ILE	CB-CG2	-7.99	1.26	1.52
3	V	268	PHE	CD1-CE1	7.99	1.62	1.38
1	E	89	ARG	C-O	7.97	1.34	1.24
3	S	264	ARG	C-O	-7.97	1.14	1.24
1	H	151	TYR	N-CA	7.96	1.56	1.46
1	B	102	ALA	CA-CB	-7.96	1.39	1.53
3	V	273	ARG	CA-C	7.96	1.64	1.52
2	C	65	GLU	CD-OE2	7.96	1.40	1.25
1	K	48	ASP	N-CA	7.96	1.56	1.46
3	S	242	ARG	C-O	-7.96	1.13	1.24
2	F	124	ASN	C-O	7.96	1.34	1.24
1	H	68	MET	CA-C	-7.96	1.43	1.52
2	C	109	VAL	N-CA	-7.95	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	60	VAL	C-O	-7.94	1.14	1.23
1	E	59	GLU	C-O	7.94	1.33	1.23
2	L	64	LEU	C-O	7.92	1.33	1.24
1	B	111	SER	C-O	7.92	1.33	1.24
2	C	144	ILE	N-CA	-7.92	1.37	1.46
1	H	35	ASN	C-O	7.91	1.33	1.23
2	L	163	LEU	CA-C	7.91	1.61	1.52
1	B	109	LEU	CA-C	-7.91	1.42	1.52
1	K	147	TRP	C-O	7.90	1.33	1.24
1	H	114	ALA	N-CA	7.89	1.56	1.46
2	L	52	GLN	N-CA	7.89	1.55	1.46
1	E	105	ILE	CA-C	-7.88	1.43	1.52
2	L	41	ASN	C-O	7.88	1.33	1.24
2	L	43	ARG	N-CA	-7.88	1.37	1.46
2	L	156	MET	CA-CB	-7.87	1.41	1.53
1	E	150	LEU	N-CA	-7.85	1.36	1.46
3	S	266	GLY	N-CA	7.85	1.57	1.45
3	S	265	VAL	C-O	-7.84	1.11	1.23
1	B	128	ASP	C-O	7.84	1.34	1.24
2	L	128	ASP	CA-C	-7.83	1.43	1.52
2	C	168	GLU	CA-C	7.83	1.63	1.52
1	E	85	ASP	N-CA	-7.83	1.34	1.46
1	K	69	ALA	C-O	7.82	1.33	1.24
3	T	281	LEU	C-O	-7.81	1.14	1.23
3	V	260	GLU	C-O	7.81	1.33	1.24
3	U	235	LYS	CB-CG	-7.81	1.29	1.52
1	B	146	ALA	C-O	-7.80	1.14	1.24
2	C	152	ARG	N-CA	-7.80	1.36	1.46
1	B	28	LYS	CE-NZ	7.79	1.72	1.49
1	K	100	SER	C-O	7.79	1.33	1.24
2	F	74	ARG	CG-CD	-7.79	1.29	1.52
1	E	22	GLU	C-O	7.78	1.33	1.24
2	F	146	VAL	C-O	7.78	1.32	1.24
2	L	169	GLY	C-O	7.78	1.34	1.23
1	H	135	THR	CA-CB	7.76	1.67	1.53
1	K	64	GLU	CD-OE1	7.76	1.40	1.25
1	E	105	ILE	C-O	7.76	1.32	1.24
3	T	302	GLU	N-CA	7.76	1.55	1.45
1	H	96	LYS	CD-CE	7.76	1.75	1.52
2	L	43	ARG	CZ-NH1	7.75	1.43	1.32
1	K	37	ARG	CZ-NH1	7.74	1.43	1.32
3	T	296	SER	CA-C	-7.74	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	145	LYS	CE-NZ	7.74	1.72	1.49
2	L	60	VAL	N-CA	-7.73	1.36	1.46
2	I	139	GLN	CD-NE2	7.73	1.49	1.33
3	V	273	ARG	CZ-NH2	7.73	1.43	1.33
2	L	54	GLY	C-O	7.73	1.34	1.23
1	B	5	SER	CA-C	7.72	1.63	1.52
1	H	32	ASP	N-CA	-7.72	1.36	1.46
1	H	139	GLN	CA-C	7.71	1.62	1.52
2	F	48	LEU	CA-C	-7.70	1.43	1.52
2	F	153	ARG	CG-CD	7.70	1.75	1.52
2	C	151	LEU	CG-CD2	-7.69	1.27	1.52
3	U	279	GLU	CD-OE2	7.68	1.40	1.25
3	S	291	ILE	CA-CB	7.68	1.65	1.54
1	E	121	PRO	CA-C	7.67	1.63	1.52
3	U	291	ILE	CA-CB	7.67	1.64	1.54
2	F	53	LYS	CD-CE	7.67	1.75	1.52
1	E	135	THR	C-O	7.66	1.34	1.24
1	K	78	LYS	CD-CE	7.66	1.75	1.52
1	K	45	GLY	N-CA	7.66	1.55	1.44
1	K	140	ALA	C-O	7.64	1.33	1.24
3	S	228	ILE	N-CA	7.64	1.55	1.46
3	S	229	PRO	C-O	7.63	1.32	1.23
3	S	261	HIS	CA-CB	-7.63	1.41	1.53
1	B	99	TRP	N-CA	7.62	1.55	1.46
2	I	92	TYR	C-O	7.60	1.33	1.24
1	E	129	VAL	CA-C	-7.60	1.42	1.53
2	C	63	GLY	C-O	-7.59	1.15	1.23
2	F	162	LYS	CA-C	-7.58	1.43	1.52
1	B	55	THR	N-CA	-7.57	1.36	1.46
1	E	93	ASP	C-O	7.57	1.33	1.24
3	U	228	ILE	N-CA	7.57	1.55	1.46
1	K	141	ILE	N-CA	7.57	1.55	1.46
2	C	73	THR	CA-CB	-7.57	1.41	1.53
2	I	55	VAL	C-O	7.56	1.33	1.24
1	E	154	ASN	C-O	-7.56	1.14	1.23
1	K	120	ASN	C-O	7.55	1.33	1.24
1	B	44	ALA	CA-CB	-7.55	1.41	1.53
1	B	45	GLY	C-O	7.55	1.34	1.24
2	C	79	ILE	N-CA	-7.55	1.37	1.46
2	F	109	VAL	N-CA	7.55	1.56	1.46
1	K	120	ASN	CB-CG	7.55	1.71	1.52
1	K	47	GLN	CA-C	7.54	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	104	GLU	C-O	-7.54	1.14	1.24
1	E	127	ASN	N-CA	7.54	1.60	1.46
1	H	39	PHE	CG-CD1	7.54	1.54	1.38
2	L	144	ILE	CA-CB	7.53	1.63	1.54
1	H	110	LEU	CG-CD2	7.53	1.77	1.52
2	I	48	LEU	N-CA	-7.53	1.36	1.46
2	L	37	LYS	N-CA	7.53	1.55	1.46
2	C	98	CYS	CA-CB	-7.52	1.43	1.53
2	L	92	TYR	CA-C	-7.52	1.43	1.52
2	C	84	ARG	CB-CG	7.52	1.75	1.52
1	E	61	PHE	C-O	7.52	1.33	1.23
3	S	263	GLN	CD-NE2	7.52	1.49	1.33
1	K	142	GLU	CB-CG	7.52	1.75	1.52
2	C	151	LEU	C-O	-7.51	1.15	1.24
2	I	159	GLU	N-CA	7.51	1.55	1.46
3	S	277	THR	CA-CB	-7.51	1.42	1.53
2	C	74	ARG	N-CA	-7.51	1.36	1.46
2	I	120	VAL	C-O	7.51	1.33	1.24
3	V	259	GLU	CG-CD	7.51	1.70	1.52
2	C	157	SER	CB-OG	7.51	1.57	1.42
2	C	164	PRO	CA-C	-7.50	1.44	1.52
3	V	266	GLY	CA-C	7.50	1.62	1.51
3	S	270	PRO	C-N	-7.50	1.25	1.33
1	B	41	VAL	CA-CB	-7.49	1.45	1.54
3	V	288	LYS	CG-CD	7.49	1.75	1.52
1	B	79	ILE	CG1-CD1	-7.47	1.22	1.51
2	C	50	GLU	CA-C	-7.47	1.43	1.52
2	F	111	PHE	C-O	-7.47	1.14	1.24
1	K	74	ARG	CA-C	-7.47	1.43	1.52
3	T	256	LYS	N-CA	7.47	1.55	1.46
1	E	99	TRP	C-O	7.46	1.34	1.23
1	K	12	ILE	CA-CB	7.46	1.62	1.54
1	B	73	VAL	N-CA	7.46	1.54	1.46
3	T	230	ASP	C-O	7.46	1.32	1.24
1	E	142	GLU	CD-OE2	7.45	1.39	1.25
3	S	285	LEU	N-CA	7.45	1.55	1.46
1	H	146	ALA	CA-CB	7.45	1.66	1.53
1	B	145	ARG	CA-CB	-7.43	1.41	1.53
2	C	34	THR	N-CA	7.43	1.55	1.46
1	H	84	VAL	CA-C	-7.43	1.44	1.52
3	V	274	SER	C-O	7.43	1.33	1.23
3	S	266	GLY	CA-C	7.43	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	ILE	CA-C	-7.43	1.43	1.52
1	K	142	GLU	CD-OE1	7.43	1.39	1.25
1	K	142	GLU	CG-CD	7.43	1.70	1.52
3	S	256	LYS	CG-CD	7.42	1.74	1.52
2	C	165	GLN	C-O	-7.41	1.13	1.23
1	B	14	LYS	CA-C	7.41	1.62	1.52
1	B	134	LYS	CA-C	7.41	1.62	1.52
3	V	280	GLN	C-O	7.41	1.33	1.24
2	L	49	GLU	CG-CD	7.40	1.70	1.52
2	I	100	PRO	C-O	-7.40	1.14	1.24
2	C	33	THR	N-CA	7.40	1.60	1.46
2	I	121	ASN	N-CA	-7.40	1.36	1.46
1	H	34	SER	CA-C	7.40	1.62	1.52
3	S	254	ASP	CG-OD1	7.39	1.39	1.25
3	T	269	ASN	CA-C	7.39	1.61	1.52
1	E	96	LYS	CD-CE	7.39	1.74	1.52
2	L	40	ARG	CD-NE	7.39	1.56	1.46
2	I	161	MET	CA-C	7.38	1.62	1.52
2	L	50	GLU	N-CA	-7.38	1.36	1.46
1	E	103	LEU	N-CA	7.37	1.54	1.45
2	I	39	PRO	N-CA	7.37	1.56	1.47
3	S	294	PHE	CA-C	7.37	1.62	1.52
1	E	143	THR	CA-C	-7.37	1.43	1.52
1	H	137	GLU	CA-C	7.37	1.62	1.52
1	K	108	VAL	C-O	7.37	1.32	1.24
2	L	38	VAL	CA-CB	7.37	1.63	1.54
2	I	37	LYS	CG-CD	7.37	1.74	1.52
3	V	280	GLN	CD-OE1	7.37	1.37	1.23
1	B	7	GLY	N-CA	-7.37	1.38	1.45
2	C	103	PRO	N-CA	-7.36	1.34	1.47
2	F	82	PRO	CA-C	7.36	1.59	1.52
1	E	87	LEU	C-O	-7.36	1.14	1.24
2	C	82	PRO	CA-C	-7.35	1.45	1.52
2	I	52	GLN	N-CA	7.35	1.55	1.46
3	T	289	GLU	C-O	7.35	1.33	1.23
3	V	291	ILE	C-O	7.33	1.32	1.24
3	T	242	ARG	CG-CD	7.33	1.74	1.52
3	S	264	ARG	CZ-NH1	7.33	1.43	1.32
1	B	142	GLU	CA-CB	-7.32	1.41	1.53
2	C	92	TYR	C-N	-7.32	1.23	1.33
1	H	156	ILE	CA-CB	7.32	1.74	1.54
2	C	115	ILE	CA-C	-7.32	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	73	THR	CA-C	-7.31	1.43	1.52
1	B	52	GLU	CA-C	-7.31	1.43	1.52
1	K	57	LYS	CG-CD	7.31	1.74	1.52
2	I	109	VAL	CA-C	-7.31	1.43	1.52
1	E	39	PHE	CA-CB	-7.30	1.42	1.53
1	K	142	GLU	N-CA	7.30	1.55	1.46
3	U	265	VAL	CA-CB	-7.30	1.44	1.55
1	B	133	TRP	CA-C	7.30	1.62	1.52
3	T	233	CYS	CA-C	-7.30	1.43	1.52
1	B	22	GLU	C-O	7.30	1.33	1.24
1	B	86	LYS	CA-CB	7.29	1.65	1.53
2	C	150	GLU	C-O	7.29	1.32	1.24
3	S	254	ASP	CG-OD2	7.29	1.39	1.25
3	T	236	ILE	CB-CG2	-7.29	1.28	1.52
1	E	91	CYS	CA-C	7.29	1.61	1.52
1	K	12	ILE	CA-C	7.29	1.61	1.52
2	L	117	MET	N-CA	7.29	1.55	1.46
3	S	264	ARG	CA-C	-7.29	1.42	1.52
1	K	5	SER	CA-C	7.28	1.62	1.52
2	F	61	SER	N-CA	7.28	1.54	1.46
1	K	98	LYS	N-CA	-7.27	1.37	1.46
2	F	146	VAL	CA-CB	7.26	1.62	1.54
3	S	255	ARG	CZ-NH2	7.26	1.42	1.33
1	H	57	LYS	CA-C	7.26	1.62	1.52
2	L	108	PHE	C-O	-7.26	1.15	1.24
3	V	286	ALA	N-CA	7.26	1.55	1.46
3	S	244	PRO	CB-CG	-7.25	1.13	1.49
1	E	24	VAL	CA-CB	-7.23	1.44	1.54
2	F	166	PRO	C-O	7.23	1.32	1.24
2	C	121	ASN	N-CA	-7.22	1.36	1.46
2	L	64	LEU	N-CA	-7.22	1.36	1.46
1	B	53	GLY	CA-C	7.22	1.62	1.51
1	H	19	LEU	C-O	7.22	1.32	1.24
3	S	273	ARG	CA-C	-7.22	1.43	1.52
1	B	105	ILE	N-CA	-7.21	1.38	1.46
1	B	94	ILE	CA-C	-7.20	1.42	1.52
1	H	24	VAL	C-O	7.20	1.33	1.24
2	F	106	PRO	N-CA	7.20	1.55	1.46
3	T	250	GLY	C-O	-7.20	1.14	1.23
1	H	45	GLY	N-CA	7.19	1.54	1.44
3	U	259	GLU	CD-OE1	7.19	1.39	1.25
1	K	141	ILE	CA-CB	7.19	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	55	VAL	CA-C	-7.19	1.43	1.52
2	F	158	LYS	N-CA	-7.19	1.36	1.46
1	B	61	PHE	CA-C	7.18	1.61	1.52
2	C	53	LYS	N-CA	7.18	1.55	1.46
2	F	53	LYS	N-CA	7.18	1.54	1.46
1	E	75	PHE	CA-CB	-7.18	1.41	1.53
2	C	66	ASP	CA-C	7.18	1.62	1.52
2	I	91	ILE	CA-C	7.18	1.60	1.53
2	I	117	MET	C-O	-7.18	1.15	1.24
3	T	256	LYS	CE-NZ	7.18	1.70	1.49
1	B	97	ASP	CA-C	-7.17	1.43	1.52
3	V	231	TYR	CA-CB	-7.17	1.40	1.53
1	B	156	ILE	C-O	7.17	1.37	1.23
1	H	57	LYS	N-CA	-7.17	1.37	1.46
1	B	29	ALA	CA-C	7.16	1.61	1.52
1	H	96	LYS	CB-CG	-7.16	1.30	1.52
2	C	153	ARG	CD-NE	7.16	1.56	1.46
3	V	262	LEU	C-O	7.15	1.32	1.24
1	H	52	GLU	C-O	7.14	1.32	1.24
2	L	113	THR	CA-CB	-7.14	1.41	1.53
2	F	137	LYS	CA-C	-7.14	1.43	1.53
2	I	136	ALA	N-CA	-7.14	1.37	1.46
2	I	101	LYS	CB-CG	-7.14	1.31	1.52
2	I	116	ASN	C-O	-7.14	1.15	1.24
3	T	271	VAL	CA-CB	-7.13	1.44	1.55
2	C	47	GLU	CD-OE1	7.13	1.38	1.25
1	H	116	LEU	N-CA	7.13	1.55	1.46
1	E	143	THR	N-CA	-7.12	1.38	1.46
3	U	273	ARG	CZ-NH1	7.11	1.42	1.32
3	S	263	GLN	CD-OE1	7.11	1.37	1.23
1	B	149	ARG	C-O	-7.11	1.15	1.24
2	L	143	SER	N-CA	-7.11	1.36	1.45
3	V	290	VAL	N-CA	7.10	1.54	1.46
3	S	295	ILE	CA-CB	7.10	1.61	1.54
1	E	104	GLN	C-O	7.10	1.31	1.23
1	E	23	PRO	C-O	7.10	1.32	1.23
1	K	44	ALA	CA-CB	7.10	1.64	1.53
1	K	65	GLU	CD-OE1	7.10	1.38	1.25
3	V	241	MET	C-O	7.10	1.32	1.23
3	S	270	PRO	C-O	-7.09	1.14	1.24
3	V	243	GLU	CD-OE1	7.08	1.38	1.25
2	C	148	LEU	N-CA	-7.08	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	119	PRO	CA-C	7.08	1.60	1.53
1	B	128	ASP	CG-OD2	7.07	1.38	1.25
2	F	91	ILE	CA-CB	-7.07	1.45	1.54
3	U	287	MET	CG-SD	7.07	1.98	1.80
2	L	88	GLU	N-CA	7.07	1.54	1.46
2	C	49	GLU	CD-OE2	7.07	1.38	1.25
2	F	132	ILE	N-CA	-7.07	1.36	1.46
2	L	65	GLU	CD-OE2	7.07	1.38	1.25
2	C	109	VAL	CA-C	7.06	1.61	1.52
1	E	97	ASP	CB-CG	7.06	1.69	1.52
1	K	70	ALA	C-O	7.05	1.32	1.24
1	E	41	VAL	C-O	-7.05	1.14	1.23
1	B	76	MET	CB-CG	-7.04	1.31	1.52
2	C	65	GLU	CD-OE1	7.04	1.38	1.25
1	B	5	SER	N-CA	7.04	1.55	1.46
2	C	77	GLY	CA-C	-7.04	1.44	1.52
2	I	80	LEU	N-CA	7.04	1.54	1.45
3	S	274	SER	C-O	-7.04	1.15	1.24
1	B	97	ASP	C-O	-7.03	1.15	1.24
2	C	110	ARG	CB-CG	-7.03	1.31	1.52
2	C	154	LEU	N-CA	-7.03	1.37	1.46
1	H	149	ARG	CZ-NH2	7.03	1.42	1.33
1	B	156	ILE	CA-CB	7.03	1.73	1.54
2	F	68	GLU	CA-C	-7.03	1.43	1.52
3	T	242	ARG	CZ-NH2	7.02	1.42	1.33
1	K	150	LEU	CB-CG	7.02	1.67	1.53
1	H	48	ASP	CG-OD1	7.02	1.38	1.25
2	I	83	PRO	C-O	7.02	1.33	1.24
1	E	112	ILE	CB-CG2	-7.01	1.29	1.52
1	K	18	ARG	CG-CD	7.01	1.73	1.52
2	F	46	GLU	CG-CD	7.01	1.69	1.52
2	C	114	LYS	CE-NZ	7.01	1.70	1.49
3	S	291	ILE	C-O	7.01	1.32	1.24
1	B	86	LYS	CE-NZ	7.00	1.70	1.49
2	I	101	LYS	CA-CB	-7.00	1.43	1.53
1	E	94	ILE	CB-CG2	6.99	1.75	1.52
2	C	43	ARG	CB-CG	-6.99	1.31	1.52
2	I	93	SER	N-CA	6.99	1.55	1.46
3	T	248	PRO	CA-C	-6.98	1.42	1.52
1	E	74	ARG	CB-CG	-6.98	1.31	1.52
1	E	113	GLN	CA-C	-6.98	1.43	1.52
3	U	293	ALA	CA-C	-6.97	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	235	LYS	C-O	-6.97	1.15	1.24
1	K	99	TRP	CE3-CZ3	6.97	1.59	1.38
1	E	8	LEU	CG-CD1	6.96	1.75	1.52
3	T	270	PRO	N-CA	-6.96	1.38	1.47
1	H	74	ARG	N-CA	6.96	1.54	1.46
3	T	247	THR	N-CA	-6.96	1.38	1.45
3	U	248	PRO	CA-C	-6.95	1.42	1.52
1	B	137	GLU	C-O	-6.95	1.15	1.24
1	K	154	ASN	C-O	6.95	1.32	1.24
2	C	153	ARG	CG-CD	6.94	1.73	1.52
1	H	12	ILE	CA-C	6.93	1.61	1.52
2	I	49	GLU	N-CA	6.93	1.54	1.46
2	C	67	ASP	CG-OD1	6.92	1.38	1.25
2	L	169	GLY	N-CA	6.92	1.55	1.45
2	F	145	LYS	C-O	6.92	1.32	1.24
1	B	58	LEU	CA-C	-6.92	1.43	1.52
2	L	49	GLU	CB-CG	6.92	1.73	1.52
1	E	132	GLN	CA-CB	-6.92	1.42	1.53
2	F	61	SER	C-O	6.91	1.32	1.23
2	I	76	THR	CB-CG2	-6.91	1.29	1.52
2	F	171	CYS	CA-CB	-6.91	1.40	1.54
1	B	123	ASP	CA-C	6.90	1.60	1.52
3	U	256	LYS	CE-NZ	6.90	1.70	1.49
1	E	76	MET	SD-CE	6.90	1.96	1.79
2	C	68	GLU	CD-OE1	6.90	1.38	1.25
3	S	278	GLN	C-O	6.90	1.32	1.24
3	T	249	SER	C-O	-6.89	1.15	1.24
1	H	70	ALA	CA-C	-6.89	1.44	1.52
2	I	157	SER	CA-C	6.89	1.62	1.52
1	E	38	TYR	CE1-CZ	6.89	1.54	1.38
1	B	68	MET	CA-CB	-6.89	1.41	1.53
2	L	78	MET	C-O	-6.88	1.15	1.23
1	B	22	GLU	CG-CD	6.88	1.69	1.52
1	K	73	VAL	C-O	6.87	1.31	1.24
2	L	84	ARG	CA-CB	6.87	1.65	1.53
1	B	116	LEU	N-CA	6.87	1.55	1.46
2	L	120	VAL	C-O	6.87	1.31	1.24
1	B	42	VAL	CB-CG2	-6.87	1.29	1.52
1	H	36	ALA	C-O	6.86	1.32	1.24
2	F	49	GLU	N-CA	6.86	1.54	1.46
2	L	37	LYS	CA-C	6.86	1.61	1.52
2	F	114	LYS	N-CA	6.85	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	73	VAL	CA-C	-6.85	1.44	1.52
1	E	123	ASP	CB-CG	6.85	1.69	1.52
2	F	60	VAL	CA-CB	-6.84	1.44	1.54
3	U	297	GLU	CA-C	6.84	1.63	1.52
3	T	279	GLU	CA-C	-6.84	1.43	1.52
3	U	283	PRO	N-CA	6.84	1.55	1.47
1	E	6	ALA	CA-CB	6.84	1.75	1.52
1	K	120	ASN	C-N	6.84	1.41	1.34
3	V	258	ILE	CA-CB	-6.84	1.46	1.54
2	C	104	GLU	C-O	-6.83	1.15	1.24
2	F	97	GLU	CD-OE2	6.83	1.38	1.25
1	H	96	LYS	CA-C	-6.83	1.46	1.53
2	I	43	ARG	CZ-NH1	6.83	1.42	1.32
2	C	123	SER	CA-CB	-6.83	1.45	1.53
3	V	251	ILE	N-CA	-6.82	1.37	1.46
2	I	110	ARG	N-CA	-6.82	1.37	1.45
3	T	272	THR	N-CA	6.82	1.54	1.46
1	K	83	ASN	CG-ND2	6.81	1.47	1.33
2	F	67	ASP	CA-C	6.81	1.61	1.52
2	F	107	PRO	N-CA	-6.81	1.40	1.46
1	H	26	GLY	N-CA	6.81	1.52	1.45
3	V	230	ASP	CA-C	6.81	1.61	1.52
1	B	57	LYS	CD-CE	6.81	1.72	1.52
3	S	264	ARG	CZ-NH2	6.81	1.42	1.33
1	B	10	ARG	CZ-NH1	6.80	1.42	1.32
3	T	255	ARG	CZ-NH2	6.80	1.42	1.33
1	H	6	ALA	C-N	6.79	1.42	1.33
2	F	78	MET	SD-CE	6.79	1.96	1.79
3	U	256	LYS	CG-CD	6.78	1.72	1.52
2	L	155	MET	CB-CG	6.78	1.72	1.52
2	F	49	GLU	CD-OE2	6.78	1.38	1.25
3	V	272	THR	N-CA	6.77	1.55	1.45
1	K	68	MET	CA-C	6.77	1.61	1.52
2	L	101	LYS	CE-NZ	6.77	1.69	1.49
2	C	154	LEU	CA-C	-6.76	1.44	1.52
2	L	80	LEU	N-CA	6.76	1.54	1.45
1	E	73	VAL	C-O	6.75	1.30	1.24
3	S	248	PRO	CA-CB	-6.75	1.43	1.53
2	C	147	VAL	CA-C	-6.75	1.44	1.52
2	I	45	LEU	C-O	6.75	1.32	1.24
1	B	76	MET	CG-SD	6.74	1.97	1.80
1	K	133	TRP	C-O	6.74	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	82	PRO	N-CA	-6.74	1.39	1.47
2	C	37	LYS	C-N	6.73	1.41	1.33
2	C	90	ARG	CA-C	-6.73	1.43	1.53
1	B	28	LYS	CD-CE	6.73	1.72	1.52
2	L	132	ILE	CB-CG1	-6.73	1.40	1.53
1	B	91	CYS	CA-C	6.73	1.61	1.52
2	F	133	SER	N-CA	-6.72	1.37	1.46
1	E	14	LYS	C-O	6.72	1.31	1.24
2	L	163	LEU	N-CA	6.71	1.57	1.46
3	T	251	ILE	C-O	-6.71	1.17	1.24
3	U	240	LEU	CA-C	-6.71	1.44	1.52
2	L	166	PRO	CA-C	-6.71	1.46	1.52
3	T	261	HIS	C-O	-6.71	1.15	1.24
3	U	233	CYS	CA-CB	-6.71	1.43	1.53
1	B	33	GLU	CD-OE2	6.71	1.38	1.25
1	H	19	LEU	CA-C	6.71	1.61	1.52
2	L	132	ILE	CA-C	6.70	1.61	1.52
3	T	258	ILE	CA-CB	-6.70	1.45	1.54
2	C	52	GLN	CD-NE2	6.70	1.47	1.33
1	K	16	THR	CA-C	-6.69	1.44	1.52
1	E	121	PRO	N-CA	6.69	1.55	1.47
2	F	163	LEU	CA-C	6.69	1.60	1.53
3	S	262	LEU	N-CA	-6.69	1.38	1.46
1	E	58	LEU	N-CA	6.68	1.54	1.45
1	H	77	THR	C-O	-6.68	1.15	1.23
2	L	147	VAL	CB-CG1	-6.68	1.30	1.52
1	E	76	MET	CA-C	6.68	1.61	1.52
2	L	117	MET	CG-SD	6.68	1.97	1.80
3	U	228	ILE	CB-CG2	6.68	1.74	1.52
1	H	70	ALA	CA-CB	-6.68	1.42	1.53
1	H	76	MET	CA-C	6.68	1.61	1.52
1	K	142	GLU	C-O	6.68	1.32	1.24
3	S	265	VAL	N-CA	-6.67	1.39	1.46
3	S	231	TYR	C-O	-6.67	1.15	1.24
2	I	59	THR	C-O	6.67	1.32	1.24
2	C	126	VAL	C-O	-6.66	1.16	1.24
2	I	67	ASP	CA-C	-6.66	1.43	1.52
1	H	98	LYS	CA-C	6.66	1.61	1.52
3	S	242	ARG	CD-NE	6.65	1.55	1.46
3	T	287	MET	N-CA	-6.65	1.38	1.46
2	C	97	GLU	CD-OE2	6.64	1.38	1.25
3	V	268	PHE	CA-C	-6.64	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	12	ILE	CA-CB	6.64	1.62	1.54
3	U	251	ILE	CA-C	-6.64	1.44	1.52
2	F	47	GLU	CA-CB	-6.64	1.42	1.53
2	I	107	PRO	C-O	-6.63	1.15	1.24
2	L	98	CYS	CA-C	-6.63	1.43	1.53
1	K	140	ALA	C-N	6.63	1.42	1.33
3	T	238	PHE	C-O	-6.63	1.15	1.24
3	U	271	VAL	CA-C	-6.63	1.44	1.52
3	V	298	ASN	CB-CG	6.63	1.68	1.52
3	V	292	ASP	CB-CG	6.63	1.68	1.52
1	E	69	ALA	CA-CB	-6.62	1.42	1.53
2	F	153	ARG	CZ-NH1	6.62	1.42	1.32
1	B	48	ASP	CA-C	6.62	1.61	1.52
1	B	8	LEU	C-N	6.62	1.42	1.33
1	E	42	VAL	CA-C	-6.62	1.44	1.52
1	B	138	ALA	CA-CB	-6.62	1.43	1.53
1	B	77	THR	CA-C	-6.61	1.44	1.53
3	S	300	TRP	CZ3-CH2	6.61	1.56	1.40
3	T	249	SER	N-CA	6.61	1.54	1.46
2	C	126	VAL	N-CA	-6.61	1.38	1.46
3	T	257	ASP	C-O	-6.60	1.16	1.24
2	F	141	SER	N-CA	6.60	1.55	1.45
1	B	11	ARG	C-O	6.60	1.31	1.24
1	K	118	ALA	CA-CB	6.60	1.60	1.53
2	F	144	ILE	CG1-CD1	6.59	1.77	1.51
1	H	68	MET	N-CA	-6.59	1.38	1.46
3	U	245	CYS	CB-SG	6.59	2.03	1.81
1	H	69	ALA	C-O	-6.59	1.15	1.23
3	U	295	ILE	CG1-CD1	6.59	1.77	1.51
2	C	105	ALA	N-CA	6.59	1.52	1.45
2	C	102	TYR	CA-CB	6.59	1.63	1.53
1	B	150	LEU	CG-CD1	6.58	1.74	1.52
1	E	120	ASN	N-CA	6.58	1.53	1.46
1	H	15	GLU	CD-OE1	6.58	1.37	1.25
1	B	27	ILE	C-O	-6.58	1.17	1.24
1	B	83	ASN	C-O	-6.58	1.15	1.24
1	B	88	GLY	CA-C	6.58	1.60	1.51
3	T	263	GLN	CG-CD	6.58	1.68	1.52
2	C	99	GLY	C-O	6.58	1.32	1.24
2	C	37	LYS	C-O	6.57	1.31	1.24
2	C	96	ILE	N-CA	-6.57	1.38	1.46
1	E	149	ARG	CA-CB	-6.57	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	124	ASN	CA-C	-6.57	1.43	1.52
2	F	169	GLY	C-O	-6.57	1.15	1.23
2	L	129	PRO	C-O	-6.57	1.15	1.24
3	U	280	GLN	CD-NE2	6.57	1.47	1.33
1	E	120	ASN	C-O	6.56	1.32	1.24
1	K	15	GLU	CD-OE1	6.56	1.37	1.25
3	S	227	ASP	CG-OD2	6.56	1.37	1.25
1	E	128	ASP	CG-OD1	6.56	1.37	1.25
3	S	235	LYS	CG-CD	-6.55	1.32	1.52
2	F	101	LYS	CB-CG	-6.55	1.32	1.52
2	L	38	VAL	CB-CG2	6.55	1.74	1.52
2	L	66	ASP	N-CA	-6.54	1.38	1.46
2	F	57	ASP	CG-OD2	6.54	1.37	1.25
2	C	120	VAL	C-O	-6.53	1.17	1.24
1	E	44	ALA	N-CA	-6.53	1.37	1.46
2	F	97	GLU	CG-CD	6.53	1.68	1.52
1	H	106	ARG	CZ-NH1	6.53	1.41	1.32
3	S	241	MET	C-O	-6.53	1.16	1.24
1	B	69	ALA	N-CA	-6.52	1.38	1.46
2	C	174	ASN	N-CA	6.52	1.58	1.46
2	I	91	ILE	CA-CB	6.52	1.60	1.53
1	K	39	PHE	CE1-CZ	6.52	1.58	1.38
3	U	234	GLY	C-O	6.52	1.32	1.23
2	C	153	ARG	N-CA	6.51	1.54	1.46
2	F	37	LYS	N-CA	6.51	1.54	1.46
1	B	79	ILE	C-O	-6.51	1.17	1.23
2	C	153	ARG	C-O	-6.51	1.16	1.24
1	K	133	TRP	CA-C	6.51	1.61	1.52
1	K	72	LYS	CA-C	6.51	1.61	1.52
2	F	49	GLU	CG-CD	6.51	1.68	1.52
2	F	105	ALA	C-N	-6.51	1.27	1.33
2	L	123	SER	CA-C	-6.50	1.44	1.52
3	S	274	SER	CB-OG	-6.50	1.29	1.42
2	C	174	ASN	CB-CG	6.50	1.68	1.52
1	H	70	ALA	N-CA	6.50	1.55	1.46
1	B	16	THR	CB-CG2	-6.49	1.31	1.52
2	F	43	ARG	CZ-NH1	6.48	1.41	1.32
3	V	284	ASN	CA-C	-6.48	1.43	1.53
1	H	20	LEU	CG-CD2	6.47	1.74	1.52
2	I	52	GLN	CD-NE2	6.47	1.46	1.33
3	S	281	LEU	N-CA	6.47	1.54	1.46
2	F	153	ARG	CZ-NH2	6.47	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	165	GLN	CA-CB	-6.47	1.44	1.53
1	K	62	LEU	N-CA	6.47	1.55	1.46
2	F	50	GLU	C-O	6.46	1.31	1.24
1	K	28	LYS	CA-C	-6.45	1.44	1.53
3	S	268	PHE	CA-C	6.45	1.60	1.52
2	L	37	LYS	C-N	6.44	1.40	1.33
3	U	292	ASP	N-CA	6.44	1.54	1.46
1	B	3	ALA	C-N	6.44	1.43	1.33
2	C	90	ARG	CZ-NH1	-6.44	1.23	1.32
2	F	84	ARG	CB-CG	6.44	1.71	1.52
1	K	60	LEU	C-O	6.44	1.31	1.24
1	B	100	SER	CA-C	-6.44	1.45	1.52
1	K	112	ILE	CA-C	6.44	1.60	1.52
1	K	72	LYS	C-O	6.43	1.31	1.24
1	B	152	ALA	CA-C	-6.43	1.44	1.52
2	L	105	ALA	CA-CB	-6.42	1.46	1.54
2	C	158	LYS	CA-CB	-6.42	1.42	1.53
3	T	259	GLU	C-O	6.42	1.31	1.24
2	I	153	ARG	CA-C	6.42	1.62	1.52
3	U	242	ARG	CA-C	6.42	1.61	1.52
1	E	101	PRO	CA-C	6.41	1.62	1.52
3	U	273	ARG	CD-NE	6.41	1.55	1.46
2	L	75	TRP	C-O	-6.41	1.15	1.23
1	E	17	GLN	N-CA	-6.40	1.38	1.46
2	I	106	PRO	CA-CB	-6.40	1.45	1.54
3	V	263	GLN	CA-C	6.40	1.61	1.53
1	B	23	PRO	C-O	6.40	1.31	1.23
2	L	84	ARG	CA-C	6.40	1.61	1.52
3	T	271	VAL	CA-C	-6.40	1.46	1.52
2	F	67	ASP	C-O	6.39	1.32	1.24
1	B	93	ASP	C-O	-6.39	1.16	1.24
2	C	101	LYS	CE-NZ	6.39	1.68	1.49
2	I	43	ARG	C-O	6.39	1.31	1.24
2	L	76	THR	C-O	-6.39	1.16	1.24
3	V	235	LYS	CE-NZ	6.39	1.68	1.49
1	B	149	ARG	CA-CB	-6.38	1.42	1.53
2	I	149	GLN	CA-C	-6.38	1.46	1.53
1	K	24	VAL	N-CA	6.38	1.54	1.46
2	C	44	LEU	CA-C	-6.38	1.44	1.52
1	E	77	THR	C-O	6.37	1.31	1.23
3	U	279	GLU	CA-C	-6.37	1.43	1.52
2	C	164	PRO	CA-CB	-6.37	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	109	LEU	N-CA	6.37	1.54	1.46
2	L	78	MET	CG-SD	6.37	1.96	1.80
3	V	233	CYS	CA-C	-6.37	1.44	1.52
2	C	101	LYS	CA-CB	-6.37	1.44	1.53
1	E	24	VAL	N-CA	6.37	1.54	1.46
1	E	69	ALA	CA-C	-6.37	1.45	1.52
1	E	62	LEU	C-O	6.37	1.30	1.25
3	T	230	ASP	CA-CB	-6.37	1.43	1.53
2	C	173	SER	C-O	6.36	1.31	1.23
1	E	21	ALA	CA-CB	6.36	1.63	1.53
2	C	90	ARG	C-O	-6.36	1.15	1.23
2	L	102	TYR	CZ-OH	6.36	1.51	1.38
3	U	274	SER	CA-CB	-6.36	1.43	1.53
1	K	93	ASP	CG-OD1	6.35	1.37	1.25
1	E	141	ILE	N-CA	-6.34	1.39	1.46
1	K	5	SER	N-CA	6.34	1.54	1.46
2	C	144	ILE	CA-C	-6.34	1.45	1.52
1	H	6	ALA	CA-C	6.34	1.66	1.52
2	L	114	LYS	C-O	6.34	1.31	1.23
2	I	136	ALA	CA-CB	-6.34	1.43	1.53
2	L	130	ARG	C-O	-6.33	1.15	1.24
1	E	102	ALA	CA-CB	6.33	1.63	1.53
1	B	58	LEU	CA-CB	-6.33	1.44	1.53
2	C	74	ARG	NE-CZ	6.33	1.40	1.33
1	K	8	LEU	N-CA	6.33	1.55	1.46
3	T	269	ASN	C-O	6.33	1.32	1.24
3	U	276	LEU	N-CA	-6.32	1.38	1.46
1	H	120	ASN	CG-OD1	6.32	1.35	1.23
2	L	134	VAL	N-CA	-6.32	1.38	1.46
1	H	137	GLU	N-CA	6.31	1.54	1.46
1	E	74	ARG	C-O	-6.31	1.16	1.23
2	C	137	LYS	CB-CG	-6.31	1.33	1.52
3	V	279	GLU	CG-CD	6.31	1.67	1.52
2	I	149	GLN	N-CA	6.30	1.53	1.46
1	H	65	GLU	CD-OE2	6.30	1.37	1.25
1	B	111	SER	CA-CB	-6.29	1.43	1.53
2	F	113	THR	N-CA	-6.29	1.38	1.46
1	E	98	LYS	CA-C	6.29	1.61	1.52
1	K	97	ASP	CA-C	6.28	1.61	1.52
1	K	122	ASP	CA-C	6.28	1.61	1.52
2	C	107	PRO	CA-CB	-6.28	1.47	1.54
3	V	287	MET	CG-SD	6.28	1.96	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	67	ASP	CA-C	-6.27	1.44	1.52
2	F	150	GLU	CD-OE2	6.27	1.37	1.25
3	S	231	TYR	N-CA	6.26	1.54	1.46
1	H	143	THR	CA-CB	6.26	1.64	1.53
1	H	47	GLN	CA-C	6.25	1.60	1.52
2	C	128	ASP	N-CA	-6.25	1.35	1.46
1	B	75	PHE	CA-CB	-6.24	1.43	1.53
3	S	227	ASP	CB-CG	6.23	1.67	1.52
3	U	243	GLU	N-CA	6.23	1.54	1.46
1	B	104	GLN	CA-C	6.23	1.60	1.52
2	C	105	ALA	CA-C	-6.22	1.45	1.52
2	F	153	ARG	NE-CZ	6.22	1.39	1.33
3	V	256	LYS	C-O	6.22	1.31	1.24
2	I	120	VAL	CA-CB	-6.22	1.46	1.53
1	K	4	GLY	CA-C	6.22	1.59	1.51
3	T	267	HIS	CA-C	-6.22	1.46	1.53
1	B	82	PRO	CA-CB	-6.21	1.45	1.53
2	I	70	MET	CA-C	-6.21	1.43	1.52
2	I	56	GLY	C-O	6.21	1.32	1.23
2	F	130	ARG	NE-CZ	6.21	1.39	1.33
3	S	239	GLU	CA-C	6.21	1.61	1.53
2	F	140	ASN	C-O	6.21	1.31	1.24
3	T	228	ILE	CG1-CD1	6.21	1.75	1.51
1	H	16	THR	N-CA	6.20	1.54	1.46
1	B	15	GLU	N-CA	-6.20	1.38	1.46
1	B	62	LEU	N-CA	-6.20	1.37	1.46
2	C	148	LEU	CA-C	-6.20	1.44	1.52
1	K	36	ALA	CA-CB	6.20	1.64	1.53
2	C	173	SER	CB-OG	6.20	1.54	1.42
3	T	302	GLU	C-O	6.20	1.31	1.23
1	K	119	PRO	CA-CB	6.19	1.59	1.53
1	E	43	ILE	C-O	-6.19	1.16	1.24
1	K	120	ASN	CA-CB	6.18	1.63	1.53
3	T	271	VAL	N-CA	-6.18	1.40	1.46
3	T	301	VAL	N-CA	6.18	1.54	1.46
2	I	99	GLY	N-CA	-6.17	1.36	1.44
1	E	6	ALA	CA-C	6.17	1.66	1.52
3	U	281	LEU	C-O	6.17	1.31	1.23
3	U	254	ASP	C-O	6.17	1.31	1.23
1	B	6	ALA	C-N	-6.17	1.27	1.34
1	B	115	LEU	N-CA	6.17	1.54	1.46
2	F	111	PHE	CA-CB	-6.17	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	84	ARG	C-O	-6.16	1.16	1.24
3	T	247	THR	CA-C	-6.16	1.45	1.52
3	T	227	ASP	N-CA	6.16	1.57	1.46
1	E	29	ALA	C-O	-6.16	1.16	1.24
1	B	74	ARG	CZ-NH2	-6.16	1.25	1.33
2	C	80	LEU	CG-CD2	-6.16	1.32	1.52
3	V	270	PRO	C-O	-6.15	1.16	1.24
1	K	83	ASN	CA-CB	6.15	1.62	1.53
2	L	112	VAL	N-CA	-6.15	1.38	1.46
3	S	253	TYR	CB-CG	6.14	1.65	1.51
1	H	142	GLU	CD-OE2	6.14	1.37	1.25
1	K	20	LEU	N-CA	6.13	1.53	1.46
2	I	138	TRP	N-CA	6.13	1.54	1.46
1	E	121	PRO	C-O	6.13	1.31	1.24
1	B	145	ARG	CA-C	-6.12	1.44	1.52
3	U	269	ASN	N-CA	-6.11	1.37	1.46
3	U	287	MET	SD-CE	6.11	1.94	1.79
2	I	37	LYS	CB-CG	6.11	1.70	1.52
1	K	122	ASP	CB-CG	6.11	1.67	1.52
3	T	301	VAL	CA-C	6.11	1.60	1.52
3	U	242	ARG	NE-CZ	6.10	1.39	1.33
1	H	142	GLU	CG-CD	6.09	1.67	1.52
3	S	254	ASP	CB-CG	6.09	1.67	1.52
3	V	270	PRO	CB-CG	6.09	1.80	1.49
3	V	259	GLU	C-O	6.09	1.31	1.24
3	U	251	ILE	CB-CG2	-6.09	1.32	1.52
2	C	74	ARG	CG-CD	6.08	1.70	1.52
2	F	53	LYS	C-O	-6.08	1.17	1.24
2	L	154	LEU	C-O	-6.08	1.16	1.24
2	L	95	LYS	CB-CG	6.08	1.70	1.52
1	H	74	ARG	C-O	-6.08	1.16	1.23
2	F	37	LYS	CE-NZ	6.07	1.67	1.49
3	U	233	CYS	CA-C	-6.07	1.45	1.52
3	U	291	ILE	C-O	6.07	1.31	1.24
1	E	102	ALA	CA-C	-6.07	1.44	1.52
1	E	93	ASP	CA-C	6.07	1.60	1.52
1	H	89	ARG	CA-CB	-6.07	1.43	1.53
2	C	107	PRO	CG-CD	-6.06	1.30	1.50
3	U	253	TYR	CG-CD2	6.06	1.52	1.39
2	F	41	ASN	CG-ND2	6.06	1.46	1.33
2	I	46	GLU	C-O	6.06	1.31	1.24
2	F	104	GLU	C-O	-6.06	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	51	PHE	CA-CB	-6.05	1.43	1.53
1	B	62	LEU	C-O	-6.05	1.16	1.24
1	E	81	HIS	C-O	6.05	1.31	1.24
2	L	115	ILE	N-CA	6.04	1.52	1.46
1	K	93	ASP	C-O	6.04	1.31	1.24
3	V	293	ALA	CA-CB	-6.04	1.42	1.53
2	C	158	LYS	CG-CD	6.04	1.70	1.52
1	E	141	ILE	CA-CB	-6.04	1.47	1.54
1	K	26	GLY	N-CA	6.04	1.54	1.45
3	S	293	ALA	CA-CB	-6.04	1.43	1.53
1	E	32	ASP	CG-OD1	6.04	1.36	1.25
3	V	289	GLU	CG-CD	6.04	1.67	1.52
1	H	137	GLU	CA-CB	6.03	1.63	1.53
2	F	108	PHE	CD2-CE2	-6.03	1.20	1.38
2	C	118	ASN	N-CA	6.03	1.53	1.46
2	I	139	GLN	C-O	6.03	1.31	1.24
2	I	159	GLU	CA-C	-6.02	1.44	1.52
1	K	154	ASN	N-CA	6.02	1.53	1.46
2	L	150	GLU	N-CA	-6.02	1.38	1.46
2	C	38	VAL	CB-CG2	6.02	1.72	1.52
2	C	57	ASP	C-O	6.01	1.31	1.24
2	F	152	ARG	CA-CB	-6.01	1.44	1.53
1	E	120	ASN	CA-C	6.01	1.58	1.52
2	L	92	TYR	N-CA	-6.01	1.38	1.45
2	C	137	LYS	CG-CD	-6.01	1.34	1.52
3	T	288	LYS	CE-NZ	6.01	1.67	1.49
2	L	102	TYR	N-CA	-6.00	1.36	1.45
2	F	49	GLU	CA-C	6.00	1.60	1.52
1	K	90	ILE	CA-CB	-6.00	1.46	1.54
3	V	273	ARG	C-O	6.00	1.35	1.24
3	S	237	SER	CA-CB	-6.00	1.43	1.53
3	U	243	GLU	CA-CB	-6.00	1.44	1.53
2	L	120	VAL	CA-CB	-6.00	1.46	1.53
2	C	55	VAL	CB-CG1	5.99	1.72	1.52
1	K	56	PHE	C-O	5.99	1.30	1.24
3	T	231	TYR	CE1-CZ	5.99	1.52	1.38
2	I	43	ARG	CA-CB	-5.99	1.44	1.53
3	S	291	ILE	CB-CG1	5.99	1.65	1.53
3	V	240	LEU	C-O	5.99	1.31	1.24
1	B	131	GLU	CG-CD	5.99	1.67	1.52
1	B	139	GLN	CB-CG	-5.99	1.34	1.52
2	C	76	THR	C-O	-5.98	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	132	ILE	CA-CB	-5.98	1.46	1.54
3	V	255	ARG	C-N	5.98	1.41	1.33
2	L	153	ARG	CZ-NH2	5.98	1.41	1.33
1	B	4	GLY	C-N	5.97	1.42	1.33
1	H	68	MET	CG-SD	5.97	1.95	1.80
2	I	50	GLU	CG-CD	5.97	1.67	1.52
3	V	281	LEU	CA-C	5.97	1.60	1.52
2	F	56	GLY	CA-C	5.97	1.60	1.51
3	S	245	CYS	N-CA	5.96	1.53	1.45
2	L	165	GLN	N-CA	5.96	1.54	1.45
1	B	145	ARG	N-CA	-5.96	1.38	1.46
3	S	279	GLU	CD-OE1	5.96	1.36	1.25
2	I	139	GLN	N-CA	5.96	1.53	1.46
2	L	113	THR	C-O	-5.96	1.16	1.23
2	F	103	PRO	CB-CG	5.95	1.74	1.51
2	L	79	ILE	CA-CB	-5.95	1.46	1.54
3	S	279	GLU	C-N	-5.95	1.26	1.33
1	B	65	GLU	CG-CD	5.95	1.67	1.52
2	C	108	PHE	CG-CD2	-5.95	1.26	1.38
2	L	94	LEU	N-CA	-5.95	1.39	1.46
1	E	70	ALA	CA-CB	-5.95	1.43	1.53
1	E	6	ALA	C-O	5.95	1.35	1.23
1	E	25	PRO	CA-C	5.95	1.59	1.52
2	L	141	SER	CA-C	5.95	1.60	1.52
2	L	149	GLN	CG-CD	5.94	1.67	1.52
2	C	39	PRO	CA-C	5.94	1.60	1.52
3	T	290	VAL	C-O	5.94	1.31	1.24
2	C	57	ASP	CB-CG	5.94	1.66	1.52
2	C	38	VAL	CA-C	5.93	1.59	1.52
3	S	236	ILE	CA-C	5.93	1.60	1.52
1	E	60	LEU	C-O	5.93	1.30	1.23
1	B	37	ARG	CA-CB	-5.93	1.42	1.53
2	C	95	LYS	CA-C	5.93	1.59	1.52
1	E	122	ASP	N-CA	5.93	1.53	1.46
2	F	97	GLU	CD-OE1	5.93	1.36	1.25
2	F	132	ILE	CG1-CD1	-5.93	1.28	1.51
1	K	65	GLU	C-O	5.93	1.31	1.24
3	S	263	GLN	C-O	-5.93	1.16	1.24
3	V	257	ASP	CA-C	-5.93	1.45	1.52
3	V	267	HIS	CA-C	-5.93	1.46	1.53
2	C	138	TRP	CB-CG	-5.92	1.31	1.50
1	E	41	VAL	CA-CB	-5.92	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	15	GLU	CD-OE2	5.92	1.36	1.25
1	K	5	SER	C-N	5.92	1.42	1.33
2	I	82	PRO	C-O	5.92	1.31	1.24
3	T	257	ASP	CA-CB	-5.92	1.44	1.53
2	I	46	GLU	CD-OE2	5.91	1.36	1.25
1	B	140	ALA	CA-CB	-5.91	1.44	1.53
1	K	72	LYS	CE-NZ	5.91	1.67	1.49
3	U	274	SER	C-O	5.91	1.31	1.24
3	V	256	LYS	CD-CE	5.91	1.70	1.52
3	S	247	THR	CA-CB	5.90	1.62	1.54
1	H	119	PRO	N-CA	5.90	1.54	1.47
2	I	104	GLU	CG-CD	5.90	1.66	1.52
3	V	240	LEU	CG-CD1	5.90	1.72	1.52
3	T	241	MET	C-O	-5.90	1.17	1.24
1	E	22	GLU	N-CA	5.90	1.52	1.46
1	H	59	GLU	CA-C	5.89	1.59	1.52
2	I	43	ARG	N-CA	-5.89	1.39	1.46
1	K	150	LEU	CA-C	5.89	1.60	1.52
2	C	139	GLN	CA-CB	-5.88	1.44	1.53
2	C	52	GLN	CD-OE1	5.88	1.34	1.23
1	H	12	ILE	C-N	5.88	1.41	1.33
1	H	43	ILE	C-O	5.88	1.32	1.24
2	L	55	VAL	C-O	-5.87	1.18	1.24
3	T	254	ASP	CA-C	-5.87	1.45	1.52
3	U	271	VAL	CB-CG1	5.87	1.72	1.52
2	C	136	ALA	CA-CB	-5.87	1.44	1.53
1	E	17	GLN	CD-OE1	5.87	1.34	1.23
3	V	245	CYS	CA-C	5.87	1.60	1.52
2	I	75	TRP	C-O	-5.87	1.16	1.23
3	S	293	ALA	CA-C	-5.87	1.45	1.52
2	F	77	GLY	C-O	5.87	1.32	1.24
3	V	242	ARG	CG-CD	5.87	1.70	1.52
3	S	290	VAL	CA-CB	-5.86	1.45	1.54
3	S	284	ASN	N-CA	-5.86	1.39	1.46
2	F	49	GLU	C-O	5.86	1.31	1.24
2	C	91	ILE	CA-CB	-5.86	1.47	1.54
1	E	153	MET	N-CA	-5.86	1.38	1.45
2	L	38	VAL	N-CA	5.86	1.53	1.46
2	F	104	GLU	CD-OE1	5.86	1.36	1.25
3	T	264	ARG	C-O	-5.85	1.16	1.24
3	T	300	TRP	C-N	5.85	1.41	1.33
1	E	151	TYR	CA-C	5.85	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	119	GLY	C-O	-5.85	1.15	1.24
1	E	92	LEU	N-CA	5.84	1.52	1.46
2	F	57	ASP	CA-C	5.83	1.60	1.52
1	B	17	GLN	N-CA	-5.83	1.38	1.46
1	H	45	GLY	C-N	5.83	1.40	1.33
3	U	280	GLN	CA-C	-5.82	1.44	1.52
2	L	174	ASN	CA-CB	5.82	1.65	1.53
1	H	102	ALA	N-CA	-5.82	1.38	1.46
2	L	161	MET	SD-CE	5.82	1.94	1.79
2	C	103	PRO	CA-C	-5.82	1.41	1.52
1	B	61	PHE	CD2-CE2	5.81	1.56	1.38
2	C	108	PHE	CA-CB	-5.81	1.44	1.53
1	K	57	LYS	CA-C	5.81	1.60	1.52
2	L	117	MET	CA-C	5.81	1.60	1.52
3	T	234	GLY	N-CA	5.81	1.53	1.45
2	F	102	TYR	N-CA	5.81	1.54	1.45
1	H	117	SER	CA-C	5.81	1.60	1.52
2	L	120	VAL	CB-CG2	-5.80	1.33	1.52
3	V	271	VAL	CA-C	-5.80	1.45	1.52
3	V	236	ILE	CA-C	5.80	1.60	1.52
1	E	105	ILE	CG1-CD1	-5.80	1.29	1.51
1	B	30	GLU	CA-CB	-5.79	1.44	1.53
2	L	77	GLY	C-O	5.79	1.31	1.23
1	E	49	SER	C-O	-5.79	1.16	1.23
1	K	105	ILE	CA-C	-5.79	1.45	1.52
3	U	236	ILE	CB-CG2	-5.79	1.33	1.52
3	V	289	GLU	CD-OE1	5.79	1.36	1.25
3	V	264	ARG	CZ-NH1	5.78	1.40	1.32
1	B	70	ALA	CA-C	-5.78	1.45	1.52
2	C	172	TYR	C-O	-5.78	1.16	1.23
2	F	108	PHE	CA-C	-5.78	1.45	1.52
3	S	268	PHE	N-CA	-5.78	1.39	1.46
1	B	103	LEU	CA-C	-5.78	1.45	1.53
1	H	142	GLU	C-O	5.78	1.31	1.24
1	B	111	SER	CA-C	-5.78	1.45	1.52
2	C	159	GLU	N-CA	5.78	1.53	1.46
2	F	39	PRO	N-CA	5.78	1.53	1.46
2	I	84	ARG	CA-CB	5.77	1.63	1.53
2	C	36	VAL	N-CA	5.77	1.53	1.46
2	L	167	PRO	C-O	5.77	1.31	1.24
1	B	64	GLU	N-CA	-5.77	1.38	1.46
1	K	77	THR	CB-CG2	5.77	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	15	GLU	CG-CD	5.77	1.66	1.52
1	H	16	THR	CA-C	5.76	1.60	1.52
2	I	55	VAL	CA-C	5.76	1.60	1.52
3	U	275	PRO	CA-C	5.76	1.59	1.52
1	B	16	THR	CA-CB	-5.76	1.43	1.53
1	K	100	SER	CA-C	5.76	1.59	1.52
2	L	50	GLU	CA-CB	-5.76	1.43	1.53
1	H	143	THR	CA-C	5.76	1.60	1.52
1	H	50	PRO	CA-C	5.76	1.60	1.52
2	F	140	ASN	CG-OD1	5.75	1.34	1.23
1	K	49	SER	CA-C	5.75	1.58	1.52
2	L	169	GLY	CA-C	5.75	1.59	1.51
1	H	104	GLN	CA-CB	-5.75	1.46	1.53
2	C	164	PRO	CB-CG	-5.74	1.21	1.49
1	K	92	LEU	N-CA	5.74	1.53	1.46
1	H	98	LYS	CB-CG	5.74	1.69	1.52
3	S	280	GLN	CA-CB	5.74	1.61	1.53
3	U	236	ILE	CG1-CD1	5.74	1.74	1.51
3	U	279	GLU	N-CA	5.74	1.52	1.46
3	U	268	PHE	CA-C	5.73	1.60	1.52
2	I	54	GLY	N-CA	5.73	1.52	1.44
2	C	128	ASP	C-O	-5.73	1.17	1.24
2	L	133	SER	CA-C	-5.73	1.45	1.52
2	F	65	GLU	N-CA	5.73	1.53	1.46
1	E	116	LEU	N-CA	-5.72	1.38	1.46
1	E	111	SER	C-O	5.72	1.30	1.24
3	T	297	GLU	N-CA	5.72	1.53	1.46
2	C	84	ARG	CZ-NH1	5.72	1.40	1.32
2	C	74	ARG	C-O	-5.72	1.17	1.24
3	S	249	SER	C-O	-5.71	1.15	1.24
3	T	301	VAL	CB-CG1	5.71	1.71	1.52
1	B	10	ARG	NE-CZ	5.71	1.39	1.33
1	H	9	PRO	N-CA	-5.71	1.40	1.47
3	V	277	THR	N-CA	5.71	1.53	1.45
2	F	37	LYS	CG-CD	5.70	1.69	1.52
3	V	273	ARG	C-N	5.70	1.41	1.33
1	H	90	ILE	CA-C	-5.70	1.45	1.52
2	C	130	ARG	N-CA	5.70	1.53	1.46
2	I	153	ARG	C-O	5.70	1.30	1.24
3	U	298	ASN	CG-OD1	5.69	1.34	1.23
2	C	139	GLN	CA-C	-5.69	1.45	1.52
2	C	124	ASN	CG-OD1	5.69	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	64	GLU	N-CA	5.69	1.53	1.46
2	I	168	GLU	CB-CG	5.69	1.69	1.52
3	S	258	ILE	CB-CG2	-5.68	1.33	1.52
2	C	41	ASN	N-CA	-5.68	1.39	1.46
3	U	289	GLU	CA-C	-5.67	1.45	1.52
1	H	10	ARG	CZ-NH2	5.67	1.40	1.33
1	H	115	LEU	N-CA	-5.67	1.39	1.46
1	E	77	THR	CA-C	5.67	1.59	1.52
1	H	74	ARG	CB-CG	-5.67	1.35	1.52
1	K	152	ALA	CA-CB	5.67	1.63	1.53
3	T	232	LEU	C-O	5.67	1.31	1.24
1	B	131	GLU	C-O	5.66	1.30	1.24
2	C	94	LEU	N-CA	5.66	1.53	1.45
2	I	101	LYS	C-O	-5.66	1.15	1.23
3	V	285	LEU	C-O	-5.66	1.17	1.24
1	K	156	ILE	N-CA	5.66	1.56	1.46
2	C	171	CYS	CA-C	-5.66	1.45	1.52
2	F	170	GLN	CD-NE2	5.66	1.45	1.33
1	K	151	TYR	C-O	5.66	1.31	1.24
2	F	37	LYS	CD-CE	5.65	1.69	1.52
3	S	252	THR	CB-OG1	5.64	1.52	1.43
2	F	105	ALA	C-O	-5.64	1.17	1.23
1	K	94	ILE	CA-C	5.64	1.59	1.52
2	F	137	LYS	C-O	5.64	1.29	1.23
2	F	172	TYR	CA-CB	-5.64	1.44	1.53
2	C	126	VAL	CB-CG1	-5.63	1.33	1.52
2	C	82	PRO	C-N	-5.63	1.26	1.33
2	F	120	VAL	N-CA	-5.63	1.39	1.46
1	K	140	ALA	CA-C	5.63	1.60	1.52
2	C	49	GLU	CG-CD	5.63	1.66	1.52
1	E	96	LYS	CE-NZ	5.63	1.66	1.49
2	F	152	ARG	C-O	-5.63	1.17	1.24
1	K	84	VAL	C-O	5.63	1.30	1.23
2	C	44	LEU	CG-CD2	-5.62	1.33	1.52
2	C	147	VAL	CA-CB	-5.62	1.47	1.54
1	H	115	LEU	CA-C	-5.62	1.45	1.52
3	U	277	THR	N-CA	5.62	1.52	1.45
2	C	117	MET	C-O	-5.62	1.16	1.23
1	E	124	PRO	C-O	5.62	1.34	1.23
1	K	7	GLY	CA-C	5.62	1.59	1.51
3	U	252	THR	C-O	-5.61	1.17	1.23
1	E	28	LYS	C-O	-5.61	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	137	LYS	N-CA	-5.61	1.38	1.46
3	T	265	VAL	CB-CG1	-5.61	1.34	1.52
3	S	273	ARG	CZ-NH1	5.60	1.40	1.32
2	C	126	VAL	CB-CG2	-5.60	1.34	1.52
1	E	86	LYS	CB-CG	5.60	1.69	1.52
1	H	19	LEU	CG-CD2	5.60	1.71	1.52
2	L	59	THR	CA-CB	5.60	1.62	1.53
2	F	43	ARG	NE-CZ	5.60	1.39	1.33
2	I	145	LYS	N-CA	5.60	1.53	1.46
2	I	126	VAL	CA-CB	-5.60	1.48	1.54
3	T	303	ASP	CA-CB	5.60	1.61	1.53
1	B	28	LYS	CA-C	-5.59	1.46	1.52
1	E	59	GLU	CA-C	-5.59	1.45	1.52
1	H	57	LYS	CE-NZ	5.59	1.66	1.49
3	U	287	MET	N-CA	-5.59	1.38	1.46
3	T	304	TYR	CE2-CZ	5.59	1.51	1.38
2	C	133	SER	CB-OG	-5.58	1.30	1.42
1	E	22	GLU	CA-C	5.58	1.60	1.52
2	L	104	GLU	CG-CD	5.58	1.66	1.52
1	E	47	GLN	CD-OE1	5.58	1.34	1.23
1	E	114	ALA	CA-C	-5.58	1.45	1.52
3	V	235	LYS	CD-CE	5.58	1.69	1.52
1	B	45	GLY	CA-C	-5.58	1.44	1.51
2	F	75	TRP	CZ3-CH2	-5.58	1.26	1.40
2	F	129	PRO	CA-C	5.58	1.59	1.52
2	I	130	ARG	N-CA	5.58	1.52	1.46
2	L	76	THR	CB-CG2	5.58	1.71	1.52
2	C	142	TYR	CZ-OH	-5.57	1.26	1.38
2	C	145	LYS	C-O	-5.57	1.17	1.24
3	S	241	MET	CA-C	-5.57	1.45	1.52
2	C	50	GLU	CD-OE2	5.57	1.35	1.25
1	H	34	SER	N-CA	5.56	1.53	1.46
2	L	49	GLU	C-O	5.56	1.30	1.24
1	E	83	ASN	C-O	5.56	1.31	1.24
2	L	101	LYS	N-CA	5.55	1.51	1.47
3	T	287	MET	CG-SD	5.55	1.94	1.80
1	E	118	ALA	N-CA	5.55	1.52	1.46
2	F	153	ARG	CA-C	-5.55	1.45	1.52
2	I	117	MET	CG-SD	5.55	1.94	1.80
2	F	106	PRO	CA-CB	-5.55	1.48	1.53
1	B	123	ASP	C-N	5.55	1.43	1.34
3	V	239	GLU	C-O	5.55	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	74	ARG	CB-CG	-5.54	1.35	1.52
1	K	57	LYS	CA-CB	5.54	1.62	1.53
1	B	102	ALA	CA-C	-5.54	1.44	1.52
1	H	68	MET	C-O	-5.53	1.17	1.24
1	K	72	LYS	CD-CE	5.53	1.69	1.52
2	L	172	TYR	CG-CD1	5.53	1.50	1.39
2	C	53	LYS	C-O	5.53	1.30	1.24
1	H	108	VAL	CB-CG2	-5.52	1.34	1.52
2	F	63	GLY	C-O	5.52	1.31	1.23
3	U	276	LEU	CG-CD2	-5.52	1.34	1.52
1	E	154	ASN	CB-CG	5.52	1.65	1.52
1	H	92	LEU	C-O	5.51	1.30	1.24
1	K	41	VAL	N-CA	5.51	1.52	1.46
3	V	237	SER	C-O	5.51	1.30	1.24
1	B	8	LEU	C-O	-5.51	1.17	1.23
1	E	137	GLU	CD-OE2	5.51	1.35	1.25
3	S	253	TYR	N-CA	-5.51	1.39	1.45
3	T	249	SER	C-N	-5.51	1.25	1.33
2	I	145	LYS	CG-CD	5.51	1.69	1.52
1	B	63	PRO	N-CA	-5.50	1.40	1.47
1	E	13	ILE	CG1-CD1	5.50	1.73	1.51
2	I	151	LEU	CA-CB	5.50	1.60	1.53
2	I	153	ARG	CD-NE	5.50	1.53	1.46
1	K	64	GLU	CG-CD	5.50	1.65	1.52
2	L	59	THR	CB-CG2	5.50	1.70	1.52
2	L	65	GLU	CD-OE1	5.50	1.35	1.25
2	L	90	ARG	CA-C	5.50	1.60	1.52
3	V	285	LEU	CG-CD1	5.50	1.70	1.52
1	E	97	ASP	CG-OD2	5.50	1.35	1.25
1	K	112	ILE	N-CA	5.50	1.53	1.46
1	E	37	ARG	CZ-NH1	5.50	1.40	1.32
2	I	158	LYS	C-O	5.50	1.30	1.24
1	E	87	LEU	CA-CB	-5.50	1.44	1.53
1	E	50	PRO	C-O	5.49	1.32	1.24
1	H	119	PRO	CB-CG	5.49	1.77	1.49
2	I	140	ASN	C-O	5.49	1.32	1.24
2	L	37	LYS	CB-CG	5.49	1.69	1.52
3	T	280	GLN	CB-CG	-5.49	1.35	1.52
3	V	273	ARG	CZ-NH1	5.49	1.40	1.32
2	C	100	PRO	C-O	-5.49	1.17	1.24
2	I	168	GLU	CA-CB	5.48	1.62	1.53
1	K	51	PHE	C-N	5.48	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	120	VAL	CB-CG2	-5.48	1.34	1.52
1	K	155	ASN	C-N	5.48	1.41	1.33
3	U	239	GLU	C-O	5.48	1.31	1.23
1	E	35	ASN	CG-ND2	5.47	1.44	1.33
3	S	282	ILE	C-O	5.47	1.28	1.23
2	F	74	ARG	CZ-NH2	5.47	1.40	1.33
2	C	95	LYS	CA-CB	-5.47	1.43	1.53
1	K	142	GLU	C-N	5.47	1.41	1.33
1	H	104	GLN	N-CA	5.46	1.54	1.46
1	H	19	LEU	N-CA	5.46	1.52	1.46
2	F	46	GLU	CD-OE1	5.46	1.35	1.25
1	K	47	GLN	CD-NE2	5.46	1.44	1.33
1	K	64	GLU	C-O	5.46	1.30	1.24
2	I	71	THR	N-CA	5.45	1.53	1.46
1	B	6	ALA	N-CA	5.45	1.52	1.45
1	E	139	GLN	N-CA	-5.45	1.39	1.46
3	T	277	THR	CA-C	-5.45	1.46	1.52
1	E	90	ILE	CA-C	-5.45	1.46	1.52
1	E	140	ALA	CA-CB	-5.45	1.44	1.53
2	F	140	ASN	N-CA	-5.45	1.39	1.46
2	I	147	VAL	C-O	-5.45	1.17	1.24
2	L	58	GLY	CA-C	5.45	1.59	1.51
3	V	252	THR	CA-C	5.45	1.59	1.52
1	E	15	GLU	CD-OE2	5.44	1.35	1.25
1	K	110	LEU	CG-CD2	5.44	1.70	1.52
3	T	242	ARG	CD-NE	5.44	1.53	1.46
1	E	85	ASP	C-O	5.44	1.30	1.24
1	E	136	ASN	CA-CB	-5.43	1.48	1.53
1	B	75	PHE	CE2-CZ	-5.43	1.22	1.38
1	E	112	ILE	C-O	-5.43	1.17	1.24
2	F	159	GLU	N-CA	5.43	1.53	1.46
3	T	286	ALA	CA-C	5.43	1.60	1.52
2	L	79	ILE	C-O	-5.43	1.17	1.24
2	F	90	ARG	CA-CB	-5.43	1.44	1.53
3	S	288	LYS	C-O	5.43	1.30	1.24
1	B	46	PRO	CA-CB	-5.43	1.46	1.53
1	B	119	PRO	CA-C	5.43	1.57	1.52
1	E	86	LYS	CA-CB	5.43	1.62	1.53
1	E	82	PRO	C-O	-5.43	1.16	1.24
2	C	147	VAL	N-CA	-5.42	1.39	1.46
3	V	229	PRO	C-O	5.42	1.34	1.23
1	H	28	LYS	CD-CE	5.42	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	294	PHE	N-CA	-5.42	1.40	1.46
3	T	286	ALA	C-N	5.42	1.40	1.33
1	E	33	GLU	CD-OE1	5.41	1.35	1.25
1	E	118	ALA	C-O	5.41	1.30	1.24
2	F	132	ILE	CA-CB	-5.41	1.46	1.53
3	S	284	ASN	CB-CG	5.41	1.65	1.52
1	B	91	CYS	N-CA	-5.41	1.39	1.46
2	F	167	PRO	C-O	-5.41	1.17	1.24
1	B	76	MET	N-CA	-5.41	1.39	1.46
3	U	267	HIS	N-CA	-5.41	1.39	1.46
3	V	278	GLN	CD-OE1	5.41	1.33	1.23
2	L	140	ASN	N-CA	-5.41	1.39	1.46
1	B	96	LYS	N-CA	5.40	1.53	1.46
3	U	283	PRO	C-O	5.40	1.29	1.23
3	V	255	ARG	CZ-NH2	5.40	1.40	1.33
1	E	6	ALA	N-CA	5.40	1.56	1.46
1	H	88	GLY	CA-C	5.40	1.59	1.51
3	U	242	ARG	CZ-NH1	5.40	1.40	1.32
3	U	242	ARG	CZ-NH2	5.40	1.40	1.33
2	I	98	CYS	C-O	-5.39	1.17	1.24
1	H	94	ILE	CA-CB	5.39	1.61	1.54
3	U	249	SER	CA-CB	5.39	1.62	1.53
1	H	89	ARG	N-CA	-5.39	1.39	1.46
1	K	156	ILE	CG1-CD1	5.39	1.72	1.51
2	C	140	ASN	C-O	5.38	1.31	1.23
1	H	50	PRO	C-O	5.38	1.30	1.24
1	K	37	ARG	CA-C	5.38	1.60	1.52
3	U	284	ASN	C-O	5.38	1.30	1.23
1	E	33	GLU	CD-OE2	5.37	1.35	1.25
1	E	127	ASN	CB-CG	5.37	1.65	1.52
2	I	70	MET	N-CA	-5.37	1.39	1.46
1	K	149	ARG	CA-C	5.37	1.59	1.52
2	L	158	LYS	CD-CE	5.37	1.68	1.52
3	V	230	ASP	C-N	5.37	1.41	1.33
2	F	128	ASP	CA-CB	-5.36	1.43	1.52
3	V	250	GLY	N-CA	5.36	1.52	1.45
1	K	40	HIS	CA-CB	5.36	1.59	1.52
1	K	83	ASN	CA-C	5.36	1.61	1.52
3	T	247	THR	CB-OG1	5.36	1.52	1.43
1	H	103	LEU	N-CA	-5.36	1.39	1.46
1	K	149	ARG	N-CA	5.36	1.53	1.46
1	B	124	PRO	CB-CG	5.35	1.76	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	GLU	CB-CG	5.35	1.68	1.52
2	F	116	ASN	CA-CB	-5.35	1.44	1.53
1	B	34	SER	CB-OG	5.34	1.52	1.42
2	F	58	GLY	C-O	-5.34	1.16	1.23
2	F	94	LEU	CA-C	-5.34	1.46	1.52
1	K	92	LEU	C-O	5.34	1.30	1.24
3	U	252	THR	N-CA	-5.34	1.39	1.46
3	S	251	ILE	N-CA	-5.34	1.40	1.46
3	T	239	GLU	CB-CG	-5.34	1.36	1.52
2	L	91	ILE	CA-C	-5.34	1.46	1.52
1	B	147	TRP	N-CA	5.33	1.53	1.46
1	E	31	PRO	C-O	5.33	1.29	1.23
1	K	20	LEU	CG-CD2	5.33	1.70	1.52
1	B	5	SER	C-N	5.33	1.42	1.33
2	F	100	PRO	N-CA	-5.33	1.40	1.47
1	H	156	ILE	N-CA	5.33	1.56	1.46
2	L	102	TYR	CA-CB	-5.33	1.44	1.53
2	L	146	VAL	CB-CG2	-5.33	1.34	1.52
2	F	73	THR	CA-CB	-5.33	1.45	1.53
1	E	87	LEU	CA-C	-5.33	1.44	1.52
1	B	29	ALA	N-CA	5.32	1.52	1.46
1	B	154	ASN	C-O	-5.32	1.17	1.24
2	L	53	LYS	CG-CD	5.32	1.68	1.52
3	U	235	LYS	CA-CB	-5.32	1.44	1.53
1	K	141	ILE	CA-C	5.32	1.59	1.52
1	K	143	THR	CB-CG2	5.32	1.70	1.52
3	T	256	LYS	C-O	5.32	1.30	1.24
3	S	291	ILE	C-N	5.32	1.41	1.33
1	B	148	THR	N-CA	-5.31	1.40	1.46
3	S	294	PHE	CD1-CE1	5.31	1.54	1.38
1	H	145	ARG	CZ-NH2	5.31	1.40	1.33
2	I	126	VAL	CA-C	-5.31	1.45	1.52
1	K	46	PRO	C-O	5.31	1.30	1.23
1	B	133	TRP	C-O	5.31	1.30	1.24
1	B	27	ILE	CA-CB	-5.30	1.47	1.54
1	H	47	GLN	C-O	5.30	1.30	1.23
2	I	132	ILE	CA-C	-5.30	1.46	1.52
1	K	47	GLN	N-CA	5.30	1.52	1.46
1	B	66	TYR	CB-CG	-5.30	1.40	1.51
2	C	93	SER	CA-C	5.30	1.58	1.52
2	F	94	LEU	N-CA	5.30	1.52	1.45
1	E	130	ALA	CA-CB	5.29	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	78	MET	CG-SD	5.29	1.94	1.80
1	K	138	ALA	CA-C	5.29	1.59	1.52
3	V	290	VAL	CA-C	5.29	1.58	1.52
1	E	96	LYS	CB-CG	5.29	1.68	1.52
1	H	28	LYS	CA-CB	5.29	1.60	1.53
3	U	288	LYS	C-O	5.28	1.30	1.24
1	E	58	LEU	CG-CD2	-5.28	1.35	1.52
2	L	156	MET	CG-SD	5.28	1.94	1.80
3	S	243	GLU	CB-CG	-5.28	1.36	1.52
1	B	148	THR	CA-CB	-5.28	1.45	1.53
2	C	120	VAL	N-CA	-5.28	1.40	1.46
2	I	62	TRP	CA-CB	-5.28	1.46	1.53
2	C	135	LEU	C-O	-5.27	1.16	1.23
1	K	111	SER	CA-C	5.27	1.59	1.52
1	E	11	ARG	CA-C	5.27	1.59	1.52
1	E	37	ARG	CB-CG	5.27	1.68	1.52
2	F	127	VAL	CB-CG2	-5.27	1.35	1.52
3	S	245	CYS	CA-CB	-5.27	1.41	1.53
2	L	96	ILE	CA-C	-5.27	1.46	1.52
3	S	274	SER	CA-CB	-5.26	1.46	1.53
3	V	259	GLU	CD-OE1	5.26	1.35	1.25
2	C	65	GLU	N-CA	5.26	1.52	1.46
1	K	67	PRO	CA-C	-5.26	1.42	1.52
1	E	148	THR	CA-CB	-5.26	1.45	1.53
1	E	58	LEU	CB-CG	-5.26	1.43	1.53
1	B	7	GLY	CA-C	5.25	1.57	1.52
3	U	280	GLN	CD-OE1	5.25	1.33	1.23
1	B	83	ASN	CA-C	-5.25	1.45	1.52
1	E	95	LEU	CA-C	-5.25	1.45	1.52
1	K	8	LEU	C-O	5.25	1.30	1.24
3	T	251	ILE	N-CA	-5.25	1.40	1.46
2	I	75	TRP	CA-C	-5.25	1.46	1.52
1	K	68	MET	CA-CB	5.24	1.62	1.53
3	U	236	ILE	N-CA	-5.24	1.39	1.46
2	C	165	GLN	C-N	-5.24	1.27	1.33
1	B	27	ILE	CA-C	5.24	1.58	1.52
2	C	138	TRP	CA-CB	-5.24	1.44	1.53
1	B	52	GLU	CA-CB	-5.23	1.44	1.53
3	S	295	ILE	N-CA	5.23	1.52	1.46
3	S	258	ILE	C-N	-5.23	1.26	1.33
1	B	152	ALA	N-CA	-5.23	1.39	1.46
1	H	61	PHE	CA-CB	-5.23	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	119	GLY	N-CA	5.23	1.53	1.45
1	K	88	GLY	C-O	5.23	1.30	1.23
1	K	89	ARG	NE-CZ	5.22	1.38	1.33
1	B	89	ARG	CZ-NH1	5.22	1.40	1.32
1	B	149	ARG	CA-C	-5.22	1.45	1.52
1	H	145	ARG	CZ-NH1	5.22	1.40	1.32
1	B	97	ASP	CB-CG	5.22	1.65	1.52
2	C	151	LEU	CG-CD1	-5.22	1.35	1.52
2	F	141	SER	C-O	5.22	1.30	1.24
3	V	263	GLN	C-N	5.22	1.41	1.33
1	K	122	ASP	C-O	5.22	1.30	1.24
1	E	72	LYS	CA-C	-5.21	1.46	1.52
3	S	281	LEU	CA-C	-5.21	1.46	1.52
1	B	146	ALA	CA-C	-5.21	1.46	1.52
2	F	88	GLU	CA-C	-5.21	1.45	1.52
3	V	237	SER	N-CA	5.21	1.52	1.46
3	U	295	ILE	CB-CG2	5.21	1.69	1.52
1	B	28	LYS	CG-CD	5.20	1.68	1.52
1	K	15	GLU	CG-CD	5.20	1.65	1.52
1	E	74	ARG	N-CA	5.20	1.52	1.46
2	L	75	TRP	N-CA	-5.20	1.39	1.45
2	L	96	ILE	CB-CG2	-5.20	1.35	1.52
2	I	153	ARG	NE-CZ	5.20	1.38	1.33
1	B	25	PRO	CA-CB	5.19	1.60	1.53
2	L	174	ASN	C-O	5.19	1.33	1.23
3	S	234	GLY	C-N	-5.19	1.26	1.33
2	I	52	GLN	CA-C	5.19	1.59	1.52
3	V	282	ILE	CA-C	5.19	1.57	1.52
3	S	261	HIS	CB-CG	-5.19	1.42	1.50
1	H	10	ARG	CZ-NH1	5.18	1.40	1.32
3	U	256	LYS	CD-CE	5.18	1.68	1.52
2	F	91	ILE	C-O	5.18	1.29	1.24
1	B	99	TRP	CE2-CZ2	-5.18	1.28	1.39
3	V	289	GLU	CA-CB	5.18	1.61	1.53
2	L	137	LYS	CB-CG	5.18	1.68	1.52
2	C	43	ARG	CA-C	5.18	1.59	1.52
2	C	172	TYR	CA-C	-5.18	1.46	1.52
1	B	52	GLU	C-N	-5.17	1.25	1.33
1	E	101	PRO	C-O	5.17	1.30	1.24
1	E	133	TRP	N-CA	-5.17	1.40	1.46
2	L	151	LEU	CA-C	-5.17	1.45	1.52
1	B	103	LEU	N-CA	5.17	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	47	GLU	CD-OE1	5.17	1.35	1.25
3	S	280	GLN	CA-C	-5.17	1.46	1.52
3	U	260	GLU	C-O	5.17	1.30	1.24
1	B	117	SER	CA-CB	-5.17	1.45	1.53
2	F	145	LYS	CB-CG	-5.17	1.36	1.52
2	L	136	ALA	N-CA	-5.17	1.40	1.46
1	E	57	LYS	N-CA	5.16	1.52	1.46
2	F	156	MET	SD-CE	5.16	1.92	1.79
1	H	58	LEU	N-CA	5.16	1.52	1.45
1	B	67	PRO	N-CA	-5.16	1.38	1.47
2	C	108	PHE	CD1-CE1	5.15	1.54	1.38
1	E	113	GLN	C-N	-5.15	1.26	1.33
3	U	265	VAL	CA-C	-5.15	1.47	1.52
2	F	55	VAL	CB-CG2	5.14	1.69	1.52
2	I	39	PRO	CG-CD	5.14	1.68	1.50
2	L	153	ARG	C-O	5.14	1.30	1.24
3	V	275	PRO	N-CA	5.14	1.53	1.47
2	I	137	LYS	CA-C	-5.14	1.45	1.52
3	S	283	PRO	C-O	-5.14	1.17	1.24
1	E	65	GLU	CD-OE1	5.14	1.35	1.25
2	L	159	GLU	CA-C	5.14	1.59	1.52
3	V	280	GLN	CD-NE2	5.14	1.44	1.33
2	F	139	GLN	C-O	5.14	1.30	1.24
1	E	53	GLY	C-O	-5.14	1.18	1.24
1	H	103	LEU	C-O	5.14	1.30	1.24
1	H	143	THR	C-O	5.14	1.30	1.24
2	L	87	TYR	C-O	5.14	1.30	1.24
2	I	72	LEU	N-CA	-5.13	1.39	1.46
1	K	123	ASP	CA-CB	5.13	1.61	1.53
2	F	54	GLY	C-N	5.13	1.40	1.33
2	F	133	SER	CA-C	5.13	1.59	1.52
3	U	229	PRO	CG-CD	5.13	1.68	1.50
1	B	151	TYR	CE1-CZ	5.12	1.50	1.38
1	E	155	ASN	C-O	5.12	1.30	1.24
2	L	112	VAL	C-O	5.12	1.29	1.23
2	L	150	GLU	CA-CB	-5.12	1.45	1.53
3	T	233	CYS	N-CA	5.12	1.52	1.45
3	U	278	GLN	CD-OE1	5.12	1.33	1.23
1	E	11	ARG	N-CA	5.12	1.52	1.46
1	B	16	THR	C-O	5.12	1.30	1.24
1	B	101	PRO	CA-C	-5.12	1.43	1.52
3	T	235	LYS	CD-CE	5.12	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	105	ALA	N-CA	5.12	1.53	1.45
1	B	92	LEU	CA-C	-5.11	1.46	1.52
1	E	65	GLU	C-O	5.11	1.30	1.24
1	H	124	PRO	CA-C	5.11	1.63	1.52
1	B	15	GLU	CA-C	-5.11	1.46	1.52
1	B	99	TRP	CZ3-CH2	5.11	1.53	1.40
2	C	92	TYR	CE2-CZ	-5.10	1.25	1.38
1	E	35	ASN	CB-CG	5.10	1.64	1.52
1	B	82	PRO	C-O	5.10	1.30	1.24
1	E	97	ASP	CG-OD1	5.10	1.35	1.25
3	U	259	GLU	CG-CD	5.10	1.64	1.52
1	B	30	GLU	CB-CG	-5.10	1.37	1.52
2	F	129	PRO	CA-CB	-5.10	1.45	1.54
1	B	10	ARG	CB-CG	5.10	1.67	1.52
1	E	53	GLY	CA-C	-5.10	1.44	1.51
2	F	73	THR	C-O	5.10	1.30	1.24
3	T	301	VAL	C-O	5.10	1.30	1.24
3	T	255	ARG	CD-NE	5.09	1.53	1.46
3	U	251	ILE	N-CA	5.09	1.51	1.46
2	I	69	ASP	C-O	-5.09	1.18	1.23
1	K	109	LEU	C-O	5.09	1.30	1.24
2	F	47	GLU	N-CA	5.09	1.52	1.46
3	U	244	PRO	CB-CG	5.09	1.75	1.49
3	T	301	VAL	CB-CG2	5.09	1.69	1.52
2	C	85	THR	C-O	-5.08	1.17	1.23
2	I	140	ASN	CA-CB	-5.08	1.44	1.53
3	U	253	TYR	CZ-OH	5.08	1.48	1.38
3	V	268	PHE	C-O	5.08	1.30	1.23
3	T	291	ILE	CA-CB	5.08	1.61	1.54
1	E	80	TYR	N-CA	-5.08	1.40	1.46
2	C	146	VAL	N-CA	5.08	1.52	1.46
1	K	99	TRP	CB-CG	5.08	1.66	1.50
3	S	242	ARG	CZ-NH1	5.08	1.39	1.32
2	L	93	SER	C-O	-5.07	1.17	1.23
3	T	238	PHE	CD2-CE2	-5.07	1.23	1.38
3	V	264	ARG	NE-CZ	5.07	1.38	1.33
3	T	304	TYR	CG-CD1	5.07	1.50	1.39
1	E	71	PRO	C-O	5.07	1.29	1.23
2	F	60	VAL	C-O	-5.07	1.17	1.23
2	C	174	ASN	CA-C	5.07	1.63	1.52
1	B	3	ALA	C-O	5.07	1.33	1.23
1	B	68	MET	CG-SD	5.07	1.93	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	91	CYS	CA-C	5.07	1.58	1.52
3	S	252	THR	N-CA	5.07	1.52	1.46
1	B	124	PRO	CA-CB	5.06	1.63	1.53
1	E	156	ILE	CA-CB	5.06	1.68	1.54
1	H	20	LEU	C-O	5.06	1.30	1.24
1	E	75	PHE	N-CA	5.06	1.52	1.45
1	K	97	ASP	CG-OD1	5.06	1.34	1.25
2	L	102	TYR	CG-CD1	-5.05	1.28	1.39
2	F	59	THR	CB-CG2	5.05	1.69	1.52
1	H	134	LYS	N-CA	5.05	1.52	1.46
3	S	280	GLN	C-O	5.05	1.30	1.24
1	K	112	ILE	C-O	5.05	1.29	1.24
3	T	266	GLY	C-N	5.04	1.40	1.33
2	C	116	ASN	CG-OD1	-5.04	1.14	1.23
1	H	140	ALA	CA-CB	-5.04	1.45	1.53
1	K	93	ASP	N-CA	5.04	1.52	1.46
1	K	87	LEU	C-O	-5.04	1.17	1.24
1	H	67	PRO	CB-CG	-5.04	1.31	1.51
1	H	86	LYS	C-O	-5.04	1.17	1.24
3	U	265	VAL	CB-CG2	-5.04	1.35	1.52
1	E	106	ARG	CG-CD	5.03	1.67	1.52
1	B	65	GLU	CD-OE2	5.03	1.34	1.25
2	C	111	PHE	C-O	-5.03	1.18	1.23
2	F	59	THR	C-O	5.03	1.30	1.24
2	I	47	GLU	N-CA	5.03	1.52	1.46
1	H	150	LEU	C-N	5.03	1.41	1.33
1	H	28	LYS	CB-CG	5.03	1.67	1.52
2	I	112	VAL	CA-C	5.03	1.58	1.52
1	E	75	PHE	C-O	5.03	1.30	1.23
2	I	137	LYS	CE-NZ	5.03	1.64	1.49
1	K	78	LYS	CE-NZ	5.03	1.64	1.49
3	T	244	PRO	CB-CG	-5.03	1.24	1.49
1	B	18	ARG	C-O	5.02	1.29	1.24
2	C	41	ASN	C-N	5.02	1.41	1.33
1	K	15	GLU	CD-OE2	5.02	1.34	1.25
1	B	32	ASP	CG-OD2	5.02	1.34	1.25
2	F	37	LYS	CA-C	5.02	1.59	1.52
3	S	248	PRO	C-N	-5.02	1.25	1.33
2	C	69	ASP	CA-C	5.02	1.59	1.53
2	L	101	LYS	CD-CE	5.02	1.67	1.52
2	I	124	ASN	CG-ND2	-5.02	1.22	1.33
3	U	249	SER	C-O	-5.02	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	247	THR	CB-OG1	-5.01	1.35	1.43
2	F	136	ALA	CA-C	5.01	1.59	1.52
1	B	79	ILE	CB-CG1	-5.01	1.43	1.53
3	V	284	ASN	C-O	5.01	1.30	1.23
2	C	160	ASN	N-CA	5.01	1.52	1.46
1	E	93	ASP	CG-OD2	5.01	1.34	1.25
2	I	38	VAL	C-O	5.01	1.30	1.24
1	K	30	GLU	CB-CG	5.01	1.67	1.52
3	U	246	ILE	CA-CB	5.01	1.61	1.54
3	V	275	PRO	C-O	5.00	1.29	1.23
1	B	106	ARG	CA-CB	-5.00	1.45	1.53
1	B	35	ASN	N-CA	5.00	1.52	1.46
1	E	63	PRO	CA-CB	5.00	1.61	1.53
2	F	111	PHE	CD1-CE1	5.00	1.53	1.38

All (1473) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	ALA	CA-C-N	-17.55	103.36	120.21
1	B	70	ALA	C-N-CA	-17.55	103.36	120.21
3	S	266	GLY	N-CA-C	17.09	133.16	112.48
1	B	7	GLY	N-CA-C	-16.95	95.45	113.58
2	F	38	VAL	CA-C-N	-16.85	103.79	120.31
2	F	38	VAL	C-N-CA	-16.85	103.79	120.31
1	H	118	ALA	CA-C-N	-16.64	102.43	119.90
1	H	118	ALA	C-N-CA	-16.64	102.43	119.90
1	B	45	GLY	CA-C-N	16.64	137.73	119.93
1	B	45	GLY	C-N-CA	16.64	137.73	119.93
2	F	105	ALA	CA-C-N	16.25	131.52	119.66
2	F	105	ALA	C-N-CA	16.25	131.52	119.66
2	C	140	ASN	N-CA-C	-16.23	92.72	113.17
1	B	22	GLU	CB-CA-C	15.59	126.87	110.65
1	K	4	GLY	N-CA-C	15.15	133.82	110.18
3	V	259	GLU	N-CA-C	-15.08	93.00	111.40
1	B	62	LEU	CA-C-N	-14.38	104.53	119.92
1	B	62	LEU	C-N-CA	-14.38	104.53	119.92
2	L	128	ASP	CA-C-N	-14.04	105.27	119.87
2	L	128	ASP	C-N-CA	-14.04	105.27	119.87
2	C	50	GLU	N-CA-C	-13.99	96.03	111.28
3	U	267	HIS	N-CA-C	-13.93	91.75	111.81
3	U	279	GLU	CA-C-N	-13.68	99.96	122.54
3	U	279	GLU	C-N-CA	-13.68	99.96	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	282	ILE	CB-CA-C	-13.67	97.60	111.00
3	S	258	ILE	CA-C-N	-13.30	102.35	120.44
3	S	258	ILE	C-N-CA	-13.30	102.35	120.44
3	S	263	GLN	CA-C-N	-13.17	101.82	121.98
3	S	263	GLN	C-N-CA	-13.17	101.82	121.98
1	B	24	VAL	CA-C-N	-12.47	107.29	119.76
1	B	24	VAL	C-N-CA	-12.47	107.29	119.76
2	F	162	LYS	CA-C-N	-12.40	103.78	120.65
2	F	162	LYS	C-N-CA	-12.40	103.78	120.65
3	S	228	ILE	CA-C-N	-12.22	108.33	120.31
3	S	228	ILE	C-N-CA	-12.22	108.33	120.31
1	B	148	THR	N-CA-C	-12.19	97.50	111.03
2	F	123	SER	N-CA-C	12.17	128.47	113.50
1	K	81	HIS	CA-C-N	-12.01	106.51	121.04
1	K	81	HIS	C-N-CA	-12.01	106.51	121.04
2	C	81	GLY	CA-C-N	-11.98	108.04	120.38
2	C	81	GLY	C-N-CA	-11.98	108.04	120.38
1	K	8	LEU	CA-C-N	11.97	134.80	119.84
1	K	8	LEU	C-N-CA	11.97	134.80	119.84
1	B	151	TYR	N-CA-C	11.86	128.11	113.17
3	U	228	ILE	CA-C-N	-11.71	105.20	119.84
3	U	228	ILE	C-N-CA	-11.71	105.20	119.84
1	E	73	VAL	N-CA-C	11.59	125.17	108.48
2	F	128	ASP	CA-C-N	-11.58	107.60	120.45
2	F	128	ASP	C-N-CA	-11.58	107.60	120.45
3	S	271	VAL	N-CA-C	-11.56	102.20	113.53
2	C	42	PHE	N-CA-C	-11.54	98.93	113.23
3	S	270	PRO	CA-C-N	-11.48	107.93	121.71
3	S	270	PRO	C-N-CA	-11.48	107.93	121.71
3	U	295	ILE	N-CA-CB	11.47	123.24	110.51
1	B	30	GLU	CA-C-N	-11.41	109.13	120.31
1	B	30	GLU	C-N-CA	-11.41	109.13	120.31
1	K	112	ILE	N-CA-C	11.34	122.02	110.23
3	S	228	ILE	N-CA-C	-11.33	84.41	108.88
3	S	265	VAL	N-CA-C	-11.33	102.01	112.43
3	T	302	GLU	N-CA-C	11.23	126.92	109.52
3	T	251	ILE	N-CA-C	-11.21	91.86	108.45
2	C	135	LEU	N-CA-C	-11.18	100.13	113.88
3	V	267	HIS	CA-C-N	-11.15	103.58	121.87
3	V	267	HIS	C-N-CA	-11.15	103.58	121.87
1	B	22	GLU	CA-C-N	11.14	131.24	119.76
1	B	22	GLU	C-N-CA	11.14	131.24	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	277	THR	N-CA-C	-11.14	92.42	109.24
3	T	271	VAL	O-C-N	-11.09	113.44	121.98
1	B	53	GLY	O-C-N	-11.09	108.29	122.70
1	E	87	LEU	N-CA-C	10.99	126.44	112.92
2	C	153	ARG	N-CA-C	-10.96	99.34	111.28
3	U	284	ASN	CA-C-N	10.92	135.29	120.54
3	U	284	ASN	C-N-CA	10.92	135.29	120.54
1	B	89	ARG	NE-CZ-NH2	-10.91	109.38	119.20
2	C	45	LEU	CA-C-N	-10.90	103.74	120.31
2	C	45	LEU	C-N-CA	-10.90	103.74	120.31
1	K	141	ILE	N-CA-C	10.79	120.76	110.30
1	E	90	ILE	CA-C-N	-10.73	105.59	122.87
1	E	90	ILE	C-N-CA	-10.73	105.59	122.87
2	C	74	ARG	CG-CD-NE	-10.70	88.47	112.00
1	B	151	TYR	CB-CA-C	-10.67	92.27	110.09
2	L	51	GLY	N-CA-C	-10.54	99.73	112.49
3	V	250	GLY	N-CA-C	-10.52	99.95	115.63
1	B	52	GLU	CA-C-N	-10.52	100.80	121.41
1	B	52	GLU	C-N-CA	-10.52	100.80	121.41
2	F	76	THR	CB-CA-C	-10.41	90.64	109.38
2	L	73	THR	CA-C-N	-10.41	105.33	122.81
2	L	73	THR	C-N-CA	-10.41	105.33	122.81
3	S	278	GLN	N-CA-C	-10.40	99.90	111.14
1	H	90	ILE	CB-CA-C	-10.40	96.32	110.98
1	H	98	LYS	O-C-N	-10.31	108.88	122.59
2	L	65	GLU	N-CA-C	-10.29	101.29	114.04
1	H	41	VAL	CB-CA-C	-10.28	97.51	111.80
2	L	106	PRO	CA-C-N	-10.28	106.99	119.84
2	L	106	PRO	C-N-CA	-10.28	106.99	119.84
3	S	296	SER	N-CA-C	-10.24	92.55	109.24
1	B	107	THR	CB-CA-C	-10.21	95.13	110.95
1	E	59	GLU	N-CA-C	-10.16	93.48	109.23
1	B	37	ARG	N-CA-C	10.16	125.20	113.01
1	K	98	LYS	N-CA-C	-10.14	94.98	110.70
1	E	104	GLN	CA-CB-CG	-10.12	93.85	114.10
2	C	89	ASN	N-CA-C	10.06	124.94	112.47
3	U	246	ILE	N-CA-C	-10.06	96.55	108.82
1	B	6	ALA	N-CA-C	10.04	125.42	109.86
2	C	61	SER	CA-C-O	-10.00	110.53	121.23
3	S	295	ILE	CA-C-N	-10.00	108.92	122.72
3	S	295	ILE	C-N-CA	-10.00	108.92	122.72
3	V	252	THR	N-CA-C	9.97	125.54	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	38	VAL	CA-C-N	-9.96	107.39	119.84
2	C	38	VAL	C-N-CA	-9.96	107.39	119.84
2	I	68	GLU	N-CA-C	-9.96	99.50	114.64
2	C	125	GLY	N-CA-C	9.93	129.41	114.61
3	S	274	SER	CA-CB-OG	-9.93	91.24	111.10
3	T	279	GLU	N-CA-C	-9.93	100.92	113.23
1	H	97	ASP	N-CA-C	-9.92	93.76	108.34
1	B	72	LYS	CA-C-N	-9.88	106.07	122.67
1	B	72	LYS	C-N-CA	-9.88	106.07	122.67
1	K	74	ARG	N-CA-C	9.80	124.43	109.23
3	U	250	GLY	CA-C-N	-9.79	106.23	122.67
3	U	250	GLY	C-N-CA	-9.79	106.23	122.67
3	U	267	HIS	CA-C-N	-9.78	106.78	122.53
3	U	267	HIS	C-N-CA	-9.78	106.78	122.53
2	C	96	ILE	N-CA-C	9.76	121.83	108.17
1	H	74	ARG	N-CA-C	9.73	124.87	108.13
3	U	298	ASN	CA-C-O	-9.71	104.30	120.80
3	T	235	LYS	N-CA-C	-9.70	101.61	113.15
3	U	271	VAL	CA-C-N	-9.69	106.86	122.26
3	U	271	VAL	C-N-CA	-9.69	106.86	122.26
2	L	40	ARG	CA-C-N	-9.65	107.31	120.44
2	L	40	ARG	C-N-CA	-9.65	107.31	120.44
2	F	90	ARG	CA-C-N	-9.63	110.33	122.37
2	F	90	ARG	C-N-CA	-9.63	110.33	122.37
3	U	276	LEU	CA-C-N	-9.63	107.36	122.87
3	U	276	LEU	C-N-CA	-9.63	107.36	122.87
3	U	228	ILE	N-CA-C	9.63	129.68	108.88
1	K	118	ALA	CA-C-N	-9.62	99.24	120.89
1	K	118	ALA	C-N-CA	-9.62	99.24	120.89
3	S	282	ILE	CB-CA-C	-9.62	100.80	110.13
2	I	130	ARG	CA-C-N	-9.59	107.75	124.82
2	I	130	ARG	C-N-CA	-9.59	107.75	124.82
2	C	172	TYR	N-CA-C	-9.59	96.09	110.28
3	V	280	GLN	CA-C-N	-9.59	108.32	122.41
3	V	280	GLN	C-N-CA	-9.59	108.32	122.41
3	V	266	GLY	CA-C-N	-9.57	107.89	122.05
3	V	266	GLY	C-N-CA	-9.57	107.89	122.05
2	C	127	VAL	N-CA-C	9.57	121.26	109.30
2	C	90	ARG	NE-CZ-NH2	9.55	127.80	119.20
3	S	272	THR	N-CA-C	-9.48	100.95	114.12
2	I	43	ARG	NE-CZ-NH2	-9.46	110.69	119.20
1	B	153	MET	CG-SD-CE	9.41	121.60	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	152	ARG	N-CA-C	-9.38	90.82	110.80
3	V	242	ARG	CA-CB-CG	-9.37	95.36	114.10
2	F	94	LEU	CA-C-N	-9.37	110.07	123.00
2	F	94	LEU	C-N-CA	-9.37	110.07	123.00
3	T	274	SER	CA-C-N	9.37	131.55	119.84
3	T	274	SER	C-N-CA	9.37	131.55	119.84
2	L	120	VAL	CB-CA-C	-9.33	98.25	111.31
2	I	81	GLY	CA-C-N	-9.33	110.78	120.38
2	I	81	GLY	C-N-CA	-9.33	110.78	120.38
3	S	295	ILE	N-CA-C	9.29	119.90	110.23
2	F	130	ARG	N-CA-C	-9.29	101.21	112.54
1	K	66	TYR	N-CA-C	-9.28	98.33	110.39
2	C	82	PRO	CB-CA-C	-9.26	99.62	110.92
2	F	106	PRO	N-CA-C	9.24	119.34	110.47
1	B	74	ARG	NE-CZ-NH2	-9.23	110.89	119.20
2	L	115	ILE	CB-CA-C	-9.21	95.96	110.69
2	F	172	TYR	N-CA-C	-9.20	95.69	110.32
2	C	47	GLU	N-CA-C	-9.20	101.49	112.89
1	K	84	VAL	N-CA-C	-9.19	95.19	107.88
3	U	287	MET	N-CA-C	-9.18	101.85	113.23
3	V	281	LEU	N-CA-C	9.13	124.06	107.99
1	K	69	ALA	N-CA-C	-9.10	91.41	110.80
1	B	61	PHE	N-CA-C	9.10	123.33	109.23
1	H	42	VAL	CA-C-N	-9.09	107.96	122.50
1	H	42	VAL	C-N-CA	-9.09	107.96	122.50
1	B	111	SER	CB-CA-C	-9.07	96.99	110.96
2	L	142	TYR	N-CA-C	9.07	124.28	109.96
2	I	56	GLY	N-CA-C	-9.06	91.70	113.18
1	B	117	SER	N-CA-C	9.06	124.47	113.23
1	B	117	SER	CA-CB-OG	-9.03	93.03	111.10
2	C	74	ARG	NE-CZ-NH2	9.01	127.31	119.20
2	C	41	ASN	CA-C-N	-9.00	105.82	121.66
2	C	41	ASN	C-N-CA	-9.00	105.82	121.66
2	L	57	ASP	N-CA-C	-8.97	98.96	110.53
2	F	106	PRO	CA-C-N	-8.96	111.17	120.85
2	F	106	PRO	C-N-CA	-8.96	111.17	120.85
1	H	70	ALA	CA-C-N	8.96	129.31	119.90
1	H	70	ALA	C-N-CA	8.96	129.31	119.90
1	B	89	ARG	NE-CZ-NH1	8.95	130.45	121.50
3	T	233	CYS	N-CA-C	8.95	123.39	109.52
2	L	132	ILE	CA-CB-CG2	8.95	125.71	110.50
2	C	131	ALA	CA-C-N	8.94	138.07	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	131	ALA	C-N-CA	8.94	138.07	121.97
1	B	94	ILE	CA-C-O	-8.94	111.01	120.57
3	S	236	ILE	O-C-N	-8.92	111.42	122.57
2	C	73	THR	CA-C-N	-8.90	110.93	122.77
2	C	73	THR	C-N-CA	-8.90	110.93	122.77
1	E	129	VAL	N-CA-C	-8.90	99.81	112.35
3	V	250	GLY	CA-C-N	-8.90	111.27	123.10
3	V	250	GLY	C-N-CA	-8.90	111.27	123.10
2	L	171	CYS	CA-CB-SG	-8.88	93.99	114.40
1	K	39	PHE	N-CA-C	8.87	122.87	108.41
2	C	130	ARG	NE-CZ-NH2	8.82	127.14	119.20
2	L	157	SER	N-CA-C	8.82	123.21	110.24
2	F	163	LEU	CB-CG-CD1	-8.82	84.23	110.70
3	S	274	SER	N-CA-C	8.82	119.74	109.60
3	T	253	TYR	CA-C-O	-8.81	111.12	120.99
2	L	137	LYS	N-CA-C	-8.80	99.88	110.44
1	B	82	PRO	CA-C-N	-8.79	108.89	122.60
1	B	82	PRO	C-N-CA	-8.79	108.89	122.60
2	C	74	ARG	N-CA-C	8.72	122.95	108.73
1	K	73	VAL	CA-C-N	-8.72	107.90	122.29
1	K	73	VAL	C-N-CA	-8.72	107.90	122.29
1	H	98	LYS	N-CA-C	8.70	129.34	110.80
3	V	296	SER	N-CA-C	-8.69	91.64	107.98
1	B	87	LEU	N-CA-C	8.67	125.33	113.37
3	S	278	GLN	N-CA-CB	-8.67	97.50	110.07
3	T	300	TRP	N-CA-C	8.67	122.66	109.23
2	F	55	VAL	CA-C-O	-8.66	112.67	121.59
1	E	78	LYS	CB-CA-C	8.66	123.95	109.84
3	U	282	ILE	N-CA-CB	-8.66	99.09	111.21
2	F	165	GLN	CA-C-N	-8.65	111.47	120.38
2	F	165	GLN	C-N-CA	-8.65	111.47	120.38
1	B	55	THR	CA-C-O	-8.64	109.91	120.54
2	I	133	SER	N-CA-C	-8.64	101.35	112.23
3	V	282	ILE	N-CA-C	8.63	117.05	109.02
3	T	282	ILE	N-CA-CB	-8.62	99.15	111.21
1	B	98	LYS	CA-C-N	-8.61	110.05	122.19
1	B	98	LYS	C-N-CA	-8.61	110.05	122.19
2	F	52	GLN	N-CA-C	8.61	120.28	111.07
1	E	111	SER	CA-CB-OG	-8.59	93.92	111.10
1	K	110	LEU	N-CA-C	-8.56	101.64	110.97
3	S	247	THR	CA-C-N	8.56	128.14	119.24
3	S	247	THR	C-N-CA	8.56	128.14	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	273	ARG	CG-CD-NE	-8.54	93.21	112.00
1	K	155	ASN	N-CA-C	-8.54	95.81	109.39
1	H	96	LYS	CB-CG-CD	-8.54	91.67	111.30
3	S	246	ILE	CG1-CB-CG2	-8.52	85.14	110.70
2	F	65	GLU	CA-C-N	-8.50	110.66	123.07
2	F	65	GLU	C-N-CA	-8.50	110.66	123.07
1	E	86	LYS	N-CA-C	-8.50	102.17	112.54
1	K	73	VAL	N-CA-C	8.50	120.72	108.48
1	E	92	LEU	CB-CA-C	-8.49	95.53	109.89
2	I	168	GLU	N-CA-CB	8.49	122.68	109.69
3	S	248	PRO	O-C-N	-8.49	113.01	122.18
1	B	66	TYR	C-N-CD	8.48	139.25	120.60
2	F	161	MET	CG-SD-CE	8.48	119.56	100.90
3	V	230	ASP	N-CA-C	8.48	128.85	110.80
1	E	73	VAL	CA-CB-CG2	-8.47	96.00	110.40
1	K	112	ILE	N-CA-CB	8.47	119.52	110.62
1	E	58	LEU	CA-C-O	-8.46	111.76	121.58
1	H	90	ILE	CA-C-N	-8.46	109.02	122.73
1	H	90	ILE	C-N-CA	-8.46	109.02	122.73
1	B	104	GLN	CA-CB-CG	-8.44	97.22	114.10
2	C	133	SER	N-CA-C	8.44	121.61	111.82
3	V	262	LEU	CA-CB-CG	-8.44	86.77	116.30
1	H	120	ASN	CA-C-N	8.44	128.56	119.28
1	H	120	ASN	C-N-CA	8.44	128.56	119.28
2	F	170	GLN	N-CA-CB	-8.41	97.63	110.42
1	B	45	GLY	O-C-N	8.41	130.18	121.77
3	S	281	LEU	CA-C-N	-8.38	116.03	123.33
3	S	281	LEU	C-N-CA	-8.38	116.03	123.33
2	C	164	PRO	CB-CA-C	-8.38	100.82	111.71
3	S	279	GLU	O-C-N	-8.36	111.47	122.59
3	U	236	ILE	CA-C-N	-8.35	108.00	122.36
3	U	236	ILE	C-N-CA	-8.35	108.00	122.36
3	T	275	PRO	N-CA-C	-8.34	95.28	112.47
3	V	272	THR	N-CA-C	-8.34	102.53	114.12
2	F	140	ASN	N-CA-CB	-8.33	96.42	110.49
1	K	123	ASP	N-CA-C	8.31	128.17	109.81
1	E	66	TYR	N-CA-C	-8.28	99.13	109.64
1	K	10	ARG	N-CA-C	-8.28	102.28	112.38
1	E	65	GLU	N-CA-C	-8.26	103.11	113.02
2	C	43	ARG	NE-CZ-NH2	-8.26	111.77	119.20
3	S	297	GLU	N-CA-C	-8.26	93.20	110.80
3	U	272	THR	N-CA-C	-8.25	103.00	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	93	SER	CA-C-N	-8.23	107.72	121.80
2	L	93	SER	C-N-CA	-8.23	107.72	121.80
2	C	164	PRO	CA-C-O	-8.18	112.68	121.27
2	C	79	ILE	CA-C-N	-8.17	110.48	122.65
2	C	79	ILE	C-N-CA	-8.17	110.48	122.65
3	T	282	ILE	CA-C-N	-8.16	111.95	120.03
3	T	282	ILE	C-N-CA	-8.16	111.95	120.03
2	L	36	VAL	CB-CA-C	-8.16	95.89	111.40
3	U	261	HIS	CA-C-N	-8.15	106.88	121.14
3	U	261	HIS	C-N-CA	-8.15	106.88	121.14
1	B	7	GLY	O-C-N	-8.15	116.19	122.71
3	U	231	TYR	N-CA-C	-8.14	102.14	113.37
3	V	275	PRO	N-CA-C	-8.12	98.43	111.19
1	H	74	ARG	CA-CB-CG	-8.12	97.85	114.10
1	K	42	VAL	CA-C-N	-8.12	112.29	122.93
1	K	42	VAL	C-N-CA	-8.12	112.29	122.93
1	B	74	ARG	NE-CZ-NH1	8.12	129.62	121.50
1	E	89	ARG	CA-C-N	-8.11	112.64	123.10
1	E	89	ARG	C-N-CA	-8.11	112.64	123.10
2	I	152	ARG	CA-C-O	-8.10	108.92	120.51
1	H	43	ILE	CG1-CB-CG2	-8.10	86.40	110.70
2	F	152	ARG	CA-C-O	-8.09	112.33	120.82
2	I	76	THR	CB-CA-C	-8.09	95.83	109.50
2	C	147	VAL	N-CA-C	8.08	118.88	110.72
2	F	137	LYS	N-CA-C	-8.07	98.51	110.06
2	F	96	ILE	CB-CA-C	-8.07	98.60	110.62
2	L	44	LEU	N-CA-C	-8.06	102.50	111.28
2	C	162	LYS	N-CA-C	-8.05	100.51	111.87
1	H	27	ILE	N-CA-C	8.04	119.43	108.17
1	E	13	ILE	CA-C-N	-8.04	109.51	120.28
1	E	13	ILE	C-N-CA	-8.04	109.51	120.28
2	I	116	ASN	N-CA-C	-8.03	95.65	108.73
3	U	297	GLU	N-CA-C	8.02	122.64	113.02
1	H	66	TYR	N-CA-C	-8.01	99.23	110.29
1	H	89	ARG	CA-CB-CG	-8.00	98.10	114.10
1	K	82	PRO	N-CA-C	-8.00	103.30	114.98
1	E	145	ARG	NE-CZ-NH1	-7.97	113.53	121.50
2	I	41	ASN	N-CA-C	7.97	122.27	112.23
3	S	257	ASP	CA-CB-CG	-7.95	104.65	112.60
1	H	90	ILE	N-CA-C	-7.94	96.88	108.71
2	C	130	ARG	NE-CZ-NH1	-7.93	113.57	121.50
2	C	87	TYR	N-CA-C	-7.91	103.65	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	284	ASN	N-CA-C	-7.91	98.70	109.54
3	U	279	GLU	N-CA-C	-7.88	103.73	112.72
1	K	72	LYS	CD-CE-NZ	-7.88	86.68	111.90
2	F	155	MET	N-CA-C	-7.88	102.68	111.82
1	E	89	ARG	CA-CB-CG	-7.86	98.39	114.10
2	F	38	VAL	CB-CA-C	-7.86	101.65	110.68
2	I	62	TRP	N-CA-C	7.85	118.25	107.73
3	S	263	GLN	N-CA-C	-7.85	103.71	113.20
3	U	264	ARG	CA-CB-CG	-7.82	98.46	114.10
2	F	62	TRP	CA-C-N	-7.82	110.12	120.91
2	F	62	TRP	C-N-CA	-7.82	110.12	120.91
2	I	155	MET	CA-C-N	7.82	131.26	120.63
2	I	155	MET	C-N-CA	7.82	131.26	120.63
2	F	63	GLY	CA-C-N	-7.82	111.17	122.19
2	F	63	GLY	C-N-CA	-7.82	111.17	122.19
3	V	267	HIS	N-CA-C	-7.82	97.90	109.62
3	U	235	LYS	CA-CB-CG	-7.81	98.48	114.10
1	K	66	TYR	CA-C-O	-7.80	112.59	120.63
2	L	149	GLN	N-CA-C	-7.80	102.40	112.23
2	F	53	LYS	CA-C-O	-7.80	112.81	121.00
1	E	39	PHE	N-CA-CB	-7.79	98.35	110.57
2	C	90	ARG	NE-CZ-NH1	-7.78	113.72	121.50
3	S	264	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	E	106	ARG	NE-CZ-NH1	-7.77	113.73	121.50
1	B	8	LEU	N-CA-CB	-7.76	99.56	110.04
2	F	66	ASP	N-CA-C	7.76	121.59	108.02
3	U	240	LEU	CB-CA-C	-7.75	97.81	109.90
2	I	52	GLN	N-CA-C	7.74	120.80	111.82
3	T	230	ASP	O-C-N	7.73	130.38	122.03
3	V	235	LYS	CB-CG-CD	7.73	129.08	111.30
2	C	153	ARG	CB-CA-C	7.73	123.62	110.79
2	L	58	GLY	CA-C-N	-7.73	106.78	121.54
2	L	58	GLY	C-N-CA	-7.73	106.78	121.54
1	H	148	THR	N-CA-C	-7.73	102.86	111.28
3	U	298	ASN	CA-C-N	7.72	131.64	116.20
3	T	245	CYS	CA-C-O	-7.72	112.41	121.44
2	C	66	ASP	O-C-N	-7.72	113.86	123.05
3	U	274	SER	CB-CA-C	-7.72	94.96	110.17
3	V	249	SER	CA-C-N	-7.72	111.33	122.29
3	V	249	SER	C-N-CA	-7.72	111.33	122.29
3	T	236	ILE	CB-CA-C	-7.71	98.65	111.29
1	B	38	TYR	CA-C-N	-7.70	110.72	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	TYR	C-N-CA	-7.70	110.72	122.81
2	I	135	LEU	N-CA-C	-7.70	104.01	113.41
3	U	274	SER	N-CA-C	7.70	126.82	109.81
1	K	28	LYS	N-CA-C	-7.69	98.56	110.17
2	L	150	GLU	N-CA-C	7.69	120.56	111.71
1	K	45	GLY	CA-C-N	-7.67	111.71	119.92
1	K	45	GLY	C-N-CA	-7.67	111.71	119.92
1	K	15	GLU	N-CA-CB	7.67	121.51	110.16
3	S	233	CYS	N-CA-CB	-7.66	98.36	110.69
2	F	55	VAL	N-CA-CB	7.65	125.37	110.45
2	I	153	ARG	N-CA-CB	7.65	122.25	109.78
1	K	129	VAL	N-CA-C	-7.64	100.62	111.17
2	I	42	PHE	N-CA-C	-7.64	101.83	112.45
2	F	132	ILE	N-CA-C	7.63	120.20	106.61
2	C	59	THR	N-CA-C	7.63	127.05	110.80
2	I	121	ASN	N-CA-C	-7.62	99.03	110.24
1	E	71	PRO	CB-CA-C	-7.61	101.00	110.98
2	F	120	VAL	N-CA-C	7.60	118.62	107.37
2	F	123	SER	CA-C-O	-7.60	110.78	119.14
1	H	52	GLU	O-C-N	7.60	130.21	122.08
2	F	119	GLY	N-CA-C	-7.60	104.72	115.43
3	V	233	CYS	N-CA-C	7.60	121.50	109.50
1	H	97	ASP	CA-C-O	-7.59	112.43	119.34
3	S	282	ILE	CA-C-N	7.59	129.33	119.84
3	S	282	ILE	C-N-CA	7.59	129.33	119.84
3	T	253	TYR	CB-CA-C	-7.58	93.79	109.94
3	U	279	GLU	CB-CA-C	-7.58	98.43	110.94
2	L	84	ARG	CA-CB-CG	7.58	129.25	114.10
2	C	92	TYR	O-C-N	-7.57	114.39	123.10
2	F	51	GLY	N-CA-C	-7.56	103.50	112.64
3	T	239	GLU	CA-CB-CG	-7.55	99.00	114.10
1	K	83	ASN	N-CA-C	7.55	121.38	112.93
1	K	94	ILE	O-C-N	-7.54	113.14	122.57
3	T	236	ILE	CA-C-N	-7.54	107.64	121.52
3	T	236	ILE	C-N-CA	-7.54	107.64	121.52
2	C	84	ARG	N-CA-C	-7.53	97.53	113.20
1	K	100	SER	N-CA-C	7.53	121.52	110.14
2	L	152	ARG	CG-CD-NE	-7.52	95.45	112.00
1	B	49	SER	CA-C-N	7.52	127.15	119.56
1	B	49	SER	C-N-CA	7.52	127.15	119.56
2	F	139	GLN	CB-CG-CD	-7.51	99.83	112.60
2	F	99	GLY	CA-C-N	-7.51	111.23	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	99	GLY	C-N-CA	-7.51	111.23	119.19
3	S	242	ARG	CA-C-N	-7.50	114.60	122.85
3	S	242	ARG	C-N-CA	-7.50	114.60	122.85
2	C	126	VAL	N-CA-C	-7.49	97.64	108.36
2	F	109	VAL	N-CA-C	7.49	118.86	107.77
2	C	78	MET	CG-SD-CE	-7.49	84.42	100.90
2	F	91	ILE	CA-C-N	-7.49	110.82	122.87
2	F	91	ILE	C-N-CA	-7.49	110.82	122.87
1	B	71	PRO	CB-CA-C	-7.49	99.92	111.22
2	F	97	GLU	N-CA-C	7.48	121.39	108.76
3	S	239	GLU	N-CA-C	7.47	120.76	109.63
2	C	153	ARG	CA-CB-CG	7.46	129.01	114.10
2	C	92	TYR	CA-C-N	-7.45	110.01	122.29
2	C	92	TYR	C-N-CA	-7.45	110.01	122.29
1	B	104	GLN	N-CA-C	7.44	118.42	108.38
1	K	72	LYS	CA-C-N	-7.44	112.79	123.06
1	K	72	LYS	C-N-CA	-7.44	112.79	123.06
2	F	102	TYR	N-CA-C	-7.44	100.02	110.29
1	B	58	LEU	CA-C-O	-7.43	112.87	121.49
1	E	86	LYS	CA-C-N	-7.43	110.76	122.65
1	E	86	LYS	C-N-CA	-7.43	110.76	122.65
1	K	22	GLU	CA-C-N	-7.41	112.58	120.66
1	K	22	GLU	C-N-CA	-7.41	112.58	120.66
2	C	76	THR	N-CA-CB	-7.40	97.61	111.00
3	V	238	PHE	CA-C-N	-7.39	112.41	122.16
3	V	238	PHE	C-N-CA	-7.39	112.41	122.16
3	T	276	LEU	CD1-CG-CD2	-7.37	94.59	110.80
1	B	123	ASP	N-CA-C	7.37	122.19	112.17
1	H	13	ILE	N-CA-C	-7.37	102.63	110.36
3	S	284	ASN	CB-CG-ND2	7.36	127.44	116.40
2	F	42	PHE	N-CA-C	-7.36	103.26	112.90
2	L	36	VAL	CA-C-N	-7.36	112.63	122.42
2	L	36	VAL	C-N-CA	-7.36	112.63	122.42
2	F	98	CYS	N-CA-C	7.36	120.72	108.73
1	K	106	ARG	NE-CZ-NH2	-7.36	112.58	119.20
2	I	103	PRO	CA-C-N	-7.35	110.88	120.44
2	I	103	PRO	C-N-CA	-7.35	110.88	120.44
1	H	31	PRO	CA-C-N	-7.35	110.83	122.73
1	H	31	PRO	C-N-CA	-7.35	110.83	122.73
2	C	103	PRO	CA-C-N	-7.34	108.47	120.72
2	C	103	PRO	C-N-CA	-7.34	108.47	120.72
3	S	259	GLU	N-CA-C	7.33	119.05	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	76	THR	CB-CA-C	-7.32	94.85	109.35
2	I	152	ARG	CA-C-N	-7.32	109.83	120.82
2	I	152	ARG	C-N-CA	-7.32	109.83	120.82
3	V	271	VAL	CB-CA-C	-7.32	103.48	110.65
3	U	291	ILE	N-CA-CB	7.31	120.48	110.54
3	S	237	SER	CA-C-N	-7.31	113.52	126.45
3	S	237	SER	C-N-CA	-7.31	113.52	126.45
3	T	236	ILE	O-C-N	-7.30	113.44	122.57
3	T	290	VAL	CB-CA-C	-7.30	99.31	111.29
1	K	24	VAL	CB-CA-C	-7.30	98.08	111.36
1	E	68	MET	CA-C-O	7.30	128.36	120.55
3	S	258	ILE	CB-CG1-CD1	-7.30	98.48	113.80
2	L	115	ILE	CA-CB-CG2	7.29	122.89	110.50
2	C	129	PRO	N-CA-C	-7.29	104.02	113.57
1	E	72	LYS	CA-C-N	-7.28	113.01	123.06
1	E	72	LYS	C-N-CA	-7.28	113.01	123.06
3	U	285	LEU	O-C-N	7.28	129.66	122.09
2	F	38	VAL	N-CA-CB	7.27	118.24	110.17
2	L	110	ARG	N-CA-CB	-7.25	99.08	111.69
2	I	36	VAL	CB-CA-C	-7.24	97.65	111.40
2	L	99	GLY	CA-C-N	-7.23	112.15	121.91
2	L	99	GLY	C-N-CA	-7.23	112.15	121.91
3	S	242	ARG	O-C-N	-7.23	112.48	122.46
2	I	97	GLU	CA-C-N	-7.23	111.61	122.74
2	I	97	GLU	C-N-CA	-7.23	111.61	122.74
3	T	274	SER	N-CA-C	-7.22	100.97	109.93
3	S	243	GLU	CB-CA-C	7.22	121.89	111.27
1	B	134	LYS	CB-CG-CD	7.21	127.89	111.30
1	B	133	TRP	N-CA-C	7.21	123.20	111.37
1	B	89	ARG	CG-CD-NE	-7.20	96.16	112.00
1	E	103	LEU	CA-C-O	-7.19	113.47	121.89
3	U	236	ILE	O-C-N	-7.19	115.01	122.20
2	F	140	ASN	CA-C-N	-7.19	110.98	121.98
2	F	140	ASN	C-N-CA	-7.19	110.98	121.98
3	T	264	ARG	NE-CZ-NH2	-7.19	112.73	119.20
1	E	102	ALA	CA-C-O	-7.19	111.71	119.97
3	U	251	ILE	CA-C-N	-7.18	111.09	122.73
3	U	251	ILE	C-N-CA	-7.18	111.09	122.73
1	B	144	ALA	CA-C-N	-7.17	109.95	120.28
1	B	144	ALA	C-N-CA	-7.17	109.95	120.28
3	S	239	GLU	CG-CD-OE2	-7.17	101.90	118.40
2	C	165	GLN	CA-C-N	7.17	127.76	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	165	GLN	C-N-CA	7.17	127.76	120.38
2	L	172	TYR	N-CA-C	-7.17	98.92	110.32
3	T	277	THR	CB-CA-C	-7.16	96.78	110.24
2	F	52	GLN	CA-C-O	-7.15	113.31	120.82
2	F	159	GLU	CA-CB-CG	7.15	128.40	114.10
3	S	282	ILE	N-CA-C	7.15	116.11	107.61
3	T	246	ILE	CB-CA-C	7.14	121.39	110.82
1	K	89	ARG	N-CA-C	-7.14	99.46	110.10
1	H	72	LYS	CA-C-N	-7.14	113.02	122.94
1	H	72	LYS	C-N-CA	-7.14	113.02	122.94
2	C	151	LEU	N-CA-C	-7.13	103.50	111.28
3	V	247	THR	N-CA-C	-7.13	97.83	109.82
1	E	153	MET	CG-SD-CE	7.13	116.59	100.90
2	F	157	SER	CA-C-N	-7.13	109.11	121.66
2	F	157	SER	C-N-CA	-7.13	109.11	121.66
3	T	241	MET	N-CA-C	7.13	120.07	109.59
1	E	153	MET	N-CA-C	-7.12	98.62	109.95
3	S	237	SER	N-CA-C	7.11	121.22	112.54
3	S	239	GLU	CB-CA-C	-7.11	99.37	113.45
3	V	232	LEU	CA-C-N	-7.11	111.53	122.62
3	V	232	LEU	C-N-CA	-7.11	111.53	122.62
1	B	24	VAL	CB-CA-C	-7.11	104.04	111.00
2	I	75	TRP	N-CA-C	7.11	121.11	109.24
2	C	76	THR	CA-C-N	-7.10	112.94	122.03
2	C	76	THR	C-N-CA	-7.10	112.94	122.03
2	L	38	VAL	N-CA-C	-7.09	93.56	108.88
2	F	51	GLY	CA-C-N	-7.08	111.23	120.44
2	F	51	GLY	C-N-CA	-7.08	111.23	120.44
1	B	8	LEU	CA-C-O	-7.08	113.35	120.64
1	H	72	LYS	CD-CE-NZ	-7.08	89.25	111.90
2	L	45	LEU	N-CA-C	7.08	119.60	111.11
1	E	42	VAL	CB-CA-C	-7.06	98.49	110.71
3	V	271	VAL	N-CA-C	-7.06	106.61	113.53
2	F	43	ARG	CB-CA-C	-7.06	98.67	110.68
1	B	53	GLY	CA-C-N	-7.06	107.57	121.41
1	B	53	GLY	C-N-CA	-7.06	107.57	121.41
1	E	134	LYS	N-CA-C	-7.05	104.70	113.38
2	L	77	GLY	N-CA-C	7.05	125.92	112.51
2	L	121	ASN	N-CA-C	7.04	120.17	110.24
3	T	249	SER	O-C-N	-7.04	113.00	122.43
1	E	78	LYS	N-CA-C	-7.03	98.58	109.76
3	S	265	VAL	N-CA-CB	-7.03	103.02	112.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	VAL	N-CA-C	7.03	119.18	108.71
1	K	129	VAL	CB-CA-C	-7.01	101.81	112.05
2	C	137	LYS	CD-CE-NZ	-7.00	89.50	111.90
3	S	273	ARG	NE-CZ-NH1	-7.00	114.50	121.50
3	U	269	ASN	CA-C-N	-6.99	111.10	119.84
3	U	269	ASN	C-N-CA	-6.99	111.10	119.84
2	C	157	SER	N-CA-C	-6.99	100.84	110.35
3	U	262	LEU	N-CA-CB	6.99	121.80	110.40
2	F	57	ASP	CB-CA-C	-6.99	96.51	110.42
1	H	91	CYS	CA-CB-SG	-6.99	98.33	114.40
1	E	90	ILE	N-CA-C	-6.99	98.40	108.53
1	H	104	GLN	CA-CB-CG	-6.98	100.13	114.10
3	T	279	GLU	CA-CB-CG	-6.98	100.15	114.10
2	C	82	PRO	N-CA-C	6.97	119.21	110.70
3	T	288	LYS	N-CA-CB	6.97	122.27	110.49
3	S	229	PRO	N-CA-C	-6.96	100.98	111.57
2	I	139	GLN	CB-CA-C	-6.96	96.07	109.37
3	S	279	GLU	CA-C-N	-6.96	111.60	122.67
3	S	279	GLU	C-N-CA	-6.96	111.60	122.67
3	T	271	VAL	N-CA-C	-6.96	106.12	111.62
1	E	38	TYR	CA-C-N	-6.95	113.41	123.00
1	E	38	TYR	C-N-CA	-6.95	113.41	123.00
2	C	115	ILE	CA-C-O	-6.95	113.91	121.28
1	H	49	SER	CA-C-N	-6.95	111.15	119.84
1	H	49	SER	C-N-CA	-6.95	111.15	119.84
3	U	258	ILE	CA-C-N	-6.95	110.98	122.79
3	U	258	ILE	C-N-CA	-6.95	110.98	122.79
1	B	51	PHE	N-CA-C	6.93	121.40	113.15
1	B	9	PRO	CA-N-CD	-6.93	102.30	112.00
2	C	153	ARG	CD-NE-CZ	6.93	134.10	124.40
3	S	260	GLU	CA-CB-CG	-6.91	100.28	114.10
1	E	100	SER	CA-CB-OG	-6.91	97.29	111.10
2	F	95	LYS	CA-C-N	-6.91	113.53	123.06
2	F	95	LYS	C-N-CA	-6.91	113.53	123.06
2	I	143	SER	CA-CB-OG	-6.90	97.29	111.10
3	V	298	ASN	CA-C-O	6.90	132.53	120.80
1	B	89	ARG	CA-C-N	-6.89	114.21	123.10
1	B	89	ARG	C-N-CA	-6.89	114.21	123.10
2	C	122	SER	CA-CB-OG	-6.88	97.33	111.10
2	C	114	LYS	CA-CB-CG	6.87	127.85	114.10
2	F	43	ARG	N-CA-C	6.87	119.64	111.33
1	K	81	HIS	N-CA-C	6.87	116.97	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	ALA	CA-C-N	-6.87	111.27	123.08
1	B	21	ALA	C-N-CA	-6.87	111.27	123.08
2	C	109	VAL	CB-CA-C	-6.87	100.30	110.33
2	L	109	VAL	CB-CA-C	-6.87	100.39	110.62
1	B	145	ARG	NE-CZ-NH2	-6.86	113.02	119.20
2	F	159	GLU	N-CA-C	-6.85	104.93	113.28
2	F	132	ILE	CB-CG1-CD1	-6.84	99.43	113.80
3	S	282	ILE	CA-C-O	-6.84	115.27	119.51
2	L	139	GLN	N-CA-CB	-6.84	99.41	110.77
3	S	263	GLN	O-C-N	-6.84	112.26	122.39
1	K	54	GLY	N-CA-C	6.84	122.38	112.60
1	H	122	ASP	N-CA-C	-6.84	96.24	110.80
2	C	110	ARG	NE-CZ-NH1	6.81	128.31	121.50
1	K	64	GLU	O-C-N	6.81	129.34	122.12
1	K	135	THR	N-CA-C	6.81	120.46	111.75
3	V	270	PRO	CA-C-N	-6.79	113.56	121.71
3	V	270	PRO	C-N-CA	-6.79	113.56	121.71
2	C	150	GLU	O-C-N	6.79	129.89	122.15
3	U	292	ASP	O-C-N	6.79	129.89	122.15
2	C	126	VAL	N-CA-CB	-6.79	102.85	110.99
2	F	145	LYS	CA-C-N	-6.78	112.02	120.56
2	F	145	LYS	C-N-CA	-6.78	112.02	120.56
1	E	49	SER	N-CA-C	-6.78	100.44	110.20
1	H	22	GLU	CA-C-N	6.77	128.30	119.84
1	H	22	GLU	C-N-CA	6.77	128.30	119.84
2	L	170	GLN	N-CA-C	-6.76	96.39	110.80
2	F	85	THR	N-CA-C	6.76	119.25	110.53
3	V	278	GLN	N-CA-C	6.76	118.65	111.28
2	C	78	MET	N-CA-CB	-6.75	99.58	111.39
3	S	260	GLU	CB-CG-CD	-6.74	101.14	112.60
3	S	260	GLU	O-C-N	6.73	129.28	122.08
2	C	64	LEU	CA-C-N	-6.73	111.48	120.63
2	C	64	LEU	C-N-CA	-6.73	111.48	120.63
1	K	46	PRO	N-CA-C	6.72	121.75	111.34
1	B	36	ALA	N-CA-C	-6.72	104.90	113.23
3	T	272	THR	N-CA-C	-6.71	105.22	113.41
1	E	49	SER	CA-C-N	6.71	126.39	119.82
1	E	49	SER	C-N-CA	6.71	126.39	119.82
3	V	251	ILE	CA-C-N	-6.71	112.55	122.41
3	V	251	ILE	C-N-CA	-6.71	112.55	122.41
2	C	122	SER	CA-C-N	-6.71	110.83	120.89
2	C	122	SER	C-N-CA	-6.71	110.83	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	70	ALA	N-CA-C	6.71	117.31	109.60
1	H	81	HIS	N-CA-CB	6.70	122.30	110.37
3	S	271	VAL	CB-CA-C	-6.70	104.08	110.65
1	E	142	GLU	CG-CD-OE1	-6.69	103.01	118.40
2	F	80	LEU	N-CA-C	6.69	119.42	109.59
3	V	265	VAL	N-CA-C	6.69	123.25	109.34
2	C	59	THR	CA-C-O	-6.68	110.96	120.51
1	B	118	ALA	N-CA-C	-6.68	95.05	109.81
3	V	245	CYS	CA-CB-SG	-6.67	99.06	114.40
1	E	74	ARG	N-CA-C	6.67	120.48	108.48
3	S	260	GLU	N-CA-C	-6.66	102.90	111.02
1	K	51	PHE	N-CA-C	6.65	120.09	112.57
2	C	89	ASN	CB-CA-C	-6.65	100.91	111.48
2	L	114	LYS	N-CA-C	-6.65	99.70	110.20
2	I	99	GLY	CA-C-N	-6.64	112.96	119.87
2	I	99	GLY	C-N-CA	-6.64	112.96	119.87
2	L	140	ASN	N-CA-C	6.64	121.22	113.18
1	H	155	ASN	N-CA-C	-6.64	98.56	108.99
2	L	82	PRO	CB-CA-C	-6.64	102.82	110.92
1	K	16	THR	CB-CA-C	-6.63	100.74	110.96
1	B	106	ARG	CA-CB-CG	-6.62	100.85	114.10
2	C	142	TYR	N-CA-C	6.62	118.55	110.41
1	E	155	ASN	CA-C-O	6.62	127.44	120.36
1	E	22	GLU	N-CA-C	6.62	120.39	108.55
2	F	174	ASN	CB-CA-C	6.61	122.66	110.10
2	L	159	GLU	N-CA-C	6.61	121.08	112.89
1	K	150	LEU	CB-CG-CD2	6.60	130.50	110.70
1	B	55	THR	CB-CA-C	-6.60	96.61	109.68
1	K	115	LEU	CA-CB-CG	-6.60	93.20	116.30
2	I	102	TYR	C-N-CD	6.60	135.11	120.60
2	F	153	ARG	CB-CA-C	-6.59	99.86	110.79
2	L	94	LEU	CA-C-N	-6.58	110.35	121.94
2	L	94	LEU	C-N-CA	-6.58	110.35	121.94
2	C	108	PHE	N-CA-CB	-6.58	100.05	109.85
1	K	91	CYS	CA-CB-SG	-6.58	99.28	114.40
2	I	74	ARG	CG-CD-NE	-6.57	97.55	112.00
2	I	130	ARG	N-CA-C	-6.56	101.43	110.35
1	K	106	ARG	CG-CD-NE	-6.56	97.57	112.00
3	U	272	THR	CA-C-O	6.56	126.26	119.05
1	B	72	LYS	CA-CB-CG	-6.55	100.99	114.10
2	L	72	LEU	N-CA-CB	-6.55	102.08	111.84
3	U	248	PRO	N-CA-C	-6.55	98.97	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	72	LEU	N-CA-C	6.55	120.55	111.90
2	F	172	TYR	O-C-N	-6.55	115.72	123.06
2	L	110	ARG	CA-CB-CG	6.55	127.19	114.10
2	L	167	PRO	CA-C-N	-6.55	108.91	122.07
2	L	167	PRO	C-N-CA	-6.55	108.91	122.07
2	F	63	GLY	N-CA-C	-6.54	101.99	110.69
2	I	74	ARG	N-CA-C	6.54	119.56	108.90
2	I	167	PRO	CA-C-O	-6.54	113.69	121.67
2	I	167	PRO	N-CA-C	-6.54	100.98	111.38
2	C	172	TYR	CA-C-N	-6.54	112.07	121.42
2	C	172	TYR	C-N-CA	-6.54	112.07	121.42
2	C	150	GLU	CB-CG-CD	-6.53	101.50	112.60
2	F	65	GLU	N-CA-C	-6.53	104.08	111.07
1	K	110	LEU	N-CA-CB	6.52	119.44	109.91
2	F	118	ASN	CA-C-O	-6.52	114.02	121.19
2	L	70	MET	CG-SD-CE	6.52	115.25	100.90
1	B	74	ARG	N-CA-C	6.51	118.11	108.60
2	L	92	TYR	CA-C-N	-6.51	111.46	122.92
2	L	92	TYR	C-N-CA	-6.51	111.46	122.92
1	B	22	GLU	CA-CB-CG	6.50	127.11	114.10
3	S	260	GLU	CA-C-O	-6.50	113.92	121.07
2	F	73	THR	CA-C-N	-6.49	113.84	122.99
2	F	73	THR	C-N-CA	-6.49	113.84	122.99
1	B	127	ASN	N-CA-C	6.49	129.17	111.00
1	H	96	LYS	CA-C-O	-6.49	113.57	120.71
2	F	53	LYS	CA-C-N	6.49	134.12	121.41
2	F	53	LYS	C-N-CA	6.49	134.12	121.41
2	L	148	LEU	N-CA-C	6.47	119.17	111.33
2	I	130	ARG	O-C-N	-6.47	114.85	122.81
2	L	38	VAL	N-CA-CB	6.47	120.27	111.21
1	B	28	LYS	N-CA-C	-6.47	99.18	109.59
2	F	102	TYR	CB-CA-C	6.47	118.17	108.86
2	F	166	PRO	N-CD-CG	-6.47	93.50	103.20
3	T	265	VAL	N-CA-C	-6.46	107.57	113.71
3	S	283	PRO	N-CA-CB	-6.46	96.47	103.25
2	C	79	ILE	N-CA-CB	-6.45	100.87	111.45
2	F	101	LYS	O-C-N	-6.45	114.02	122.59
2	I	68	GLU	CB-CA-C	6.45	119.02	109.29
3	V	260	GLU	O-C-N	6.45	128.79	122.09
1	K	105	ILE	CB-CA-C	-6.44	100.73	111.29
1	K	155	ASN	CA-C-N	6.44	133.30	121.70
1	K	155	ASN	C-N-CA	6.44	133.30	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	14	LYS	N-CA-C	6.44	118.30	111.28
3	S	230	ASP	O-C-N	6.44	129.04	122.09
1	K	62	LEU	CA-C-N	-6.44	114.03	120.21
1	K	62	LEU	C-N-CA	-6.44	114.03	120.21
1	K	89	ARG	NE-CZ-NH2	6.44	124.99	119.20
3	S	285	LEU	CA-C-N	-6.43	109.97	120.72
3	S	285	LEU	C-N-CA	-6.43	109.97	120.72
1	H	11	ARG	N-CA-C	-6.43	104.31	111.71
3	S	236	ILE	CA-C-N	-6.43	109.98	120.72
3	S	236	ILE	C-N-CA	-6.43	109.98	120.72
2	C	79	ILE	CB-CA-C	-6.43	99.59	110.71
1	E	73	VAL	CA-C-N	-6.43	110.71	121.89
1	E	73	VAL	C-N-CA	-6.43	110.71	121.89
2	I	173	SER	N-CA-C	6.43	120.13	109.46
1	H	115	LEU	N-CA-C	-6.42	104.20	111.07
1	H	89	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	K	11	ARG	CA-CB-CG	-6.41	101.27	114.10
2	C	89	ASN	CA-C-N	-6.41	109.15	122.03
2	C	89	ASN	C-N-CA	-6.41	109.15	122.03
1	E	145	ARG	N-CA-C	6.41	118.34	111.36
2	C	53	LYS	CA-CB-CG	6.40	126.89	114.10
2	C	149	GLN	CA-C-N	-6.40	111.21	120.29
2	C	149	GLN	C-N-CA	-6.40	111.21	120.29
2	I	138	TRP	CA-C-N	6.39	132.53	122.94
2	I	138	TRP	C-N-CA	6.39	132.53	122.94
3	V	272	THR	CA-C-N	-6.39	113.77	125.02
3	V	272	THR	C-N-CA	-6.39	113.77	125.02
2	F	171	CYS	N-CA-C	6.39	118.89	109.24
3	V	282	ILE	CB-CG1-CD1	-6.38	100.40	113.80
3	U	260	GLU	CA-C-N	-6.38	111.10	120.28
3	U	260	GLU	C-N-CA	-6.38	111.10	120.28
1	H	88	GLY	N-CA-C	6.37	123.84	115.36
2	I	168	GLU	CB-CG-CD	6.37	123.43	112.60
2	F	62	TRP	O-C-N	-6.37	117.15	123.46
3	T	278	GLN	CA-C-O	6.37	127.27	119.11
2	F	160	ASN	N-CA-C	6.36	122.51	114.31
1	K	62	LEU	CA-CB-CG	-6.35	94.06	116.30
1	H	68	MET	N-CA-C	-6.35	103.98	111.03
1	E	153	MET	CB-CG-SD	-6.34	93.68	112.70
3	T	273	ARG	CB-CA-C	-6.34	101.57	111.39
1	B	35	ASN	CA-C-O	6.34	127.20	120.36
1	E	85	ASP	CB-CG-OD1	6.33	132.96	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	131	GLU	N-CA-C	-6.33	104.07	110.97
2	F	139	GLN	N-CA-CB	-6.32	99.80	110.49
1	B	150	LEU	CA-CB-CG	6.32	138.41	116.30
2	I	38	VAL	CB-CA-C	-6.32	99.86	111.36
2	L	169	GLY	CA-C-N	-6.32	109.48	121.54
2	L	169	GLY	C-N-CA	-6.32	109.48	121.54
2	L	156	MET	CG-SD-CE	6.31	114.79	100.90
3	S	269	ASN	CA-C-N	6.31	127.73	119.84
3	S	269	ASN	C-N-CA	6.31	127.73	119.84
2	L	105	ALA	CA-C-N	-6.31	113.88	120.38
2	L	105	ALA	C-N-CA	-6.31	113.88	120.38
3	V	279	GLU	CB-CA-C	-6.31	97.87	110.42
1	E	25	PRO	CA-C-O	-6.30	114.45	121.32
3	V	298	ASN	N-CA-C	-6.30	93.36	111.00
1	B	149	ARG	N-CA-C	6.30	119.81	111.75
3	S	264	ARG	CB-CG-CD	-6.30	96.81	111.30
1	B	22	GLU	CG-CD-OE1	6.30	132.88	118.40
2	C	171	CYS	CB-CA-C	-6.29	96.23	109.38
2	C	34	THR	CB-CA-C	6.29	122.94	110.42
1	H	152	ALA	N-CA-C	6.29	118.22	111.36
1	K	147	TRP	N-CA-C	6.29	124.20	110.80
1	B	24	VAL	N-CA-CB	6.29	116.47	109.99
2	C	83	PRO	CB-CA-C	-6.28	103.58	111.56
3	S	255	ARG	CG-CD-NE	6.28	125.82	112.00
3	S	262	LEU	CA-C-O	-6.28	114.23	120.70
2	C	65	GLU	N-CA-CB	6.28	119.08	109.98
2	C	67	ASP	CB-CG-OD2	-6.26	103.99	118.40
1	K	31	PRO	O-C-N	6.26	130.64	123.00
2	C	132	ILE	CA-C-O	6.26	128.60	120.78
1	H	151	TYR	N-CA-C	6.26	121.10	112.90
2	I	47	GLU	CA-C-N	-6.26	109.59	121.54
2	I	47	GLU	C-N-CA	-6.26	109.59	121.54
1	K	16	THR	N-CA-C	-6.26	104.15	110.97
1	K	95	LEU	N-CA-C	-6.26	105.13	112.89
3	S	271	VAL	CA-C-N	-6.25	112.41	122.23
3	S	271	VAL	C-N-CA	-6.25	112.41	122.23
2	F	60	VAL	CB-CA-C	-6.25	101.57	110.82
2	C	143	SER	CA-CB-OG	-6.25	98.61	111.10
2	C	98	CYS	CA-C-N	-6.24	112.07	121.87
2	C	98	CYS	C-N-CA	-6.24	112.07	121.87
1	B	123	ASP	O-C-N	6.24	124.58	120.27
2	L	102	TYR	N-CA-C	-6.24	101.03	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	139	GLN	CB-CA-C	-6.24	99.67	109.72
3	S	237	SER	CA-CB-OG	-6.24	98.62	111.10
1	E	120	ASN	N-CA-C	6.24	122.31	108.27
2	L	40	ARG	N-CA-C	-6.24	104.48	111.28
1	E	151	TYR	CA-CB-CG	6.24	125.12	113.90
3	V	248	PRO	CB-CA-C	-6.24	101.27	111.56
3	V	241	MET	CB-CA-C	6.23	119.86	109.89
2	L	52	GLN	N-CA-C	6.22	118.57	111.11
3	T	239	GLU	N-CA-C	6.22	118.55	110.53
3	T	249	SER	CA-C-O	6.22	127.03	119.38
2	L	64	LEU	CA-C-N	-6.22	111.42	122.42
2	L	64	LEU	C-N-CA	-6.22	111.42	122.42
2	F	80	LEU	CB-CG-CD1	-6.21	92.06	110.70
2	L	173	SER	CA-CB-OG	-6.21	98.67	111.10
2	L	145	LYS	CB-CG-CD	6.21	125.59	111.30
1	E	28	LYS	O-C-N	-6.21	115.42	122.68
3	T	292	ASP	CB-CA-C	-6.21	98.07	110.42
2	F	171	CYS	CA-CB-SG	-6.20	100.13	114.40
1	E	40	HIS	N-CA-C	6.19	118.06	109.15
2	C	38	VAL	CA-CB-CG1	6.19	120.92	110.40
1	K	152	ALA	N-CA-C	-6.18	105.38	113.17
1	B	66	TYR	CA-C-N	-6.17	112.18	127.00
1	B	66	TYR	C-N-CA	-6.17	112.18	127.00
1	E	46	PRO	N-CA-C	6.17	125.19	112.47
1	B	57	LYS	CA-C-N	-6.17	112.03	123.01
1	B	57	LYS	C-N-CA	-6.17	112.03	123.01
1	E	16	THR	N-CA-C	-6.17	104.62	111.71
3	S	268	PHE	O-C-N	-6.16	116.83	123.42
3	V	268	PHE	CA-CB-CG	-6.16	107.64	113.80
1	H	89	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	H	120	ASN	N-CA-C	6.16	123.42	109.81
3	T	269	ASN	CA-C-N	6.16	127.53	119.84
3	T	269	ASN	C-N-CA	6.16	127.53	119.84
1	H	62	LEU	CB-CA-C	-6.15	99.94	109.85
1	E	24	VAL	CB-CA-C	-6.15	100.17	111.36
1	K	82	PRO	CA-C-O	6.14	125.32	118.38
1	K	112	ILE	CB-CA-C	-6.14	103.84	111.70
3	V	252	THR	CA-CB-CG2	-6.14	100.06	110.50
2	C	127	VAL	CB-CA-C	-6.14	102.18	111.33
2	C	102	TYR	N-CA-C	-6.14	101.61	110.08
2	L	101	LYS	CB-CG-CD	-6.14	97.19	111.30
3	S	240	LEU	CA-C-O	-6.14	113.86	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	291	ILE	O-C-N	6.14	127.82	121.87
2	L	54	GLY	CA-C-N	-6.13	113.88	122.71
2	L	54	GLY	C-N-CA	-6.13	113.88	122.71
1	K	31	PRO	CB-CA-C	-6.13	102.92	110.95
2	C	155	MET	CG-SD-CE	6.12	114.37	100.90
2	F	159	GLU	CA-C-N	-6.12	112.63	122.24
2	F	159	GLU	C-N-CA	-6.12	112.63	122.24
2	L	105	ALA	CA-C-O	-6.12	114.58	120.64
2	I	48	LEU	CA-C-N	6.11	129.99	120.82
2	I	48	LEU	C-N-CA	6.11	129.99	120.82
1	E	135	THR	N-CA-C	6.11	121.67	113.72
3	U	273	ARG	CA-C-O	-6.11	111.77	120.51
2	C	66	ASP	CA-C-N	-6.11	112.70	122.66
2	C	66	ASP	C-N-CA	-6.11	112.70	122.66
1	E	92	LEU	O-C-N	6.10	130.38	123.42
1	E	134	LYS	CB-CA-C	6.10	120.26	109.65
3	S	259	GLU	N-CA-CB	6.09	118.91	110.07
1	H	17	GLN	CA-CB-CG	-6.09	101.92	114.10
2	L	143	SER	CA-C-N	-6.09	111.95	120.53
2	L	143	SER	C-N-CA	-6.09	111.95	120.53
2	I	49	GLU	O-C-N	6.08	129.11	122.11
2	C	91	ILE	N-CA-CB	-6.08	103.02	111.41
2	L	131	ALA	CA-C-N	-6.08	111.03	121.97
2	L	131	ALA	C-N-CA	-6.08	111.03	121.97
1	E	96	LYS	CB-CG-CD	6.08	125.27	111.30
3	U	280	GLN	N-CA-C	-6.07	105.52	113.17
2	L	132	ILE	CB-CG1-CD1	-6.07	101.06	113.80
3	V	242	ARG	CA-C-N	-6.07	115.81	123.15
3	V	242	ARG	C-N-CA	-6.07	115.81	123.15
2	L	125	GLY	N-CA-C	6.06	127.54	113.18
1	B	132	GLN	N-CA-CB	-6.05	101.20	110.16
1	E	78	LYS	CB-CG-CD	6.05	125.22	111.30
1	E	119	PRO	N-CA-C	-6.05	101.59	111.15
3	S	270	PRO	O-C-N	-6.05	114.47	122.64
2	I	152	ARG	N-CA-CB	6.05	120.72	110.49
3	V	245	CYS	O-C-N	-6.05	116.58	123.48
1	H	95	LEU	CB-CG-CD1	-6.04	92.57	110.70
2	F	163	LEU	CA-C-N	6.04	127.39	119.84
2	F	163	LEU	C-N-CA	6.04	127.39	119.84
1	K	144	ALA	O-C-N	6.03	128.30	122.03
1	K	129	VAL	O-C-N	6.03	127.99	121.90
2	C	145	LYS	N-CA-C	-6.03	103.88	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	150	LEU	CA-C-N	6.03	132.61	121.52
1	H	150	LEU	C-N-CA	6.03	132.61	121.52
1	E	101	PRO	CA-C-O	6.03	126.49	118.90
1	B	93	ASP	N-CA-C	-6.02	104.63	111.07
3	U	283	PRO	CB-CA-C	-6.02	103.69	111.46
3	V	267	HIS	CA-C-O	-6.02	114.86	122.63
2	C	33	THR	N-CA-C	6.01	127.84	111.00
3	U	243	GLU	N-CA-C	6.01	123.10	109.81
2	I	112	VAL	N-CA-C	6.01	116.67	110.36
3	T	292	ASP	N-CA-C	6.01	123.61	110.80
2	C	84	ARG	CG-CD-NE	-6.01	98.78	112.00
2	C	71	THR	N-CA-C	-6.00	105.92	113.18
1	H	69	ALA	N-CA-CB	-6.00	101.15	109.97
1	K	81	HIS	O-C-N	-6.00	117.15	121.83
2	I	111	PHE	CA-C-O	-5.99	113.87	120.70
2	F	57	ASP	CA-C-N	-5.99	109.67	121.41
2	F	57	ASP	C-N-CA	-5.99	109.67	121.41
1	E	64	GLU	CB-CA-C	-5.98	98.52	110.42
1	H	16	THR	OG1-CB-CG2	-5.98	97.34	109.30
1	E	132	GLN	CB-CA-C	-5.98	100.69	110.85
1	B	142	GLU	CA-CB-CG	-5.98	102.15	114.10
1	E	66	TYR	CB-CA-C	-5.98	100.08	109.52
1	B	136	ASN	CA-CB-CG	-5.97	106.63	112.60
2	C	168	GLU	N-CA-C	5.97	123.53	110.80
3	T	245	CYS	CA-C-N	-5.97	114.31	122.92
3	T	245	CYS	C-N-CA	-5.97	114.31	122.92
1	H	19	LEU	N-CA-C	5.97	117.46	111.07
3	S	231	TYR	N-CA-C	5.97	123.52	110.80
1	B	77	THR	N-CA-CB	-5.97	101.73	110.26
1	B	53	GLY	N-CA-C	5.96	127.31	113.18
3	S	267	HIS	CA-CB-CG	-5.96	107.84	113.80
1	E	140	ALA	CA-C-N	-5.96	112.93	120.56
1	E	140	ALA	C-N-CA	-5.96	112.93	120.56
3	V	264	ARG	CG-CD-NE	-5.96	98.90	112.00
3	T	249	SER	CA-C-N	-5.96	109.74	121.41
3	T	249	SER	C-N-CA	-5.96	109.74	121.41
1	B	68	MET	CG-SD-CE	-5.95	87.80	100.90
1	B	73	VAL	CB-CA-C	-5.95	101.65	110.82
2	C	169	GLY	CA-C-N	-5.95	110.82	120.87
2	C	169	GLY	C-N-CA	-5.95	110.82	120.87
1	E	14	LYS	CB-CA-C	5.95	120.66	110.79
1	K	106	ARG	N-CA-CB	5.94	118.97	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	64	LEU	CA-C-O	-5.93	113.84	120.54
1	H	32	ASP	N-CA-C	-5.93	99.33	109.24
1	B	135	THR	N-CA-C	-5.92	104.40	111.69
3	S	256	LYS	CA-CB-CG	-5.92	102.25	114.10
1	K	98	LYS	CA-C-N	-5.92	114.55	122.72
1	K	98	LYS	C-N-CA	-5.92	114.55	122.72
2	L	55	VAL	N-CA-C	5.92	117.21	108.45
1	B	69	ALA	N-CA-CB	-5.92	100.42	111.13
1	H	30	GLU	CB-CA-C	-5.92	101.88	109.92
1	B	60	LEU	N-CA-CB	-5.90	101.41	110.85
1	B	89	ARG	CD-NE-CZ	5.90	132.66	124.40
2	C	95	LYS	CG-CD-CE	-5.90	97.73	111.30
1	B	57	LYS	CA-C-O	-5.90	114.14	120.92
2	C	154	LEU	CB-CG-CD1	-5.90	93.01	110.70
2	C	58	GLY	N-CA-C	-5.89	107.60	115.32
2	F	117	MET	CA-C-N	-5.89	112.34	120.71
2	F	117	MET	C-N-CA	-5.89	112.34	120.71
1	B	102	ALA	CA-C-N	-5.89	110.88	122.02
1	B	102	ALA	C-N-CA	-5.89	110.88	122.02
2	F	47	GLU	CA-CB-CG	-5.89	102.32	114.10
1	B	26	GLY	N-CA-C	5.88	127.12	113.18
2	L	130	ARG	CB-CG-CD	-5.88	97.77	111.30
1	H	47	GLN	CA-CB-CG	5.88	125.86	114.10
2	F	47	GLU	CB-CA-C	5.88	120.67	110.68
1	H	57	LYS	O-C-N	-5.88	115.56	122.96
3	V	277	THR	CA-C-N	5.87	128.15	120.28
3	V	277	THR	C-N-CA	5.87	128.15	120.28
1	K	60	LEU	CD1-CG-CD2	5.87	123.71	110.80
3	V	259	GLU	CA-CB-CG	5.87	125.84	114.10
1	E	12	ILE	N-CA-C	-5.87	104.79	110.42
2	F	90	ARG	N-CA-C	-5.87	98.30	108.69
1	H	101	PRO	CB-CA-C	-5.87	101.88	111.56
3	T	272	THR	OG1-CB-CG2	-5.87	97.56	109.30
2	L	89	ASN	N-CA-C	5.87	123.30	110.80
2	C	63	GLY	O-C-N	-5.86	116.58	123.55
2	I	139	GLN	CB-CG-CD	-5.85	102.66	112.60
1	B	65	GLU	CG-CD-OE2	-5.84	104.96	118.40
1	B	129	VAL	N-CA-C	-5.84	104.63	111.00
1	E	28	LYS	N-CA-CB	-5.84	101.54	110.42
1	E	148	THR	CA-C-O	-5.84	114.65	121.07
3	T	243	GLU	CA-C-O	5.84	128.16	120.16
1	H	148	THR	CB-CA-C	-5.83	101.11	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	90	ILE	CA-C-N	-5.83	114.96	123.00
1	K	90	ILE	C-N-CA	-5.83	114.96	123.00
2	L	149	GLN	CA-C-O	5.83	126.67	119.79
2	L	163	LEU	N-CA-C	5.83	118.07	109.50
2	F	39	PRO	CA-C-O	-5.83	114.89	122.12
1	H	137	GLU	CA-CB-CG	5.83	125.75	114.10
2	C	42	PHE	N-CA-CB	5.82	119.53	110.44
1	B	32	ASP	CB-CA-C	-5.82	101.82	110.67
1	E	116	LEU	CA-C-N	-5.82	113.47	122.49
1	E	116	LEU	C-N-CA	-5.82	113.47	122.49
1	K	18	ARG	CB-CA-C	5.82	120.57	110.79
1	B	45	GLY	CA-C-O	-5.82	113.20	121.52
2	C	78	MET	CA-C-N	-5.82	114.33	122.71
2	C	78	MET	C-N-CA	-5.82	114.33	122.71
1	K	119	PRO	CA-C-O	-5.82	115.04	123.07
2	F	50	GLU	CB-CA-C	5.82	120.74	110.85
2	L	80	LEU	CA-C-N	-5.82	112.74	121.87
2	L	80	LEU	C-N-CA	-5.82	112.74	121.87
1	K	57	LYS	CB-CG-CD	5.81	124.67	111.30
2	L	78	MET	N-CA-C	5.80	118.00	109.24
1	E	102	ALA	CA-C-N	-5.80	110.37	122.03
1	E	102	ALA	C-N-CA	-5.80	110.37	122.03
1	H	57	LYS	CA-C-N	-5.80	113.49	122.59
1	H	57	LYS	C-N-CA	-5.80	113.49	122.59
1	E	41	VAL	N-CA-C	5.79	118.08	109.17
1	H	80	TYR	N-CA-C	-5.79	102.34	110.50
2	F	44	LEU	CA-C-N	-5.79	111.95	120.28
2	F	44	LEU	C-N-CA	-5.79	111.95	120.28
3	T	246	ILE	CA-C-O	-5.78	115.77	121.67
2	C	68	GLU	CG-CD-OE2	-5.78	105.11	118.40
1	B	17	GLN	CB-CG-CD	-5.77	102.79	112.60
1	B	89	ARG	CA-CB-CG	-5.77	102.55	114.10
3	S	241	MET	CA-C-N	-5.76	111.05	121.14
3	S	241	MET	C-N-CA	-5.76	111.05	121.14
1	E	107	THR	CB-CA-C	-5.75	101.82	110.90
3	T	279	GLU	CA-C-O	-5.75	112.55	119.27
3	T	291	ILE	CA-CB-CG1	5.74	120.16	110.40
2	C	130	ARG	CA-C-N	-5.74	110.58	121.54
2	C	130	ARG	C-N-CA	-5.74	110.58	121.54
2	L	81	GLY	CA-C-N	5.74	126.29	120.38
2	L	81	GLY	C-N-CA	5.74	126.29	120.38
2	C	169	GLY	O-C-N	-5.73	115.11	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	56	PHE	CA-C-O	5.73	126.42	120.40
1	B	64	GLU	N-CA-C	5.73	123.00	110.80
2	L	112	VAL	N-CA-C	-5.73	106.10	111.48
3	U	264	ARG	N-CA-C	5.73	123.00	110.80
1	H	11	ARG	CA-C-N	-5.72	113.24	120.56
1	H	11	ARG	C-N-CA	-5.72	113.24	120.56
3	V	258	ILE	CB-CG1-CD1	-5.72	101.79	113.80
3	V	279	GLU	CA-C-O	-5.72	112.33	120.51
2	L	37	LYS	CA-C-O	-5.72	114.46	120.58
1	B	34	SER	CB-CA-C	5.72	121.80	110.42
3	U	295	ILE	CB-CA-C	-5.71	104.57	111.88
2	C	76	THR	O-C-N	-5.71	116.30	123.27
2	L	141	SER	CA-C-N	-5.71	111.49	123.20
2	L	141	SER	C-N-CA	-5.71	111.49	123.20
1	K	97	ASP	CA-C-N	-5.71	113.76	122.21
1	K	97	ASP	C-N-CA	-5.71	113.76	122.21
1	B	112	ILE	CA-C-O	-5.69	115.13	121.05
2	C	174	ASN	CA-C-O	-5.69	103.93	121.00
2	C	157	SER	CA-C-O	-5.69	115.52	121.55
1	K	57	LYS	CG-CD-CE	5.69	124.38	111.30
3	S	245	CYS	CA-CB-SG	-5.68	101.33	114.40
1	K	82	PRO	CB-CA-C	5.68	116.87	109.89
2	C	65	GLU	CA-C-N	5.67	130.22	122.84
2	C	65	GLU	C-N-CA	5.67	130.22	122.84
1	H	42	VAL	O-C-N	-5.67	117.87	122.97
1	H	91	CYS	CA-C-O	5.67	127.18	120.66
1	B	87	LEU	CB-CG-CD2	-5.67	93.70	110.70
1	E	27	ILE	N-CA-C	5.67	116.03	107.75
1	K	61	PHE	CA-C-O	-5.67	114.70	120.71
1	B	68	MET	CB-CA-C	-5.67	99.28	110.27
2	I	170	GLN	CB-CG-CD	-5.67	102.97	112.60
2	I	158	LYS	N-CA-CB	5.66	118.22	110.01
1	K	11	ARG	O-C-N	5.66	127.92	122.03
3	T	229	PRO	CA-C-N	-5.66	112.93	120.63
3	T	229	PRO	C-N-CA	-5.66	112.93	120.63
2	I	138	TRP	N-CA-C	5.66	122.85	110.80
2	C	44	LEU	O-C-N	5.65	128.11	122.12
1	E	153	MET	CB-CA-C	5.65	119.72	109.37
2	F	95	LYS	O-C-N	-5.65	116.62	123.29
2	C	45	LEU	N-CA-C	-5.65	105.21	111.71
2	C	150	GLU	CG-CD-OE1	-5.65	105.41	118.40
1	H	104	GLN	N-CA-C	5.64	115.56	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	275	PRO	O-C-N	-5.64	115.02	122.64
3	T	288	LYS	CB-CG-CD	5.64	124.28	111.30
1	B	91	CYS	CA-CB-SG	-5.64	101.42	114.40
2	C	138	TRP	CA-C-N	5.64	133.01	122.74
2	C	138	TRP	C-N-CA	5.64	133.01	122.74
3	S	267	HIS	N-CA-C	5.64	122.82	110.80
3	U	284	ASN	N-CA-C	-5.64	96.99	107.71
1	B	13	ILE	N-CA-CB	5.64	117.15	110.55
2	C	134	VAL	CA-CB-CG1	5.64	119.99	110.40
3	S	264	ARG	CB-CA-C	-5.64	100.02	109.27
1	B	52	GLU	CB-CA-C	-5.64	99.20	110.42
1	H	58	LEU	N-CA-C	5.63	118.25	109.52
1	H	91	CYS	N-CA-C	5.63	118.65	109.24
2	I	46	GLU	N-CA-CB	5.63	120.01	110.49
1	B	73	VAL	CA-CB-CG2	-5.63	100.83	110.40
3	T	230	ASP	CA-CB-CG	-5.63	106.97	112.60
3	T	245	CYS	CA-CB-SG	-5.63	101.45	114.40
2	L	153	ARG	NH1-CZ-NH2	5.63	126.62	119.30
2	L	41	ASN	CA-C-N	5.62	129.26	120.82
2	L	41	ASN	C-N-CA	5.62	129.26	120.82
3	V	231	TYR	N-CA-C	-5.62	105.52	112.38
1	B	155	ASN	CA-C-N	5.62	131.82	121.70
1	B	155	ASN	C-N-CA	5.62	131.82	121.70
2	C	102	TYR	CA-C-O	-5.62	114.58	120.70
2	C	135	LEU	CA-C-O	5.62	125.59	119.24
1	E	69	ALA	CA-C-O	-5.62	114.97	121.15
2	F	54	GLY	CA-C-O	-5.62	110.80	120.57
2	F	52	GLN	CA-CB-CG	-5.62	102.87	114.10
2	F	117	MET	CB-CG-SD	-5.62	95.86	112.70
1	K	72	LYS	CB-CA-C	5.62	119.50	110.29
2	C	141	SER	CA-C-O	5.61	126.29	119.11
2	C	133	SER	CA-CB-OG	-5.60	99.89	111.10
1	E	130	ALA	CA-C-N	-5.58	113.28	120.65
1	E	130	ALA	C-N-CA	-5.58	113.28	120.65
1	K	61	PHE	CB-CA-C	-5.58	99.34	109.38
3	T	303	ASP	CA-C-N	5.58	131.74	121.70
3	T	303	ASP	C-N-CA	5.58	131.74	121.70
1	E	98	LYS	N-CA-C	5.58	118.87	112.57
2	F	146	VAL	CA-C-N	-5.58	112.50	120.42
2	F	146	VAL	C-N-CA	-5.58	112.50	120.42
2	I	172	TYR	N-CA-C	5.58	122.68	110.80
1	H	58	LEU	CA-C-N	-5.57	114.58	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	58	LEU	C-N-CA	-5.57	114.58	122.94
2	I	166	PRO	CA-CB-CG	-5.57	93.91	104.50
3	S	233	CYS	CA-CB-SG	-5.57	101.58	114.40
2	C	91	ILE	CA-C-O	-5.57	114.54	120.39
1	E	12	ILE	CB-CG1-CD1	5.57	125.50	113.80
3	S	273	ARG	CA-C-N	-5.57	112.44	120.51
3	S	273	ARG	C-N-CA	-5.57	112.44	120.51
2	C	89	ASN	CA-C-O	-5.57	113.42	120.55
1	H	59	GLU	N-CA-C	5.57	118.47	109.40
2	F	43	ARG	CB-CG-CD	5.56	124.10	111.30
3	S	280	GLN	N-CA-C	-5.56	105.81	112.59
3	U	239	GLU	CA-C-N	5.56	128.65	120.82
3	U	239	GLU	C-N-CA	5.56	128.65	120.82
2	I	156	MET	N-CA-C	-5.55	104.87	111.03
1	B	19	LEU	CD1-CG-CD2	5.55	123.00	110.80
1	K	136	ASN	N-CA-C	5.55	117.75	107.60
1	E	53	GLY	CA-C-N	-5.54	110.55	121.41
1	E	53	GLY	C-N-CA	-5.54	110.55	121.41
2	C	80	LEU	N-CA-C	5.54	118.85	109.76
1	K	138	ALA	N-CA-C	5.54	117.76	111.11
3	U	265	VAL	N-CA-CB	-5.54	107.10	111.64
3	U	240	LEU	N-CA-CB	-5.54	101.22	109.69
1	K	156	ILE	CA-CB-CG1	5.54	119.81	110.40
3	U	267	HIS	N-CA-CB	5.54	118.55	110.25
1	B	57	LYS	CG-CD-CE	-5.53	98.58	111.30
1	B	64	GLU	CB-CG-CD	-5.53	103.20	112.60
1	E	21	ALA	N-CA-C	-5.53	105.25	111.28
1	K	8	LEU	N-CA-CB	5.53	120.21	110.37
1	K	82	PRO	CA-C-N	5.53	131.82	122.65
1	K	82	PRO	C-N-CA	5.53	131.82	122.65
1	E	134	LYS	CA-C-N	-5.52	113.48	122.26
1	E	134	LYS	C-N-CA	-5.52	113.48	122.26
1	E	39	PHE	CA-C-O	-5.52	114.36	120.38
3	S	243	GLU	N-CA-C	-5.52	99.37	108.75
1	B	19	LEU	CB-CG-CD2	-5.52	94.14	110.70
3	V	272	THR	CA-C-O	5.51	124.97	118.90
1	B	34	SER	CA-C-O	-5.51	112.63	120.51
2	F	158	LYS	N-CA-CB	5.51	119.04	110.44
2	F	153	ARG	N-CA-CB	5.51	118.22	110.12
1	H	84	VAL	CA-C-O	-5.51	114.44	120.72
2	C	82	PRO	CA-C-N	5.50	125.51	119.90
2	C	82	PRO	C-N-CA	5.50	125.51	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	163	LEU	CB-CG-CD1	-5.50	94.19	110.70
1	B	139	GLN	N-CA-C	-5.50	105.28	111.28
1	H	11	ARG	CB-CA-C	-5.50	100.45	110.63
2	I	78	MET	CB-CG-SD	-5.50	96.20	112.70
1	H	43	ILE	CA-C-N	-5.50	113.07	120.82
1	H	43	ILE	C-N-CA	-5.50	113.07	120.82
3	S	242	ARG	N-CA-C	5.50	119.71	112.89
2	F	93	SER	N-CA-C	5.49	118.51	109.72
2	F	173	SER	CA-CB-OG	-5.49	100.12	111.10
2	L	147	VAL	CA-C-N	-5.49	112.86	120.38
2	L	147	VAL	C-N-CA	-5.49	112.86	120.38
3	S	270	PRO	CB-CA-C	-5.49	102.50	111.56
3	U	239	GLU	N-CA-C	-5.49	101.41	109.81
2	C	152	ARG	NE-CZ-NH1	-5.49	116.01	121.50
3	S	236	ILE	N-CA-CB	-5.49	102.18	111.23
3	V	260	GLU	CB-CA-C	-5.49	102.03	110.81
1	B	84	VAL	CB-CA-C	-5.48	102.66	110.83
2	C	146	VAL	CA-C-N	-5.48	112.64	120.42
2	C	146	VAL	C-N-CA	-5.48	112.64	120.42
3	U	233	CYS	CA-CB-SG	-5.48	101.79	114.40
1	E	42	VAL	CA-C-N	-5.48	114.47	122.68
1	E	42	VAL	C-N-CA	-5.48	114.47	122.68
2	L	58	GLY	O-C-N	-5.48	115.58	122.70
1	B	92	LEU	CA-C-N	5.47	127.56	120.44
1	B	92	LEU	C-N-CA	5.47	127.56	120.44
1	E	75	PHE	CB-CA-C	-5.47	99.47	109.54
3	S	239	GLU	N-CA-CB	-5.47	99.39	109.18
3	S	276	LEU	CA-C-N	-5.47	113.72	122.53
3	S	276	LEU	C-N-CA	-5.47	113.72	122.53
3	V	256	LYS	N-CA-C	-5.47	104.55	111.11
1	K	106	ARG	NH1-CZ-NH2	5.47	126.41	119.30
2	L	65	GLU	CA-CB-CG	-5.46	103.17	114.10
2	F	74	ARG	CA-CB-CG	-5.46	103.18	114.10
1	B	74	ARG	CB-CG-CD	-5.46	98.75	111.30
2	C	75	TRP	N-CA-C	5.46	117.81	109.95
1	B	74	ARG	CB-CA-C	-5.45	100.49	111.17
2	C	116	ASN	CA-C-O	5.45	126.73	120.84
3	V	256	LYS	O-C-N	5.45	127.75	122.09
3	S	274	SER	N-CA-CB	-5.44	101.75	109.75
1	B	94	ILE	N-CA-CB	5.44	119.95	110.65
1	K	149	ARG	NE-CZ-NH2	-5.44	114.31	119.20
1	B	70	ALA	O-C-N	-5.44	115.44	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	LYS	CD-CE-NZ	-5.43	94.51	111.90
3	V	294	PHE	N-CA-C	-5.43	106.78	113.41
2	C	98	CYS	CB-CA-C	-5.43	101.28	110.19
3	U	237	SER	CB-CA-C	5.43	117.82	109.03
3	U	246	ILE	CG1-CB-CG2	-5.43	94.42	110.70
3	V	251	ILE	N-CA-C	5.43	115.67	107.75
2	C	112	VAL	CA-CB-CG2	-5.42	101.18	110.40
2	C	142	TYR	CA-C-O	-5.42	115.81	121.99
1	H	46	PRO	CA-C-N	-5.42	113.25	120.90
1	H	46	PRO	C-N-CA	-5.42	113.25	120.90
1	K	110	LEU	CA-C-N	-5.42	112.07	120.31
1	K	110	LEU	C-N-CA	-5.42	112.07	120.31
3	S	272	THR	CA-C-O	5.42	124.86	118.90
2	C	60	VAL	CB-CA-C	-5.42	102.01	110.52
2	C	84	ARG	CA-CB-CG	5.42	124.93	114.10
2	F	168	GLU	CB-CA-C	-5.41	99.19	110.40
1	B	131	GLU	N-CA-C	-5.41	102.50	111.37
2	C	110	ARG	N-CA-C	5.41	118.37	109.72
2	F	101	LYS	N-CA-C	5.40	122.31	110.80
1	H	80	TYR	CA-C-O	-5.40	115.67	121.56
3	S	239	GLU	CG-CD-OE1	5.40	130.83	118.40
3	T	296	SER	CA-CB-OG	-5.40	100.30	111.10
1	B	148	THR	CA-C-O	-5.39	115.34	120.90
1	B	150	LEU	CA-C-O	-5.39	115.14	120.80
1	H	95	LEU	O-C-N	5.39	128.61	122.25
2	F	78	MET	CG-SD-CE	5.39	112.76	100.90
2	L	130	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	K	19	LEU	CA-CB-CG	-5.39	97.43	116.30
2	C	142	TYR	N-CA-CB	-5.39	103.00	110.38
1	H	136	ASN	CA-C-N	5.39	131.83	121.54
1	H	136	ASN	C-N-CA	5.39	131.83	121.54
3	S	233	CYS	N-CA-C	5.38	118.26	109.59
2	L	54	GLY	N-CA-C	-5.38	100.43	113.18
2	C	137	LYS	CA-CB-CG	-5.38	103.34	114.10
2	C	158	LYS	O-C-N	-5.38	116.07	122.20
2	I	152	ARG	NE-CZ-NH2	5.37	124.04	119.20
2	L	106	PRO	N-CA-C	5.37	117.25	110.70
2	C	158	LYS	CD-CE-NZ	-5.37	94.72	111.90
2	F	102	TYR	CA-CB-CG	5.37	123.56	113.90
2	I	159	GLU	N-CA-C	5.37	122.23	110.80
1	E	135	THR	CA-C-O	5.37	124.95	119.05
1	E	106	ARG	NH1-CZ-NH2	5.36	126.27	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	112	ILE	CA-C-N	-5.36	112.68	120.29
1	H	112	ILE	C-N-CA	-5.36	112.68	120.29
1	B	77	THR	CB-CA-C	-5.36	98.55	109.65
1	E	41	VAL	CA-C-O	-5.36	115.93	121.93
2	I	133	SER	CA-CB-OG	-5.36	100.38	111.10
1	H	29	ALA	N-CA-C	5.36	118.13	109.40
3	S	240	LEU	N-CA-C	-5.36	100.96	109.96
1	K	58	LEU	N-CA-C	5.36	118.01	109.81
2	L	48	LEU	CB-CA-C	-5.36	99.76	110.42
3	T	247	THR	CA-CB-OG1	5.36	117.64	109.60
2	C	45	LEU	CA-CB-CG	-5.35	97.56	116.30
1	H	99	TRP	CB-CA-C	-5.35	100.48	109.53
2	I	104	GLU	N-CA-C	5.35	116.80	111.07
3	U	242	ARG	CA-C-O	-5.35	112.86	120.51
3	U	243	GLU	CA-C-N	-5.35	114.08	120.13
3	U	243	GLU	C-N-CA	-5.35	114.08	120.13
2	C	153	ARG	NE-CZ-NH1	5.35	126.85	121.50
2	L	101	LYS	CD-CE-NZ	-5.35	94.79	111.90
1	B	46	PRO	CB-CA-C	-5.35	104.85	111.64
1	H	129	VAL	N-CA-C	-5.35	103.79	111.17
2	F	173	SER	N-CA-C	5.34	116.84	109.15
3	T	246	ILE	CA-C-N	-5.34	112.98	123.56
3	T	246	ILE	C-N-CA	-5.34	112.98	123.56
2	F	130	ARG	CA-C-N	-5.34	114.21	122.49
2	F	130	ARG	C-N-CA	-5.34	114.21	122.49
3	T	264	ARG	CA-C-N	-5.34	114.05	121.53
3	T	264	ARG	C-N-CA	-5.34	114.05	121.53
2	L	165	GLN	N-CA-C	5.34	118.27	110.10
1	H	82	PRO	CB-CG-CD	-5.33	89.03	106.10
2	I	125	GLY	N-CA-C	5.33	125.82	113.18
2	I	171	CYS	N-CA-C	5.33	122.16	110.80
1	H	98	LYS	CD-CE-NZ	5.33	128.95	111.90
2	L	160	ASN	CA-CB-CG	-5.33	107.27	112.60
1	B	62	LEU	N-CA-C	5.32	121.57	109.81
2	F	131	ALA	CA-C-N	-5.32	116.36	123.17
2	F	131	ALA	C-N-CA	-5.32	116.36	123.17
1	B	135	THR	N-CA-CB	-5.32	102.27	110.20
2	F	89	ASN	CA-C-N	-5.32	113.39	122.33
2	F	89	ASN	C-N-CA	-5.32	113.39	122.33
3	S	248	PRO	CA-C-N	-5.32	109.07	121.52
3	S	248	PRO	C-N-CA	-5.32	109.07	121.52
1	K	13	ILE	N-CA-C	-5.32	105.20	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	65	GLU	CB-CA-C	-5.31	102.54	110.88
3	V	289	GLU	N-CA-CB	5.31	118.12	110.20
1	B	38	TYR	N-CA-CB	-5.31	102.24	110.57
1	E	22	GLU	CA-CB-CG	-5.31	103.49	114.10
2	F	156	MET	N-CA-C	5.30	119.50	113.19
1	B	9	PRO	CB-CG-CD	-5.30	89.14	106.10
2	C	75	TRP	CB-CA-C	-5.30	101.35	111.48
1	E	149	ARG	CA-CB-CG	5.30	124.70	114.10
1	K	31	PRO	N-CA-C	-5.30	103.46	111.41
2	C	151	LEU	CD1-CG-CD2	-5.29	99.15	110.80
2	L	87	TYR	CA-C-N	-5.29	113.36	120.87
2	L	87	TYR	C-N-CA	-5.29	113.36	120.87
1	B	98	LYS	N-CA-C	-5.29	106.01	113.20
2	C	48	LEU	CB-CA-C	5.29	119.27	110.81
3	S	287	MET	CG-SD-CE	-5.29	89.27	100.90
3	V	243	GLU	N-CA-CB	-5.29	102.64	110.99
1	B	86	LYS	N-CA-C	-5.28	105.98	112.90
2	I	70	MET	CG-SD-CE	5.28	112.52	100.90
2	F	93	SER	CA-CB-OG	-5.28	100.54	111.10
3	T	281	LEU	CA-C-O	-5.28	115.25	121.16
3	S	268	PHE	CA-C-O	5.28	126.88	121.23
1	H	141	ILE	N-CA-CB	5.28	118.50	110.58
1	H	115	LEU	CA-C-O	-5.27	115.28	120.82
2	I	123	SER	N-CA-C	-5.27	104.97	111.40
1	B	106	ARG	CG-CD-NE	-5.27	100.40	112.00
2	C	114	LYS	CA-C-O	-5.27	115.68	120.95
1	E	69	ALA	N-CA-CB	-5.27	101.31	109.69
2	F	101	LYS	CA-CB-CG	-5.27	103.56	114.10
3	T	258	ILE	CG1-CB-CG2	5.27	126.50	110.70
3	U	263	GLN	CB-CG-CD	-5.26	103.65	112.60
3	V	247	THR	N-CA-CB	-5.26	100.97	110.39
2	C	44	LEU	CA-C-O	-5.26	114.97	120.55
2	L	50	GLU	CA-CB-CG	-5.26	103.58	114.10
2	C	165	GLN	CA-CB-CG	-5.26	103.59	114.10
2	F	55	VAL	CB-CA-C	5.26	118.53	111.28
3	T	234	GLY	CA-C-N	-5.26	111.80	122.31
3	T	234	GLY	C-N-CA	-5.26	111.80	122.31
1	B	71	PRO	N-CA-C	5.25	118.57	111.22
2	I	128	ASP	CA-C-N	-5.25	113.13	118.85
2	I	128	ASP	C-N-CA	-5.25	113.13	118.85
1	H	30	GLU	CA-C-N	-5.25	113.28	119.84
1	H	30	GLU	C-N-CA	-5.25	113.28	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	91	ILE	N-CA-CB	5.24	116.98	111.00
1	E	76	MET	CB-CG-SD	-5.24	96.97	112.70
1	H	29	ALA	CA-C-N	-5.24	112.49	122.08
1	H	29	ALA	C-N-CA	-5.24	112.49	122.08
1	E	98	LYS	CD-CE-NZ	-5.24	95.13	111.90
2	I	127	VAL	N-CA-C	5.24	116.13	108.58
3	V	285	LEU	CA-C-O	-5.24	115.00	120.55
2	C	81	GLY	O-C-N	-5.24	116.53	121.77
2	I	111	PHE	N-CA-C	5.24	117.93	107.62
1	H	74	ARG	NH1-CZ-NH2	5.23	126.10	119.30
3	U	256	LYS	N-CA-C	-5.23	105.75	111.82
1	B	14	LYS	CG-CD-CE	-5.23	99.27	111.30
1	H	31	PRO	CB-CA-C	-5.23	102.93	111.56
1	E	66	TYR	O-C-N	5.23	126.69	121.30
1	B	44	ALA	CA-C-N	-5.23	113.66	121.87
1	B	44	ALA	C-N-CA	-5.23	113.66	121.87
2	L	76	THR	N-CA-C	5.23	116.93	108.41
1	B	121	PRO	CA-C-N	-5.22	114.80	123.37
1	B	121	PRO	C-N-CA	-5.22	114.80	123.37
2	I	139	GLN	N-CA-C	5.22	117.91	109.40
3	U	272	THR	CA-C-N	-5.22	111.57	121.54
3	U	272	THR	C-N-CA	-5.22	111.57	121.54
3	T	257	ASP	CB-CG-OD2	-5.22	106.40	118.40
3	V	262	LEU	CB-CG-CD1	-5.22	95.04	110.70
2	F	63	GLY	CA-C-O	5.22	126.83	121.35
3	V	261	HIS	N-CA-CB	5.22	117.53	109.91
1	E	113	GLN	N-CA-CB	-5.21	101.74	110.39
1	B	154	ASN	CA-C-N	5.21	131.49	121.54
1	B	154	ASN	C-N-CA	5.21	131.49	121.54
3	V	269	ASN	CA-C-N	5.21	126.35	119.84
3	V	269	ASN	C-N-CA	5.21	126.35	119.84
2	C	95	LYS	CA-C-N	-5.21	116.73	123.19
2	C	95	LYS	C-N-CA	-5.21	116.73	123.19
3	V	235	LYS	O-C-N	-5.20	115.67	122.59
1	B	145	ARG	CA-CB-CG	-5.20	103.70	114.10
1	B	122	ASP	CA-C-N	5.20	125.60	119.83
1	B	122	ASP	C-N-CA	5.20	125.60	119.83
2	F	161	MET	CA-C-N	-5.20	114.36	122.37
2	F	161	MET	C-N-CA	-5.20	114.36	122.37
1	K	80	TYR	CA-C-O	-5.20	115.51	120.92
3	U	294	PHE	CA-C-O	-5.20	115.35	121.07
1	E	132	GLN	CA-C-O	5.20	125.93	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	239	GLU	N-CA-C	5.19	118.26	108.65
3	T	244	PRO	O-C-N	-5.19	116.30	122.89
2	F	108	PHE	N-CA-C	-5.19	100.85	109.46
3	V	269	ASN	CA-C-O	5.19	124.27	119.24
1	B	10	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	E	93	ASP	CA-C-O	5.19	127.93	120.51
2	L	173	SER	N-CA-C	5.18	117.69	109.24
3	V	244	PRO	CB-CA-C	-5.18	105.11	111.64
1	H	110	LEU	CB-CG-CD1	-5.18	95.16	110.70
2	C	171	CYS	CA-CB-SG	-5.18	102.49	114.40
2	F	43	ARG	CG-CD-NE	-5.18	100.61	112.00
1	H	43	ILE	N-CA-CB	5.17	117.70	110.56
1	K	94	ILE	N-CA-C	5.17	120.10	109.34
1	B	47	GLN	O-C-N	5.17	128.96	122.86
1	B	116	LEU	CA-C-N	-5.17	112.57	121.66
1	B	116	LEU	C-N-CA	-5.17	112.57	121.66
1	H	10	ARG	CA-C-N	-5.17	112.84	120.28
1	H	10	ARG	C-N-CA	-5.17	112.84	120.28
2	C	153	ARG	NH1-CZ-NH2	-5.16	112.59	119.30
3	U	278	GLN	N-CA-C	5.16	121.80	110.80
2	F	50	GLU	N-CA-C	-5.16	105.73	111.36
3	U	255	ARG	CB-CG-CD	5.16	123.17	111.30
1	H	150	LEU	CA-C-O	-5.16	115.40	121.07
3	U	257	ASP	CA-CB-CG	-5.16	107.44	112.60
2	F	60	VAL	N-CA-C	-5.16	101.27	108.80
1	H	100	SER	N-CA-CB	-5.16	100.41	110.10
1	B	6	ALA	O-C-N	-5.15	115.23	121.83
3	S	275	PRO	CA-C-N	-5.15	111.70	121.54
3	S	275	PRO	C-N-CA	-5.15	111.70	121.54
2	L	157	SER	CA-CB-OG	-5.15	100.80	111.10
2	L	169	GLY	N-CA-C	-5.15	100.97	113.18
3	V	285	LEU	N-CA-CB	5.15	117.69	110.12
3	U	280	GLN	O-C-N	5.15	128.78	122.34
2	L	74	ARG	N-CA-C	5.14	117.98	109.85
3	V	246	ILE	CB-CA-C	-5.14	102.86	111.29
3	T	265	VAL	CA-C-N	-5.14	112.89	122.56
3	T	265	VAL	C-N-CA	-5.14	112.89	122.56
1	E	155	ASN	CA-C-N	5.14	130.95	121.70
1	E	155	ASN	C-N-CA	5.14	130.95	121.70
3	S	232	LEU	CD1-CG-CD2	-5.14	99.50	110.80
1	E	68	MET	N-CA-CB	-5.13	102.53	110.13
2	F	127	VAL	CA-C-N	-5.13	114.01	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	127	VAL	C-N-CA	-5.13	114.01	121.20
3	V	291	ILE	CB-CA-C	-5.13	102.87	111.29
1	B	5	SER	N-CA-C	5.13	121.73	110.80
2	L	160	ASN	CA-C-N	5.13	131.34	121.54
2	L	160	ASN	C-N-CA	5.13	131.34	121.54
2	F	37	LYS	CA-C-O	-5.12	113.18	120.51
1	B	91	CYS	N-CA-C	5.12	117.00	107.99
2	C	116	ASN	CA-C-N	-5.12	112.94	121.64
2	C	116	ASN	C-N-CA	-5.12	112.94	121.64
1	E	78	LYS	N-CA-CB	5.12	117.88	109.95
1	H	102	ALA	N-CA-C	-5.12	107.17	113.41
3	V	274	SER	N-CA-CB	5.12	117.58	110.11
1	H	76	MET	CG-SD-CE	-5.11	89.65	100.90
1	H	62	LEU	N-CA-C	5.11	119.87	109.60
1	K	68	MET	CG-SD-CE	-5.11	89.66	100.90
3	U	255	ARG	CA-CB-CG	-5.11	103.89	114.10
3	U	264	ARG	CA-C-N	-5.11	117.75	123.16
3	U	264	ARG	C-N-CA	-5.11	117.75	123.16
3	S	260	GLU	CB-CA-C	-5.10	102.80	110.92
3	V	280	GLN	N-CA-CB	5.10	117.87	110.47
1	B	19	LEU	N-CA-C	5.10	116.84	111.28
2	F	109	VAL	CB-CA-C	-5.10	103.54	110.42
2	I	84	ARG	N-CA-C	-5.10	99.94	110.80
2	L	146	VAL	N-CA-C	-5.10	105.87	110.82
3	S	287	MET	N-CA-C	-5.10	105.81	112.23
2	C	91	ILE	N-CA-C	-5.10	100.98	108.11
2	C	60	VAL	CA-C-O	-5.09	116.65	121.64
2	F	89	ASN	O-C-N	-5.09	117.12	123.33
2	F	140	ASN	CB-CA-C	5.09	120.55	110.42
3	U	275	PRO	CA-C-N	-5.09	113.83	121.86
3	U	275	PRO	C-N-CA	-5.09	113.83	121.86
1	B	27	ILE	CB-CA-C	-5.08	103.04	110.62
3	V	257	ASP	CA-C-N	-5.08	113.11	121.19
3	V	257	ASP	C-N-CA	-5.08	113.11	121.19
1	E	78	LYS	CA-CB-CG	5.08	124.26	114.10
2	F	78	MET	CA-C-O	-5.08	115.17	121.06
3	S	258	ILE	CA-CB-CG1	-5.08	101.77	110.40
3	V	247	THR	CA-C-O	-5.08	115.43	120.66
1	B	66	TYR	CA-C-O	-5.07	115.45	119.71
1	H	23	PRO	CA-C-N	-5.07	112.74	122.13
1	H	23	PRO	C-N-CA	-5.07	112.74	122.13
2	L	93	SER	CA-CB-OG	-5.07	100.95	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	GLY	N-CA-C	-5.07	101.99	112.34
1	B	153	MET	CB-CG-SD	-5.07	97.49	112.70
1	K	133	TRP	CA-CB-CG	-5.07	103.97	113.60
2	F	44	LEU	N-CA-C	-5.07	105.45	111.69
2	C	110	ARG	NH1-CZ-NH2	-5.07	112.71	119.30
1	K	74	ARG	O-C-N	5.07	129.15	123.27
3	U	290	VAL	CA-C-O	5.07	127.11	120.78
2	C	126	VAL	CA-C-O	-5.07	115.15	120.57
3	U	228	ILE	N-CA-CB	-5.06	104.12	111.21
2	F	56	GLY	N-CA-C	5.06	125.17	113.18
1	E	145	ARG	CB-CG-CD	-5.06	99.66	111.30
2	I	64	LEU	N-CA-CB	5.06	117.41	109.97
1	B	145	ARG	N-CA-C	-5.06	105.89	111.71
1	B	108	VAL	CA-C-N	-5.06	113.00	120.28
1	B	108	VAL	C-N-CA	-5.06	113.00	120.28
2	F	59	THR	CA-C-N	-5.05	115.64	122.92
2	F	59	THR	C-N-CA	-5.05	115.64	122.92
2	C	50	GLU	CA-C-N	-5.05	114.44	120.00
2	C	50	GLU	C-N-CA	-5.05	114.44	120.00
2	F	110	ARG	N-CA-C	5.05	117.48	109.50
2	C	124	ASN	CB-CG-ND2	-5.05	108.82	116.40
1	K	93	ASP	CA-C-N	-5.05	112.88	121.97
1	K	93	ASP	C-N-CA	-5.05	112.88	121.97
2	F	45	LEU	CA-C-N	-5.05	111.95	120.58
2	F	45	LEU	C-N-CA	-5.05	111.95	120.58
1	E	18	ARG	NE-CZ-NH1	-5.04	116.45	121.50
2	C	132	ILE	N-CA-C	5.04	119.83	109.34
1	H	14	LYS	N-CA-C	5.04	116.78	111.28
2	L	170	GLN	CA-C-N	5.04	131.17	121.54
2	L	170	GLN	C-N-CA	5.04	131.17	121.54
1	H	47	GLN	CB-CA-C	5.04	117.81	109.70
3	S	268	PHE	N-CA-C	5.04	116.50	108.79
3	S	233	CYS	O-C-N	-5.04	116.81	123.21
2	F	74	ARG	CA-C-N	-5.04	114.76	122.62
2	F	74	ARG	C-N-CA	-5.04	114.76	122.62
1	H	142	GLU	CB-CA-C	5.04	120.44	110.42
2	I	98	CYS	CB-CA-C	-5.03	100.59	109.70
3	S	255	ARG	NE-CZ-NH2	5.03	123.73	119.20
2	F	108	PHE	CD1-CE1-CZ	-5.03	110.94	120.00
3	S	282	ILE	O-C-N	5.03	126.19	121.11
1	H	73	VAL	N-CA-C	5.03	115.95	108.46
2	I	75	TRP	CB-CA-C	-5.03	99.40	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	228	ILE	CG1-CB-CG2	-5.02	95.63	110.70
1	B	7	GLY	CA-C-O	5.02	124.10	119.83
2	C	72	LEU	CD1-CG-CD2	-5.02	99.75	110.80
2	L	43	ARG	N-CA-CB	-5.02	102.73	110.01
3	V	253	TYR	N-CA-C	5.02	121.49	110.80
2	C	38	VAL	CB-CA-C	5.02	120.49	111.36
1	B	112	ILE	CA-C-N	-5.01	111.25	121.18
1	B	112	ILE	C-N-CA	-5.01	111.25	121.18
3	V	259	GLU	O-C-N	5.01	128.24	122.17
1	E	97	ASP	O-C-N	-5.01	115.93	122.59
1	E	132	GLN	CB-CG-CD	-5.01	104.08	112.60
2	L	40	ARG	NH1-CZ-NH2	5.01	125.81	119.30
1	B	93	ASP	N-CA-CB	-5.01	102.75	110.01
1	H	100	SER	O-C-N	-5.01	116.69	121.20
1	E	148	THR	N-CA-CB	5.00	117.43	109.82
3	U	237	SER	N-CA-C	-5.00	107.72	113.88
2	F	93	SER	CB-CA-C	-5.00	99.47	109.33
1	H	96	LYS	N-CA-C	5.00	120.27	110.56
3	U	290	VAL	CA-CB-CG2	5.00	118.91	110.40
2	F	93	SER	CA-C-N	-5.00	114.82	122.62
2	F	93	SER	C-N-CA	-5.00	114.82	122.62

There are no chirality outliers.

All (73) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	117	SER	Peptide
1	B	154	ASN	Peptide
1	B	29	ALA	Peptide
1	B	5	SER	Peptide
1	B	6	ALA	Peptide
1	B	76	MET	Peptide
1	B	97	ASP	Peptide
2	C	102	TYR	Mainchain
2	C	131	ALA	Peptide
2	C	173	SER	Peptide
2	C	33	THR	Peptide
2	C	56	GLY	Peptide
2	C	75	TRP	Mainchain
1	E	128	ASP	Peptide
1	E	154	ASN	Peptide
1	E	155	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	E	63	PRO	Peptide
1	E	64	GLU	Peptide
1	E	69	ALA	Peptide
2	F	141	SER	Peptide
2	F	47	GLU	Mainchain
2	F	56	GLY	Peptide
2	F	58	GLY	Peptide
1	H	123	ASP	Peptide
1	H	34	SER	Peptide
1	H	44	ALA	Peptide
1	H	7	GLY	Peptide
1	H	80	TYR	Peptide
1	H	88	GLY	Peptide
1	H	91	CYS	Peptide
2	I	102	TYR	Peptide
2	I	132	ILE	Peptide
2	I	151	LEU	Peptide
2	I	54	GLY	Peptide
2	I	55	VAL	Peptide
2	I	56	GLY	Peptide
2	I	58	GLY	Peptide
2	I	62	TRP	Peptide
2	I	67	ASP	Peptide
2	I	77	GLY	Peptide
2	I	81	GLY	Peptide
2	I	87	TYR	Peptide
2	I	88	GLU	Peptide
1	K	102	ALA	Peptide
1	K	131	GLU	Peptide
1	K	133	TRP	Peptide
1	K	147	TRP	Peptide
1	K	150	LEU	Peptide
1	K	153	MET	Peptide
1	K	154	ASN	Peptide
1	K	23	PRO	Peptide
1	K	4	GLY	Peptide
1	K	52	GLU	Peptide
1	K	57	LYS	Peptide
1	K	63	PRO	Peptide
1	K	68	MET	Peptide
1	K	7	GLY	Peptide
1	K	76	MET	Peptide

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Mol	Chain	Res	Type	Group
1	K	85	ASP	Peptide
1	K	97	ASP	Peptide
2	L	169	GLY	Peptide
2	L	170	GLN	Peptide
2	L	39	PRO	Peptide
3	S	228	ILE	Mainchain
3	S	235	LYS	Peptide
3	S	291	ILE	Peptide
3	S	298	ASN	Peptide
3	T	249	SER	Peptide
3	U	227	ASP	Peptide
3	U	228	ILE	Peptide
3	U	250	GLY	Peptide
3	V	229	PRO	Peptide
3	V	245	CYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1202	0	1209	147	1
1	E	1187	0	1196	153	1
1	H	1187	0	1196	195	1
1	K	1202	0	1209	221	1
2	C	1123	0	1121	133	1
2	F	1109	0	1114	143	0
2	I	1109	0	1114	159	0
2	L	1109	0	1114	132	1
3	S	598	0	584	91	0
3	T	634	0	612	92	0
3	U	577	0	569	142	0
3	V	564	0	557	116	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	E	3	0	0	0	0
4	F	7	0	0	1	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1	0	0	0	0
4	S	6	0	0	0	0
4	T	2	0	0	1	0
4	U	1	0	0	0	0
4	V	3	0	0	1	0
All	All	11636	0	11595	1649	3

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 71.

All (1649) 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:E:96:LYS:CD	1:E:96:LYS:CE	1.74	1.65
3:U:228:ILE:CG2	3:U:228:ILE:CB	1.74	1.64
3:V:288:LYS:CD	3:V:288:LYS:CG	1.74	1.63
1:E:8:LEU:CD1	1:E:8:LEU:CG	1.75	1.63
1:H:110:LEU:CD2	1:H:110:LEU:CG	1.77	1.62
1:K:78:LYS:CE	1:K:78:LYS:CD	1.75	1.62
3:T:242:ARG:CD	3:T:242:ARG:CG	1.74	1.62
2:L:145:LYS:CE	2:L:145:LYS:CD	1.77	1.61
2:C:84:ARG:CG	2:C:84:ARG:CB	1.75	1.61
1:K:156:ILE:CB	1:K:156:ILE:CA	1.78	1.60
1:E:94:ILE:CB	1:E:94:ILE:CG2	1.75	1.60
1:E:96:LYS:CD	1:E:96:LYS:CG	1.77	1.60
3:S:256:LYS:CD	3:S:256:LYS:CG	1.74	1.60
1:E:6:ALA:CB	1:E:6:ALA:CA	1.75	1.60
2:I:37:LYS:CE	2:I:37:LYS:CD	1.79	1.60
1:K:142:GLU:CG	1:K:142:GLU:CB	1.75	1.59
1:E:149:ARG:CG	1:E:149:ARG:CD	1.76	1.59
2:F:53:LYS:CD	2:F:53:LYS:CE	1.75	1.59
2:F:144:ILE:CD1	2:F:144:ILE:CG1	1.77	1.59
1:H:96:LYS:CE	1:H:96:LYS:CD	1.75	1.59
1:K:150:LEU:CG	1:K:150:LEU:CD2	1.79	1.58
2:C:159:GLU:CB	2:C:159:GLU:CG	1.80	1.58
2:C:159:GLU:CG	2:C:159:GLU:CD	1.74	1.58
1:E:78:LYS:CG	1:E:78:LYS:CB	1.78	1.58
2:I:37:LYS:CD	2:I:37:LYS:CG	1.74	1.58
3:S:242:ARG:CD	3:S:242:ARG:CG	1.82	1.58
3:U:252:THR:CB	3:U:252:THR:CA	1.74	1.58
3:U:295:ILE:CG1	3:U:295:ILE:CD1	1.77	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:270:PRO:CB	3:V:270:PRO:CG	1.80	1.58
1:B:124:PRO:CB	1:B:124:PRO:CG	1.76	1.57
3:T:301:VAL:CB	3:T:301:VAL:CA	1.76	1.57
3:T:228:ILE:CD1	3:T:228:ILE:CG1	1.76	1.57
1:K:106:ARG:CG	1:K:106:ARG:CD	1.78	1.56
3:U:295:ILE:CA	3:U:295:ILE:CB	1.75	1.56
3:V:248:PRO:CG	3:V:248:PRO:CD	1.79	1.56
2:F:153:ARG:CD	2:F:153:ARG:CG	1.75	1.56
2:C:53:LYS:CG	2:C:53:LYS:CD	1.78	1.55
2:F:37:LYS:NZ	2:F:37:LYS:CE	1.67	1.55
1:K:57:LYS:CG	1:K:57:LYS:CB	1.78	1.55
2:L:101:LYS:CE	2:L:101:LYS:NZ	1.69	1.55
3:T:288:LYS:CE	3:T:288:LYS:CD	1.78	1.55
1:B:22:GLU:CG	1:B:22:GLU:CB	1.76	1.55
1:B:86:LYS:CE	1:B:86:LYS:NZ	1.70	1.54
2:F:55:VAL:CB	2:F:55:VAL:CG1	1.81	1.54
2:C:153:ARG:CG	2:C:153:ARG:CB	1.81	1.53
2:L:84:ARG:CB	2:L:84:ARG:CG	1.76	1.53
3:U:256:LYS:NZ	3:U:256:LYS:CE	1.70	1.53
2:C:101:LYS:CE	2:C:101:LYS:NZ	1.68	1.52
1:B:28:LYS:NZ	1:B:28:LYS:CE	1.72	1.52
2:F:55:VAL:CB	2:F:55:VAL:CA	1.85	1.52
3:V:235:LYS:CE	3:V:235:LYS:NZ	1.68	1.51
3:T:288:LYS:CD	3:T:288:LYS:CG	1.85	1.51
3:T:256:LYS:CE	3:T:256:LYS:NZ	1.70	1.51
1:H:65:GLU:CD	1:H:65:GLU:CG	1.83	1.51
1:E:86:LYS:NZ	1:E:86:LYS:CE	1.74	1.50
2:C:114:LYS:CE	2:C:114:LYS:NZ	1.70	1.50
1:E:78:LYS:CG	1:E:78:LYS:CD	1.87	1.49
2:I:152:ARG:CD	2:I:152:ARG:CG	1.88	1.49
2:C:145:LYS:CE	2:C:145:LYS:NZ	1.72	1.49
3:U:245:CYS:CB	3:U:245:CYS:SG	2.03	1.47
1:B:134:LYS:NZ	1:B:134:LYS:CE	1.76	1.46
3:U:244:PRO:CB	3:U:244:PRO:CG	1.75	1.46
1:H:98:LYS:NZ	1:H:98:LYS:CE	1.78	1.46
2:F:95:LYS:NZ	2:F:95:LYS:CE	1.77	1.46
2:C:34:THR:CB	2:C:34:THR:CA	1.93	1.45
1:E:78:LYS:CE	1:E:78:LYS:NZ	1.80	1.43
1:H:119:PRO:CG	1:H:119:PRO:CB	1.77	1.43
2:C:53:LYS:CE	2:C:53:LYS:NZ	1.84	1.39
2:C:78:MET:SD	2:C:78:MET:CE	2.13	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:11:ARG:NH2	1:K:67:PRO:HG2	1.36	1.35
1:H:81:HIS:HD2	1:H:83:ASN:ND2	1.30	1.30
1:H:81:HIS:CD2	1:H:83:ASN:ND2	2.05	1.23
2:C:131:ALA:CB	2:C:131:ALA:CA	2.16	1.23
3:V:261:HIS:CE1	3:V:270:PRO:HG3	1.76	1.21
1:B:35:ASN:C	1:B:35:ASN:HD22	1.47	1.19
2:F:37:LYS:HZ2	2:F:37:LYS:HA	1.06	1.17
2:L:92:TYR:CE2	2:L:115:ILE:HG22	1.80	1.17
2:L:114:LYS:HD2	2:L:170:GLN:HB2	1.25	1.16
2:C:132:ILE:C	2:C:132:ILE:HD13	1.70	1.16
3:T:277:THR:HG22	3:T:279:GLU:H	0.99	1.13
2:L:156:MET:O	2:L:161:MET:HG3	1.47	1.13
2:L:153:ARG:HG3	2:L:153:ARG:HH11	1.13	1.12
1:K:43:ILE:HD12	1:K:58:LEU:HD21	1.28	1.11
2:L:153:ARG:HA	2:L:156:MET:HE3	1.31	1.11
1:H:54:GLY:CA	1:H:152:ALA:HB1	1.81	1.11
2:F:130:ARG:HG3	2:F:130:ARG:HH11	1.16	1.10
1:H:54:GLY:HA3	1:H:152:ALA:HB1	1.19	1.09
1:H:54:GLY:HA3	1:H:152:ALA:CB	1.81	1.09
2:C:55:VAL:HG13	2:C:57:ASP:O	1.50	1.09
1:H:124:PRO:CB	1:H:130:ALA:HB1	1.83	1.09
1:H:81:HIS:CD2	1:H:83:ASN:HD21	1.67	1.08
1:B:81:HIS:CD2	1:B:83:ASN:H	1.72	1.07
2:I:152:ARG:HG3	2:I:152:ARG:HH11	1.15	1.07
2:I:84:ARG:HH11	2:I:84:ARG:HB2	1.19	1.07
2:I:159:GLU:HA	2:I:159:GLU:OE1	1.33	1.06
2:I:130:ARG:O	2:I:131:ALA:HB3	1.43	1.06
1:H:76:MET:O	2:I:70:MET:HE3	1.53	1.06
1:K:81:HIS:CD2	1:K:83:ASN:HB2	1.88	1.06
3:V:268:PHE:O	3:V:270:PRO:HD3	1.56	1.06
1:H:50:PRO:HG3	1:H:141:ILE:HG23	1.35	1.05
1:E:149:ARG:CG	1:E:149:ARG:HH11	1.68	1.05
2:I:67:ASP:OD1	2:I:67:ASP:N	1.89	1.04
2:I:82:PRO:CB	2:I:85:THR:HG21	1.86	1.04
1:K:144:ALA:O	1:K:147:TRP:HB2	1.56	1.04
2:L:40:ARG:HG2	2:L:40:ARG:HH21	0.95	1.04
3:V:261:HIS:ND1	3:V:270:PRO:HG3	1.71	1.03
2:L:67:ASP:O	2:L:68:GLU:HG3	1.58	1.03
2:L:115:ILE:HG12	2:L:115:ILE:O	1.56	1.03
3:T:277:THR:HG22	3:T:278:GLN:N	1.74	1.03
3:U:228:ILE:HG13	3:U:228:ILE:O	1.54	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:PRO:HB3	1:H:130:ALA:HB1	1.06	1.02
1:H:92:LEU:O	1:H:95:LEU:HB2	1.58	1.02
3:T:277:THR:CG2	3:T:278:GLN:N	2.21	1.02
2:L:82:PRO:HA	2:L:152:ARG:NH2	1.74	1.02
3:S:247:THR:HG22	3:S:251:ILE:H	1.17	1.02
2:I:84:ARG:HB2	2:I:84:ARG:NH1	1.74	1.01
1:K:128:ASP:OD2	1:K:128:ASP:N	1.86	1.01
2:C:114:LYS:HA	2:C:172:TYR:CE1	1.95	1.01
3:U:277:THR:H	3:U:280:GLN:NE2	1.57	1.01
1:K:142:GLU:O	1:K:144:ALA:N	1.95	1.00
3:V:282:ILE:HD13	3:V:282:ILE:N	1.75	1.00
1:H:65:GLU:HG2	1:H:69:ALA:HB2	1.39	1.00
2:F:37:LYS:NZ	2:F:37:LYS:HA	1.76	0.99
1:B:150:LEU:HD13	1:B:151:TYR:CZ	1.98	0.99
1:E:149:ARG:HH11	1:E:149:ARG:HG2	1.26	0.98
2:I:79:ILE:HG21	2:I:155:MET:HE1	1.44	0.98
1:K:143:THR:O	1:K:147:TRP:CD1	2.16	0.98
3:T:277:THR:HG22	3:T:279:GLU:N	1.77	0.98
2:F:168:GLU:HG2	2:F:169:GLY:N	1.78	0.98
3:V:247:THR:HG23	3:V:249:SER:H	1.26	0.98
2:I:55:VAL:O	2:I:57:ASP:N	1.98	0.97
1:E:122:ASP:HB3	1:E:134:LYS:NZ	1.78	0.97
1:H:65:GLU:CG	1:H:69:ALA:HB2	1.94	0.97
2:C:130:ARG:HH21	2:F:121:ASN:HA	1.27	0.97
2:I:82:PRO:HB2	2:I:85:THR:HG21	1.44	0.97
2:I:159:GLU:OE1	2:I:159:GLU:CA	2.12	0.97
1:E:65:GLU:HG2	1:E:69:ALA:HB2	1.44	0.97
1:B:35:ASN:HD22	1:B:36:ALA:N	1.61	0.96
2:L:161:MET:CE	2:L:162:LYS:HZ2	1.78	0.96
2:L:40:ARG:HG2	2:L:40:ARG:NH2	1.73	0.96
3:U:234:GLY:HA3	3:U:237:SER:HB3	1.47	0.96
2:L:118:ASN:HD22	2:L:160:ASN:HD21	0.99	0.96
2:L:40:ARG:HH21	2:L:40:ARG:CG	1.79	0.95
2:C:74:ARG:NH2	2:C:97:GLU:OE1	2.00	0.94
2:C:76:THR:HG22	2:C:76:THR:O	1.66	0.94
1:B:81:HIS:HD2	1:B:83:ASN:H	0.95	0.93
2:F:55:VAL:CB	2:F:55:VAL:HA	1.98	0.93
2:I:92:TYR:CE1	2:I:115:ILE:HD12	2.04	0.93
3:U:245:CYS:SG	3:U:255:ARG:HG3	2.08	0.93
2:L:153:ARG:HA	2:L:156:MET:CE	1.99	0.92
1:K:46:PRO:HD3	1:K:116:LEU:CD1	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:58:LEU:HB2	1:K:74:ARG:O	1.69	0.92
3:S:259:GLU:O	3:S:263:GLN:NE2	2.00	0.92
1:K:15:GLU:OE2	1:K:66:TYR:OH	1.85	0.92
3:T:299:GLY:O	3:T:300:TRP:CE3	2.23	0.92
1:B:128:ASP:N	1:B:128:ASP:OD2	2.01	0.92
1:H:58:LEU:HB3	1:H:75:PHE:HA	1.49	0.92
3:U:262:LEU:CD2	3:U:276:LEU:O	2.18	0.91
1:H:50:PRO:HG3	1:H:141:ILE:CG2	1.99	0.91
2:L:153:ARG:HH11	2:L:153:ARG:CG	1.83	0.91
1:K:50:PRO:HG3	1:K:141:ILE:CD1	1.99	0.91
1:K:11:ARG:NH2	1:K:67:PRO:CG	2.32	0.91
1:K:35:ASN:C	1:K:35:ASN:HD22	1.78	0.91
3:S:257:ASP:OD2	3:S:257:ASP:N	1.99	0.91
1:E:38:TYR:OH	1:E:59:GLU:OE1	1.89	0.91
2:I:152:ARG:CG	2:I:152:ARG:HH11	1.83	0.90
1:K:60:LEU:HD12	1:K:73:VAL:HG11	1.52	0.90
3:U:258:ILE:HG13	3:U:258:ILE:O	1.67	0.90
1:H:50:PRO:CG	1:H:141:ILE:HG23	2.02	0.90
2:L:92:TYR:CE2	2:L:115:ILE:CG2	2.55	0.90
3:V:246:ILE:HG13	3:V:247:THR:H	1.36	0.90
2:F:65:GLU:OE2	2:F:95:LYS:HE2	1.72	0.90
2:F:44:LEU:HD21	2:F:102:TYR:CE2	2.07	0.90
1:E:122:ASP:HB3	1:E:134:LYS:HZ2	1.35	0.89
1:H:81:HIS:HD2	1:H:83:ASN:HD21	0.93	0.89
2:C:132:ILE:C	2:C:132:ILE:CD1	2.45	0.89
3:T:277:THR:CG2	3:T:279:GLU:H	1.85	0.89
1:K:81:HIS:CD2	1:K:82:PRO:HD3	2.08	0.89
1:B:68:MET:HE1	3:S:261:HIS:HA	1.54	0.89
2:I:84:ARG:HH11	2:I:84:ARG:CB	1.85	0.89
2:I:93:SER:C	2:I:94:LEU:HD12	1.97	0.89
2:F:168:GLU:HG2	2:F:169:GLY:H	1.33	0.89
2:L:118:ASN:HD22	2:L:160:ASN:ND2	1.71	0.89
1:K:50:PRO:HG3	1:K:141:ILE:HD12	1.54	0.89
1:H:110:LEU:CD2	1:H:110:LEU:HG	2.02	0.88
1:K:27:ILE:HD11	1:K:113:GLN:HB3	1.55	0.88
3:V:272:THR:O	3:V:273:ARG:HB2	1.70	0.88
1:K:60:LEU:HD12	1:K:73:VAL:CG1	2.03	0.88
1:K:143:THR:O	1:K:147:TRP:HD1	1.53	0.88
3:U:227:ASP:HA	3:U:228:ILE:CG2	2.04	0.88
1:H:53:GLY:HA3	1:H:153:MET:HE3	1.56	0.88
1:K:81:HIS:CD2	1:K:82:PRO:CD	2.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:ARG:CG	1:E:149:ARG:NH1	2.36	0.88
2:I:79:ILE:HG21	2:I:155:MET:CE	2.03	0.87
3:U:247:THR:O	3:U:249:SER:N	2.07	0.87
3:U:269:ASN:O	3:U:271:VAL:N	2.08	0.87
1:E:8:LEU:HG	1:E:9:PRO:HD2	1.55	0.86
3:V:253:TYR:OH	3:V:270:PRO:HB2	1.75	0.86
2:I:170:GLN:O	2:I:171:CYS:HB3	1.71	0.86
3:S:297:GLU:C	3:S:297:GLU:OE1	2.18	0.86
1:B:35:ASN:C	1:B:35:ASN:ND2	2.26	0.86
1:H:65:GLU:HG2	1:H:69:ALA:CB	2.05	0.86
2:F:132:ILE:O	2:F:132:ILE:HG12	1.73	0.86
1:H:28:LYS:O	1:H:41:VAL:HA	1.74	0.86
1:E:78:LYS:HG2	1:E:147:TRP:CZ3	2.10	0.86
1:K:29:ALA:HB2	1:K:41:VAL:HG13	1.56	0.86
3:S:247:THR:HG22	3:S:251:ILE:N	1.91	0.86
1:E:35:ASN:ND2	1:E:37:ARG:H	1.73	0.86
2:C:53:LYS:NZ	2:C:53:LYS:HG2	1.90	0.85
3:U:247:THR:HG22	3:U:249:SER:H	1.41	0.85
2:F:130:ARG:HG3	2:F:130:ARG:NH1	1.87	0.85
1:H:124:PRO:HB3	1:H:130:ALA:CB	2.01	0.85
3:U:262:LEU:HD22	3:U:276:LEU:O	1.77	0.85
1:K:146:ALA:O	1:K:149:ARG:N	2.08	0.85
2:C:53:LYS:HG2	2:C:53:LYS:HZ2	1.42	0.84
2:F:56:GLY:O	2:F:57:ASP:O	1.93	0.84
2:I:140:ASN:HD22	2:I:141:SER:N	1.74	0.84
1:H:76:MET:C	2:I:70:MET:HE3	2.03	0.84
2:I:79:ILE:CG2	2:I:155:MET:HE1	2.07	0.84
2:I:140:ASN:HD22	2:I:140:ASN:C	1.81	0.84
2:I:83:PRO:HA	2:I:88:GLU:OE1	1.78	0.84
2:L:132:ILE:O	2:L:132:ILE:HG13	1.68	0.83
2:F:118:ASN:HD22	2:F:160:ASN:ND2	1.76	0.83
1:K:56:PHE:CE1	1:K:79:ILE:CD1	2.62	0.83
2:I:152:ARG:HG3	2:I:152:ARG:NH1	1.92	0.83
1:K:46:PRO:HD3	1:K:116:LEU:HD13	1.58	0.83
1:K:109:LEU:HD23	1:K:109:LEU:N	1.91	0.83
3:S:230:ASP:O	3:S:233:CYS:HB2	1.78	0.83
1:K:43:ILE:CD1	1:K:58:LEU:HD21	2.08	0.83
3:S:247:THR:O	3:S:250:GLY:N	2.11	0.83
1:B:38:TYR:HE1	1:B:40:HIS:CE1	1.96	0.83
2:F:163:LEU:O	2:F:165:GLN:NE2	2.11	0.83
3:S:259:GLU:C	3:S:263:GLN:HE21	1.87	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:227:ASP:HA	3:U:228:ILE:HG22	1.61	0.83
3:U:287:MET:HE2	3:V:287:MET:SD	2.19	0.83
1:K:53:GLY:HA2	1:K:153:MET:HE3	1.59	0.82
1:H:103:LEU:HD22	1:H:107:THR:HG21	1.62	0.82
2:I:82:PRO:HB3	2:I:85:THR:HG21	1.58	0.82
1:E:51:PHE:CE2	1:E:79:ILE:HD11	2.13	0.82
1:K:68:MET:CE	3:V:265:VAL:HG23	2.10	0.82
1:K:76:MET:O	2:L:70:MET:HE2	1.79	0.82
1:K:86:LYS:O	1:K:87:LEU:HD23	1.78	0.82
3:U:228:ILE:O	3:U:228:ILE:CG1	2.28	0.82
3:V:282:ILE:HD13	3:V:282:ILE:H	1.41	0.82
1:B:81:HIS:HD2	1:B:83:ASN:N	1.76	0.82
1:H:111:SER:O	1:H:115:LEU:HB2	1.80	0.82
2:L:37:LYS:HB2	2:L:37:LYS:NZ	1.95	0.82
1:H:131:GLU:HG3	1:H:132:GLN:N	1.93	0.82
1:H:91:CYS:HB2	1:H:96:LYS:NZ	1.93	0.82
3:U:277:THR:H	3:U:280:GLN:HE21	1.25	0.82
1:E:35:ASN:HD22	1:E:37:ARG:H	1.26	0.82
1:H:81:HIS:CD2	1:H:83:ASN:HD22	1.93	0.82
2:F:37:LYS:HZ2	2:F:37:LYS:CA	1.91	0.81
2:I:114:LYS:CD	2:I:171:CYS:HA	2.11	0.81
1:K:51:PHE:N	1:K:51:PHE:CD1	2.48	0.81
1:K:56:PHE:CE1	1:K:79:ILE:HD12	2.15	0.81
1:K:56:PHE:CD1	1:K:79:ILE:HD12	2.16	0.81
1:E:64:GLU:HA	1:E:64:GLU:OE1	1.77	0.81
2:F:167:PRO:HG2	2:F:170:GLN:HE22	1.44	0.81
1:H:119:PRO:O	1:H:121:PRO:HD2	1.79	0.81
2:I:132:ILE:HG22	2:I:132:ILE:O	1.79	0.81
3:V:269:ASN:HA	3:V:276:LEU:HD23	1.61	0.81
1:K:128:ASP:HA	1:K:131:GLU:HB2	1.60	0.81
1:H:32:ASP:HB2	1:H:40:HIS:NE2	1.96	0.81
2:I:130:ARG:O	2:I:131:ALA:CB	2.11	0.81
1:E:72:LYS:O	1:E:73:VAL:HG23	1.81	0.81
2:F:81:GLY:HA3	2:F:87:TYR:O	1.81	0.81
2:I:152:ARG:CG	2:I:152:ARG:NH1	2.42	0.81
1:B:154:ASN:HB2	1:B:156:ILE:HG12	1.60	0.81
1:H:53:GLY:HA3	1:H:153:MET:CE	2.11	0.81
2:L:140:ASN:HD22	2:L:141:SER:N	1.77	0.81
2:I:40:ARG:HH21	2:I:40:ARG:HG2	1.43	0.80
2:L:161:MET:CE	2:L:162:LYS:NZ	2.43	0.80
1:K:106:ARG:CG	1:K:106:ARG:NE	2.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:LEU:HD13	1:E:151:TYR:CE1	2.16	0.80
1:B:130:ALA:O	1:B:131:GLU:C	2.23	0.80
3:S:233:CYS:HA	3:S:239:GLU:O	1.82	0.80
1:H:131:GLU:HG3	1:H:132:GLN:H	1.47	0.79
1:H:121:PRO:C	1:H:123:ASP:H	1.90	0.79
1:H:141:ILE:O	1:H:144:ALA:HB3	1.82	0.79
3:U:242:ARG:HG3	3:U:242:ARG:HH11	1.46	0.79
2:C:165:GLN:HB3	2:C:166:PRO:HD2	1.62	0.79
2:F:167:PRO:HB2	2:F:170:GLN:NE2	1.98	0.79
3:V:247:THR:CG2	3:V:249:SER:H	1.96	0.79
2:C:132:ILE:HD13	2:C:132:ILE:O	1.83	0.78
1:E:64:GLU:OE1	1:E:64:GLU:CA	2.29	0.78
1:H:27:ILE:CG1	1:H:43:ILE:HG13	2.13	0.78
3:U:272:THR:O	3:U:273:ARG:HB2	1.83	0.78
1:K:59:GLU:HB3	1:K:76:MET:CE	2.13	0.78
2:C:84:ARG:HB3	2:C:84:ARG:HE	1.49	0.78
2:F:44:LEU:HD21	2:F:102:TYR:HE2	1.48	0.78
1:E:44:ALA:O	1:E:46:PRO:HD3	1.83	0.78
1:H:38:TYR:OH	1:H:59:GLU:OE1	2.01	0.78
1:H:133:TRP:CD1	1:H:133:TRP:C	2.60	0.78
2:L:157:SER:O	2:L:158:LYS:C	2.26	0.78
2:I:43:ARG:NH2	2:I:143:SER:HB3	1.98	0.78
1:K:35:ASN:C	1:K:35:ASN:ND2	2.41	0.78
1:K:142:GLU:O	1:K:145:ARG:N	2.17	0.78
3:V:261:HIS:CE1	3:V:270:PRO:CG	2.63	0.78
2:F:168:GLU:CG	2:F:169:GLY:H	1.96	0.78
3:S:229:PRO:HD2	3:S:232:LEU:HD22	1.66	0.78
3:V:234:GLY:O	3:V:236:ILE:N	2.16	0.78
1:E:98:LYS:O	3:U:273:ARG:NH2	2.17	0.78
2:I:94:LEU:HD12	2:I:94:LEU:N	1.97	0.78
1:E:65:GLU:O	1:E:68:MET:N	2.17	0.78
2:L:50:GLU:OE1	2:L:145:LYS:HE3	1.84	0.78
2:L:92:TYR:HE2	2:L:115:ILE:HG22	1.43	0.78
2:C:47:GLU:OE1	2:C:143:SER:HB2	1.83	0.77
1:H:124:PRO:HG3	1:H:134:LYS:HE3	1.66	0.77
1:H:150:LEU:C	1:H:150:LEU:HD23	2.09	0.77
2:C:53:LYS:CG	2:C:53:LYS:CE	2.62	0.77
1:B:153:MET:O	1:B:154:ASN:ND2	2.18	0.77
3:S:246:ILE:HG13	3:S:247:THR:H	1.49	0.77
2:F:37:LYS:NZ	2:F:37:LYS:CA	2.47	0.77
3:V:261:HIS:C	3:V:261:HIS:CD2	2.62	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:288:LYS:CD	3:V:288:LYS:CB	2.62	0.77
1:K:136:ASN:C	1:K:136:ASN:HD22	1.92	0.77
3:T:290:VAL:O	3:T:293:ALA:HB3	1.85	0.77
2:F:57:ASP:OD1	2:F:59:THR:HB	1.85	0.77
3:U:228:ILE:CG2	3:U:228:ILE:HB	2.08	0.77
2:I:161:MET:HE3	2:I:162:LYS:NZ	2.00	0.77
3:U:233:CYS:HA	3:U:239:GLU:O	1.85	0.77
3:U:247:THR:C	3:U:249:SER:H	1.91	0.77
3:U:287:MET:HE1	3:V:290:VAL:HG23	1.65	0.77
2:L:40:ARG:NH2	2:L:40:ARG:CG	2.45	0.77
3:T:243:GLU:HG2	3:T:255:ARG:HB2	1.65	0.77
1:E:24:VAL:HG13	1:E:25:PRO:HD2	1.67	0.76
1:E:149:ARG:CD	1:E:149:ARG:CB	2.63	0.76
1:K:11:ARG:CZ	1:K:67:PRO:HG2	2.14	0.76
1:H:149:ARG:HA	1:H:153:MET:SD	2.25	0.76
3:S:276:LEU:HD12	3:S:277:THR:N	1.99	0.76
1:B:9:PRO:HD2	1:B:12:ILE:HD12	1.67	0.76
3:V:246:ILE:CG1	3:V:247:THR:H	1.98	0.76
3:V:246:ILE:CG1	3:V:247:THR:N	2.48	0.76
1:H:64:GLU:HG3	1:H:65:GLU:H	1.51	0.75
2:L:101:LYS:NZ	2:L:101:LYS:CD	2.48	0.75
1:K:76:MET:O	2:L:70:MET:CE	2.34	0.75
1:K:82:PRO:HB3	1:K:130:ALA:HA	1.68	0.75
3:S:233:CYS:O	3:S:241:MET:HE2	1.87	0.75
1:B:77:THR:HG22	1:B:78:LYS:N	2.02	0.74
1:H:91:CYS:HB2	1:H:96:LYS:HZ2	1.48	0.74
2:I:40:ARG:HG3	2:I:102:TYR:O	1.88	0.74
1:B:116:LEU:N	1:B:116:LEU:HD23	2.02	0.74
2:L:126:VAL:HG12	2:L:127:VAL:N	2.01	0.74
1:H:127:ASN:O	1:H:130:ALA:HB3	1.86	0.74
1:H:14:LYS:HD3	1:H:18:ARG:HH21	1.50	0.74
3:V:247:THR:HG21	3:V:269:ASN:HD21	1.53	0.74
1:H:92:LEU:HD13	1:H:115:LEU:HD22	1.70	0.74
2:L:140:ASN:HD22	2:L:140:ASN:C	1.96	0.74
3:T:269:ASN:HD22	3:T:271:VAL:H	1.33	0.74
1:B:106:ARG:O	1:B:106:ARG:HG2	1.88	0.73
2:F:40:ARG:HB2	2:F:102:TYR:O	1.88	0.73
3:U:247:THR:C	3:U:249:SER:N	2.32	0.73
2:F:139:GLN:O	2:F:141:SER:N	2.21	0.73
3:V:247:THR:HG22	3:V:251:ILE:H	1.54	0.73
1:K:11:ARG:HH22	1:K:67:PRO:HG2	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:241:MET:HE2	3:T:253:TYR:C	2.13	0.73
3:T:274:SER:C	3:T:275:PRO:O	2.22	0.73
1:K:81:HIS:HD2	1:K:83:ASN:HB2	1.50	0.73
1:H:27:ILE:HG12	1:H:43:ILE:HG13	1.69	0.73
3:V:282:ILE:N	3:V:282:ILE:CD1	2.51	0.73
1:H:57:LYS:HB3	1:H:76:MET:HB2	1.71	0.73
2:C:130:ARG:O	2:C:131:ALA:C	2.32	0.73
2:I:152:ARG:N	2:I:155:MET:HG3	2.04	0.73
1:K:46:PRO:HD3	1:K:116:LEU:HD12	1.68	0.73
3:V:246:ILE:HG13	3:V:247:THR:N	2.03	0.72
1:B:62:LEU:HD11	1:B:105:ILE:HD11	1.70	0.72
1:E:81:HIS:HD2	1:E:83:ASN:H	1.36	0.72
2:F:160:ASN:HB3	2:F:163:LEU:CD1	2.19	0.72
1:B:78:LYS:HD2	1:B:151:TYR:CZ	2.24	0.72
2:C:53:LYS:CG	2:C:53:LYS:NZ	2.51	0.72
3:V:247:THR:HG21	3:V:269:ASN:ND2	2.04	0.72
2:C:87:TYR:CE2	2:C:115:ILE:HD11	2.24	0.72
2:I:161:MET:HE3	2:I:162:LYS:HZ2	1.53	0.72
2:L:111:PHE:CE1	2:L:115:ILE:HD12	2.23	0.72
3:S:259:GLU:C	3:S:263:GLN:NE2	2.45	0.71
3:S:286:ALA:O	3:S:290:VAL:HG23	1.90	0.71
1:B:127:ASN:ND2	1:B:130:ALA:H	1.86	0.71
1:E:51:PHE:N	1:E:51:PHE:CD1	2.56	0.71
3:U:268:PHE:HD1	3:U:273:ARG:HA	1.56	0.71
3:U:295:ILE:CB	3:U:295:ILE:C	2.62	0.71
2:I:114:LYS:CG	2:I:171:CYS:HA	2.20	0.71
3:U:287:MET:HE3	3:V:286:ALA:C	2.16	0.71
1:B:114:ALA:O	1:B:117:SER:N	2.21	0.71
1:K:43:ILE:HD12	1:K:58:LEU:CD2	2.14	0.71
2:L:145:LYS:O	2:L:149:GLN:HG3	1.90	0.71
2:L:53:LYS:HD3	2:L:53:LYS:N	2.05	0.71
2:L:126:VAL:CG1	2:L:127:VAL:N	2.53	0.71
1:H:76:MET:O	2:I:70:MET:CE	2.36	0.71
2:L:59:THR:O	2:L:60:VAL:HG13	1.90	0.71
2:L:153:ARG:CA	2:L:156:MET:HE3	2.17	0.71
1:K:11:ARG:HH21	1:K:67:PRO:HG2	1.53	0.71
2:L:114:LYS:CD	2:L:170:GLN:HB2	2.14	0.71
3:T:231:TYR:CD1	3:T:232:LEU:HD13	2.25	0.71
2:C:123:SER:O	2:C:172:TYR:CD2	2.44	0.71
2:F:128:ASP:C	2:F:128:ASP:OD1	2.33	0.71
1:H:20:LEU:O	1:H:22:GLU:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:258:ILE:HG13	3:V:258:ILE:O	1.91	0.71
2:C:158:LYS:HG3	2:C:159:GLU:N	2.05	0.70
1:E:29:ALA:C	1:E:30:GLU:HG3	2.14	0.70
1:E:51:PHE:CD2	1:E:79:ILE:HD11	2.26	0.70
3:U:277:THR:N	3:U:280:GLN:HE21	1.89	0.70
2:C:132:ILE:CD1	2:C:132:ILE:O	2.39	0.70
2:L:153:ARG:CG	2:L:153:ARG:NH1	2.49	0.70
1:B:134:LYS:NZ	1:B:134:LYS:CG	2.54	0.70
1:E:127:ASN:HD22	1:E:127:ASN:C	1.98	0.70
1:H:32:ASP:HB2	1:H:40:HIS:HE2	1.55	0.70
2:L:153:ARG:HG3	2:L:153:ARG:NH1	1.95	0.70
3:T:277:THR:CG2	3:T:278:GLN:H	2.03	0.70
3:U:254:ASP:OD1	3:U:255:ARG:N	2.23	0.70
1:B:35:ASN:ND2	1:B:36:ALA:N	2.37	0.70
2:F:105:ALA:HB1	2:F:106:PRO:HD2	1.72	0.70
2:F:140:ASN:C	2:F:140:ASN:HD22	1.99	0.70
2:I:132:ILE:HG23	2:I:134:VAL:CG1	2.22	0.70
1:K:37:ARG:HG2	1:K:62:LEU:HB2	1.74	0.70
1:B:119:PRO:O	1:B:121:PRO:HD3	1.90	0.70
2:F:138:TRP:CG	2:F:139:GLN:H	2.09	0.70
1:H:121:PRO:C	1:H:123:ASP:N	2.48	0.70
2:I:62:TRP:CH2	2:I:145:LYS:HB3	2.26	0.70
1:B:29:ALA:C	1:B:30:GLU:HG3	2.16	0.70
1:H:131:GLU:CG	1:H:132:GLN:N	2.54	0.70
1:H:136:ASN:HB3	1:H:139:GLN:HB3	1.73	0.70
2:C:78:MET:CE	2:C:78:MET:CG	2.70	0.70
3:U:247:THR:HG22	3:U:249:SER:HB2	1.72	0.70
1:B:88:GLY:N	2:C:70:MET:HE3	2.06	0.70
1:K:128:ASP:O	1:K:131:GLU:N	2.25	0.70
3:T:241:MET:CE	3:T:253:TYR:CA	2.70	0.70
1:B:74:ARG:HG3	1:B:75:PHE:O	1.92	0.69
3:S:236:ILE:HG22	3:S:237:SER:N	2.07	0.69
3:U:251:ILE:HG22	3:U:253:TYR:CE1	2.27	0.69
3:U:284:ASN:HD21	3:V:284:ASN:HD21	1.40	0.69
1:B:24:VAL:HG12	1:B:25:PRO:N	2.05	0.69
1:K:58:LEU:CB	1:K:74:ARG:O	2.39	0.69
3:U:252:THR:CB	3:U:252:THR:C	2.61	0.69
1:B:21:ALA:O	1:B:23:PRO:HD3	1.92	0.69
2:I:90:ARG:HH11	2:I:168:GLU:HA	1.57	0.69
1:K:59:GLU:HB3	1:K:76:MET:HE2	1.73	0.69
2:C:84:ARG:CB	2:C:84:ARG:HE	2.03	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:129:PRO:O	2:I:136:ALA:HB2	1.92	0.69
3:S:267:HIS:N	3:S:267:HIS:CD2	2.49	0.69
2:F:160:ASN:HB3	2:F:163:LEU:HD11	1.73	0.69
2:L:114:LYS:HA	2:L:172:TYR:CE1	2.28	0.69
3:S:237:SER:O	3:S:238:PHE:HB2	1.91	0.69
3:S:272:THR:C	3:S:274:SER:H	1.98	0.69
1:H:96:LYS:CE	1:H:96:LYS:CG	2.69	0.69
1:H:121:PRO:O	1:H:123:ASP:N	2.25	0.69
1:H:131:GLU:O	1:H:132:GLN:C	2.36	0.69
1:K:28:LYS:O	1:K:41:VAL:HG13	1.93	0.69
1:K:51:PHE:HD1	1:K:51:PHE:H	1.38	0.69
2:F:132:ILE:O	2:F:133:SER:C	2.34	0.69
2:I:132:ILE:HG23	2:I:134:VAL:HG13	1.75	0.69
1:K:28:LYS:NZ	1:K:28:LYS:HB3	2.08	0.69
2:F:114:LYS:HE3	2:F:170:GLN:OE1	1.92	0.69
3:U:252:THR:CA	3:U:252:THR:CG2	2.71	0.69
2:C:150:GLU:OE2	2:C:153:ARG:HD2	1.93	0.68
2:F:166:PRO:C	2:F:167:PRO:O	2.36	0.68
3:U:277:THR:N	3:U:280:GLN:NE2	2.36	0.68
3:V:268:PHE:O	3:V:270:PRO:CD	2.39	0.68
2:F:140:ASN:C	2:F:140:ASN:ND2	2.50	0.68
1:H:53:GLY:CA	1:H:153:MET:HE3	2.23	0.68
1:K:142:GLU:CG	1:K:142:GLU:CA	2.72	0.68
1:K:128:ASP:CA	1:K:131:GLU:HB2	2.24	0.68
3:U:248:PRO:HD2	3:U:276:LEU:HD11	1.74	0.68
2:F:118:ASN:H	2:F:160:ASN:ND2	1.92	0.68
1:K:109:LEU:HD23	1:K:109:LEU:H	1.57	0.68
1:K:139:GLN:O	1:K:140:ALA:C	2.37	0.68
2:F:43:ARG:NH2	2:F:142:TYR:O	2.25	0.68
3:T:246:ILE:HG13	3:T:247:THR:N	2.06	0.68
1:H:12:ILE:HD13	1:H:62:LEU:HD13	1.75	0.68
3:T:237:SER:HB3	3:T:257:ASP:OD2	1.94	0.68
2:C:80:LEU:N	2:C:80:LEU:HD13	2.09	0.67
2:C:130:ARG:NH2	2:F:121:ASN:HA	2.06	0.67
1:K:49:SER:O	1:K:51:PHE:N	2.27	0.67
1:K:68:MET:HE3	3:V:265:VAL:HG23	1.76	0.67
1:H:148:THR:O	1:H:152:ALA:HB3	1.95	0.67
3:T:301:VAL:CB	3:T:301:VAL:HA	2.13	0.67
1:B:150:LEU:HD13	1:B:151:TYR:CE1	2.29	0.67
1:E:35:ASN:HD22	1:E:35:ASN:C	2.02	0.67
1:H:83:ASN:ND2	1:H:83:ASN:N	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:82:PRO:CD	1:K:83:ASN:H	1.99	0.67
2:L:111:PHE:CD1	2:L:115:ILE:HD12	2.29	0.67
2:L:143:SER:OG	2:L:146:VAL:HG23	1.94	0.67
3:T:242:ARG:CD	3:T:242:ARG:CB	2.72	0.67
1:B:88:GLY:N	2:C:70:MET:CE	2.57	0.67
2:I:60:VAL:HG22	2:I:148:LEU:HB3	1.76	0.67
1:B:52:GLU:O	1:B:53:GLY:C	2.35	0.67
1:B:56:PHE:O	1:B:58:LEU:HD23	1.95	0.67
2:C:42:PHE:O	2:C:46:GLU:HG3	1.94	0.67
2:F:153:ARG:CD	2:F:153:ARG:CB	2.72	0.67
3:T:277:THR:HG23	3:T:278:GLN:H	1.59	0.67
3:U:256:LYS:NZ	3:U:256:LYS:CD	2.57	0.67
2:L:65:GLU:O	2:L:65:GLU:HG2	1.94	0.67
1:K:121:PRO:HB3	1:K:133:TRP:HB3	1.77	0.67
2:I:144:ILE:O	2:I:148:LEU:HD12	1.95	0.67
1:K:13:ILE:HG22	1:K:17:GLN:NE2	2.10	0.67
1:K:114:ALA:O	1:K:115:LEU:C	2.38	0.67
1:B:15:GLU:OE1	1:B:104:GLN:HB2	1.94	0.66
2:L:82:PRO:CA	2:L:152:ARG:NH2	2.54	0.66
2:L:161:MET:HE3	2:L:162:LYS:HZ2	1.59	0.66
3:U:247:THR:HG22	3:U:249:SER:N	2.10	0.66
1:K:105:ILE:O	1:K:108:VAL:N	2.27	0.66
2:I:132:ILE:CG2	2:I:134:VAL:HG13	2.25	0.66
3:T:287:MET:O	3:T:289:GLU:N	2.29	0.66
1:E:47:GLN:O	1:E:48:ASP:HB2	1.94	0.66
1:H:24:VAL:O	1:H:26:GLY:N	2.29	0.66
2:L:37:LYS:HB2	2:L:37:LYS:HZ2	1.58	0.66
1:H:133:TRP:C	1:H:133:TRP:HD1	2.02	0.66
1:K:128:ASP:C	1:K:130:ALA:N	2.51	0.66
3:U:241:MET:HG2	3:U:254:ASP:HB2	1.77	0.66
2:C:78:MET:HB2	2:C:78:MET:HE2	1.76	0.66
2:F:36:VAL:HG23	2:F:36:VAL:O	1.96	0.66
2:F:66:ASP:C	2:F:66:ASP:OD2	2.39	0.66
1:H:97:ASP:O	1:H:99:TRP:N	2.28	0.66
1:B:83:ASN:HB3	1:B:91:CYS:HB3	1.78	0.66
1:B:86:LYS:HD3	2:C:68:GLU:HG2	1.77	0.66
1:E:58:LEU:N	1:E:58:LEU:HD12	2.11	0.66
2:F:80:LEU:O	2:F:81:GLY:C	2.33	0.66
1:H:24:VAL:O	1:H:25:PRO:C	2.38	0.66
3:T:242:ARG:CG	3:T:242:ARG:NE	2.59	0.66
3:U:227:ASP:HA	3:U:228:ILE:HG23	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:LYS:O	2:C:37:LYS:HG3	1.96	0.66
3:V:243:GLU:OE1	3:V:256:LYS:CE	2.44	0.66
2:C:101:LYS:NZ	2:C:101:LYS:CD	2.57	0.66
2:I:40:ARG:HG2	2:I:40:ARG:NH2	2.11	0.66
3:S:267:HIS:CD2	3:S:267:HIS:H	2.14	0.66
1:K:156:ILE:CA	1:K:156:ILE:HB	2.12	0.66
1:H:43:ILE:HG22	1:H:44:ALA:O	1.95	0.65
2:I:87:TYR:CD1	2:I:155:MET:HB3	2.31	0.65
1:K:142:GLU:O	1:K:143:THR:C	2.39	0.65
1:E:94:ILE:CG2	1:E:94:ILE:CG1	2.71	0.65
2:I:131:ALA:O	2:I:132:ILE:HG13	1.95	0.65
2:F:114:LYS:HE2	2:F:170:GLN:HG2	1.78	0.65
2:C:82:PRO:HG2	2:C:85:THR:HG21	1.77	0.65
2:F:167:PRO:HB2	2:F:170:GLN:HE21	1.60	0.65
1:B:35:ASN:HD21	1:B:37:ARG:HB2	1.61	0.65
1:B:134:LYS:NZ	1:B:134:LYS:CD	2.60	0.65
1:K:46:PRO:HG2	1:K:116:LEU:HB3	1.79	0.65
1:B:127:ASN:C	1:B:127:ASN:HD22	2.04	0.65
2:C:140:ASN:C	2:C:140:ASN:ND2	2.54	0.65
1:B:11:ARG:NH2	1:B:67:PRO:CG	2.60	0.65
2:C:55:VAL:CG1	2:C:57:ASP:O	2.39	0.65
1:H:142:GLU:O	1:H:145:ARG:N	2.24	0.65
3:T:231:TYR:HD1	3:T:232:LEU:HD13	1.60	0.65
1:B:50:PRO:O	1:B:145:ARG:HG3	1.96	0.65
2:C:127:VAL:HG12	2:C:128:ASP:N	2.10	0.65
3:T:232:LEU:O	3:T:240:LEU:HA	1.97	0.65
1:E:73:VAL:HG12	1:E:90:ILE:HD13	1.78	0.64
1:E:153:MET:O	1:E:154:ASN:C	2.40	0.64
2:F:114:LYS:CE	2:F:170:GLN:HG2	2.28	0.64
2:F:138:TRP:CG	2:F:139:GLN:N	2.63	0.64
2:L:61:SER:HB3	2:L:78:MET:HG3	1.77	0.64
1:B:96:LYS:HB3	1:B:97:ASP:OD1	1.97	0.64
1:E:35:ASN:HD22	1:E:37:ARG:N	1.95	0.64
2:I:114:LYS:HG3	2:I:172:TYR:H	1.63	0.64
1:K:150:LEU:CD2	1:K:150:LEU:HG	2.15	0.64
3:V:253:TYR:CD1	3:V:258:ILE:HD13	2.33	0.64
1:B:144:ALA:O	1:B:145:ARG:C	2.37	0.64
1:E:8:LEU:CD1	1:E:8:LEU:CB	2.72	0.64
2:I:154:LEU:O	2:I:157:SER:HB3	1.97	0.64
1:K:150:LEU:CD2	1:K:150:LEU:CD1	2.76	0.64
2:L:157:SER:O	2:L:159:GLU:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:ASP:O	1:E:35:ASN:N	2.30	0.64
2:I:114:LYS:HG3	2:I:171:CYS:HA	1.80	0.64
2:I:152:ARG:O	2:I:153:ARG:C	2.41	0.64
2:C:118:ASN:H	2:C:160:ASN:HD21	1.46	0.63
2:F:44:LEU:CD2	2:F:102:TYR:HE2	2.10	0.63
3:U:268:PHE:HB2	3:U:273:ARG:O	1.98	0.63
2:C:114:LYS:HA	2:C:172:TYR:CZ	2.32	0.63
1:H:14:LYS:NZ	3:T:228:ILE:HD12	2.12	0.63
2:L:50:GLU:OE1	2:L:55:VAL:HG21	1.98	0.63
3:U:247:THR:O	3:U:248:PRO:C	2.42	0.63
3:U:247:THR:CG2	3:U:249:SER:HB2	2.26	0.63
2:C:101:LYS:O	2:C:104:GLU:N	2.31	0.63
1:H:84:VAL:HG12	1:H:88:GLY:HA2	1.80	0.63
1:H:146:ALA:O	1:H:149:ARG:HB3	1.98	0.63
3:T:241:MET:CE	3:T:253:TYR:HA	2.29	0.63
3:T:277:THR:HG23	3:T:278:GLN:N	2.13	0.63
1:B:154:ASN:HB2	1:B:156:ILE:CG1	2.28	0.63
1:H:15:GLU:OE1	1:H:104:GLN:HB2	1.98	0.63
1:H:73:VAL:HG12	1:H:90:ILE:CD1	2.29	0.63
1:B:38:TYR:HD2	2:C:39:PRO:HG3	1.62	0.63
1:E:127:ASN:ND2	1:E:130:ALA:H	1.97	0.63
1:H:93:ASP:OD1	1:H:94:ILE:N	2.31	0.63
2:L:40:ARG:HB2	2:L:102:TYR:O	1.99	0.63
2:F:167:PRO:CG	2:F:170:GLN:HE22	2.10	0.63
3:V:253:TYR:CZ	3:V:270:PRO:HB2	2.34	0.63
1:K:28:LYS:HB3	1:K:28:LYS:HZ2	1.64	0.63
1:K:78:LYS:NZ	1:K:147:TRP:CH2	2.60	0.63
1:K:149:ARG:O	1:K:150:LEU:C	2.42	0.63
2:C:159:GLU:CG	2:C:159:GLU:CA	2.73	0.63
1:K:81:HIS:O	1:K:129:VAL:HG11	1.99	0.63
3:S:261:HIS:C	3:S:261:HIS:CD2	2.75	0.63
2:I:40:ARG:HH21	2:I:40:ARG:CG	2.11	0.62
3:V:229:PRO:O	3:V:230:ASP:HB3	1.99	0.62
1:H:58:LEU:N	1:H:58:LEU:CD2	2.62	0.62
1:H:91:CYS:O	1:H:91:CYS:SG	2.54	0.62
1:E:80:TYR:HB2	1:E:147:TRP:CE3	2.34	0.62
1:H:58:LEU:N	1:H:58:LEU:HD22	2.14	0.62
1:H:65:GLU:CG	1:H:69:ALA:CB	2.71	0.62
1:K:144:ALA:O	1:K:147:TRP:CB	2.42	0.62
3:T:237:SER:O	3:T:238:PHE:HB2	1.97	0.62
3:T:241:MET:HE3	3:T:253:TYR:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:297:GLU:O	3:T:298:ASN:C	2.39	0.62
3:U:242:ARG:O	3:U:243:GLU:HB2	2.00	0.62
3:U:262:LEU:HD21	3:U:276:LEU:HD23	1.82	0.62
3:U:284:ASN:ND2	3:V:284:ASN:HD21	1.95	0.62
1:H:76:MET:C	2:I:70:MET:CE	2.72	0.62
1:K:104:GLN:HG3	1:K:106:ARG:H	1.65	0.62
3:S:276:LEU:HD12	3:S:277:THR:H	1.63	0.62
3:U:231:TYR:CD1	3:U:232:LEU:CD2	2.83	0.62
3:U:247:THR:O	3:U:250:GLY:N	2.32	0.62
3:U:289:GLU:OE1	3:V:231:TYR:HB3	1.99	0.62
3:V:261:HIS:C	3:V:261:HIS:HD2	2.07	0.62
1:B:81:HIS:NE2	1:B:83:ASN:ND2	2.47	0.62
2:F:144:ILE:CD1	2:F:144:ILE:CB	2.72	0.62
1:E:99:TRP:C	3:U:273:ARG:HH22	2.07	0.62
2:F:53:LYS:CE	2:F:53:LYS:CG	2.77	0.62
1:K:80:TYR:HB3	1:K:144:ALA:HA	1.81	0.62
2:L:54:GLY:O	2:L:55:VAL:HG23	1.98	0.62
3:V:234:GLY:C	3:V:236:ILE:H	2.08	0.62
1:B:127:ASN:HB2	1:B:128:ASP:OD2	1.99	0.62
2:C:129:PRO:C	2:C:130:ARG:O	2.41	0.62
2:I:152:ARG:H	2:I:155:MET:HG3	1.65	0.62
3:T:269:ASN:HB3	3:T:273:ARG:H	1.63	0.62
3:U:269:ASN:CG	3:U:272:THR:HG1	2.07	0.62
2:F:47:GLU:OE1	2:F:143:SER:HB2	1.99	0.62
2:F:95:LYS:N	2:F:110:ARG:O	2.29	0.62
3:U:287:MET:HE3	3:V:287:MET:N	2.15	0.61
1:B:28:LYS:HE2	1:B:30:GLU:OE2	1.99	0.61
1:E:104:GLN:O	1:E:107:THR:N	2.33	0.61
2:F:168:GLU:CG	2:F:169:GLY:N	2.45	0.61
1:K:78:LYS:CD	1:K:78:LYS:NZ	2.61	0.61
3:U:245:CYS:SG	3:U:245:CYS:CA	2.85	0.61
3:S:243:GLU:HG2	3:S:255:ARG:HB3	1.82	0.61
3:U:285:LEU:HB2	3:V:250:GLY:O	2.00	0.61
2:I:153:ARG:O	2:I:156:MET:HB2	2.01	0.61
1:K:80:TYR:HD2	1:K:144:ALA:HB2	1.65	0.61
3:U:269:ASN:O	3:U:270:PRO:C	2.41	0.61
2:L:53:LYS:N	2:L:53:LYS:CD	2.62	0.61
1:H:127:ASN:OD1	1:H:128:ASP:N	2.34	0.61
3:U:287:MET:HE1	3:V:290:VAL:CG2	2.31	0.61
2:C:53:LYS:CD	2:C:53:LYS:CB	2.76	0.61
1:E:141:ILE:HG22	1:E:142:GLU:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:LEU:HD13	1:E:151:TYR:CD1	2.36	0.61
1:B:24:VAL:HG13	1:B:25:PRO:HD2	1.83	0.61
2:F:118:ASN:HD22	2:F:160:ASN:HD22	1.47	0.61
2:I:114:LYS:HD3	2:I:171:CYS:HA	1.83	0.61
1:E:6:ALA:CB	1:E:6:ALA:HA	2.18	0.61
1:H:9:PRO:HG2	1:H:12:ILE:HG13	1.82	0.61
3:S:233:CYS:C	3:S:241:MET:HE2	2.26	0.61
1:B:87:LEU:C	2:C:70:MET:HE3	2.26	0.60
2:I:130:ARG:HG3	2:I:130:ARG:HH11	1.66	0.60
1:B:137:GLU:O	1:B:138:ALA:C	2.42	0.60
1:H:66:TYR:CD1	1:H:67:PRO:HA	2.36	0.60
1:K:120:ASN:OD1	1:K:122:ASP:CG	2.44	0.60
2:F:50:GLU:OE2	2:F:145:LYS:NZ	2.34	0.60
1:H:119:PRO:O	1:H:121:PRO:CD	2.48	0.60
3:T:242:ARG:HG2	3:T:303:ASP:OD2	2.01	0.60
1:B:147:TRP:O	1:B:151:TYR:HD1	1.82	0.60
3:U:295:ILE:CA	3:U:295:ILE:HB	2.16	0.60
1:H:54:GLY:CA	1:H:152:ALA:CB	2.57	0.60
3:S:296:SER:O	3:S:297:GLU:HB2	2.01	0.60
2:F:44:LEU:HD21	2:F:102:TYR:CD2	2.36	0.60
1:H:19:LEU:HD23	1:H:23:PRO:HA	1.81	0.60
2:L:111:PHE:CD1	2:L:115:ILE:CD1	2.84	0.60
1:K:128:ASP:C	1:K:131:GLU:H	2.09	0.60
3:S:231:TYR:CD1	3:S:232:LEU:HD13	2.37	0.60
3:U:247:THR:CG2	3:U:249:SER:H	2.13	0.60
3:U:289:GLU:O	3:U:292:ASP:N	2.34	0.60
1:B:104:GLN:O	1:B:105:ILE:C	2.40	0.60
1:H:70:ALA:HB1	1:H:71:PRO:HD2	1.83	0.60
2:L:67:ASP:O	2:L:68:GLU:CG	2.44	0.60
3:U:266:GLY:C	3:U:268:PHE:H	2.08	0.60
3:V:271:VAL:CG1	3:V:271:VAL:O	2.49	0.60
2:C:33:THR:O	2:C:34:THR:O	2.20	0.60
1:E:121:PRO:O	1:E:122:ASP:OD1	2.19	0.60
2:F:139:GLN:HB3	2:F:142:TYR:CE1	2.36	0.60
3:S:292:ASP:O	3:S:293:ALA:O	2.20	0.60
1:B:123:ASP:N	1:B:124:PRO:HA	2.17	0.60
1:H:150:LEU:C	1:H:150:LEU:CD2	2.75	0.60
3:S:284:ASN:O	3:S:284:ASN:OD1	2.20	0.60
3:V:237:SER:C	3:V:239:GLU:H	2.10	0.60
1:B:65:GLU:O	1:B:66:TYR:C	2.44	0.59
3:S:247:THR:HG21	3:S:269:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:291:ILE:O	3:T:294:PHE:N	2.35	0.59
3:U:228:ILE:CG2	3:U:228:ILE:CA	2.77	0.59
3:U:252:THR:CB	3:U:252:THR:N	2.58	0.59
3:U:269:ASN:OD1	3:U:272:THR:N	2.33	0.59
1:K:156:ILE:CB	1:K:156:ILE:HA	2.17	0.59
3:T:253:TYR:OH	3:T:270:PRO:HB2	2.02	0.59
1:B:154:ASN:CB	1:B:156:ILE:HG12	2.32	0.59
2:C:82:PRO:HG2	2:C:85:THR:CG2	2.32	0.59
1:E:8:LEU:CD1	1:E:8:LEU:HG	2.15	0.59
1:E:76:MET:C	2:F:70:MET:HE1	2.27	0.59
1:B:59:GLU:HG3	1:B:59:GLU:O	2.02	0.59
1:E:70:ALA:HB1	1:E:71:PRO:HD2	1.83	0.59
1:H:127:ASN:OD1	1:H:127:ASN:C	2.44	0.59
3:S:272:THR:C	3:S:274:SER:N	2.58	0.59
3:T:299:GLY:O	3:T:300:TRP:HE3	1.81	0.59
2:F:65:GLU:OE2	2:F:95:LYS:CE	2.48	0.59
3:V:243:GLU:OE2	3:V:255:ARG:HD2	2.01	0.59
1:E:24:VAL:CG1	1:E:25:PRO:HD2	2.32	0.59
1:H:14:LYS:HD3	1:H:18:ARG:NH2	2.16	0.59
2:L:118:ASN:ND2	2:L:160:ASN:HD21	1.84	0.59
2:L:143:SER:O	2:L:144:ILE:C	2.44	0.59
3:T:243:GLU:HG2	3:T:255:ARG:CB	2.33	0.59
1:E:28:LYS:HG3	1:E:29:ALA:N	2.18	0.59
1:K:68:MET:HE3	1:K:68:MET:HA	1.85	0.59
1:K:136:ASN:C	1:K:136:ASN:ND2	2.57	0.59
1:B:47:GLN:HA	1:B:52:GLU:HG3	1.85	0.58
3:U:230:ASP:C	3:U:232:LEU:H	2.11	0.58
3:U:233:CYS:CA	3:U:239:GLU:O	2.51	0.58
1:K:86:LYS:C	1:K:87:LEU:HD23	2.28	0.58
2:I:157:SER:OG	2:I:159:GLU:HB2	2.03	0.58
3:U:289:GLU:OE1	3:V:231:TYR:CB	2.51	0.58
1:E:84:VAL:HA	1:E:89:ARG:O	2.03	0.58
2:I:63:GLY:O	2:I:75:TRP:HE3	1.87	0.58
3:T:246:ILE:HG13	3:T:247:THR:H	1.65	0.58
2:C:129:PRO:O	2:C:130:ARG:O	2.21	0.58
3:V:236:ILE:O	3:V:238:PHE:HD1	1.85	0.58
1:B:27:ILE:HG21	1:B:109:LEU:HD13	1.86	0.58
2:F:118:ASN:ND2	2:F:160:ASN:HD22	2.02	0.58
1:K:7:GLY:H	1:K:8:LEU:HB3	1.68	0.58
3:T:247:THR:O	3:T:250:GLY:HA2	2.03	0.58
1:H:141:ILE:O	1:H:142:GLU:O	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:58:LEU:CD2	1:K:58:LEU:N	2.66	0.58
3:T:292:ASP:HA	3:T:295:ILE:HG13	1.86	0.58
1:B:155:ASN:OD1	1:B:155:ASN:N	2.19	0.58
2:C:34:THR:CB	2:C:34:THR:HA	2.22	0.58
2:C:123:SER:O	2:C:172:TYR:HD2	1.87	0.58
3:S:229:PRO:HD2	3:S:232:LEU:CD2	2.33	0.58
3:S:246:ILE:HG13	3:S:247:THR:N	2.19	0.58
2:C:94:LEU:HD12	2:C:94:LEU:N	2.18	0.58
2:L:43:ARG:HG2	2:L:103:PRO:HG3	1.85	0.58
3:S:271:VAL:HG12	3:S:271:VAL:O	2.04	0.58
2:C:78:MET:CE	2:C:78:MET:HB2	2.33	0.58
2:F:73:THR:HG22	2:F:73:THR:O	2.01	0.57
2:L:128:ASP:O	2:L:129:PRO:C	2.40	0.57
1:H:134:LYS:HG2	1:H:135:THR:H	1.67	0.57
3:U:236:ILE:O	3:U:236:ILE:HG22	2.04	0.57
2:C:153:ARG:O	2:C:156:MET:HG3	2.03	0.57
1:H:142:GLU:HG2	1:H:145:ARG:HH12	1.69	0.57
3:T:303:ASP:CG	3:T:304:TYR:N	2.62	0.57
1:E:35:ASN:ND2	1:E:37:ARG:N	2.49	0.57
3:U:231:TYR:CE1	3:U:232:LEU:HD23	2.39	0.57
3:V:236:ILE:O	3:V:237:SER:C	2.48	0.57
1:B:98:LYS:N	1:B:98:LYS:CD	2.67	0.57
1:E:60:LEU:HA	1:E:73:VAL:CG2	2.34	0.57
1:E:67:PRO:O	1:E:101:PRO:HB3	2.04	0.57
2:I:156:MET:O	2:I:157:SER:O	2.23	0.57
1:K:95:LEU:HD21	1:K:108:VAL:CG1	2.34	0.57
2:L:48:LEU:O	2:L:52:GLN:HG3	2.05	0.57
1:B:24:VAL:CG1	1:B:25:PRO:N	2.67	0.57
2:F:158:LYS:HD2	2:F:159:GLU:OE1	2.05	0.57
2:I:90:ARG:HH11	2:I:168:GLU:CA	2.17	0.57
1:K:49:SER:O	1:K:50:PRO:C	2.47	0.57
3:T:287:MET:O	3:T:288:LYS:C	2.48	0.57
1:B:4:GLY:O	1:B:5:SER:HB3	2.04	0.57
2:F:82:PRO:HG2	2:F:85:THR:HG21	1.87	0.57
1:H:24:VAL:HG13	1:H:25:PRO:HD2	1.87	0.57
2:I:46:GLU:O	2:I:48:LEU:N	2.37	0.57
2:I:102:TYR:CD1	2:I:103:PRO:HA	2.40	0.57
2:I:140:ASN:C	2:I:140:ASN:ND2	2.52	0.57
1:K:54:GLY:HA3	1:K:152:ALA:HB1	1.87	0.57
1:K:120:ASN:OD1	1:K:122:ASP:CB	2.53	0.57
1:K:147:TRP:O	1:K:151:TYR:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:227:ASP:O	3:S:228:ILE:HG13	2.05	0.57
1:B:68:MET:HE3	3:S:265:VAL:HG23	1.87	0.56
1:E:63:PRO:HG2	1:E:69:ALA:HB1	1.87	0.56
1:H:128:ASP:CG	1:H:129:VAL:N	2.63	0.56
2:I:132:ILE:HG22	2:I:135:LEU:HB2	1.86	0.56
1:K:46:PRO:CD	1:K:116:LEU:HD13	2.31	0.56
1:K:80:TYR:HE2	1:K:140:ALA:HA	1.70	0.56
3:S:254:ASP:O	3:S:255:ARG:C	2.46	0.56
3:T:242:ARG:N	3:T:254:ASP:OD2	2.37	0.56
1:B:134:LYS:NZ	1:B:134:LYS:CB	2.68	0.56
1:B:134:LYS:HB2	1:B:134:LYS:HZ2	1.69	0.56
2:C:144:ILE:O	2:C:145:LYS:C	2.46	0.56
1:K:35:ASN:HD22	1:K:36:ALA:N	2.03	0.56
1:K:97:ASP:C	1:K:99:TRP:H	2.13	0.56
3:U:287:MET:CE	3:V:286:ALA:C	2.78	0.56
1:B:68:MET:HE3	3:S:265:VAL:CG2	2.35	0.56
2:C:156:MET:O	2:C:157:SER:C	2.45	0.56
1:H:10:ARG:O	1:H:11:ARG:C	2.46	0.56
1:H:46:PRO:CG	1:H:116:LEU:HB2	2.35	0.56
3:T:247:THR:O	3:T:248:PRO:C	2.47	0.56
3:T:287:MET:C	3:T:289:GLU:N	2.63	0.56
3:U:261:HIS:C	3:U:261:HIS:CD2	2.83	0.56
3:V:276:LEU:HA	3:V:280:GLN:OE1	2.05	0.56
2:L:161:MET:HE1	2:L:162:LYS:HZ2	1.69	0.56
3:U:278:GLN:HB3	3:U:279:GLU:OE2	2.06	0.56
3:V:245:CYS:HB2	3:V:283:PRO:HA	1.88	0.56
1:H:81:HIS:HB3	1:H:84:VAL:HG23	1.88	0.56
2:I:43:ARG:HH22	2:I:143:SER:HB3	1.71	0.56
3:S:297:GLU:OE1	3:S:298:ASN:CG	2.49	0.56
2:F:43:ARG:HG3	2:F:103:PRO:HG2	1.88	0.56
1:H:81:HIS:HE1	1:H:116:LEU:HA	1.69	0.56
1:K:97:ASP:C	1:K:99:TRP:N	2.61	0.56
3:S:257:ASP:C	3:S:259:GLU:N	2.63	0.56
3:U:295:ILE:CB	3:U:295:ILE:HA	2.18	0.56
3:V:231:TYR:HD1	3:V:232:LEU:N	2.03	0.56
1:B:77:THR:CG2	1:B:78:LYS:N	2.64	0.56
1:H:81:HIS:CD2	1:H:82:PRO:CD	2.89	0.56
1:K:81:HIS:NE2	1:K:83:ASN:HB2	2.18	0.56
1:K:93:ASP:OD1	1:K:93:ASP:N	2.39	0.56
2:L:115:ILE:HD11	2:L:120:VAL:HG11	1.87	0.56
1:E:8:LEU:HG	1:E:9:PRO:CD	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:VAL:HG12	1:H:90:ILE:HD11	1.87	0.56
3:U:231:TYR:CE1	3:U:232:LEU:CD2	2.89	0.56
2:F:118:ASN:ND2	2:F:160:ASN:ND2	2.52	0.56
1:H:53:GLY:C	1:H:153:MET:HE3	2.31	0.56
2:L:80:LEU:HD12	2:L:80:LEU:N	2.20	0.56
3:U:234:GLY:C	3:U:237:SER:H	2.14	0.56
1:B:88:GLY:CA	2:C:70:MET:HE1	2.36	0.55
3:V:246:ILE:HA	3:V:252:THR:HG23	1.87	0.55
2:C:129:PRO:HG2	2:C:130:ARG:N	2.22	0.55
1:E:57:LYS:C	1:E:58:LEU:HD12	2.32	0.55
1:H:142:GLU:O	1:H:143:THR:C	2.48	0.55
1:K:14:LYS:HE3	1:K:18:ARG:HH22	1.72	0.55
3:S:258:ILE:HG23	3:S:259:GLU:N	2.20	0.55
3:V:271:VAL:O	3:V:271:VAL:HG12	2.06	0.55
3:V:288:LYS:CG	3:V:288:LYS:CE	2.79	0.55
2:C:35:GLY:O	2:C:36:VAL:HB	2.07	0.55
1:E:128:ASP:O	1:E:131:GLU:HB3	2.07	0.55
3:T:289:GLU:O	3:T:290:VAL:C	2.50	0.55
3:V:284:ASN:CG	3:V:287:MET:HB2	2.32	0.55
2:C:132:ILE:HD13	2:C:133:SER:N	2.16	0.55
2:I:115:ILE:HG23	2:I:120:VAL:HG11	1.88	0.55
1:K:32:ASP:OD2	1:K:33:GLU:N	2.39	0.55
3:T:276:LEU:O	3:T:276:LEU:HG	1.97	0.55
2:L:84:ARG:NE	2:L:84:ARG:HB3	2.22	0.55
2:C:37:LYS:O	2:C:37:LYS:CG	2.54	0.55
1:B:62:LEU:O	1:B:63:PRO:C	2.41	0.55
2:C:84:ARG:CB	2:C:84:ARG:NE	2.69	0.55
1:E:150:LEU:CD1	1:E:151:TYR:CE1	2.89	0.55
1:K:50:PRO:CG	1:K:141:ILE:HD12	2.33	0.55
1:K:86:LYS:HD2	2:L:68:GLU:HG2	1.87	0.55
3:S:293:ALA:O	3:S:294:PHE:C	2.49	0.55
3:U:250:GLY:HA3	3:V:285:LEU:CD1	2.36	0.55
1:E:123:ASP:H	1:E:124:PRO:HA	1.72	0.55
2:F:36:VAL:O	2:F:36:VAL:CG2	2.54	0.55
2:I:55:VAL:O	2:I:56:GLY:C	2.43	0.55
1:K:156:ILE:CB	1:K:156:ILE:C	2.75	0.55
2:L:67:ASP:OD2	2:L:67:ASP:N	2.40	0.55
3:V:229:PRO:O	3:V:230:ASP:CB	2.55	0.55
3:V:232:LEU:O	3:V:241:MET:HE2	2.07	0.55
1:E:149:ARG:CG	1:E:149:ARG:NE	2.65	0.55
2:I:69:ASP:O	2:I:70:MET:C	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:94:LEU:N	2:I:94:LEU:CD1	2.65	0.55
3:U:256:LYS:NZ	3:U:256:LYS:CG	2.70	0.55
2:C:163:LEU:O	2:C:165:GLN:NE2	2.36	0.55
1:H:73:VAL:CG1	1:H:74:ARG:N	2.70	0.55
1:H:93:ASP:C	1:H:95:LEU:H	2.15	0.55
1:H:132:GLN:O	1:H:133:TRP:C	2.49	0.55
3:S:292:ASP:O	3:S:293:ALA:C	2.45	0.55
3:V:287:MET:O	3:V:290:VAL:N	2.40	0.55
2:C:53:LYS:O	2:C:54:GLY:O	2.25	0.54
2:C:57:ASP:OD1	2:C:59:THR:CG2	2.55	0.54
1:K:81:HIS:HD2	1:K:83:ASN:H	1.54	0.54
1:B:11:ARG:NH2	1:B:67:PRO:HG2	2.22	0.54
1:E:150:LEU:HD13	1:E:151:TYR:CZ	2.42	0.54
3:T:294:PHE:C	3:T:294:PHE:CD2	2.85	0.54
2:F:166:PRO:O	2:F:167:PRO:C	2.50	0.54
2:I:130:ARG:HG3	2:I:130:ARG:NH1	2.21	0.54
3:S:253:TYR:OH	3:S:271:VAL:HG23	2.07	0.54
1:H:141:ILE:O	1:H:142:GLU:C	2.48	0.54
1:H:148:THR:HG22	1:H:152:ALA:CB	2.38	0.54
2:I:161:MET:CE	2:I:162:LYS:NZ	2.70	0.54
1:K:65:GLU:O	1:K:68:MET:N	2.40	0.54
2:L:145:LYS:CE	2:L:145:LYS:CG	2.75	0.54
3:S:247:THR:HG21	3:S:251:ILE:HB	1.89	0.54
1:B:123:ASP:HB2	1:B:124:PRO:C	2.33	0.54
2:F:133:SER:OG	2:F:134:VAL:N	2.40	0.54
1:H:117:SER:O	1:H:119:PRO:HD3	2.07	0.54
2:L:82:PRO:HA	2:L:152:ARG:HH21	1.69	0.54
2:F:157:SER:O	2:F:161:MET:HG2	2.08	0.54
1:K:14:LYS:HE3	1:K:18:ARG:NH2	2.23	0.54
2:L:84:ARG:CB	2:L:84:ARG:NE	2.70	0.54
2:C:167:PRO:O	2:C:168:GLU:C	2.51	0.54
1:E:130:ALA:O	1:E:131:GLU:C	2.49	0.54
1:H:135:THR:C	1:H:136:ASN:OD1	2.51	0.54
1:K:32:ASP:HB3	1:K:35:ASN:O	2.08	0.54
3:T:295:ILE:HD12	3:T:296:SER:OG	2.07	0.54
3:U:231:TYR:CD1	3:U:232:LEU:HD23	2.43	0.54
1:B:61:PHE:CE1	2:C:39:PRO:HD3	2.42	0.54
1:E:43:ILE:HG22	1:E:44:ALA:N	2.23	0.54
1:H:58:LEU:HD13	1:H:75:PHE:CD2	2.42	0.54
2:I:36:VAL:HG12	2:I:37:LYS:N	2.13	0.54
3:V:277:THR:HG23	3:V:280:GLN:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ASN:ND2	1:B:154:ASN:O	2.41	0.54
3:V:236:ILE:O	3:V:238:PHE:N	2.41	0.54
3:V:290:VAL:O	3:V:291:ILE:C	2.52	0.54
2:C:45:LEU:O	2:C:49:GLU:HG3	2.08	0.53
2:C:57:ASP:OD1	2:C:59:THR:HG21	2.07	0.53
2:F:53:LYS:CD	2:F:53:LYS:NZ	2.69	0.53
1:H:15:GLU:OE2	1:H:66:TYR:OH	2.25	0.53
1:K:74:ARG:NH1	2:L:41:ASN:HD22	2.06	0.53
3:S:229:PRO:CD	3:S:232:LEU:HD22	2.36	0.53
3:S:297:GLU:OE1	3:S:298:ASN:OD1	2.25	0.53
3:U:250:GLY:HA3	3:V:285:LEU:HD12	1.90	0.53
3:U:262:LEU:HD23	3:U:276:LEU:O	2.04	0.53
1:B:11:ARG:NH2	1:B:67:PRO:HG3	2.23	0.53
1:E:122:ASP:CG	1:E:122:ASP:O	2.51	0.53
1:K:27:ILE:HD11	1:K:113:GLN:CB	2.35	0.53
3:T:269:ASN:O	3:T:273:ARG:N	2.40	0.53
2:F:81:GLY:CA	2:F:87:TYR:O	2.53	0.53
2:I:132:ILE:O	2:I:136:ALA:N	2.41	0.53
1:K:32:ASP:OD2	1:K:32:ASP:C	2.50	0.53
3:V:231:TYR:CD1	3:V:232:LEU:N	2.76	0.53
1:E:38:TYR:HE1	1:E:40:HIS:CE1	2.26	0.53
1:H:65:GLU:HG3	1:H:69:ALA:H	1.73	0.53
2:I:36:VAL:CG1	2:I:37:LYS:N	2.68	0.53
2:I:92:TYR:CZ	2:I:115:ILE:HD12	2.43	0.53
3:V:232:LEU:C	3:V:241:MET:HE2	2.33	0.53
3:V:237:SER:C	3:V:239:GLU:N	2.58	0.53
1:B:127:ASN:HD21	1:B:130:ALA:H	1.57	0.53
2:L:82:PRO:HA	2:L:152:ARG:HH22	1.67	0.53
2:L:118:ASN:ND2	2:L:160:ASN:ND2	2.51	0.53
3:T:254:ASP:O	3:T:258:ILE:HG22	2.07	0.53
3:T:303:ASP:CG	3:T:304:TYR:H	2.16	0.53
3:U:230:ASP:C	3:U:232:LEU:N	2.63	0.53
2:C:78:MET:CE	2:C:78:MET:CB	2.87	0.53
2:F:160:ASN:HB3	2:F:163:LEU:HD12	1.90	0.53
1:H:138:ALA:HA	1:H:141:ILE:HG13	1.91	0.53
3:S:296:SER:O	3:S:297:GLU:CB	2.55	0.53
1:E:122:ASP:HB3	1:E:134:LYS:HZ1	1.67	0.53
2:F:59:THR:HG23	2:F:60:VAL:HG13	1.89	0.53
1:E:81:HIS:CD2	1:E:83:ASN:H	2.21	0.53
1:H:64:GLU:HG3	1:H:65:GLU:N	2.22	0.53
2:I:63:GLY:O	2:I:75:TRP:CE3	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:110:ARG:HB2	2:I:126:VAL:HA	1.91	0.53
1:K:128:ASP:O	1:K:129:VAL:C	2.52	0.53
1:B:154:ASN:HB2	1:B:156:ILE:CD1	2.38	0.53
2:L:49:GLU:O	2:L:50:GLU:C	2.51	0.53
2:L:66:ASP:O	2:L:69:ASP:HB3	2.09	0.53
2:C:174:ASN:HB2	4:F:2002:HOH:O	2.09	0.52
1:H:83:ASN:ND2	1:H:83:ASN:H	2.04	0.52
1:K:39:PHE:HB2	1:K:60:LEU:HB3	1.91	0.52
1:K:93:ASP:O	1:K:96:LYS:N	2.42	0.52
1:B:136:ASN:C	1:B:136:ASN:HD22	2.05	0.52
2:C:80:LEU:N	2:C:80:LEU:CD1	2.72	0.52
2:I:161:MET:CE	2:I:162:LYS:HZ3	2.21	0.52
3:S:261:HIS:CE1	3:S:270:PRO:HG3	2.44	0.52
1:B:127:ASN:ND2	1:B:127:ASN:C	2.67	0.52
2:C:132:ILE:HD12	2:C:135:LEU:HB2	1.90	0.52
1:E:96:LYS:O	1:E:97:ASP:C	2.52	0.52
2:F:145:LYS:O	2:F:146:VAL:C	2.49	0.52
1:H:65:GLU:O	1:H:68:MET:HB2	2.09	0.52
1:K:28:LYS:O	1:K:41:VAL:CG1	2.56	0.52
2:L:37:LYS:HE3	2:L:104:GLU:CD	2.34	0.52
2:L:140:ASN:C	2:L:140:ASN:ND2	2.61	0.52
2:L:161:MET:HE2	2:L:162:LYS:NZ	2.24	0.52
1:E:89:ARG:HD3	2:F:45:LEU:CD2	2.39	0.52
2:F:62:TRP:CH2	2:F:145:LYS:HB2	2.45	0.52
1:K:145:ARG:HG2	1:K:149:ARG:NH1	2.25	0.52
1:B:79:ILE:HG13	1:B:80:TYR:N	2.24	0.52
1:B:98:LYS:N	1:B:98:LYS:HD3	2.25	0.52
1:E:70:ALA:HA	1:E:99:TRP:CE2	2.44	0.52
2:I:79:ILE:CG2	2:I:155:MET:CE	2.79	0.52
1:K:13:ILE:HG22	1:K:17:GLN:HE21	1.74	0.52
1:K:51:PHE:CD2	1:K:79:ILE:HD11	2.45	0.52
1:H:50:PRO:CB	1:H:141:ILE:HG23	2.39	0.52
1:H:65:GLU:OE1	3:T:264:ARG:NH2	2.43	0.52
3:U:286:ALA:O	3:U:290:VAL:HG23	2.10	0.52
2:C:51:GLY:HA2	2:C:62:TRP:CZ2	2.45	0.52
2:F:118:ASN:H	2:F:160:ASN:HD22	1.58	0.52
2:I:152:ARG:CG	2:I:152:ARG:NE	2.70	0.52
1:K:37:ARG:CG	1:K:62:LEU:HB2	2.38	0.52
2:L:37:LYS:HE3	2:L:104:GLU:OE2	2.09	0.52
2:L:79:ILE:HG21	2:L:155:MET:HE1	1.92	0.52
3:V:243:GLU:OE1	3:V:256:LYS:HE3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:ALA:O	1:E:30:GLU:HG3	2.10	0.52
1:E:94:ILE:CG2	1:E:94:ILE:CD1	2.87	0.52
1:E:149:ARG:CG	1:E:149:ARG:CZ	2.87	0.52
2:F:166:PRO:O	2:F:167:PRO:O	2.27	0.52
1:H:97:ASP:OD2	1:H:97:ASP:N	2.40	0.52
2:L:84:ARG:CB	2:L:84:ARG:CD	2.82	0.52
3:S:257:ASP:O	3:S:258:ILE:C	2.50	0.52
1:E:29:ALA:O	1:E:30:GLU:CG	2.58	0.52
2:I:67:ASP:O	2:I:68:GLU:HG3	2.10	0.52
2:I:79:ILE:HD13	2:I:151:LEU:O	2.10	0.52
3:U:246:ILE:HA	3:U:251:ILE:O	2.10	0.52
1:B:88:GLY:HA3	2:C:70:MET:HE1	1.91	0.52
2:F:96:ILE:HG22	2:F:97:GLU:N	2.23	0.52
2:L:161:MET:HE1	2:L:162:LYS:NZ	2.24	0.52
3:S:246:ILE:HA	3:S:251:ILE:O	2.10	0.52
3:U:228:ILE:CG2	3:U:228:ILE:N	2.72	0.52
3:U:251:ILE:HG22	3:U:253:TYR:CZ	2.45	0.52
1:B:24:VAL:CG1	1:B:25:PRO:CD	2.88	0.51
1:B:38:TYR:CE1	1:B:40:HIS:CE1	2.87	0.51
2:C:50:GLU:OE1	2:C:145:LYS:HE2	2.10	0.51
1:H:20:LEU:HD21	1:H:31:PRO:HD2	1.91	0.51
1:H:145:ARG:O	1:H:146:ALA:C	2.53	0.51
1:K:82:PRO:CD	1:K:83:ASN:N	2.68	0.51
1:K:103:LEU:HD22	1:K:107:THR:HG21	1.92	0.51
2:I:43:ARG:NH1	2:I:140:ASN:O	2.42	0.51
3:V:282:ILE:HG22	3:V:283:PRO:O	2.10	0.51
2:F:167:PRO:CB	2:F:170:GLN:NE2	2.72	0.51
2:I:87:TYR:HD1	2:I:155:MET:HB3	1.75	0.51
1:K:120:ASN:CG	1:K:120:ASN:O	2.53	0.51
3:U:247:THR:HG21	3:U:269:ASN:ND2	2.26	0.51
1:B:24:VAL:HG13	1:B:25:PRO:CD	2.41	0.51
1:B:80:TYR:CE1	1:B:129:VAL:HG13	2.46	0.51
2:F:139:GLN:HB3	2:F:142:TYR:CD1	2.45	0.51
1:K:39:PHE:N	1:K:60:LEU:O	2.42	0.51
1:K:61:PHE:CZ	2:L:38:VAL:HA	2.45	0.51
1:K:81:HIS:HD2	1:K:83:ASN:CB	2.21	0.51
1:B:38:TYR:CD2	2:C:39:PRO:HG3	2.43	0.51
1:E:60:LEU:HA	1:E:73:VAL:HG23	1.92	0.51
1:E:74:ARG:HH21	2:F:41:ASN:ND2	2.08	0.51
2:I:60:VAL:CG1	2:I:61:SER:N	2.71	0.51
2:I:85:THR:HA	2:I:161:MET:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:58:LEU:CD2	1:K:58:LEU:H	2.23	0.51
2:L:116:ASN:O	2:L:117:MET:HB2	2.10	0.51
3:T:241:MET:HE2	3:T:253:TYR:CA	2.40	0.51
3:U:227:ASP:CA	3:U:228:ILE:HG23	2.39	0.51
1:E:24:VAL:HG12	1:E:25:PRO:N	2.23	0.51
2:L:50:GLU:OE1	2:L:145:LYS:CE	2.58	0.51
2:L:115:ILE:O	2:L:115:ILE:CG1	2.43	0.51
3:U:266:GLY:C	3:U:268:PHE:N	2.61	0.51
3:V:234:GLY:C	3:V:236:ILE:N	2.68	0.51
2:C:127:VAL:CG1	2:C:128:ASP:N	2.74	0.51
1:E:79:ILE:HG13	1:E:80:TYR:N	2.25	0.51
1:E:122:ASP:OD1	1:E:122:ASP:O	2.28	0.51
2:F:137:LYS:O	2:F:138:TRP:C	2.53	0.51
2:I:102:TYR:CG	2:I:103:PRO:HA	2.46	0.51
1:K:56:PHE:CE1	1:K:79:ILE:HD11	2.46	0.51
2:L:113:THR:HG22	2:L:114:LYS:O	2.11	0.51
1:B:87:LEU:C	2:C:70:MET:CE	2.84	0.51
1:B:149:ARG:HA	1:B:153:MET:HG3	1.91	0.51
1:E:127:ASN:HD21	1:E:130:ALA:H	1.57	0.51
1:H:142:GLU:HG2	1:H:145:ARG:NH1	2.26	0.51
3:S:268:PHE:HD1	3:S:273:ARG:HA	1.75	0.51
1:E:60:LEU:HG	1:E:73:VAL:CG2	2.41	0.50
1:H:51:PHE:HB3	1:H:56:PHE:CZ	2.45	0.50
2:L:62:TRP:CH2	2:L:145:LYS:HB2	2.46	0.50
2:L:91:ILE:N	2:L:91:ILE:HD12	2.25	0.50
1:K:78:LYS:CE	1:K:78:LYS:CG	2.80	0.50
1:B:24:VAL:CG1	1:B:25:PRO:HD2	2.40	0.50
2:I:162:LYS:O	2:I:163:LEU:O	2.29	0.50
2:L:37:LYS:NZ	2:L:37:LYS:CB	2.70	0.50
3:T:300:TRP:O	3:T:301:VAL:O	2.29	0.50
2:I:42:PHE:HA	2:I:45:LEU:HB2	1.94	0.50
1:K:104:GLN:HG3	1:K:106:ARG:N	2.26	0.50
1:B:65:GLU:O	1:B:68:MET:N	2.44	0.50
1:E:79:ILE:CG2	1:E:84:VAL:HG11	2.42	0.50
3:S:268:PHE:O	3:S:270:PRO:HD3	2.11	0.50
2:F:168:GLU:O	2:F:169:GLY:C	2.54	0.50
1:K:74:ARG:HG3	1:K:75:PHE:O	2.10	0.50
2:L:55:VAL:HG13	2:L:56:GLY:N	2.26	0.50
3:T:241:MET:CE	3:T:253:TYR:C	2.81	0.50
1:B:50:PRO:HB3	1:B:141:ILE:HG23	1.94	0.50
1:B:135:THR:HG22	1:B:136:ASN:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:80:LEU:O	2:C:81:GLY:C	2.55	0.50
1:K:29:ALA:CB	1:K:41:VAL:HG13	2.35	0.50
3:U:284:ASN:O	3:U:287:MET:HB2	2.12	0.50
1:B:151:TYR:CD1	1:B:151:TYR:N	2.74	0.50
1:E:29:ALA:C	1:E:30:GLU:CG	2.84	0.50
1:H:12:ILE:HD13	1:H:62:LEU:CD1	2.40	0.50
2:I:152:ARG:CG	2:I:152:ARG:CZ	2.89	0.50
2:L:92:TYR:CZ	2:L:115:ILE:HG22	2.41	0.50
3:T:234:GLY:C	3:T:236:ILE:H	2.20	0.50
3:T:291:ILE:O	3:T:292:ASP:C	2.55	0.50
3:U:231:TYR:HD1	3:U:232:LEU:HD22	1.76	0.50
1:E:89:ARG:HD3	2:F:45:LEU:HD21	1.94	0.50
1:H:46:PRO:HB2	1:H:49:SER:HB3	1.94	0.50
1:H:68:MET:HE3	3:T:260:GLU:HB3	1.94	0.50
2:I:118:ASN:HD22	2:I:160:ASN:ND2	2.10	0.50
3:S:253:TYR:CD1	3:S:258:ILE:HD13	2.47	0.50
3:T:287:MET:C	3:T:289:GLU:H	2.20	0.50
2:F:50:GLU:O	2:F:51:GLY:C	2.55	0.49
2:F:61:SER:O	2:F:62:TRP:HB3	2.12	0.49
1:K:49:SER:HB3	1:K:117:SER:HB3	1.93	0.49
1:K:139:GLN:O	1:K:141:ILE:N	2.45	0.49
1:H:85:ASP:O	1:H:86:LYS:C	2.55	0.49
2:I:81:GLY:HA3	2:I:87:TYR:O	2.12	0.49
2:I:143:SER:H	2:I:146:VAL:HB	1.76	0.49
1:K:29:ALA:HA	1:K:41:VAL:HA	1.94	0.49
1:K:48:ASP:N	1:K:48:ASP:OD1	2.45	0.49
3:V:231:TYR:CD1	3:V:231:TYR:C	2.88	0.49
1:E:108:VAL:O	1:E:109:LEU:C	2.52	0.49
1:K:81:HIS:CD2	1:K:83:ASN:CB	2.79	0.49
3:S:272:THR:O	3:S:274:SER:N	2.46	0.49
3:V:236:ILE:HG22	3:V:237:SER:N	2.27	0.49
2:I:78:MET:SD	2:I:78:MET:C	2.94	0.49
1:K:82:PRO:HB3	1:K:130:ALA:CA	2.42	0.49
1:K:130:ALA:O	1:K:131:GLU:O	2.30	0.49
2:L:106:PRO:HB3	2:L:135:LEU:HD23	1.95	0.49
2:F:128:ASP:OD1	2:F:129:PRO:N	2.45	0.49
1:K:82:PRO:HD2	1:K:83:ASN:H	1.73	0.49
1:B:121:PRO:O	1:B:130:ALA:HB1	2.12	0.49
1:E:14:LYS:HE2	3:U:238:PHE:O	2.13	0.49
1:E:66:TYR:CD1	1:E:67:PRO:HA	2.47	0.49
2:F:61:SER:HB3	2:F:78:MET:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:94:ILE:HA	1:K:98:LYS:O	2.12	0.49
2:L:147:VAL:O	2:L:148:LEU:C	2.52	0.49
3:S:256:LYS:CD	3:S:256:LYS:CB	2.81	0.49
1:B:8:LEU:HD12	1:B:9:PRO:CD	2.43	0.49
1:H:14:LYS:HZ1	3:T:228:ILE:HD12	1.77	0.49
2:C:54:GLY:O	2:C:55:VAL:HB	2.13	0.49
2:F:138:TRP:CD1	2:F:139:GLN:H	2.31	0.49
3:S:297:GLU:OE1	3:S:297:GLU:O	2.31	0.49
3:T:236:ILE:O	3:T:236:ILE:HG22	2.07	0.49
3:T:258:ILE:HG13	3:T:258:ILE:O	2.13	0.49
2:C:145:LYS:O	2:C:149:GLN:HG3	2.12	0.49
2:I:43:ARG:HH21	2:I:143:SER:HB3	1.74	0.49
2:I:156:MET:O	2:I:157:SER:C	2.56	0.49
1:K:9:PRO:HB2	1:K:12:ILE:HD12	1.95	0.49
1:K:78:LYS:HZ2	1:K:147:TRP:HH2	1.49	0.49
1:K:95:LEU:HD21	1:K:108:VAL:HG13	1.95	0.49
3:U:261:HIS:CD2	3:U:261:HIS:O	2.66	0.49
2:C:99:GLY:HA3	2:F:174:ASN:HD22	1.78	0.48
1:E:78:LYS:HG2	1:E:147:TRP:HZ3	1.70	0.48
2:F:66:ASP:OD2	2:F:67:ASP:N	2.46	0.48
1:H:128:ASP:C	1:H:130:ALA:N	2.68	0.48
1:H:131:GLU:OE1	1:H:135:THR:OG1	2.30	0.48
1:E:28:LYS:HG3	1:E:29:ALA:H	1.77	0.48
1:E:70:ALA:HB1	1:E:71:PRO:CD	2.43	0.48
2:F:81:GLY:H	2:F:90:ARG:H	1.60	0.48
1:K:103:LEU:CD2	1:K:107:THR:HG21	2.43	0.48
1:B:114:ALA:C	1:B:117:SER:H	2.20	0.48
1:E:15:GLU:C	1:E:17:GLN:N	2.65	0.48
1:E:72:LYS:HB3	2:F:42:PHE:CE1	2.49	0.48
2:L:61:SER:HB3	2:L:78:MET:CG	2.43	0.48
3:U:284:ASN:HD21	3:V:284:ASN:ND2	2.06	0.48
3:U:290:VAL:O	3:U:291:ILE:C	2.56	0.48
2:F:121:ASN:HB3	2:F:124:ASN:OD1	2.14	0.48
2:I:80:LEU:HD13	2:I:90:ARG:O	2.13	0.48
3:S:256:LYS:CG	3:S:256:LYS:CE	2.83	0.48
3:T:262:LEU:HD23	3:T:267:HIS:HA	1.96	0.48
2:F:114:LYS:HA	2:F:172:TYR:CE1	2.48	0.48
2:F:138:TRP:CD1	2:F:139:GLN:N	2.81	0.48
2:I:88:GLU:O	2:I:89:ASN:C	2.56	0.48
1:K:58:LEU:HD13	1:K:75:PHE:CE2	2.49	0.48
3:S:288:LYS:O	3:S:292:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:246:ILE:HG12	3:U:247:THR:H	1.78	0.48
3:U:247:THR:HG22	3:U:249:SER:CB	2.40	0.48
3:U:277:THR:HG23	3:U:280:GLN:NE2	2.28	0.48
2:F:61:SER:CB	2:F:78:MET:HB3	2.44	0.48
1:H:18:ARG:HG2	1:H:18:ARG:HH11	1.78	0.48
1:H:102:ALA:HB2	3:T:270:PRO:HB3	1.93	0.48
3:T:290:VAL:O	3:T:291:ILE:O	2.31	0.48
3:U:286:ALA:HB2	3:V:252:THR:OG1	2.13	0.48
1:B:74:ARG:CG	1:B:75:PHE:N	2.73	0.48
1:B:136:ASN:C	1:B:136:ASN:ND2	2.65	0.48
1:K:12:ILE:O	1:K:13:ILE:C	2.56	0.48
3:U:231:TYR:CD1	3:U:232:LEU:HD22	2.48	0.48
3:U:295:ILE:CG1	3:U:295:ILE:CA	2.81	0.48
1:H:22:GLU:O	1:H:22:GLU:HG2	2.13	0.48
2:I:47:GLU:O	2:I:48:LEU:C	2.53	0.48
1:K:105:ILE:O	1:K:106:ARG:C	2.56	0.48
1:B:127:ASN:ND2	1:B:129:VAL:H	2.12	0.48
2:C:174:ASN:OXT	2:F:100:PRO:HG2	2.13	0.48
1:H:35:ASN:HB3	1:H:38:TYR:HB3	1.96	0.48
2:I:95:LYS:HD2	2:I:112:VAL:CG2	2.43	0.48
2:I:171:CYS:O	2:I:171:CYS:SG	2.71	0.48
3:T:243:GLU:N	3:T:244:PRO:HD3	2.29	0.48
3:T:298:ASN:C	3:T:298:ASN:ND2	2.72	0.48
1:B:21:ALA:C	1:B:23:PRO:HD3	2.38	0.48
1:E:39:PHE:CD1	1:E:39:PHE:N	2.82	0.48
2:F:56:GLY:C	2:F:57:ASP:O	2.56	0.48
1:H:84:VAL:CG1	1:H:88:GLY:HA2	2.43	0.48
1:H:92:LEU:HB3	1:H:95:LEU:HD12	1.96	0.48
1:H:116:LEU:HA	1:H:116:LEU:HD23	1.49	0.48
2:I:102:TYR:C	2:I:102:TYR:CD2	2.90	0.48
1:K:120:ASN:OD1	1:K:122:ASP:HB2	2.13	0.48
2:L:153:ARG:O	2:L:156:MET:N	2.35	0.48
2:C:81:GLY:HA3	2:C:87:TYR:O	2.14	0.47
1:K:82:PRO:HD2	1:K:83:ASN:N	2.29	0.47
1:K:142:GLU:CB	1:K:142:GLU:CD	2.80	0.47
2:L:157:SER:C	2:L:159:GLU:N	2.71	0.47
3:U:248:PRO:HA	3:V:282:ILE:HG13	1.95	0.47
2:C:45:LEU:O	2:C:46:GLU:C	2.48	0.47
1:H:49:SER:O	1:H:50:PRO:C	2.55	0.47
2:I:132:ILE:O	2:I:135:LEU:HB2	2.14	0.47
1:K:75:PHE:HB2	1:K:88:GLY:CA	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:LYS:NZ	2:C:145:LYS:CD	2.71	0.47
1:H:6:ALA:N	1:H:8:LEU:HD23	2.29	0.47
2:I:40:ARG:HG2	2:I:44:LEU:HD12	1.96	0.47
1:K:145:ARG:HG2	1:K:149:ARG:HH12	1.79	0.47
3:U:260:GLU:O	3:U:261:HIS:C	2.56	0.47
1:B:111:SER:O	1:B:114:ALA:N	2.44	0.47
2:C:129:PRO:HG2	2:C:130:ARG:H	1.78	0.47
2:C:153:ARG:CB	2:C:153:ARG:CD	2.86	0.47
1:E:115:LEU:O	1:E:116:LEU:C	2.57	0.47
1:E:127:ASN:ND2	1:E:129:VAL:H	2.11	0.47
1:H:64:GLU:HB3	2:I:36:VAL:HG21	1.96	0.47
2:L:86:ILE:HG12	2:L:86:ILE:O	2.14	0.47
3:S:295:ILE:HG22	3:S:296:SER:N	2.29	0.47
3:T:282:ILE:HG22	3:T:283:PRO:O	2.13	0.47
3:V:267:HIS:HB3	3:V:276:LEU:O	2.14	0.47
1:B:74:ARG:HG3	1:B:75:PHE:N	2.29	0.47
1:B:85:ASP:C	1:B:85:ASP:OD1	2.57	0.47
1:B:134:LYS:CG	1:B:134:LYS:HZ3	2.24	0.47
2:F:162:LYS:O	2:F:163:LEU:C	2.47	0.47
1:H:46:PRO:HG3	1:H:116:LEU:HB2	1.95	0.47
1:K:60:LEU:HA	1:K:73:VAL:HG12	1.96	0.47
1:E:94:ILE:CG2	1:E:94:ILE:CA	2.81	0.47
1:E:132:GLN:O	1:E:133:TRP:C	2.58	0.47
2:L:40:ARG:HD2	2:L:102:TYR:H	1.78	0.47
3:U:290:VAL:HG11	3:V:290:VAL:HG11	1.95	0.47
3:V:259:GLU:O	3:V:262:LEU:HB2	2.14	0.47
1:B:52:GLU:O	1:B:54:GLY:N	2.47	0.47
1:B:107:THR:HB	1:B:108:VAL:H	1.45	0.47
1:B:131:GLU:HA	1:B:131:GLU:OE1	2.15	0.47
1:H:155:ASN:N	1:H:155:ASN:OD1	2.48	0.47
2:I:161:MET:HE2	2:I:162:LYS:HD2	1.96	0.47
1:K:24:VAL:HG11	1:K:27:ILE:HD12	1.96	0.47
1:K:46:PRO:CD	1:K:116:LEU:CD1	2.83	0.47
1:K:74:ARG:HH12	2:L:41:ASN:HD22	1.61	0.47
1:K:116:LEU:C	1:K:118:ALA:H	2.22	0.47
3:U:284:ASN:C	3:U:284:ASN:OD1	2.56	0.47
1:B:53:GLY:HA3	1:B:153:MET:HE2	1.97	0.47
2:C:48:LEU:HD12	2:C:48:LEU:HA	1.69	0.47
2:I:82:PRO:HB3	2:I:85:THR:CG2	2.38	0.47
2:I:115:ILE:CG2	2:I:120:VAL:HG11	2.45	0.47
2:L:126:VAL:CG1	2:L:127:VAL:H	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:277:THR:HG23	3:U:280:GLN:HE21	1.79	0.47
2:F:137:LYS:C	2:F:138:TRP:O	2.57	0.47
1:H:24:VAL:HG22	1:H:106:ARG:NH1	2.30	0.47
1:H:65:GLU:HG3	1:H:69:ALA:HB2	1.93	0.47
2:I:82:PRO:HD3	2:I:152:ARG:HG2	1.97	0.47
2:I:132:ILE:HG21	2:I:135:LEU:HD12	1.97	0.47
2:L:80:LEU:N	2:L:80:LEU:CD1	2.78	0.47
3:U:235:LYS:O	3:U:238:PHE:HE1	1.97	0.47
3:U:250:GLY:CA	3:V:285:LEU:HD12	2.44	0.47
3:V:237:SER:HB2	3:V:257:ASP:OD2	2.15	0.47
1:B:97:ASP:C	1:B:99:TRP:N	2.72	0.46
1:K:134:LYS:C	1:K:134:LYS:CD	2.88	0.46
3:S:258:ILE:HD12	3:S:258:ILE:HA	1.62	0.46
3:U:284:ASN:ND2	3:V:284:ASN:ND2	2.63	0.46
1:E:51:PHE:CD2	1:E:79:ILE:CD1	2.98	0.46
2:I:132:ILE:O	2:I:135:LEU:N	2.39	0.46
2:L:82:PRO:CA	2:L:152:ARG:HH21	2.25	0.46
2:L:106:PRO:HB3	2:L:135:LEU:CD2	2.45	0.46
3:T:236:ILE:HB	4:T:2002:HOH:O	2.15	0.46
3:U:242:ARG:O	3:U:243:GLU:CB	2.63	0.46
1:B:130:ALA:O	1:B:131:GLU:O	2.33	0.46
2:C:49:GLU:C	2:C:51:GLY:N	2.60	0.46
2:C:53:LYS:CD	2:C:53:LYS:NZ	2.73	0.46
2:C:86:ILE:HB	2:C:161:MET:O	2.15	0.46
1:K:77:THR:HG23	1:K:151:TYR:O	2.15	0.46
3:T:234:GLY:HA3	3:T:237:SER:H	1.81	0.46
2:C:83:PRO:HB2	2:C:84:ARG:HG2	1.98	0.46
2:F:120:VAL:O	2:F:121:ASN:C	2.57	0.46
1:H:20:LEU:O	1:H:21:ALA:C	2.58	0.46
1:H:78:LYS:HE2	1:H:78:LYS:HB3	1.40	0.46
1:H:131:GLU:O	1:H:134:LYS:HG2	2.15	0.46
2:I:46:GLU:C	2:I:48:LEU:N	2.73	0.46
1:K:74:ARG:HB2	1:K:88:GLY:O	2.14	0.46
1:H:65:GLU:HB2	3:T:264:ARG:HH22	1.81	0.46
2:I:61:SER:C	2:I:62:TRP:HE3	2.23	0.46
2:I:114:LYS:HA	2:I:172:TYR:CE1	2.51	0.46
1:K:93:ASP:O	1:K:94:ILE:C	2.58	0.46
1:K:142:GLU:C	1:K:144:ALA:N	2.73	0.46
3:V:255:ARG:O	3:V:256:LYS:C	2.58	0.46
1:B:41:VAL:HB	1:B:58:LEU:HB2	1.96	0.46
2:I:96:ILE:HG23	2:I:109:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:13:ILE:O	1:K:17:GLN:HB2	2.16	0.46
2:L:83:PRO:HA	2:L:88:GLU:HB3	1.97	0.46
3:T:235:LYS:HA	3:T:235:LYS:HD2	1.46	0.46
2:C:97:GLU:HB3	2:C:108:PHE:HB2	1.97	0.46
1:H:65:GLU:HG3	1:H:65:GLU:O	2.16	0.46
2:I:39:PRO:O	2:I:40:ARG:C	2.58	0.46
2:I:139:GLN:HB2	2:I:142:TYR:CG	2.51	0.46
2:L:45:LEU:HD23	2:L:45:LEU:HA	1.71	0.46
2:L:81:GLY:HA2	2:L:82:PRO:HD2	1.66	0.46
3:S:248:PRO:O	3:S:249:SER:C	2.54	0.46
3:V:247:THR:CG2	3:V:269:ASN:ND2	2.78	0.46
2:C:165:GLN:CB	2:C:166:PRO:HD2	2.34	0.46
1:E:38:TYR:CE1	1:E:40:HIS:CE1	3.03	0.46
2:F:142:TYR:N	2:F:142:TYR:CD2	2.83	0.46
1:H:81:HIS:CE1	1:H:116:LEU:HA	2.49	0.46
2:I:113:THR:HA	2:I:171:CYS:CB	2.45	0.46
2:C:49:GLU:O	2:C:50:GLU:C	2.55	0.46
1:E:43:ILE:CG2	1:E:44:ALA:N	2.79	0.46
1:K:68:MET:CE	3:V:265:VAL:CG2	2.90	0.46
1:K:134:LYS:C	1:K:134:LYS:HD2	2.41	0.46
2:L:85:THR:CG2	2:L:155:MET:O	2.64	0.46
3:V:247:THR:HG23	3:V:249:SER:N	2.10	0.46
2:F:105:ALA:CB	2:F:106:PRO:HD2	2.36	0.45
3:S:278:GLN:NE2	3:S:281:LEU:HD12	2.31	0.45
1:B:97:ASP:OD1	1:B:97:ASP:N	2.48	0.45
2:I:88:GLU:O	2:I:89:ASN:O	2.34	0.45
2:I:139:GLN:C	2:I:141:SER:H	2.23	0.45
1:K:100:SER:C	1:K:102:ALA:H	2.24	0.45
2:L:37:LYS:HB2	2:L:37:LYS:HZ3	1.81	0.45
3:V:258:ILE:O	3:V:258:ILE:CG1	2.59	0.45
1:B:4:GLY:O	1:B:5:SER:CB	2.63	0.45
2:C:114:LYS:HZ2	2:C:170:GLN:HE21	1.64	0.45
1:K:15:GLU:OE1	1:K:104:GLN:HB2	2.16	0.45
3:S:247:THR:O	3:S:250:GLY:CA	2.64	0.45
3:S:291:ILE:O	3:S:292:ASP:C	2.59	0.45
3:U:263:GLN:HB3	3:U:264:ARG:H	1.58	0.45
1:E:49:SER:HB2	1:E:51:PHE:HD1	1.81	0.45
2:F:165:GLN:HB3	2:F:166:PRO:CD	2.47	0.45
1:H:24:VAL:CG1	1:H:25:PRO:HD2	2.46	0.45
1:K:41:VAL:O	1:K:58:LEU:HD23	2.17	0.45
3:V:269:ASN:CA	3:V:276:LEU:HD23	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.71	0.45
2:F:50:GLU:HG3	2:F:62:TRP:HZ2	1.81	0.45
1:K:81:HIS:CD2	1:K:82:PRO:HD2	2.49	0.45
3:S:247:THR:HG21	3:S:269:ASN:ND2	2.31	0.45
3:S:258:ILE:CG2	3:S:259:GLU:N	2.76	0.45
3:T:298:ASN:ND2	3:T:300:TRP:CE3	2.85	0.45
3:U:234:GLY:H	3:U:241:MET:HG3	1.81	0.45
3:U:234:GLY:N	3:U:241:MET:HG3	2.31	0.45
1:E:71:PRO:HD3	1:E:99:TRP:CH2	2.52	0.45
1:E:100:SER:H	1:E:103:LEU:CD1	2.30	0.45
1:H:81:HIS:HA	1:H:82:PRO:HD3	1.73	0.45
2:I:56:GLY:C	2:I:58:GLY:N	2.74	0.45
3:S:287:MET:CA	3:S:287:MET:HE3	2.36	0.45
1:B:51:PHE:CE2	1:B:79:ILE:HD11	2.52	0.45
1:E:149:ARG:HG2	1:E:149:ARG:NH1	2.09	0.45
3:V:235:LYS:NZ	3:V:235:LYS:CD	2.75	0.45
3:V:245:CYS:CB	3:V:283:PRO:HA	2.45	0.45
1:B:96:LYS:CB	1:B:97:ASP:OD1	2.64	0.45
2:F:80:LEU:HA	2:F:80:LEU:HD13	1.36	0.45
2:I:73:THR:HG22	2:I:74:ARG:HG2	1.99	0.45
1:K:73:VAL:O	1:K:74:ARG:CB	2.63	0.45
1:B:98:LYS:HA	1:B:98:LYS:HD2	1.62	0.45
1:E:51:PHE:CE2	1:E:79:ILE:CD1	2.94	0.45
1:E:78:LYS:HG2	1:E:147:TRP:CE3	2.52	0.45
1:H:148:THR:O	1:H:152:ALA:CB	2.64	0.45
2:I:144:ILE:HG22	2:I:148:LEU:HD12	1.98	0.45
3:T:298:ASN:C	3:T:298:ASN:HD22	2.25	0.45
3:V:237:SER:OG	3:V:239:GLU:HG2	2.17	0.45
1:B:115:LEU:O	1:B:116:LEU:C	2.60	0.45
1:E:73:VAL:HG11	1:E:112:ILE:HD11	1.99	0.45
1:H:32:ASP:HB2	1:H:40:HIS:CD2	2.51	0.45
1:H:81:HIS:CD2	1:H:82:PRO:HD2	2.51	0.45
2:L:82:PRO:O	2:L:85:THR:OG1	2.35	0.45
3:T:254:ASP:OD1	3:T:255:ARG:N	2.49	0.45
1:H:109:LEU:HA	1:H:109:LEU:HD23	1.54	0.44
1:K:68:MET:CE	3:V:261:HIS:HA	2.47	0.44
1:K:78:LYS:HG2	1:K:147:TRP:CZ3	2.53	0.44
1:K:80:TYR:CB	1:K:144:ALA:HA	2.46	0.44
1:K:82:PRO:HA	1:K:129:VAL:HB	1.99	0.44
3:T:253:TYR:OH	3:T:269:ASN:ND2	2.50	0.44
3:U:233:CYS:C	3:U:241:MET:HE2	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:278:GLN:O	3:V:279:GLU:C	2.58	0.44
1:H:78:LYS:HE2	1:H:147:TRP:CZ3	2.52	0.44
1:K:109:LEU:H	1:K:109:LEU:CD2	2.27	0.44
2:L:79:ILE:HG21	2:L:155:MET:CE	2.47	0.44
3:S:231:TYR:CD1	3:S:232:LEU:CD1	3.01	0.44
3:U:285:LEU:HB2	4:V:2003:HOH:O	2.16	0.44
2:C:75:TRP:CD1	2:C:75:TRP:N	2.85	0.44
1:E:127:ASN:C	1:E:127:ASN:ND2	2.66	0.44
1:K:67:PRO:C	1:K:69:ALA:H	2.25	0.44
3:U:293:ALA:HB3	3:U:294:PHE:H	1.37	0.44
3:V:294:PHE:CD2	3:V:294:PHE:C	2.95	0.44
2:C:44:LEU:HD23	2:C:44:LEU:HA	1.78	0.44
1:E:35:ASN:ND2	1:E:35:ASN:C	2.72	0.44
1:E:104:GLN:O	1:E:105:ILE:C	2.60	0.44
1:K:49:SER:CB	1:K:117:SER:HB3	2.48	0.44
3:U:257:ASP:OD2	3:U:257:ASP:N	2.49	0.44
3:V:254:ASP:O	3:V:255:ARG:C	2.60	0.44
1:B:22:GLU:CB	1:B:22:GLU:CD	2.84	0.44
1:B:118:ALA:N	1:B:119:PRO:HD3	2.32	0.44
1:H:82:PRO:HD2	1:H:83:ASN:HD21	1.83	0.44
1:E:51:PHE:HD1	1:E:51:PHE:H	1.64	0.44
1:H:115:LEU:HD12	1:H:115:LEU:HA	1.62	0.44
2:I:120:VAL:O	2:I:121:ASN:C	2.59	0.44
1:K:87:LEU:HD23	1:K:87:LEU:HA	1.71	0.44
3:V:269:ASN:C	3:V:269:ASN:OD1	2.59	0.44
2:C:143:SER:O	2:C:146:VAL:N	2.50	0.44
1:E:106:ARG:HH11	1:E:106:ARG:HD3	1.41	0.44
1:E:123:ASP:H	1:E:124:PRO:CA	2.31	0.44
2:I:82:PRO:HA	2:I:83:PRO:HD3	1.70	0.44
2:I:144:ILE:CG2	2:I:148:LEU:HD12	2.47	0.44
2:I:163:LEU:HA	2:I:164:PRO:HD2	1.74	0.44
3:S:247:THR:CG2	3:S:251:ILE:HB	2.47	0.44
3:V:236:ILE:O	3:V:238:PHE:CD1	2.70	0.44
1:H:10:ARG:C	1:H:12:ILE:N	2.75	0.44
1:H:44:ALA:O	1:H:46:PRO:HD3	2.18	0.44
2:I:56:GLY:O	2:I:58:GLY:N	2.51	0.44
2:I:137:LYS:O	2:I:138:TRP:C	2.61	0.44
1:K:58:LEU:N	1:K:58:LEU:HD22	2.32	0.44
3:V:254:ASP:C	3:V:254:ASP:OD1	2.61	0.44
2:C:87:TYR:O	2:C:88:GLU:C	2.61	0.44
2:C:174:ASN:O	2:F:101:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:229:PRO:CG	3:S:232:LEU:HD22	2.47	0.44
1:E:24:VAL:CG1	1:E:25:PRO:CD	2.96	0.43
1:E:118:ALA:O	1:E:119:PRO:C	2.60	0.43
2:I:140:ASN:ND2	2:I:140:ASN:N	2.62	0.43
2:L:55:VAL:CG1	2:L:56:GLY:N	2.76	0.43
2:L:98:CYS:O	2:L:99:GLY:O	2.35	0.43
1:E:76:MET:C	2:F:70:MET:CE	2.91	0.43
2:F:62:TRP:CZ3	2:F:145:LYS:HB2	2.53	0.43
1:K:37:ARG:HG2	1:K:62:LEU:O	2.18	0.43
1:K:80:TYR:HB2	1:K:147:TRP:CD2	2.53	0.43
1:K:123:ASP:HB2	1:K:124:PRO:O	2.18	0.43
3:U:261:HIS:CE1	3:U:270:PRO:HG3	2.53	0.43
3:U:262:LEU:CD2	3:U:276:LEU:HB3	2.49	0.43
1:E:12:ILE:HD11	1:E:66:TYR:HD2	1.82	0.43
2:I:135:LEU:HD23	2:I:135:LEU:HA	1.48	0.43
2:I:168:GLU:HG2	2:I:169:GLY:N	2.33	0.43
3:V:284:ASN:OD1	3:V:287:MET:HB2	2.18	0.43
1:B:29:ALA:O	1:B:30:GLU:HG3	2.17	0.43
1:E:15:GLU:O	1:E:16:THR:C	2.60	0.43
1:E:60:LEU:HG	1:E:73:VAL:HG21	2.00	0.43
1:H:32:ASP:CB	1:H:40:HIS:HE2	2.26	0.43
1:H:117:SER:O	1:H:119:PRO:CD	2.66	0.43
2:I:113:THR:HA	2:I:171:CYS:HB2	2.00	0.43
3:U:266:GLY:HA3	3:U:268:PHE:CD2	2.54	0.43
3:V:268:PHE:N	3:V:268:PHE:CD2	2.86	0.43
1:B:154:ASN:CA	1:B:156:ILE:HG12	2.49	0.43
2:C:152:ARG:O	2:C:153:ARG:C	2.62	0.43
1:E:92:LEU:HD12	1:E:95:LEU:CD1	2.48	0.43
2:F:96:ILE:CG2	2:F:97:GLU:N	2.77	0.43
1:H:18:ARG:HH11	1:H:18:ARG:CG	2.32	0.43
1:H:95:LEU:HD23	1:H:95:LEU:HA	1.48	0.43
1:H:117:SER:C	1:H:119:PRO:HD3	2.44	0.43
2:I:114:LYS:H	2:I:171:CYS:CB	2.32	0.43
2:I:130:ARG:HH11	2:I:130:ARG:CG	2.30	0.43
2:I:151:LEU:O	2:I:152:ARG:HB2	2.18	0.43
1:K:20:LEU:O	1:K:21:ALA:C	2.60	0.43
1:K:150:LEU:HB3	1:K:151:TYR:CD1	2.54	0.43
2:C:85:THR:C	2:C:87:TYR:H	2.26	0.43
1:E:18:ARG:O	1:E:22:GLU:N	2.51	0.43
2:F:40:ARG:NE	2:F:99:GLY:O	2.49	0.43
2:I:45:LEU:HD23	2:I:45:LEU:HA	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:63:GLY:C	2:I:75:TRP:CE3	2.96	0.43
1:K:50:PRO:HG2	1:K:51:PHE:CE1	2.54	0.43
2:L:140:ASN:C	2:L:142:TYR:N	2.76	0.43
3:U:262:LEU:HA	3:U:266:GLY:O	2.18	0.43
3:U:268:PHE:CD1	3:U:273:ARG:HA	2.44	0.43
3:U:287:MET:HE3	3:V:286:ALA:CB	2.48	0.43
3:V:261:HIS:O	3:V:262:LEU:C	2.61	0.43
2:C:128:ASP:OD1	2:C:128:ASP:C	2.62	0.43
1:E:78:LYS:NZ	2:F:68:GLU:HB3	2.33	0.43
2:F:83:PRO:HA	2:F:88:GLU:CD	2.43	0.43
2:I:82:PRO:HD3	2:I:152:ARG:NH1	2.33	0.43
3:S:257:ASP:O	3:S:259:GLU:N	2.51	0.43
3:V:237:SER:CB	3:V:257:ASP:OD2	2.67	0.43
2:C:149:GLN:HG3	2:C:149:GLN:H	1.54	0.43
1:E:24:VAL:HG12	1:E:25:PRO:O	2.18	0.43
1:H:14:LYS:O	1:H:18:ARG:HD3	2.18	0.43
1:H:47:GLN:O	1:H:48:ASP:HB2	2.18	0.43
1:H:113:GLN:C	1:H:115:LEU:N	2.75	0.43
2:I:142:TYR:O	2:I:143:SER:HB3	2.17	0.43
2:L:99:GLY:C	2:L:101:LYS:H	2.26	0.43
3:S:275:PRO:O	3:S:276:LEU:HB2	2.19	0.43
3:V:245:CYS:O	3:V:245:CYS:SG	2.76	0.43
1:H:22:GLU:HA	1:H:23:PRO:HD3	1.65	0.43
1:H:131:GLU:OE1	1:H:131:GLU:C	2.61	0.43
2:I:145:LYS:HG3	2:I:146:VAL:N	2.33	0.43
3:S:267:HIS:N	3:S:267:HIS:HD2	2.12	0.43
2:F:132:ILE:HG21	2:F:132:ILE:HD12	1.49	0.43
1:K:80:TYR:CE2	1:K:140:ALA:O	2.71	0.43
1:K:84:VAL:HG12	1:K:85:ASP:O	2.19	0.43
3:S:240:LEU:HD12	3:S:240:LEU:HA	1.86	0.43
3:T:263:GLN:H	3:T:263:GLN:HG2	1.61	0.43
1:B:134:LYS:NZ	1:B:134:LYS:HB2	2.30	0.42
2:C:75:TRP:HB2	2:C:96:ILE:HB	2.01	0.42
1:E:128:ASP:C	1:E:131:GLU:H	2.27	0.42
2:F:134:VAL:HB	2:F:150:GLU:HG3	2.01	0.42
3:T:288:LYS:CD	3:T:288:LYS:NZ	2.76	0.42
1:B:18:ARG:O	1:B:22:GLU:N	2.50	0.42
1:B:97:ASP:C	1:B:99:TRP:H	2.26	0.42
1:E:22:GLU:HA	1:E:23:PRO:HD3	1.64	0.42
1:E:51:PHE:O	1:E:52:GLU:C	2.62	0.42
1:E:121:PRO:O	1:E:122:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:64:LEU:HD23	2:I:64:LEU:HA	1.77	0.42
1:K:148:THR:O	1:K:152:ALA:HB3	2.19	0.42
2:L:93:SER:O	2:L:94:LEU:HG	2.19	0.42
3:U:289:GLU:OE1	3:V:231:TYR:HB2	2.19	0.42
3:U:290:VAL:O	3:U:293:ALA:HB3	2.18	0.42
2:C:129:PRO:CG	2:C:130:ARG:N	2.81	0.42
2:C:167:PRO:HG3	2:C:170:GLN:OE1	2.19	0.42
1:E:94:ILE:CD1	1:E:94:ILE:HG21	2.49	0.42
2:I:83:PRO:CA	2:I:88:GLU:OE1	2.61	0.42
2:L:132:ILE:O	2:L:132:ILE:CG1	2.52	0.42
3:U:242:ARG:HG3	3:U:242:ARG:NH1	2.23	0.42
3:U:264:ARG:HE	3:U:264:ARG:HB3	1.57	0.42
2:C:78:MET:HE2	2:C:78:MET:CB	2.46	0.42
2:F:82:PRO:O	2:F:88:GLU:HA	2.20	0.42
1:K:62:LEU:HD23	1:K:62:LEU:HA	1.46	0.42
2:L:44:LEU:O	2:L:47:GLU:N	2.52	0.42
2:L:50:GLU:O	2:L:50:GLU:HG2	2.19	0.42
3:T:230:ASP:O	3:T:233:CYS:N	2.51	0.42
1:B:66:TYR:CG	1:B:67:PRO:HA	2.55	0.42
1:B:116:LEU:HD23	1:B:116:LEU:H	1.81	0.42
2:C:115:ILE:HG13	2:C:116:ASN:N	2.35	0.42
2:F:132:ILE:HG23	2:F:132:ILE:HD13	1.53	0.42
2:F:151:LEU:HA	2:F:151:LEU:HD23	1.90	0.42
1:K:43:ILE:HD13	1:K:58:LEU:HD11	2.01	0.42
1:K:54:GLY:HA3	1:K:152:ALA:CB	2.48	0.42
1:K:59:GLU:OE2	1:K:74:ARG:NH1	2.46	0.42
1:K:144:ALA:C	1:K:147:TRP:HB2	2.38	0.42
2:L:52:GLN:C	2:L:54:GLY:H	2.27	0.42
3:S:265:VAL:O	3:S:265:VAL:HG12	2.19	0.42
3:S:284:ASN:ND2	3:S:287:MET:HG3	2.34	0.42
3:T:277:THR:HG22	3:T:278:GLN:CA	2.47	0.42
3:V:230:ASP:O	3:V:233:CYS:N	2.52	0.42
1:H:91:CYS:HB2	1:H:96:LYS:HZ1	1.77	0.42
2:I:60:VAL:HG13	2:I:61:SER:N	2.35	0.42
2:I:114:LYS:HD3	2:I:170:GLN:OE1	2.20	0.42
1:K:19:LEU:HD23	1:K:19:LEU:HA	1.36	0.42
3:S:282:ILE:HG23	3:S:283:PRO:HD2	2.01	0.42
3:U:236:ILE:O	3:U:236:ILE:CG2	2.65	0.42
1:B:100:SER:HA	1:B:101:PRO:HD3	1.90	0.42
1:B:150:LEU:HB3	1:B:151:TYR:CD1	2.55	0.42
1:B:150:LEU:CD1	1:B:151:TYR:CE1	2.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:ALA:HB2	1:E:99:TRP:CD2	2.55	0.42
2:L:113:THR:HG22	2:L:114:LYS:N	2.34	0.42
3:T:229:PRO:HD2	3:T:232:LEU:HD22	2.01	0.42
1:B:11:ARG:HD3	1:B:67:PRO:HG3	2.02	0.42
2:C:129:PRO:O	2:C:130:ARG:C	2.62	0.42
2:C:165:GLN:H	2:C:165:GLN:HG2	1.55	0.42
1:E:149:ARG:NH1	1:E:149:ARG:HG3	2.27	0.42
2:I:85:THR:O	2:I:88:GLU:HG3	2.20	0.42
1:K:72:LYS:HZ2	1:K:72:LYS:HG2	1.63	0.42
1:K:128:ASP:C	1:K:130:ALA:H	2.26	0.42
1:B:134:LYS:CB	1:B:134:LYS:HZ3	2.33	0.42
1:E:128:ASP:O	1:E:131:GLU:N	2.52	0.42
2:F:80:LEU:HD22	2:F:80:LEU:N	2.35	0.42
2:F:124:ASN:OD1	2:F:124:ASN:N	2.53	0.42
1:H:53:GLY:CA	1:H:153:MET:CE	2.87	0.42
1:H:54:GLY:HA3	1:H:148:THR:HG22	2.02	0.42
1:H:114:ALA:O	1:H:115:LEU:C	2.62	0.42
3:S:229:PRO:HG2	3:S:232:LEU:HD22	2.01	0.42
3:T:231:TYR:HD1	3:T:232:LEU:CD1	2.27	0.42
3:U:274:SER:HA	3:U:275:PRO:HD3	1.85	0.42
1:E:15:GLU:OE1	1:E:104:GLN:HB2	2.20	0.42
1:E:61:PHE:CE1	2:F:39:PRO:HD3	2.55	0.42
1:K:105:ILE:HB	1:K:106:ARG:H	1.68	0.42
2:L:132:ILE:HG21	2:L:132:ILE:HD13	1.64	0.42
2:L:139:GLN:HB3	2:L:142:TYR:CE1	2.54	0.42
3:S:273:ARG:O	3:S:274:SER:C	2.62	0.42
1:B:10:ARG:O	1:B:11:ARG:C	2.63	0.41
2:C:132:ILE:HD12	2:C:132:ILE:HG23	1.95	0.41
2:F:153:ARG:HD2	2:F:153:ARG:N	2.35	0.41
2:I:167:PRO:HG2	2:I:170:GLN:NE2	2.34	0.41
1:K:128:ASP:O	1:K:130:ALA:N	2.52	0.41
3:S:282:ILE:HG22	3:S:283:PRO:N	2.35	0.41
3:V:262:LEU:HD23	3:V:266:GLY:O	2.20	0.41
1:H:127:ASN:OD1	1:H:129:VAL:N	2.53	0.41
1:H:134:LYS:CG	1:H:135:THR:N	2.83	0.41
2:I:73:THR:HG22	2:I:74:ARG:CG	2.50	0.41
1:K:16:THR:O	1:K:17:GLN:C	2.62	0.41
2:L:54:GLY:O	2:L:55:VAL:CG2	2.68	0.41
2:L:153:ARG:NH1	2:L:153:ARG:CB	2.83	0.41
3:U:238:PHE:CD1	3:U:238:PHE:N	2.88	0.41
3:U:295:ILE:C	3:U:295:ILE:CG2	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ALA:HB1	1:B:8:LEU:H	1.85	0.41
1:H:93:ASP:O	1:H:95:LEU:N	2.54	0.41
1:E:14:LYS:O	1:E:17:GLN:HB2	2.20	0.41
1:E:15:GLU:C	1:E:17:GLN:H	2.28	0.41
2:F:44:LEU:CD2	2:F:102:TYR:CE2	2.87	0.41
1:H:73:VAL:O	1:H:90:ILE:HD12	2.21	0.41
3:T:293:ALA:HB3	3:T:294:PHE:H	1.62	0.41
1:B:66:TYR:CD1	1:B:67:PRO:HA	2.55	0.41
1:H:80:TYR:CZ	1:H:129:VAL:HG13	2.56	0.41
1:H:93:ASP:C	1:H:95:LEU:N	2.77	0.41
1:K:38:TYR:C	1:K:39:PHE:CD1	2.99	0.41
3:S:237:SER:O	3:S:238:PHE:CB	2.52	0.41
1:E:59:GLU:O	1:E:59:GLU:HG3	2.19	0.41
2:F:129:PRO:C	2:F:131:ALA:N	2.72	0.41
2:F:148:LEU:O	2:F:149:GLN:C	2.61	0.41
1:H:27:ILE:HD12	1:H:113:GLN:OE1	2.20	0.41
1:H:150:LEU:HD22	1:H:151:TYR:CG	2.56	0.41
1:K:5:SER:O	1:K:8:LEU:HD22	2.20	0.41
1:K:18:ARG:HG3	1:K:18:ARG:HH11	1.85	0.41
1:K:66:TYR:CD1	1:K:67:PRO:HA	2.55	0.41
3:V:236:ILE:HD13	3:V:236:ILE:HG21	1.84	0.41
2:C:161:MET:HE3	2:C:161:MET:HB3	1.65	0.41
2:F:44:LEU:O	2:F:45:LEU:C	2.60	0.41
1:H:20:LEU:C	1:H:22:GLU:N	2.78	0.41
2:I:86:ILE:O	2:I:86:ILE:HG13	2.20	0.41
1:K:92:LEU:HA	1:K:92:LEU:HD23	1.56	0.41
2:L:58:GLY:O	2:L:59:THR:HB	2.20	0.41
3:S:297:GLU:OE1	3:S:297:GLU:CA	2.68	0.41
3:T:253:TYR:CE2	3:T:270:PRO:HG2	2.56	0.41
3:U:269:ASN:C	3:U:271:VAL:N	2.77	0.41
1:E:74:ARG:NH2	2:F:41:ASN:ND2	2.69	0.41
2:F:83:PRO:HA	2:F:88:GLU:OE1	2.21	0.41
1:H:50:PRO:HB3	1:H:141:ILE:HG23	2.02	0.41
3:S:227:ASP:C	3:S:228:ILE:HG13	2.45	0.41
3:U:245:CYS:O	3:U:252:THR:HA	2.20	0.41
3:U:261:HIS:ND1	3:U:270:PRO:HG3	2.35	0.41
1:B:9:PRO:O	1:B:13:ILE:HD12	2.21	0.41
1:B:101:PRO:HG2	3:S:261:HIS:ND1	2.36	0.41
2:C:96:ILE:HG22	2:C:97:GLU:N	2.33	0.41
1:E:58:LEU:HG	1:E:75:PHE:HA	2.03	0.41
2:F:119:GLY:O	2:F:127:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:129:PRO:O	2:F:130:ARG:C	2.56	0.41
2:I:49:GLU:HA	2:I:52:GLN:HE21	1.85	0.41
2:L:40:ARG:HG3	2:L:44:LEU:HD11	2.02	0.41
2:L:87:TYR:CE1	2:L:155:MET:HB3	2.56	0.41
2:L:104:GLU:HA	2:L:104:GLU:OE1	2.21	0.41
3:S:236:ILE:O	3:S:237:SER:C	2.62	0.41
3:U:227:ASP:CA	3:U:228:ILE:CG2	2.87	0.41
3:V:264:ARG:O	3:V:265:VAL:C	2.64	0.41
1:H:17:GLN:HE21	1:H:17:GLN:HB3	1.70	0.41
1:H:50:PRO:HG3	1:H:141:ILE:HG21	1.93	0.41
1:H:70:ALA:HB1	1:H:71:PRO:CD	2.50	0.41
1:K:43:ILE:CD1	1:K:58:LEU:HD11	2.51	0.41
1:K:93:ASP:HB2	1:K:98:LYS:HB2	2.03	0.41
3:S:268:PHE:HA	3:S:276:LEU:HB3	2.03	0.41
1:B:68:MET:HE3	1:B:68:MET:HB3	1.92	0.40
2:F:80:LEU:N	2:F:80:LEU:CD2	2.85	0.40
2:I:114:LYS:N	2:I:171:CYS:HB2	2.37	0.40
1:K:84:VAL:HG13	1:K:88:GLY:HA2	2.03	0.40
1:K:115:LEU:HD12	1:K:115:LEU:HA	1.29	0.40
3:S:293:ALA:HB2	3:T:231:TYR:CE2	2.57	0.40
3:U:266:GLY:HA3	3:U:268:PHE:CE2	2.55	0.40
3:U:272:THR:O	3:U:273:ARG:CB	2.55	0.40
2:C:114:LYS:NZ	2:C:170:GLN:NE2	2.69	0.40
1:E:141:ILE:O	1:E:144:ALA:HB3	2.21	0.40
1:E:149:ARG:CD	1:E:149:ARG:HB2	2.48	0.40
1:E:150:LEU:CD1	1:E:151:TYR:CZ	3.03	0.40
2:F:37:LYS:CA	2:F:37:LYS:HZ3	2.28	0.40
2:F:103:PRO:O	2:F:104:GLU:C	2.63	0.40
1:H:50:PRO:HB3	1:H:144:ALA:HB1	2.03	0.40
2:I:45:LEU:O	2:I:46:GLU:O	2.39	0.40
1:K:85:ASP:OD2	1:K:89:ARG:HB2	2.21	0.40
3:V:262:LEU:HD23	3:V:262:LEU:HA	1.76	0.40
2:C:79:ILE:HD13	2:C:79:ILE:HG21	1.82	0.40
2:F:66:ASP:O	2:F:68:GLU:N	2.54	0.40
2:I:139:GLN:HB2	2:I:142:TYR:CD2	2.56	0.40
1:K:49:SER:C	1:K:51:PHE:N	2.79	0.40
1:K:67:PRO:C	1:K:69:ALA:N	2.79	0.40
3:S:247:THR:HG22	3:S:251:ILE:CA	2.50	0.40
3:V:262:LEU:HD23	3:V:267:HIS:HA	2.04	0.40
1:B:134:LYS:HZ3	1:B:134:LYS:HG2	1.87	0.40
2:C:85:THR:C	2:C:87:TYR:N	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:ILE:HD12	2:C:86:ILE:HA	1.90	0.40
2:C:132:ILE:O	2:C:132:ILE:HD12	2.17	0.40
1:E:131:GLU:HG3	1:E:132:GLN:N	2.37	0.40
2:F:73:THR:O	2:F:73:THR:CG2	2.60	0.40
1:H:62:LEU:HD21	1:H:105:ILE:HD11	2.04	0.40
1:K:27:ILE:HG13	1:K:113:GLN:OE1	2.22	0.40
1:K:64:GLU:H	1:K:64:GLU:HG2	1.65	0.40
1:K:95:LEU:HD21	1:K:108:VAL:HG11	2.03	0.40
2:L:37:LYS:CB	2:L:37:LYS:HZ3	2.34	0.40
3:T:260:GLU:O	3:T:261:HIS:C	2.61	0.40
3:U:286:ALA:CB	3:V:252:THR:OG1	2.70	0.40
1:B:70:ALA:O	1:B:71:PRO:C	2.52	0.40
1:B:122:ASP:OD2	1:B:122:ASP:N	2.55	0.40
2:C:158:LYS:CB	2:C:158:LYS:HZ2	2.35	0.40
1:E:44:ALA:O	1:E:46:PRO:CD	2.62	0.40
1:E:73:VAL:CG1	1:E:90:ILE:HD13	2.50	0.40
1:H:11:ARG:O	1:H:11:ARG:HG2	2.21	0.40
1:H:73:VAL:HG12	1:H:74:ARG:N	2.37	0.40
2:L:130:ARG:H	2:L:130:ARG:HG3	1.75	0.40
3:T:301:VAL:CA	3:T:301:VAL:CG2	2.89	0.40
3:V:230:ASP:CG	3:V:231:TYR:N	2.74	0.40
3:V:240:LEU:HD12	3:V:240:LEU:HA	1.85	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ALA:O	2:C:142:TYR:OH[2_555]	2.08	0.12
1:E:65:GLU:OE1	2:L:158:LYS:NZ[2_556]	2.16	0.04
1:H:142:GLU:OE2	1:K:145:ARG:NH1[3_434]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	B	148/154 (96%)	114 (77%)	28 (19%)	6 (4%)	2	9
1	E	145/154 (94%)	122 (84%)	13 (9%)	10 (7%)	1	2
1	H	145/154 (94%)	103 (71%)	23 (16%)	19 (13%)	0	0
1	K	148/154 (96%)	92 (62%)	27 (18%)	29 (20%)	0	0
2	C	140/142 (99%)	114 (81%)	12 (9%)	14 (10%)	0	1
2	F	137/142 (96%)	113 (82%)	12 (9%)	12 (9%)	0	1
2	I	137/142 (96%)	94 (69%)	20 (15%)	23 (17%)	0	0
2	L	137/142 (96%)	106 (77%)	17 (12%)	14 (10%)	0	1
3	S	73/78 (94%)	47 (64%)	15 (20%)	11 (15%)	0	0
3	T	76/78 (97%)	52 (68%)	14 (18%)	10 (13%)	0	0
3	U	71/78 (91%)	49 (69%)	14 (20%)	8 (11%)	0	1
3	V	69/78 (88%)	47 (68%)	10 (14%)	12 (17%)	0	0
All	All	1426/1496 (95%)	1053 (74%)	205 (14%)	168 (12%)	0	1

All (168) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	5	SER
1	B	137	GLU
2	C	34	THR
2	C	54	GLY
2	C	55	VAL
2	C	132	ILE
1	E	52	GLU
1	E	64	GLU
1	E	123	ASP
1	E	137	GLU
2	F	56	GLY
2	F	57	ASP
2	F	69	ASP
2	F	169	GLY
1	H	81	HIS
1	H	98	LYS
1	H	118	ALA
1	H	131	GLU
1	H	137	GLU
1	H	144	ALA

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Mol	Chain	Res	Type
2	I	57	ASP
2	I	78	MET
2	I	89	ASN
2	I	138	TRP
2	I	152	ARG
2	I	157	SER
2	I	159	GLU
2	I	162	LYS
2	I	172	TYR
1	K	5	SER
1	K	26	GLY
1	K	48	ASP
1	K	86	LYS
1	K	97	ASP
1	K	116	LEU
1	K	123	ASP
1	K	131	GLU
1	K	132	GLN
1	K	134	LYS
1	K	140	ALA
1	K	142	GLU
1	K	143	THR
1	K	146	ALA
1	K	147	TRP
1	K	154	ASN
2	L	60	VAL
2	L	68	GLU
2	L	99	GLY
3	S	231	TYR
3	S	258	ILE
3	S	267	HIS
3	S	285	LEU
3	S	292	ASP
3	S	293	ALA
3	S	294	PHE
3	T	231	TYR
3	T	291	ILE
3	T	297	GLU
3	T	301	VAL
3	U	243	GLU
3	U	263	GLN
3	U	264	ARG

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Mol	Chain	Res	Type
3	U	278	GLN
3	V	230	ASP
3	V	235	LYS
3	V	237	SER
3	V	264	ARG
1	B	48	ASP
1	B	97	ASP
2	C	53	LYS
2	C	56	GLY
2	C	57	ASP
2	C	81	GLY
2	C	130	ARG
2	C	131	ALA
1	E	93	ASP
1	E	122	ASP
1	E	128	ASP
2	F	140	ASN
2	F	142	TYR
1	H	21	ALA
1	H	65	GLU
1	H	143	THR
2	I	56	GLY
2	I	58	GLY
2	I	59	THR
2	I	84	ARG
2	I	132	ILE
2	I	163	LEU
1	K	29	ALA
1	K	92	LEU
1	K	133	TRP
2	L	125	GLY
2	L	138	TRP
2	L	154	LEU
2	L	169	GLY
3	S	279	GLU
3	S	297	GLU
3	T	248	PRO
3	T	288	LYS
3	T	293	ALA
3	U	293	ALA
3	V	232	LEU
3	V	265	VAL

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Mol	Chain	Res	Type
3	V	270	PRO
3	V	287	MET
3	V	291	ILE
3	V	297	GLU
1	B	52	GLU
2	C	59	THR
1	E	9	PRO
2	F	67	ASP
2	F	133	SER
2	F	138	TRP
2	F	161	MET
2	F	167	PRO
1	H	34	SER
1	H	45	GLY
1	H	116	LEU
1	H	132	GLN
2	I	46	GLU
2	I	150	GLU
1	K	53	GLY
1	K	78	LYS
1	K	105	ILE
1	K	109	LEU
2	L	64	LEU
2	L	117	MET
2	L	161	MET
3	U	270	PRO
3	V	288	LYS
1	B	53	GLY
2	C	36	VAL
2	C	88	GLU
2	C	155	MET
2	F	84	ARG
1	H	25	PRO
1	H	135	THR
2	I	50	GLU
2	I	171	CYS
1	K	50	PRO
1	K	77	THR
1	K	120	ASN
1	K	139	GLN
2	L	49	GLU
2	L	158	LYS

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Mol	Chain	Res	Type
3	S	255	ARG
3	U	274	SER
1	E	18	ARG
1	H	23	PRO
2	I	60	VAL
2	I	82	PRO
2	L	59	THR
2	L	89	ASN
3	U	234	GLY
1	H	50	PRO
1	H	89	ARG
2	I	45	LEU
2	I	103	PRO
1	K	8	LEU
1	K	93	ASP
3	T	270	PRO
3	V	236	ILE
3	S	236	ILE
3	T	295	ILE
1	H	79	ILE
3	T	275	PRO
1	E	121	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	B	128/129 (99%)	89 (70%)	39 (30%)	0	1
1	E	127/129 (98%)	92 (72%)	35 (28%)	0	1
1	H	127/129 (98%)	92 (72%)	35 (28%)	0	1
1	K	128/129 (99%)	90 (70%)	38 (30%)	0	1
2	C	125/127 (98%)	95 (76%)	30 (24%)	1	2
2	F	125/127 (98%)	96 (77%)	29 (23%)	1	3
2	I	125/127 (98%)	79 (63%)	46 (37%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	125/127 (98%)	89 (71%)	36 (29%)	0	1
3	S	68/72 (94%)	48 (71%)	20 (29%)	0	1
3	T	72/72 (100%)	52 (72%)	20 (28%)	0	1
3	U	66/72 (92%)	53 (80%)	13 (20%)	1	5
3	V	65/72 (90%)	35 (54%)	30 (46%)	0	0
All	All	1281/1312 (98%)	910 (71%)	371 (29%)	0	1

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	LEU
1	B	9	PRO
1	B	20	LEU
1	B	22	GLU
1	B	28	LYS
1	B	34	SER
1	B	35	ASN
1	B	58	LEU
1	B	64	GLU
1	B	65	GLU
1	B	73	VAL
1	B	74	ARG
1	B	76	MET
1	B	78	LYS
1	B	79	ILE
1	B	83	ASN
1	B	86	LYS
1	B	90	ILE
1	B	93	ASP
1	B	94	ILE
1	B	96	LYS
1	B	97	ASP
1	B	98	LYS
1	B	110	LEU
1	B	115	LEU
1	B	116	LEU
1	B	117	SER
1	B	122	ASP
1	B	127	ASN
1	B	128	ASP

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Mol	Chain	Res	Type
1	B	133	TRP
1	B	134	LYS
1	B	135	THR
1	B	142	GLU
1	B	148	THR
1	B	150	LEU
1	B	154	ASN
1	B	155	ASN
1	B	156	ILE
2	C	38	VAL
2	C	43	ARG
2	C	53	LYS
2	C	55	VAL
2	C	57	ASP
2	C	59	THR
2	C	61	SER
2	C	71	THR
2	C	74	ARG
2	C	76	THR
2	C	78	MET
2	C	80	LEU
2	C	84	ARG
2	C	88	GLU
2	C	89	ASN
2	C	95	LYS
2	C	115	ILE
2	C	126	VAL
2	C	132	ILE
2	C	133	SER
2	C	134	VAL
2	C	137	LYS
2	C	141	SER
2	C	145	LYS
2	C	147	VAL
2	C	158	LYS
2	C	160	ASN
2	C	161	MET
2	C	163	LEU
2	C	173	SER
1	E	10	ARG
1	E	13	ILE
1	E	14	LYS

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Mol	Chain	Res	Type
1	E	18	ARG
1	E	19	LEU
1	E	28	LYS
1	E	34	SER
1	E	35	ASN
1	E	51	PHE
1	E	64	GLU
1	E	65	GLU
1	E	72	LYS
1	E	73	VAL
1	E	74	ARG
1	E	76	MET
1	E	79	ILE
1	E	86	LYS
1	E	90	ILE
1	E	91	CYS
1	E	94	ILE
1	E	96	LYS
1	E	98	LYS
1	E	103	LEU
1	E	111	SER
1	E	116	LEU
1	E	117	SER
1	E	127	ASN
1	E	131	GLU
1	E	134	LYS
1	E	135	THR
1	E	136	ASN
1	E	141	ILE
1	E	149	ARG
1	E	150	LEU
1	E	156	ILE
2	F	37	LYS
2	F	43	ARG
2	F	50	GLU
2	F	52	GLN
2	F	53	LYS
2	F	55	VAL
2	F	61	SER
2	F	64	LEU
2	F	67	ASP
2	F	71	THR

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Mol	Chain	Res	Type
2	F	72	LEU
2	F	86	ILE
2	F	97	GLU
2	F	114	LYS
2	F	123	SER
2	F	124	ASN
2	F	129	PRO
2	F	130	ARG
2	F	132	ILE
2	F	134	VAL
2	F	135	LEU
2	F	140	ASN
2	F	153	ARG
2	F	157	SER
2	F	158	LYS
2	F	159	GLU
2	F	160	ASN
2	F	162	LYS
2	F	174	ASN
1	H	8	LEU
1	H	10	ARG
1	H	12	ILE
1	H	13	ILE
1	H	16	THR
1	H	18	ARG
1	H	19	LEU
1	H	27	ILE
1	H	30	GLU
1	H	32	ASP
1	H	47	GLN
1	H	57	LYS
1	H	58	LEU
1	H	61	PHE
1	H	65	GLU
1	H	78	LYS
1	H	79	ILE
1	H	83	ASN
1	H	84	VAL
1	H	87	LEU
1	H	96	LYS
1	H	100	SER
1	H	108	VAL

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Mol	Chain	Res	Type
1	H	110	LEU
1	H	111	SER
1	H	117	SER
1	H	127	ASN
1	H	128	ASP
1	H	131	GLU
1	H	134	LYS
1	H	143	THR
1	H	145	ARG
1	H	150	LEU
1	H	155	ASN
1	H	156	ILE
2	I	37	LYS
2	I	38	VAL
2	I	47	GLU
2	I	49	GLU
2	I	53	LYS
2	I	55	VAL
2	I	60	VAL
2	I	64	LEU
2	I	66	ASP
2	I	67	ASP
2	I	70	MET
2	I	72	LEU
2	I	74	ARG
2	I	76	THR
2	I	78	MET
2	I	80	LEU
2	I	82	PRO
2	I	84	ARG
2	I	88	GLU
2	I	89	ASN
2	I	90	ARG
2	I	91	ILE
2	I	93	SER
2	I	95	LYS
2	I	97	GLU
2	I	101	LYS
2	I	103	PRO
2	I	110	ARG
2	I	130	ARG
2	I	132	ILE

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Mol	Chain	Res	Type
2	I	134	VAL
2	I	137	LYS
2	I	140	ASN
2	I	141	SER
2	I	145	LYS
2	I	147	VAL
2	I	151	LEU
2	I	152	ARG
2	I	153	ARG
2	I	159	GLU
2	I	160	ASN
2	I	161	MET
2	I	163	LEU
2	I	165	GLN
2	I	166	PRO
2	I	170	GLN
1	K	5	SER
1	K	8	LEU
1	K	9	PRO
1	K	10	ARG
1	K	15	GLU
1	K	16	THR
1	K	18	ARG
1	K	20	LEU
1	K	28	LYS
1	K	35	ASN
1	K	37	ARG
1	K	43	ILE
1	K	48	ASP
1	K	51	PHE
1	K	58	LEU
1	K	64	GLU
1	K	66	TYR
1	K	74	ARG
1	K	76	MET
1	K	78	LYS
1	K	92	LEU
1	K	93	ASP
1	K	94	ILE
1	K	96	LYS
1	K	98	LYS
1	K	100	SER

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Mol	Chain	Res	Type
1	K	105	ILE
1	K	106	ARG
1	K	107	THR
1	K	117	SER
1	K	122	ASP
1	K	127	ASN
1	K	128	ASP
1	K	134	LYS
1	K	142	GLU
1	K	150	LEU
1	K	155	ASN
1	K	156	ILE
2	L	36	VAL
2	L	37	LYS
2	L	40	ARG
2	L	41	ASN
2	L	48	LEU
2	L	49	GLU
2	L	52	GLN
2	L	53	LYS
2	L	55	VAL
2	L	59	THR
2	L	60	VAL
2	L	64	LEU
2	L	67	ASP
2	L	70	MET
2	L	78	MET
2	L	80	LEU
2	L	84	ARG
2	L	104	GLU
2	L	115	ILE
2	L	130	ARG
2	L	132	ILE
2	L	134	VAL
2	L	140	ASN
2	L	142	TYR
2	L	145	LYS
2	L	151	LEU
2	L	153	ARG
2	L	155	MET
2	L	158	LYS
2	L	159	GLU

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Mol	Chain	Res	Type
2	L	161	MET
2	L	162	LYS
2	L	166	PRO
2	L	167	PRO
2	L	171	CYS
2	L	173	SER
3	S	228	ILE
3	S	230	ASP
3	S	242	ARG
3	S	243	GLU
3	S	244	PRO
3	S	246	ILE
3	S	249	SER
3	S	252	THR
3	S	256	LYS
3	S	263	GLN
3	S	264	ARG
3	S	270	PRO
3	S	278	GLN
3	S	279	GLU
3	S	283	PRO
3	S	285	LEU
3	S	287	MET
3	S	288	LYS
3	S	295	ILE
3	S	297	GLU
3	T	227	ASP
3	T	230	ASP
3	T	232	LEU
3	T	235	LYS
3	T	241	MET
3	T	246	ILE
3	T	249	SER
3	T	258	ILE
3	T	263	GLN
3	T	269	ASN
3	T	270	PRO
3	T	274	SER
3	T	276	LEU
3	T	277	THR
3	T	278	GLN
3	T	279	GLU

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Mol	Chain	Res	Type
3	T	288	LYS
3	T	295	ILE
3	T	298	ASN
3	T	301	VAL
3	U	228	ILE
3	U	229	PRO
3	U	242	ARG
3	U	243	GLU
3	U	247	THR
3	U	249	SER
3	U	251	ILE
3	U	260	GLU
3	U	262	LEU
3	U	263	GLN
3	U	291	ILE
3	U	296	SER
3	U	297	GLU
3	V	229	PRO
3	V	232	LEU
3	V	235	LYS
3	V	240	LEU
3	V	241	MET
3	V	242	ARG
3	V	246	ILE
3	V	247	THR
3	V	248	PRO
3	V	252	THR
3	V	256	LYS
3	V	258	ILE
3	V	261	HIS
3	V	263	GLN
3	V	264	ARG
3	V	270	PRO
3	V	273	ARG
3	V	276	LEU
3	V	277	THR
3	V	278	GLN
3	V	279	GLU
3	V	280	GLN
3	V	282	ILE
3	V	285	LEU
3	V	287	MET

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Mol	Chain	Res	Type
3	V	288	LYS
3	V	290	VAL
3	V	291	ILE
3	V	294	PHE
3	V	295	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	GLN
1	B	35	ASN
1	B	83	ASN
1	B	104	GLN
1	B	127	ASN
1	B	136	ASN
2	C	52	GLN
2	C	140	ASN
2	C	160	ASN
2	C	170	GLN
2	C	174	ASN
1	E	35	ASN
1	E	40	HIS
1	E	47	GLN
1	E	81	HIS
1	E	113	GLN
1	E	120	ASN
1	E	127	ASN
1	E	136	ASN
1	E	139	GLN
1	E	154	ASN
2	F	41	ASN
2	F	140	ASN
2	F	160	ASN
2	F	170	GLN
2	F	174	ASN
1	H	17	GLN
1	H	81	HIS
1	H	83	ASN
1	H	154	ASN
2	I	52	GLN
2	I	89	ASN
2	I	140	ASN

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Mol	Chain	Res	Type
2	I	160	ASN
1	K	17	GLN
1	K	35	ASN
1	K	81	HIS
1	K	83	ASN
1	K	104	GLN
1	K	127	ASN
1	K	136	ASN
1	K	154	ASN
2	L	41	ASN
2	L	140	ASN
2	L	160	ASN
2	L	165	GLN
3	S	263	GLN
3	S	278	GLN
3	T	263	GLN
3	T	269	ASN
3	T	298	ASN
3	U	280	GLN
3	U	284	ASN
3	U	298	ASN
3	V	263	GLN
3	V	298	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	152/154 (98%)	-0.01	3 (1%) 65 56	2, 2, 12, 28	0
1	E	149/154 (96%)	0.17	4 (2%) 56 47	2, 2, 18, 32	0
1	H	149/154 (96%)	-0.40	2 (1%) 75 67	2, 2, 20, 27	0
1	K	152/154 (98%)	0.15	4 (2%) 57 48	2, 3, 29, 38	0
2	C	142/142 (100%)	0.54	6 (4%) 40 32	2, 2, 10, 28	0
2	F	139/142 (97%)	-0.50	1 (0%) 84 79	2, 2, 10, 20	0
2	I	139/142 (97%)	-0.33	0 100 100	2, 2, 10, 17	0
2	L	139/142 (97%)	-0.02	1 (0%) 84 79	2, 2, 10, 13	0
3	S	75/78 (96%)	-0.57	0 100 100	2, 2, 17, 21	0
3	T	78/78 (100%)	-0.54	2 (2%) 57 48	2, 2, 50, 59	0
3	U	73/78 (93%)	-0.55	0 100 100	2, 2, 11, 17	0
3	V	71/78 (91%)	-0.48	0 100 100	2, 3, 14, 27	0
All	All	1458/1496 (97%)	-0.15	23 (1%) 70 62	2, 2, 18, 59	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	34	THR	5.5
1	B	124	PRO	5.0
2	C	58	GLY	3.8
1	H	6	ALA	3.7
1	E	6	ALA	3.2
2	C	33	THR	3.1
3	T	303	ASP	2.9
3	T	301	VAL	2.9
1	B	3	ALA	2.9
1	E	156	ILE	2.8
1	K	156	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	124	PRO	2.6
1	K	3	ALA	2.4
2	F	61	SER	2.3
1	E	26	GLY	2.3
1	E	124	PRO	2.2
1	B	156	ILE	2.2
2	C	158	LYS	2.2
2	C	173	SER	2.2
1	K	135	THR	2.1
2	C	57	ASP	2.1
1	K	124	PRO	2.0
2	L	58	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.