Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 12:54 AM GMT

PDB ID	:	2C2V
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

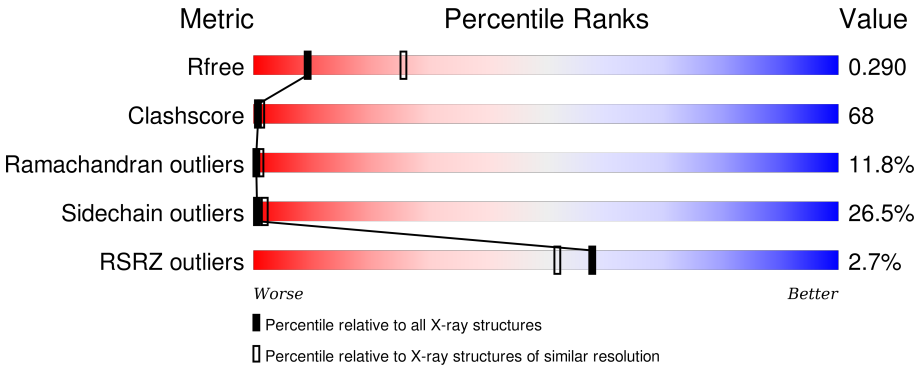
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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% 6% 38% 37% 18%
1	E	154	2% 16% 26% 40% 14%
1	H	154	3% 5% 31% 47% 14%
1	K	154	11% 7% 28% 37% 27%
2	C	142	2% 13% 38% 36% 13%

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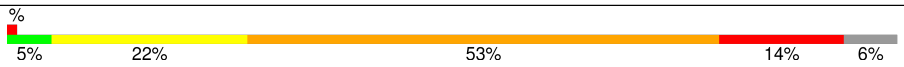
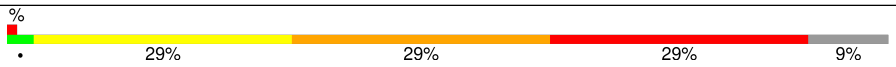
Mol	Chain	Length	Quality of chain
2	F	142	
2	I	142	
2	L	142	
3	S	78	
3	T	78	
3	U	78	
3	V	78	

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 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	SER	MET	CONFLICT	UNP P61089
K	5	SER	MET	CONFLICT	UNP P61089

- 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			
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			

- Molecule 3 is a protein called CARBOXY TERMINUS OF HSP70-INTERACTING PROTEIN.

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			

- Molecule 4 is water.

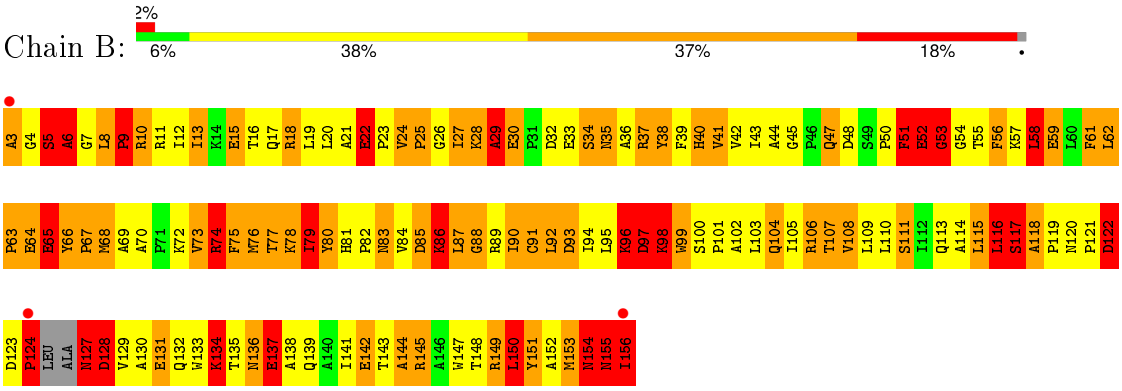
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total	O	0	0
			5	5		
4	C	5	Total	O	0	0
			5	5		
4	E	3	Total	O	0	0
			3	3		
4	F	7	Total	O	0	0
			7	7		
4	H	1	Total	O	0	0
			1	1		
4	I	1	Total	O	0	0
			1	1		
4	L	1	Total	O	0	0
			1	1		
4	S	6	Total	O	0	0
			6	6		
4	T	2	Total	O	0	0
			2	2		
4	U	1	Total	O	0	0
			1	1		
4	V	3	Total	O	0	0
			3	3		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

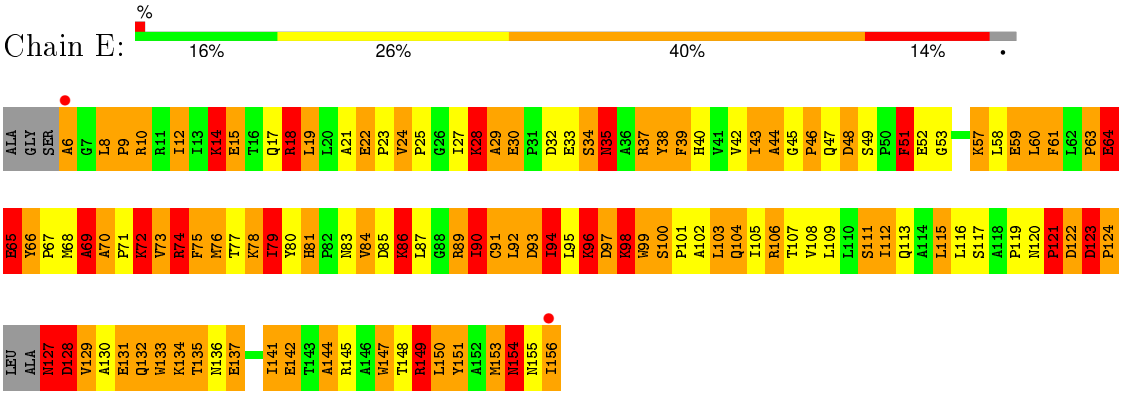
- Molecule 1: UBIQUITIN-CONJUGATING ENZYME E2 N

Chain B:



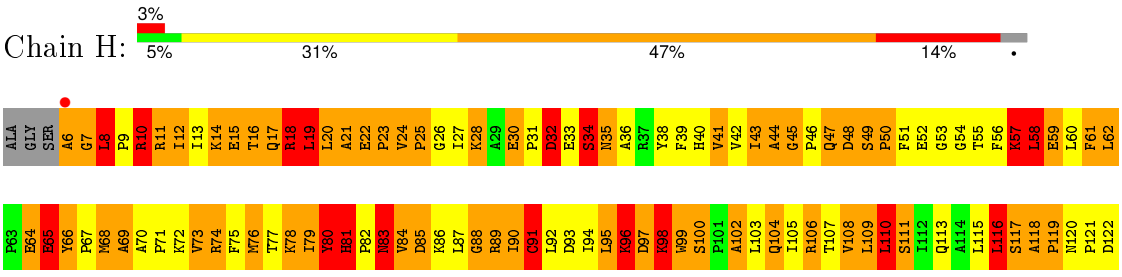
- Molecule 1: UBIQUITIN-CONJUGATING ENZYME E2 N

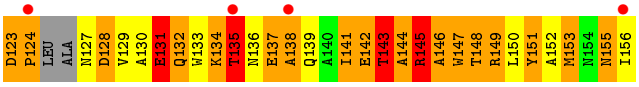
Chain E:



- Molecule 1: UBIQUITIN-CONJUGATING ENZYME E2 N

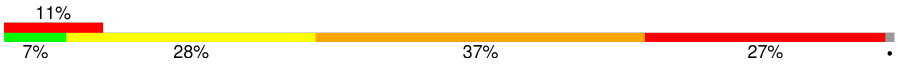
Chain H:

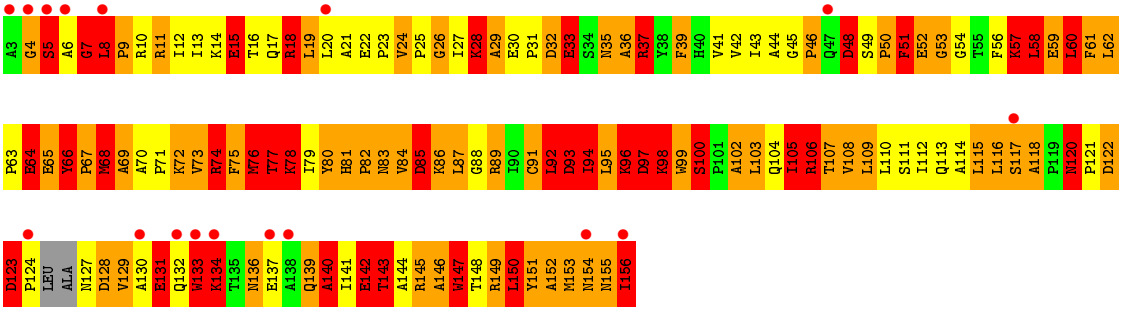




• Molecule 1: UBIQUITIN-CONJUGATING ENZYME E2 N

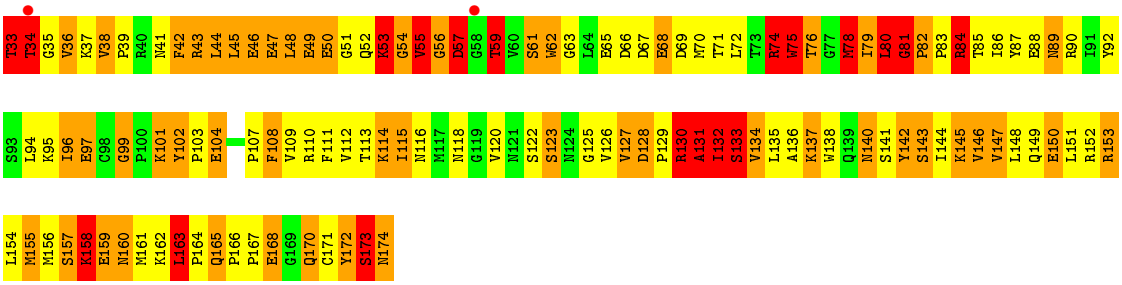
Chain K:





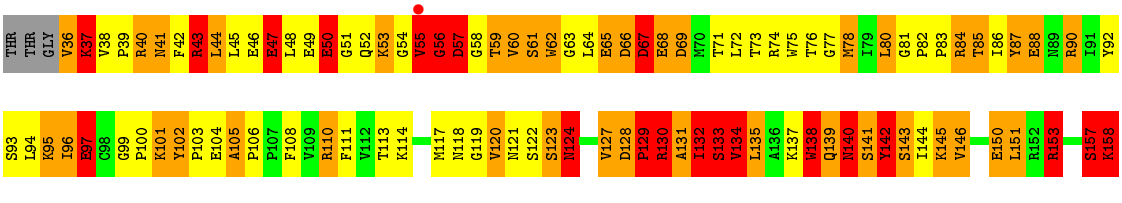
• Molecule 2: UBIQUITIN-CONJUGATING ENZYME E2 VARIANT 1

Chain C:



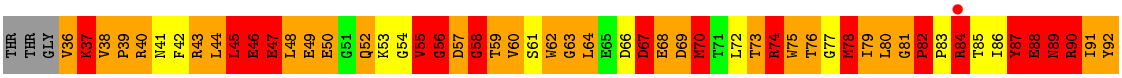
• Molecule 2: UBIQUITIN-CONJUGATING ENZYME E2 VARIANT 1

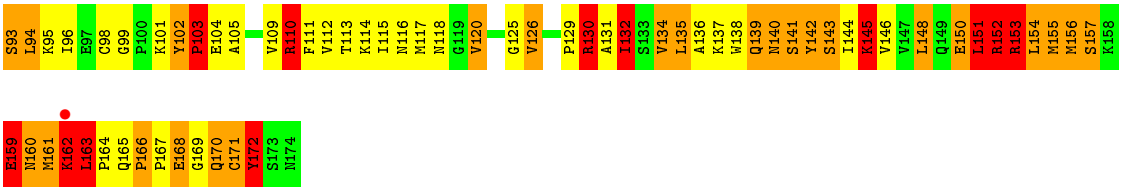
Chain F:



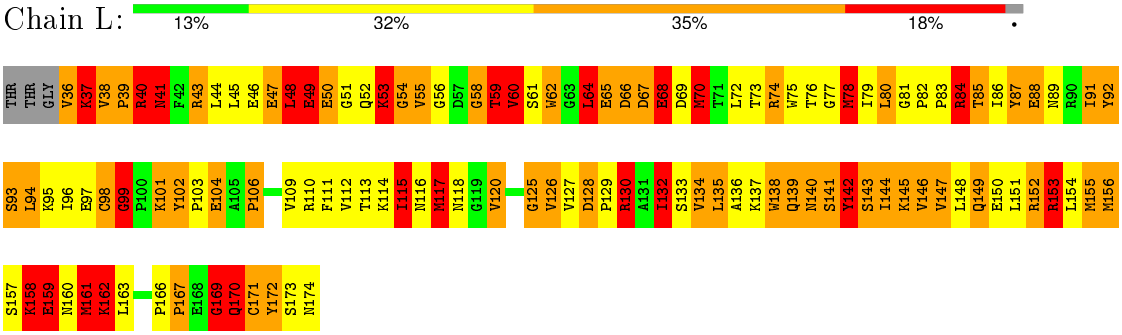
• Molecule 2: UBIQUITIN-CONJUGATING ENZYME E2 VARIANT 1

Chain I:

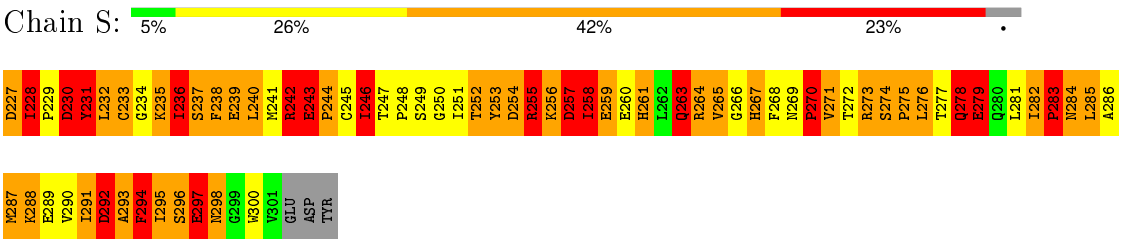




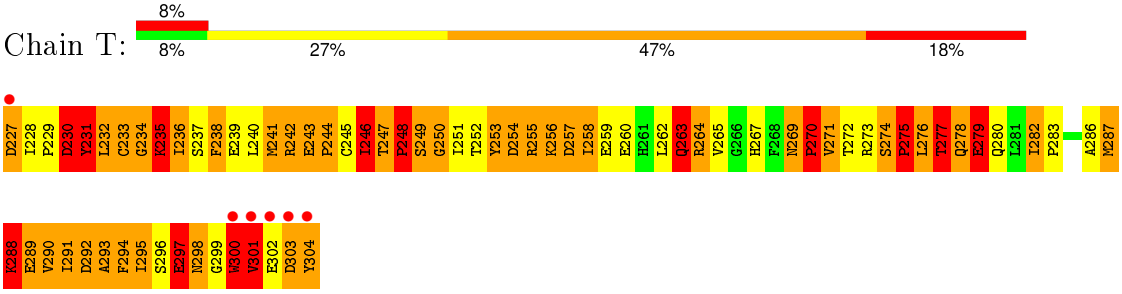
• Molecule 2: UBIQUITIN-CONJUGATING ENZYME E2 VARIANT 1



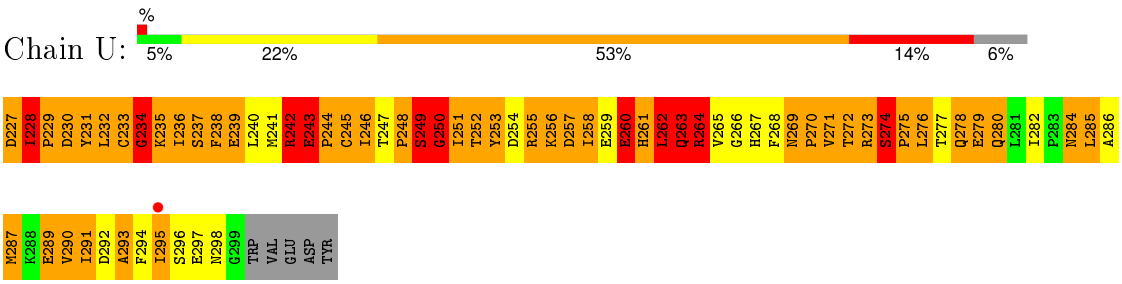
• Molecule 3: CARBOXY TERMINUS OF HSP70-INTERACTING PROTEIN



• Molecule 3: CARBOXY TERMINUS OF HSP70-INTERACTING PROTEIN

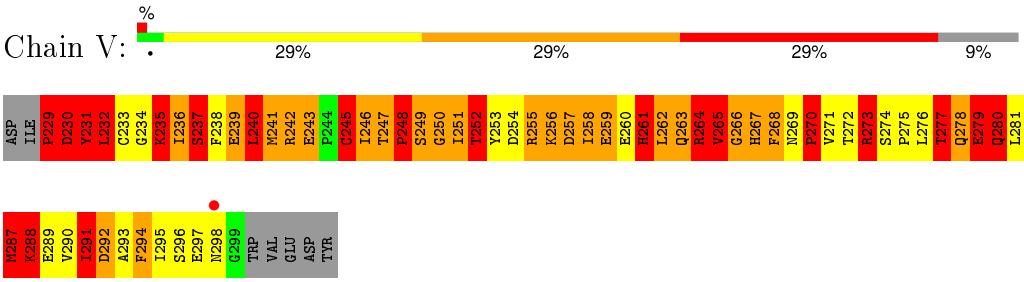


• Molecule 3: CARBOXY TERMINUS OF HSP70-INTERACTING PROTEIN



• Molecule 3: CARBOXY TERMINUS OF HSP70-INTERACTING PROTEIN

Chain V:


%
29%
29%
29%
9%
ASP ILE P229 D230 V231 L232 C233 G234 K235 I236 S237 F238 E239 L240 M241 R242 E243 P244 C245 I246 T247 P248 S249 G250 I251 T252 Y253 D254 R255 K256 D257 I258 E259 E260 H261 L262 Q263 R264 V265 G266 H267 F268 N269 P270 V271 T272 R273 S274 P275 L276 T277 Q278 E279 Q280 L281 I282 P283 N284 L285 A286
M287 K288 E289 V290 I291 D292 A293 F294 I295 S296 E297 N298 G299 TRP VAL GLU ASP TYR

4 Data and refinement statistics (i)

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 37.40 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.3 (196.12-2.90) 95.4 (37.40-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.30%)	DCC
Wilson B-factor (Å^2)	64.0	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 52095 reflections	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	3.41	160/1231 (13.0%)	2.68	86/1673 (5.1%)
1	E	3.07	115/1216 (9.5%)	2.33	62/1653 (3.8%)
1	H	2.87	99/1216 (8.1%)	2.29	61/1653 (3.7%)
1	K	3.07	114/1231 (9.3%)	2.29	65/1673 (3.9%)
2	C	3.59	140/1147 (12.2%)	2.73	88/1551 (5.7%)
2	F	3.13	108/1133 (9.5%)	2.43	75/1532 (4.9%)
2	I	2.61	68/1133 (6.0%)	2.17	49/1532 (3.2%)
2	L	2.82	92/1133 (8.1%)	2.32	62/1532 (4.0%)
3	S	3.46	83/612 (13.6%)	2.81	61/831 (7.3%)
3	T	3.20	78/649 (12.0%)	2.47	44/880 (5.0%)
3	U	3.14	60/589 (10.2%)	2.44	45/799 (5.6%)
3	V	3.32	74/576 (12.8%)	2.43	36/780 (4.6%)
All	All	3.13	1191/11866 (10.0%)	2.44	734/16089 (4.6%)

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 (1191) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	131	ALA	CA-CB	30.67	2.16	1.52
1	B	142	GLU	CD-OE2	26.58	1.54	1.25
1	K	142	GLU	CD-OE2	22.60	1.50	1.25
1	H	65	GLU	CG-CD	20.68	1.82	1.51
3	S	243	GLU	CD-OE1	19.09	1.46	1.25
1	E	15	GLU	CD-OE1	18.40	1.45	1.25
1	B	142	GLU	CD-OE1	16.06	1.43	1.25
3	V	289	GLU	CD-OE2	15.58	1.42	1.25
3	S	239	GLU	CD-OE1	15.45	1.42	1.25
2	C	34	THR	CA-CB	15.37	1.93	1.53
1	B	65	GLU	CD-OE1	15.36	1.42	1.25
2	C	159	GLU	CG-CD	15.03	1.74	1.51
2	C	146	VAL	CB-CG2	-14.90	1.21	1.52
2	C	49	GLU	CD-OE1	14.85	1.42	1.25
3	U	279	GLU	CG-CD	14.77	1.74	1.51
2	C	159	GLU	CB-CG	14.74	1.80	1.52
2	I	152	ARG	CG-CD	14.55	1.88	1.51
1	E	145	ARG	CZ-NH2	14.49	1.51	1.33
2	F	55	VAL	CA-CB	14.47	1.85	1.54
2	C	53	LYS	CE-NZ	14.06	1.84	1.49
1	B	142	GLU	CB-CG	-13.97	1.25	1.52
3	V	243	GLU	CD-OE2	13.80	1.40	1.25
2	F	55	VAL	CB-CG1	13.69	1.81	1.52
2	C	65	GLU	CD-OE2	13.48	1.40	1.25
1	K	64	GLU	CD-OE1	13.14	1.40	1.25
2	C	127	VAL	CB-CG2	-13.12	1.25	1.52
1	H	69	ALA	CA-CB	-13.09	1.25	1.52
3	U	279	GLU	CD-OE2	12.99	1.40	1.25
1	B	22	GLU	CB-CG	12.78	1.76	1.52
1	E	142	GLU	CD-OE2	12.60	1.39	1.25
3	V	259	GLU	CG-CD	12.58	1.70	1.51
1	K	142	GLU	CD-OE1	12.56	1.39	1.25
1	E	78	LYS	CE-NZ	12.51	1.80	1.49
1	E	38	TYR	CE1-CZ	12.49	1.54	1.38
3	U	239	GLU	CB-CG	-12.47	1.28	1.52
1	K	142	GLU	CG-CD	12.45	1.70	1.51
1	K	99	TRP	CE3-CZ3	12.41	1.59	1.38
2	L	49	GLU	CG-CD	12.40	1.70	1.51
2	F	174	ASN	C-O	12.40	1.47	1.23
2	C	108	PHE	CB-CG	-12.33	1.30	1.51
3	S	242	ARG	CG-CD	12.22	1.82	1.51
3	U	245	CYS	CB-SG	12.21	2.03	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	259	GLU	CD-OE1	12.15	1.39	1.25
2	C	47	GLU	CD-OE1	12.04	1.38	1.25
1	K	142	GLU	CB-CG	12.03	1.75	1.52
1	K	65	GLU	CD-OE1	11.99	1.38	1.25
3	V	243	GLU	CD-OE1	11.96	1.38	1.25
2	C	49	GLU	CD-OE2	11.94	1.38	1.25
2	L	65	GLU	CD-OE2	11.94	1.38	1.25
2	C	65	GLU	CD-OE1	11.90	1.38	1.25
2	F	74	ARG	CZ-NH1	11.80	1.48	1.33
1	H	98	LYS	CE-NZ	11.78	1.78	1.49
2	F	46	GLU	CG-CD	11.75	1.69	1.51
3	V	268	PHE	CD1-CE1	11.68	1.62	1.39
2	C	68	GLU	CD-OE1	11.64	1.38	1.25
2	F	97	GLU	CD-OE2	11.53	1.38	1.25
1	B	22	GLU	CG-CD	11.53	1.69	1.51
2	F	95	LYS	CE-NZ	11.52	1.77	1.49
1	K	149	ARG	CZ-NH1	11.52	1.48	1.33
2	I	37	LYS	CD-CE	11.48	1.79	1.51
2	C	157	SER	CB-OG	11.47	1.57	1.42
2	F	49	GLU	CD-OE2	11.44	1.38	1.25
1	E	45	GLY	C-O	-11.41	1.05	1.23
1	B	33	GLU	CD-OE2	11.31	1.38	1.25
2	C	97	GLU	CD-OE2	11.20	1.38	1.25
3	V	266	GLY	C-O	11.12	1.41	1.23
3	S	236	ILE	CA-CB	-11.11	1.29	1.54
1	H	15	GLU	CD-OE1	11.10	1.37	1.25
2	L	49	GLU	CB-CG	11.09	1.73	1.52
1	K	15	GLU	CD-OE1	11.05	1.37	1.25
1	K	39	PHE	CE1-CZ	10.97	1.58	1.37
2	F	97	GLU	CG-CD	10.95	1.68	1.51
1	B	42	VAL	CB-CG2	-10.93	1.29	1.52
2	F	49	GLU	CG-CD	10.91	1.68	1.51
3	T	231	TYR	CE1-CZ	10.83	1.52	1.38
1	B	134	LYS	CE-NZ	10.81	1.76	1.49
1	E	6	ALA	CA-CB	10.80	1.75	1.52
3	T	288	LYS	CD-CE	10.74	1.78	1.51
2	L	147	VAL	CB-CG1	-10.65	1.30	1.52
1	H	39	PHE	CG-CD1	10.62	1.54	1.38
1	H	65	GLU	CD-OE2	10.61	1.37	1.25
3	V	279	GLU	CG-CD	10.58	1.67	1.51
3	S	300	TRP	CZ3-CH2	10.58	1.56	1.40
2	F	150	GLU	CD-OE2	10.55	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	153	ARG	CB-CG	10.52	1.80	1.52
1	K	106	ARG	CG-CD	10.48	1.78	1.51
1	H	149	ARG	CZ-NH1	10.43	1.46	1.33
1	K	156	ILE	CA-CB	10.36	1.78	1.54
1	H	142	GLU	CD-OE2	10.33	1.37	1.25
2	L	145	LYS	CD-CE	10.31	1.77	1.51
1	E	78	LYS	CG-CD	10.30	1.87	1.52
3	T	301	VAL	CA-CB	10.30	1.76	1.54
1	H	142	GLU	CG-CD	10.22	1.67	1.51
3	U	250	GLY	C-O	10.22	1.40	1.23
2	C	138	TRP	CB-CG	-10.20	1.31	1.50
1	E	86	LYS	CE-NZ	10.17	1.74	1.49
1	B	144	ALA	CA-CB	-10.17	1.31	1.52
2	L	38	VAL	CB-CG2	10.15	1.74	1.52
1	B	6	ALA	CA-CB	-10.14	1.31	1.52
1	B	145	ARG	CZ-NH1	10.13	1.46	1.33
2	L	40	ARG	CZ-NH2	10.13	1.46	1.33
3	V	289	GLU	CG-CD	10.13	1.67	1.51
3	T	304	TYR	CE2-CZ	10.09	1.51	1.38
3	S	274	SER	CB-OG	-10.08	1.29	1.42
1	B	131	GLU	CG-CD	10.04	1.67	1.51
2	I	50	GLU	CG-CD	10.02	1.67	1.51
3	S	279	GLU	CD-OE1	10.02	1.36	1.25
1	B	65	GLU	CG-CD	9.98	1.67	1.51
2	F	97	GLU	CD-OE1	9.96	1.36	1.25
1	H	15	GLU	CD-OE2	9.95	1.36	1.25
3	U	253	TYR	CG-CD2	9.95	1.52	1.39
2	I	46	GLU	CD-OE2	9.94	1.36	1.25
1	H	98	LYS	C-O	-9.92	1.04	1.23
2	I	104	GLU	CG-CD	9.90	1.66	1.51
1	E	149	ARG	CG-CD	9.89	1.76	1.51
2	F	104	GLU	CD-OE1	9.84	1.36	1.25
3	T	288	LYS	CG-CD	9.84	1.85	1.52
3	S	263	GLN	CG-CD	9.84	1.73	1.51
1	H	96	LYS	CD-CE	9.79	1.75	1.51
3	V	289	GLU	CD-OE1	9.72	1.36	1.25
3	S	235	LYS	CB-CG	-9.71	1.26	1.52
2	F	53	LYS	CD-CE	9.68	1.75	1.51
1	E	15	GLU	CG-CD	9.68	1.66	1.51
1	K	78	LYS	CD-CE	9.68	1.75	1.51
2	C	92	TYR	CE2-CZ	-9.65	1.25	1.38
2	C	43	ARG	CZ-NH1	9.65	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	57	LYS	CB-CG	9.64	1.78	1.52
2	F	105	ALA	CA-CB	-9.59	1.32	1.52
1	E	78	LYS	CB-CG	9.57	1.78	1.52
2	F	120	VAL	CA-CB	-9.53	1.34	1.54
3	S	234	GLY	N-CA	9.52	1.60	1.46
1	B	28	LYS	CE-NZ	9.46	1.72	1.49
1	B	34	SER	CA-CB	9.46	1.67	1.52
2	C	173	SER	CB-OG	9.45	1.54	1.42
2	C	49	GLU	CG-CD	9.45	1.66	1.51
2	F	153	ARG	CG-CD	9.44	1.75	1.51
2	C	41	ASN	C-O	9.41	1.41	1.23
2	F	55	VAL	N-CA	9.40	1.65	1.46
2	C	145	LYS	CE-NZ	9.40	1.72	1.49
3	T	246	ILE	CB-CG2	-9.38	1.23	1.52
2	L	104	GLU	CG-CD	9.37	1.66	1.51
2	F	108	PHE	CD2-CE2	-9.35	1.20	1.39
1	E	96	LYS	CD-CE	9.34	1.74	1.51
2	C	50	GLU	CD-OE2	9.34	1.35	1.25
2	C	38	VAL	CB-CG2	9.31	1.72	1.52
2	C	174	ASN	C-OXT	9.31	1.41	1.23
2	C	55	VAL	CB-CG1	9.27	1.72	1.52
2	L	120	VAL	CB-CG2	-9.27	1.33	1.52
1	E	145	ARG	CZ-NH1	9.26	1.45	1.33
1	E	137	GLU	CD-OE2	9.24	1.35	1.25
1	K	64	GLU	CG-CD	9.24	1.65	1.51
2	L	65	GLU	CD-OE1	9.23	1.35	1.25
1	B	151	TYR	CE1-CZ	9.23	1.50	1.38
1	K	21	ALA	CA-CB	9.20	1.71	1.52
2	F	46	GLU	CD-OE1	9.15	1.35	1.25
2	F	74	ARG	CG-CD	-9.14	1.29	1.51
2	I	168	GLU	CB-CG	9.14	1.69	1.52
1	E	15	GLU	CD-OE2	9.12	1.35	1.25
3	U	271	VAL	CB-CG1	9.08	1.72	1.52
2	L	172	TYR	CG-CD1	9.08	1.50	1.39
1	E	33	GLU	CD-OE1	9.08	1.35	1.25
3	U	295	ILE	CA-CB	9.03	1.75	1.54
1	E	33	GLU	CD-OE2	9.01	1.35	1.25
3	S	253	TYR	CB-CG	9.01	1.65	1.51
3	T	242	ARG	CG-CD	9.00	1.74	1.51
2	C	126	VAL	CB-CG1	-9.00	1.33	1.52
3	T	265	VAL	CB-CG1	-8.95	1.34	1.52
2	C	126	VAL	CB-CG2	-8.95	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	84	ARG	CB-CG	8.93	1.76	1.52
2	C	69	ASP	C-O	8.84	1.40	1.23
3	T	301	VAL	CB-CG1	8.83	1.71	1.52
1	H	108	VAL	CB-CG2	-8.82	1.34	1.52
3	V	259	GLU	CD-OE1	8.82	1.35	1.25
1	B	156	ILE	C-OXT	8.80	1.40	1.23
2	F	174	ASN	C-OXT	8.79	1.40	1.23
2	L	153	ARG	CZ-NH1	8.77	1.44	1.33
3	T	255	ARG	CZ-NH1	8.76	1.44	1.33
2	I	120	VAL	CB-CG2	-8.75	1.34	1.52
1	K	99	TRP	CB-CG	8.74	1.66	1.50
1	K	15	GLU	CG-CD	8.74	1.65	1.51
3	T	256	LYS	CE-NZ	8.73	1.70	1.49
3	S	300	TRP	N-CA	8.72	1.63	1.46
3	T	286	ALA	CA-CB	-8.71	1.34	1.52
3	V	248	PRO	CG-CD	8.71	1.79	1.50
2	F	102	TYR	CD2-CE2	-8.71	1.26	1.39
3	U	235	LYS	CB-CG	-8.71	1.29	1.52
2	C	133	SER	CB-OG	-8.66	1.30	1.42
2	L	47	GLU	CD-OE1	8.66	1.35	1.25
1	K	145	ARG	CZ-NH2	8.65	1.44	1.33
1	B	57	LYS	CD-CE	8.65	1.72	1.51
1	K	120	ASN	CB-CG	8.64	1.71	1.51
1	B	80	TYR	CD2-CE2	-8.62	1.26	1.39
1	K	18	ARG	CG-CD	8.62	1.73	1.51
2	F	40	ARG	C-O	8.61	1.39	1.23
1	B	64	GLU	CB-CG	8.61	1.68	1.52
2	C	132	ILE	CB-CG2	-8.61	1.26	1.52
1	E	65	GLU	CD-OE1	8.61	1.35	1.25
2	L	138	TRP	C-O	-8.59	1.07	1.23
3	T	248	PRO	C-O	-8.58	1.06	1.23
1	B	10	ARG	CZ-NH2	8.57	1.44	1.33
3	U	259	GLU	CG-CD	8.57	1.64	1.51
1	B	28	LYS	CD-CE	8.56	1.72	1.51
1	E	89	ARG	CZ-NH1	8.56	1.44	1.33
1	E	144	ALA	CA-CB	-8.55	1.34	1.52
1	E	97	ASP	CB-CG	8.54	1.69	1.51
2	C	62	TRP	CB-CG	8.53	1.65	1.50
2	C	114	LYS	CE-NZ	8.53	1.70	1.49
2	C	153	ARG	CG-CD	8.53	1.73	1.51
1	B	86	LYS	CE-NZ	8.53	1.70	1.49
2	L	146	VAL	CB-CG2	-8.52	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	75	TRP	CZ3-CH2	-8.46	1.26	1.40
2	C	38	VAL	N-CA	8.46	1.63	1.46
2	L	87	TYR	CD2-CE2	8.45	1.52	1.39
2	F	127	VAL	CB-CG2	-8.42	1.35	1.52
1	B	61	PHE	CD2-CE2	8.42	1.56	1.39
1	B	65	GLU	CD-OE2	8.42	1.34	1.25
1	H	156	ILE	CA-CB	8.42	1.74	1.54
1	K	15	GLU	CD-OE2	8.40	1.34	1.25
3	U	256	LYS	CE-NZ	8.40	1.70	1.49
3	V	230	ASP	C-O	8.38	1.39	1.23
1	H	16	THR	C-O	8.36	1.39	1.23
2	I	50	GLU	CD-OE1	8.35	1.34	1.25
1	K	80	TYR	CE2-CZ	8.35	1.49	1.38
3	T	304	TYR	CG-CD1	8.35	1.50	1.39
2	F	139	GLN	N-CA	-8.33	1.29	1.46
3	V	279	GLU	CD-OE1	8.33	1.34	1.25
2	C	84	ARG	CB-CG	8.32	1.75	1.52
1	E	123	ASP	CB-CG	8.29	1.69	1.51
3	T	286	ALA	C-O	8.29	1.39	1.23
2	I	63	GLY	N-CA	8.28	1.58	1.46
3	T	239	GLU	CB-CG	-8.28	1.36	1.52
1	K	6	ALA	CA-CB	8.26	1.69	1.52
2	C	108	PHE	CG-CD2	-8.26	1.26	1.38
2	C	75	TRP	CG-CD1	8.25	1.48	1.36
1	K	143	THR	CB-OG1	8.24	1.59	1.43
2	L	101	LYS	CE-NZ	8.24	1.69	1.49
1	K	7	GLY	N-CA	8.23	1.58	1.46
1	B	99	TRP	CZ3-CH2	8.23	1.53	1.40
2	C	97	GLU	CG-CD	8.22	1.64	1.51
3	V	239	GLU	CD-OE2	8.19	1.34	1.25
3	S	243	GLU	CB-CG	-8.18	1.36	1.52
1	B	66	TYR	CE1-CZ	-8.17	1.27	1.38
2	C	81	GLY	C-O	-8.16	1.10	1.23
1	B	34	SER	CB-OG	8.14	1.52	1.42
3	U	252	THR	CA-CB	8.14	1.74	1.53
1	B	131	GLU	CD-OE1	8.12	1.34	1.25
2	L	43	ARG	CZ-NH1	8.12	1.43	1.33
1	B	72	LYS	CA-C	-8.11	1.31	1.52
1	H	142	GLU	CD-OE1	8.11	1.34	1.25
1	K	37	ARG	CZ-NH1	8.11	1.43	1.33
1	H	109	LEU	C-O	8.08	1.38	1.23
1	B	93	ASP	CG-OD1	8.08	1.44	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	50	GLU	CA-C	8.07	1.74	1.52
1	B	156	ILE	CA-CB	8.07	1.73	1.54
1	K	30	GLU	CB-CG	8.06	1.67	1.52
3	U	265	VAL	CB-CG2	-8.06	1.35	1.52
1	K	64	GLU	CD-OE2	8.04	1.34	1.25
3	V	273	ARG	CZ-NH2	8.04	1.43	1.33
2	F	68	GLU	CD-OE2	8.03	1.34	1.25
1	B	33	GLU	CD-OE1	8.03	1.34	1.25
3	V	292	ASP	CB-CG	8.03	1.68	1.51
2	I	105	ALA	CA-CB	-8.02	1.35	1.52
2	L	102	TYR	CG-CD1	-8.01	1.28	1.39
1	H	96	LYS	CB-CG	-7.99	1.30	1.52
2	L	102	TYR	CZ-OH	7.97	1.51	1.37
2	I	101	LYS	CB-CG	-7.97	1.31	1.52
2	L	136	ALA	CA-CB	-7.96	1.35	1.52
3	S	266	GLY	N-CA	7.96	1.57	1.46
2	F	46	GLU	CD-OE2	7.95	1.34	1.25
2	F	55	VAL	CB-CG2	7.94	1.69	1.52
1	H	33	GLU	CD-OE1	7.94	1.34	1.25
2	L	142	TYR	CG-CD2	7.94	1.49	1.39
1	K	61	PHE	CE2-CZ	7.91	1.52	1.37
3	T	238	PHE	CD2-CE2	-7.91	1.23	1.39
1	B	30	GLU	CB-CG	-7.90	1.37	1.52
1	B	75	PHE	CE2-CZ	-7.89	1.22	1.37
3	T	236	ILE	CB-CG2	-7.86	1.28	1.52
3	T	301	VAL	CB-CG2	7.85	1.69	1.52
1	B	124	PRO	N-CA	7.85	1.60	1.47
2	C	110	ARG	CB-CG	-7.85	1.31	1.52
2	F	150	GLU	CD-OE1	7.84	1.34	1.25
3	U	279	GLU	CD-OE1	7.84	1.34	1.25
3	S	294	PHE	CE2-CZ	7.84	1.52	1.37
1	H	55	THR	C-O	7.83	1.38	1.23
1	E	65	GLU	CG-CD	7.82	1.63	1.51
2	C	63	GLY	N-CA	-7.82	1.34	1.46
1	K	155	ASN	C-O	7.82	1.38	1.23
1	K	151	TYR	CE1-CZ	7.81	1.48	1.38
1	B	64	GLU	CG-CD	7.81	1.63	1.51
2	C	43	ARG	CB-CG	-7.80	1.31	1.52
1	E	65	GLU	CD-OE2	7.80	1.34	1.25
2	C	38	VAL	C-O	7.80	1.38	1.23
1	E	74	ARG	CB-CG	-7.79	1.31	1.52
2	C	101	LYS	CE-NZ	7.79	1.68	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	150	GLU	CD-OE2	7.79	1.34	1.25
3	V	235	LYS	CE-NZ	7.78	1.68	1.49
3	S	289	GLU	CD-OE2	7.77	1.34	1.25
1	B	66	TYR	CB-CG	-7.77	1.40	1.51
1	B	95	LEU	CA-CB	-7.77	1.35	1.53
3	U	258	ILE	CA-CB	-7.77	1.36	1.54
1	B	30	GLU	CD-OE2	7.76	1.34	1.25
3	T	270	PRO	CA-C	-7.76	1.37	1.52
1	H	118	ALA	CA-CB	7.75	1.68	1.52
1	E	100	SER	CB-OG	-7.74	1.32	1.42
3	V	265	VAL	CB-CG2	-7.72	1.36	1.52
3	T	243	GLU	CG-CD	7.69	1.63	1.51
1	E	137	GLU	CG-CD	7.69	1.63	1.51
1	H	7	GLY	N-CA	7.69	1.57	1.46
2	C	65	GLU	CG-CD	7.68	1.63	1.51
3	T	259	GLU	CG-CD	7.68	1.63	1.51
3	S	279	GLU	C-O	-7.67	1.08	1.23
3	S	294	PHE	CD1-CE1	7.67	1.54	1.39
1	B	111	SER	CB-OG	-7.67	1.32	1.42
3	S	264	ARG	CZ-NH1	7.66	1.43	1.33
1	K	4	GLY	N-CA	7.66	1.57	1.46
1	B	156	ILE	C-O	7.65	1.37	1.23
1	B	30	GLU	CD-OE1	7.64	1.34	1.25
3	V	298	ASN	CB-CG	7.64	1.68	1.51
2	C	53	LYS	CG-CD	7.62	1.78	1.52
1	E	44	ALA	CA-CB	-7.61	1.36	1.52
1	K	150	LEU	CG-CD2	7.59	1.79	1.51
3	T	263	GLN	CG-CD	7.58	1.68	1.51
3	T	294	PHE	CE1-CZ	7.57	1.51	1.37
3	S	255	ARG	CZ-NH2	7.57	1.42	1.33
3	V	256	LYS	CD-CE	7.57	1.70	1.51
1	E	112	ILE	CB-CG2	-7.56	1.29	1.52
3	S	227	ASP	CB-CG	7.56	1.67	1.51
2	F	56	GLY	N-CA	7.55	1.57	1.46
2	C	153	ARG	NE-CZ	7.54	1.42	1.33
3	V	249	SER	CB-OG	7.53	1.52	1.42
2	L	75	TRP	CB-CG	-7.53	1.36	1.50
3	V	245	CYS	C-O	-7.51	1.09	1.23
3	V	292	ASP	CG-OD1	7.50	1.42	1.25
2	C	174	ASN	CB-CG	7.50	1.68	1.51
2	C	74	ARG	CG-CD	7.50	1.70	1.51
3	U	260	GLU	CD-OE2	7.47	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	TYR	N-CA	-7.46	1.31	1.46
3	S	300	TRP	CB-CG	7.46	1.63	1.50
2	L	134	VAL	CB-CG2	-7.45	1.37	1.52
3	U	253	TYR	CE1-CZ	7.45	1.48	1.38
2	I	98	CYS	CA-C	-7.45	1.33	1.52
2	F	104	GLU	CB-CG	7.45	1.66	1.52
2	C	108	PHE	CD1-CE1	7.43	1.54	1.39
1	B	37	ARG	CD-NE	-7.43	1.33	1.46
2	I	168	GLU	CG-CD	7.43	1.63	1.51
3	U	273	ARG	CZ-NH1	7.43	1.42	1.33
1	K	122	ASP	CB-CG	7.42	1.67	1.51
3	S	233	CYS	CA-CB	-7.42	1.37	1.53
1	H	39	PHE	CD1-CE1	-7.41	1.24	1.39
2	F	37	LYS	CE-NZ	7.41	1.67	1.49
1	E	129	VAL	CA-CB	-7.41	1.39	1.54
2	I	76	THR	CA-CB	-7.41	1.34	1.53
1	E	96	LYS	CG-CD	7.40	1.77	1.52
3	S	254	ASP	CB-CG	7.39	1.67	1.51
1	K	80	TYR	CG-CD1	7.39	1.48	1.39
1	H	33	GLU	CG-CD	7.38	1.63	1.51
1	B	131	GLU	CB-CG	7.37	1.66	1.52
2	C	103	PRO	N-CA	-7.36	1.34	1.47
1	B	131	GLU	CD-OE2	7.36	1.33	1.25
2	C	142	TYR	CD2-CE2	-7.36	1.28	1.39
1	B	77	THR	CA-CB	-7.35	1.34	1.53
1	E	94	ILE	CB-CG2	7.34	1.75	1.52
2	F	138	TRP	CE3-CZ3	7.34	1.50	1.38
1	H	149	ARG	CZ-NH2	7.34	1.42	1.33
3	T	242	ARG	CZ-NH2	7.33	1.42	1.33
3	T	243	GLU	CD-OE2	7.33	1.33	1.25
3	T	288	LYS	CE-NZ	7.33	1.67	1.49
1	B	120	ASN	C-O	7.33	1.37	1.23
2	C	170	GLN	C-O	7.33	1.37	1.23
2	I	104	GLU	CD-OE1	7.33	1.33	1.25
2	C	33	THR	CA-C	7.32	1.72	1.52
2	L	106	PRO	CA-C	-7.32	1.38	1.52
2	F	101	LYS	CB-CG	-7.31	1.32	1.52
3	S	244	PRO	CB-CG	-7.31	1.13	1.50
1	B	41	VAL	CB-CG1	-7.30	1.37	1.52
3	V	237	SER	CB-OG	7.29	1.51	1.42
3	V	235	LYS	CA-C	7.28	1.71	1.52
2	F	60	VAL	CB-CG2	-7.28	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	63	GLY	N-CA	-7.28	1.35	1.46
1	E	27	ILE	CA-CB	-7.26	1.38	1.54
2	F	37	LYS	CD-CE	7.26	1.69	1.51
1	B	80	TYR	CD1-CE1	-7.25	1.28	1.39
3	V	294	PHE	CE1-CZ	7.25	1.51	1.37
2	F	65	GLU	CG-CD	7.25	1.62	1.51
3	V	242	ARG	CG-CD	7.24	1.70	1.51
2	C	46	GLU	CD-OE2	7.24	1.33	1.25
2	C	57	ASP	CB-CG	7.21	1.66	1.51
2	F	38	VAL	C-O	7.21	1.37	1.23
1	K	72	LYS	CE-NZ	7.21	1.67	1.49
1	B	137	GLU	CB-CG	7.20	1.65	1.52
2	F	111	PHE	CD1-CE1	7.20	1.53	1.39
1	K	65	GLU	CG-CD	7.20	1.62	1.51
3	V	255	ARG	C-O	7.20	1.37	1.23
1	H	66	TYR	CG-CD2	-7.19	1.29	1.39
1	B	56	PHE	N-CA	-7.18	1.31	1.46
1	E	38	TYR	CG-CD1	7.18	1.48	1.39
1	B	73	VAL	CB-CG2	-7.18	1.37	1.52
2	C	46	GLU	CD-OE1	7.18	1.33	1.25
3	V	235	LYS	CD-CE	7.17	1.69	1.51
2	C	90	ARG	CZ-NH1	-7.17	1.23	1.33
1	K	51	PHE	CE2-CZ	7.15	1.50	1.37
3	S	271	VAL	CB-CG1	-7.15	1.37	1.52
2	F	74	ARG	NE-CZ	7.15	1.42	1.33
1	B	69	ALA	CA-CB	-7.14	1.37	1.52
1	B	75	PHE	CB-CG	-7.14	1.39	1.51
1	H	64	GLU	CD-OE1	7.13	1.33	1.25
2	I	43	ARG	CZ-NH1	7.13	1.42	1.33
1	K	123	ASP	N-CA	7.12	1.60	1.46
2	F	84	ARG	CB-CG	7.12	1.71	1.52
3	S	253	TYR	CE1-CZ	-7.12	1.29	1.38
3	T	276	LEU	C-O	-7.12	1.09	1.23
2	L	98	CYS	CB-SG	7.12	1.94	1.82
1	K	72	LYS	CD-CE	7.11	1.69	1.51
3	S	257	ASP	CG-OD2	7.11	1.41	1.25
3	S	264	ARG	CZ-NH2	7.11	1.42	1.33
1	E	127	ASN	N-CA	7.11	1.60	1.46
3	T	303	ASP	C-O	7.11	1.36	1.23
3	T	255	ARG	CZ-NH2	7.11	1.42	1.33
2	C	50	GLU	CG-CD	7.10	1.62	1.51
1	B	10	ARG	CZ-NH1	7.09	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	ALA	CA-CB	-7.09	1.37	1.52
1	E	147	TRP	CE3-CZ3	7.07	1.50	1.38
1	H	22	GLU	CD-OE1	7.07	1.33	1.25
1	H	17	GLN	CA-CB	-7.05	1.38	1.53
1	H	49	SER	CB-OG	7.05	1.51	1.42
2	C	137	LYS	CB-CG	-7.05	1.33	1.52
1	B	15	GLU	CD-OE1	7.04	1.33	1.25
1	E	105	ILE	N-CA	-7.04	1.32	1.46
1	K	30	GLU	CD-OE1	7.04	1.33	1.25
3	U	228	ILE	CB-CG2	7.01	1.74	1.52
1	H	11	ARG	C-O	7.01	1.36	1.23
1	H	36	ALA	CA-CB	-7.00	1.37	1.52
1	K	33	GLU	CG-CD	6.99	1.62	1.51
1	B	5	SER	CB-OG	6.99	1.51	1.42
1	H	28	LYS	CD-CE	6.99	1.68	1.51
1	E	129	VAL	CB-CG1	-6.98	1.38	1.52
2	C	33	THR	N-CA	6.98	1.60	1.46
2	I	55	VAL	CB-CG1	6.97	1.67	1.52
1	B	9	PRO	C-O	6.97	1.37	1.23
1	E	34	SER	CB-OG	6.97	1.51	1.42
3	T	231	TYR	CD1-CE1	6.97	1.49	1.39
1	H	131	GLU	CG-CD	6.96	1.62	1.51
3	S	245	CYS	CB-SG	-6.96	1.70	1.82
3	U	259	GLU	CD-OE2	6.95	1.33	1.25
1	B	70	ALA	C-N	-6.93	1.21	1.34
2	L	158	LYS	CD-CE	6.92	1.68	1.51
3	T	277	THR	C-O	-6.92	1.10	1.23
1	H	81	HIS	N-CA	6.92	1.60	1.46
1	E	97	ASP	CA-C	6.92	1.71	1.52
1	E	79	ILE	CA-CB	6.91	1.70	1.54
1	H	110	LEU	CG-CD2	6.91	1.77	1.51
2	F	153	ARG	CZ-NH1	6.90	1.42	1.33
1	H	7	GLY	CA-C	6.90	1.62	1.51
2	L	149	GLN	CG-CD	6.89	1.67	1.51
1	H	12	ILE	C-O	6.89	1.36	1.23
3	S	270	PRO	CA-C	-6.88	1.39	1.52
2	C	127	VAL	CA-CB	-6.88	1.40	1.54
1	H	6	ALA	CA-CB	6.88	1.66	1.52
2	L	91	ILE	C-O	-6.88	1.10	1.23
2	F	104	GLU	CG-CD	6.88	1.62	1.51
1	E	96	LYS	CE-NZ	6.87	1.66	1.49
1	E	113	GLN	C-O	-6.87	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	260	GLU	CD-OE1	6.87	1.33	1.25
3	V	261	HIS	C-O	6.85	1.36	1.23
2	I	76	THR	CB-CG2	-6.85	1.29	1.52
1	H	80	TYR	CE1-CZ	-6.84	1.29	1.38
1	H	22	GLU	CG-CD	6.84	1.62	1.51
2	C	114	LYS	C-O	-6.84	1.10	1.23
1	H	57	LYS	CE-NZ	6.83	1.66	1.49
2	F	127	VAL	CA-CB	-6.83	1.40	1.54
1	E	33	GLU	CG-CD	6.82	1.62	1.51
1	H	15	GLU	C-O	6.81	1.36	1.23
2	C	142	TYR	CG-CD1	6.81	1.48	1.39
1	B	22	GLU	CD-OE1	6.81	1.33	1.25
1	B	113	GLN	C-O	-6.80	1.10	1.23
1	H	106	ARG	CZ-NH1	6.80	1.41	1.33
3	U	289	GLU	CD-OE2	6.80	1.33	1.25
1	B	22	GLU	CA-CB	6.78	1.68	1.53
2	F	153	ARG	CZ-NH2	6.78	1.41	1.33
2	L	150	GLU	CD-OE2	6.78	1.33	1.25
2	C	142	TYR	CZ-OH	-6.77	1.26	1.37
1	B	92	LEU	N-CA	6.76	1.59	1.46
2	I	49	GLU	CG-CD	6.76	1.62	1.51
2	F	43	ARG	CZ-NH1	6.75	1.41	1.33
2	I	37	LYS	CB-CG	6.75	1.70	1.52
3	V	265	VAL	CB-CG1	6.75	1.67	1.52
2	C	147	VAL	CB-CG2	-6.74	1.38	1.52
2	L	169	GLY	C-O	6.74	1.34	1.23
3	U	253	TYR	CD1-CE1	6.73	1.49	1.39
3	S	270	PRO	CA-CB	-6.72	1.40	1.53
1	B	33	GLU	CG-CD	6.72	1.62	1.51
1	H	84	VAL	CA-CB	-6.72	1.40	1.54
2	L	95	LYS	CB-CG	6.72	1.70	1.52
2	L	50	GLU	CD-OE2	6.72	1.33	1.25
3	S	231	TYR	CB-CG	6.71	1.61	1.51
2	L	155	MET	CB-CG	6.70	1.72	1.51
3	U	256	LYS	CD-CE	6.70	1.68	1.51
2	I	50	GLU	CD-OE2	6.70	1.33	1.25
1	K	57	LYS	C-O	6.69	1.36	1.23
2	L	54	GLY	C-O	6.69	1.34	1.23
1	B	139	GLN	CB-CG	-6.69	1.34	1.52
3	S	237	SER	CA-CB	-6.68	1.43	1.52
1	K	6	ALA	N-CA	6.68	1.59	1.46
2	C	151	LEU	CG-CD2	-6.67	1.27	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	155	ASN	C-O	6.67	1.36	1.23
2	F	142	TYR	CD2-CE2	-6.67	1.29	1.39
1	E	75	PHE	CB-CG	-6.66	1.40	1.51
1	B	72	LYS	CA-CB	-6.66	1.39	1.53
1	E	156	ILE	CA-C	6.66	1.70	1.52
2	I	139	GLN	CD-NE2	6.66	1.49	1.32
1	B	56	PHE	C-O	6.65	1.35	1.23
3	U	287	MET	CG-SD	6.65	1.98	1.81
1	B	85	ASP	CG-OD2	6.64	1.40	1.25
1	B	66	TYR	CA-CB	-6.63	1.39	1.53
3	S	271	VAL	CB-CG2	6.63	1.66	1.52
1	K	22	GLU	CB-CG	6.63	1.64	1.52
1	K	59	GLU	CD-OE2	6.63	1.32	1.25
3	V	266	GLY	CA-C	6.63	1.62	1.51
3	T	235	LYS	CD-CE	6.62	1.67	1.51
3	V	288	LYS	CG-CD	6.61	1.75	1.52
2	L	143	SER	CB-OG	6.60	1.50	1.42
1	B	84	VAL	C-O	-6.59	1.10	1.23
3	V	273	ARG	C-O	6.59	1.35	1.23
1	B	13	ILE	CA-CB	6.59	1.70	1.54
1	E	70	ALA	N-CA	6.58	1.59	1.46
2	I	153	ARG	N-CA	6.58	1.59	1.46
3	U	251	ILE	CB-CG2	-6.58	1.32	1.52
1	B	40	HIS	N-CA	-6.56	1.33	1.46
1	B	45	GLY	C-O	6.56	1.34	1.23
1	K	11	ARG	C-O	6.56	1.35	1.23
3	S	256	LYS	CG-CD	6.55	1.74	1.52
3	S	231	TYR	CG-CD1	6.55	1.47	1.39
3	S	275	PRO	N-CA	6.55	1.58	1.47
3	U	231	TYR	CG-CD2	6.55	1.47	1.39
3	T	253	TYR	N-CA	-6.54	1.33	1.46
2	C	131	ALA	CA-C	6.54	1.70	1.52
2	I	99	GLY	N-CA	-6.53	1.36	1.46
2	L	68	GLU	CG-CD	6.53	1.61	1.51
3	T	243	GLU	CD-OE1	6.53	1.32	1.25
2	L	49	GLU	CD-OE1	6.53	1.32	1.25
3	S	279	GLU	CD-OE2	6.53	1.32	1.25
1	H	83	ASN	C-O	6.51	1.35	1.23
1	H	66	TYR	CB-CG	-6.50	1.41	1.51
2	L	101	LYS	CD-CE	6.50	1.67	1.51
1	B	59	GLU	CB-CG	-6.50	1.39	1.52
2	I	37	LYS	CG-CD	6.50	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	260	GLU	CB-CG	-6.50	1.39	1.52
3	V	282	ILE	CA-CB	6.49	1.69	1.54
1	E	92	LEU	C-O	6.49	1.35	1.23
1	E	91	CYS	N-CA	-6.49	1.33	1.46
3	T	244	PRO	CA-C	6.48	1.65	1.52
1	H	146	ALA	CA-CB	6.48	1.66	1.52
3	S	263	GLN	CD-NE2	6.47	1.49	1.32
1	B	33	GLU	N-CA	6.46	1.59	1.46
1	B	108	VAL	CB-CG2	-6.46	1.39	1.52
2	F	95	LYS	CD-CE	6.46	1.67	1.51
3	U	243	GLU	CG-CD	6.46	1.61	1.51
1	B	56	PHE	CE2-CZ	-6.45	1.25	1.37
1	K	57	LYS	CG-CD	6.45	1.74	1.52
1	B	107	THR	N-CA	-6.45	1.33	1.46
1	K	59	GLU	CG-CD	6.45	1.61	1.51
1	K	70	ALA	CA-CB	-6.44	1.39	1.52
3	U	251	ILE	CA-CB	6.44	1.69	1.54
2	L	87	TYR	CD1-CE1	6.44	1.49	1.39
2	C	145	LYS	CD-CE	6.44	1.67	1.51
1	E	154	ASN	CB-CG	6.43	1.65	1.51
1	H	84	VAL	CB-CG2	-6.43	1.39	1.52
3	V	274	SER	CB-OG	6.43	1.50	1.42
1	B	16	THR	CB-CG2	-6.43	1.31	1.52
1	K	18	ARG	C-O	6.42	1.35	1.23
3	T	270	PRO	C-O	-6.42	1.10	1.23
2	F	57	ASP	N-CA	6.42	1.59	1.46
2	L	126	VAL	CB-CG2	-6.41	1.39	1.52
2	C	147	VAL	CB-CG1	-6.41	1.39	1.52
2	I	75	TRP	CE3-CZ3	6.40	1.49	1.38
2	C	92	TYR	C-O	-6.40	1.11	1.23
1	E	8	LEU	CG-CD1	6.40	1.75	1.51
2	I	91	ILE	C-O	6.40	1.35	1.23
3	U	253	TYR	CZ-OH	6.40	1.48	1.37
2	C	78	MET	SD-CE	6.39	2.13	1.77
2	F	36	VAL	CB-CG2	6.39	1.66	1.52
1	H	131	GLU	CB-CG	6.39	1.64	1.52
1	H	39	PHE	CD2-CE2	-6.39	1.26	1.39
1	B	53	GLY	CA-C	6.38	1.62	1.51
2	C	49	GLU	CA-C	-6.38	1.36	1.52
3	U	274	SER	CA-CB	-6.38	1.43	1.52
3	T	238	PHE	CD1-CE1	-6.38	1.26	1.39
1	E	6	ALA	C-O	6.36	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	104	GLU	CD-OE2	6.36	1.32	1.25
1	B	97	ASP	CB-CG	6.36	1.65	1.51
2	C	109	VAL	CA-CB	-6.36	1.41	1.54
3	T	290	VAL	CA-CB	-6.35	1.41	1.54
2	C	45	LEU	CA-CB	-6.35	1.39	1.53
1	H	98	LYS	CB-CG	6.34	1.69	1.52
1	B	86	LYS	CD-CE	6.34	1.67	1.51
1	B	99	TRP	CE2-CZ2	-6.34	1.28	1.39
3	U	265	VAL	CB-CG1	-6.34	1.39	1.52
2	L	85	THR	N-CA	6.34	1.59	1.46
1	H	74	ARG	CB-CG	-6.33	1.35	1.52
1	B	76	MET	CG-SD	6.33	1.97	1.81
3	S	284	ASN	CB-CG	6.32	1.65	1.51
2	C	126	VAL	CA-C	-6.30	1.36	1.52
2	L	143	SER	CA-CB	6.30	1.62	1.52
2	I	159	GLU	CD-OE1	6.30	1.32	1.25
3	T	238	PHE	CE2-CZ	-6.30	1.25	1.37
1	E	99	TRP	CA-CB	-6.29	1.40	1.53
1	K	81	HIS	N-CA	6.29	1.58	1.46
3	V	264	ARG	C-O	6.29	1.35	1.23
3	U	231	TYR	CE2-CZ	6.29	1.46	1.38
2	L	153	ARG	CZ-NH2	6.29	1.41	1.33
2	I	68	GLU	CD-OE2	6.28	1.32	1.25
1	E	127	ASN	CB-CG	6.28	1.65	1.51
1	H	73	VAL	CB-CG2	-6.27	1.39	1.52
1	B	75	PHE	CG-CD1	-6.27	1.29	1.38
1	B	111	SER	CA-CB	-6.27	1.43	1.52
2	L	117	MET	CG-SD	6.27	1.97	1.81
2	I	150	GLU	CD-OE1	6.26	1.32	1.25
1	B	34	SER	C-O	-6.26	1.11	1.23
1	B	76	MET	CB-CG	-6.26	1.31	1.51
3	U	236	ILE	CB-CG2	-6.26	1.33	1.52
1	H	61	PHE	CG-CD1	6.25	1.48	1.38
1	E	106	ARG	CG-CD	6.24	1.67	1.51
2	L	169	GLY	N-CA	6.24	1.55	1.46
3	S	231	TYR	CD2-CE2	6.24	1.48	1.39
3	T	282	ILE	CA-CB	-6.24	1.40	1.54
1	B	17	GLN	CA-CB	-6.24	1.40	1.53
2	C	92	TYR	CD2-CE2	-6.24	1.29	1.39
3	T	271	VAL	CB-CG1	-6.23	1.39	1.52
1	K	28	LYS	CD-CE	6.22	1.66	1.51
1	H	14	LYS	CD-CE	6.22	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	68	GLU	CB-CG	6.22	1.64	1.52
2	C	107	PRO	CG-CD	-6.22	1.30	1.50
2	L	62	TRP	CB-CG	6.22	1.61	1.50
1	B	43	ILE	C-O	-6.21	1.11	1.23
2	C	113	THR	C-O	-6.21	1.11	1.23
1	B	3	ALA	CA-CB	6.21	1.65	1.52
1	E	72	LYS	CD-CE	6.21	1.66	1.51
1	E	78	LYS	CD-CE	6.20	1.66	1.51
2	I	47	GLU	CD-OE1	6.20	1.32	1.25
2	F	74	ARG	CB-CG	-6.20	1.35	1.52
1	B	151	TYR	CG-CD1	6.19	1.47	1.39
1	E	86	LYS	CB-CG	6.19	1.69	1.52
2	I	41	ASN	C-O	6.19	1.35	1.23
1	K	71	PRO	C-O	6.18	1.35	1.23
2	L	152	ARG	CG-CD	6.18	1.67	1.51
3	V	280	GLN	CD-OE1	6.18	1.37	1.24
1	K	112	ILE	CA-CB	6.17	1.69	1.54
3	S	248	PRO	CA-C	-6.17	1.40	1.52
3	U	275	PRO	C-O	6.16	1.35	1.23
3	U	279	GLU	C-O	6.16	1.35	1.23
1	K	134	LYS	CA-C	6.15	1.69	1.52
1	K	78	LYS	CE-NZ	6.15	1.64	1.49
2	I	137	LYS	CE-NZ	6.15	1.64	1.49
2	C	174	ASN	N-CA	6.15	1.58	1.46
2	I	49	GLU	CD-OE1	6.14	1.32	1.25
3	S	258	ILE	CB-CG2	-6.14	1.33	1.52
3	U	249	SER	CA-CB	6.14	1.62	1.52
1	B	152	ALA	CA-CB	-6.14	1.39	1.52
1	B	80	TYR	CE1-CZ	-6.14	1.30	1.38
3	T	280	GLN	CB-CG	-6.14	1.35	1.52
1	K	120	ASN	N-CA	6.12	1.58	1.46
1	K	39	PHE	CE2-CZ	6.12	1.49	1.37
2	F	165	GLN	CA-CB	-6.12	1.40	1.53
3	S	265	VAL	C-O	-6.12	1.11	1.23
2	C	102	TYR	CE1-CZ	-6.11	1.30	1.38
3	S	254	ASP	CG-OD1	6.11	1.39	1.25
2	I	38	VAL	N-CA	6.11	1.58	1.46
2	I	88	GLU	CD-OE1	6.10	1.32	1.25
1	K	45	GLY	N-CA	6.10	1.55	1.46
1	H	65	GLU	CB-CG	6.10	1.63	1.52
1	K	99	TRP	C-O	6.10	1.34	1.23
1	H	58	LEU	CA-C	-6.10	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	45	LEU	N-CA	6.10	1.58	1.46
3	S	283	PRO	CA-CB	-6.09	1.41	1.53
1	B	70	ALA	C-O	-6.08	1.11	1.23
2	C	104	GLU	CD-OE1	6.08	1.32	1.25
2	F	40	ARG	CG-CD	6.08	1.67	1.51
3	V	231	TYR	CA-CB	-6.06	1.40	1.53
2	L	37	LYS	CB-CG	6.06	1.69	1.52
2	F	172	TYR	CE1-CZ	6.06	1.46	1.38
1	K	22	GLU	CD-OE1	6.06	1.32	1.25
3	S	294	PHE	CG-CD1	6.06	1.47	1.38
1	B	150	LEU	CG-CD1	6.06	1.74	1.51
2	F	65	GLU	CA-C	-6.06	1.37	1.52
1	K	46	PRO	N-CA	6.05	1.57	1.47
3	V	231	TYR	CB-CG	-6.05	1.42	1.51
2	I	137	LYS	C-O	-6.05	1.11	1.23
1	E	22	GLU	CD-OE1	6.05	1.32	1.25
2	C	47	GLU	CD-OE2	6.04	1.32	1.25
3	S	253	TYR	CD2-CE2	-6.03	1.30	1.39
3	U	238	PHE	CG-CD1	6.03	1.47	1.38
3	V	270	PRO	CB-CG	6.03	1.80	1.50
2	C	82	PRO	C-O	-6.03	1.11	1.23
3	S	254	ASP	CG-OD2	6.03	1.39	1.25
1	B	39	PHE	CD2-CE2	-6.02	1.27	1.39
2	C	61	SER	C-O	-6.02	1.11	1.23
2	C	112	VAL	CB-CG2	6.01	1.65	1.52
1	B	102	ALA	CA-CB	-6.01	1.39	1.52
1	E	76	MET	C-O	-6.01	1.11	1.23
1	K	75	PHE	C-O	6.00	1.34	1.23
1	H	18	ARG	CG-CD	6.00	1.67	1.51
1	K	52	GLU	N-CA	6.00	1.58	1.46
1	K	80	TYR	CG-CD2	6.00	1.47	1.39
1	H	34	SER	CB-OG	6.00	1.50	1.42
3	V	264	ARG	CZ-NH1	6.00	1.40	1.33
1	E	61	PHE	CE1-CZ	-5.99	1.25	1.37
2	I	132	ILE	CA-CB	-5.99	1.41	1.54
3	U	256	LYS	CG-CD	5.99	1.72	1.52
1	E	35	ASN	CB-CG	5.98	1.64	1.51
3	S	278	GLN	N-CA	-5.98	1.34	1.46
1	H	10	ARG	CZ-NH2	5.98	1.40	1.33
2	L	104	GLU	CB-CG	5.97	1.63	1.52
2	L	78	MET	CG-SD	5.97	1.96	1.81
1	K	89	ARG	C-O	5.97	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	39	PRO	N-CA	5.96	1.57	1.47
2	L	40	ARG	CD-NE	5.96	1.56	1.46
1	H	20	LEU	CG-CD2	5.96	1.74	1.51
3	S	294	PHE	CD2-CE2	5.96	1.51	1.39
3	S	256	LYS	N-CA	5.96	1.58	1.46
3	S	263	GLN	CD-OE1	5.96	1.37	1.24
2	F	171	CYS	CA-CB	-5.95	1.40	1.53
1	K	133	TRP	CZ3-CH2	5.95	1.49	1.40
3	V	279	GLU	CD-OE2	5.95	1.32	1.25
1	K	30	GLU	CG-CD	5.95	1.60	1.51
3	T	247	THR	C-O	-5.94	1.12	1.23
1	H	147	TRP	CE3-CZ3	5.94	1.48	1.38
3	V	264	ARG	CA-C	5.94	1.68	1.52
1	B	73	VAL	CB-CG1	-5.93	1.40	1.52
1	E	22	GLU	CD-OE2	5.93	1.32	1.25
2	F	102	TYR	CD1-CE1	-5.93	1.30	1.39
2	C	84	ARG	CZ-NH1	5.93	1.40	1.33
2	C	111	PHE	CE2-CZ	-5.92	1.26	1.37
2	C	159	GLU	CD-OE1	5.92	1.32	1.25
2	L	126	VAL	CA-CB	-5.91	1.42	1.54
2	C	38	VAL	CA-CB	5.90	1.67	1.54
3	T	250	GLY	C-O	-5.90	1.14	1.23
3	V	267	HIS	C-O	5.90	1.34	1.23
1	B	78	LYS	CE-NZ	5.90	1.63	1.49
3	V	273	ARG	CG-CD	5.90	1.66	1.51
3	S	252	THR	CA-CB	5.89	1.68	1.53
1	H	99	TRP	CD2-CE2	5.89	1.48	1.41
1	K	83	ASN	CG-ND2	5.88	1.47	1.32
3	V	287	MET	CG-SD	5.88	1.96	1.81
3	T	255	ARG	CG-CD	5.88	1.66	1.51
3	T	253	TYR	C-O	-5.88	1.12	1.23
2	C	42	PHE	CE1-CZ	5.86	1.48	1.37
2	C	164	PRO	C-O	-5.86	1.11	1.23
3	T	297	GLU	CD-OE2	5.86	1.32	1.25
1	B	74	ARG	CZ-NH2	-5.85	1.25	1.33
1	E	14	LYS	CA-C	5.84	1.68	1.52
3	S	243	GLU	CD-OE2	5.84	1.32	1.25
1	B	128	ASP	CG-OD2	5.84	1.38	1.25
1	B	142	GLU	CA-CB	-5.84	1.41	1.53
1	K	155	ASN	CA-C	5.84	1.68	1.52
1	E	96	LYS	CB-CG	5.84	1.68	1.52
1	K	77	THR	CB-CG2	5.83	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	145	ARG	CA-CB	-5.83	1.41	1.53
1	K	44	ALA	CA-CB	5.83	1.64	1.52
3	V	231	TYR	CZ-OH	5.83	1.47	1.37
2	C	103	PRO	CA-C	-5.82	1.41	1.52
1	E	37	ARG	CB-CG	5.82	1.68	1.52
3	T	259	GLU	CD-OE1	5.82	1.32	1.25
2	F	77	GLY	C-O	5.81	1.32	1.23
2	I	37	LYS	N-CA	5.81	1.57	1.46
2	C	164	PRO	CB-CG	-5.80	1.21	1.50
2	L	144	ILE	C-O	5.80	1.34	1.23
3	S	273	ARG	CZ-NH1	5.80	1.40	1.33
2	F	124	ASN	N-CA	5.80	1.57	1.46
3	T	227	ASP	N-CA	5.80	1.57	1.46
2	F	134	VAL	CB-CG2	-5.80	1.40	1.52
1	H	48	ASP	CG-OD1	5.80	1.38	1.25
2	C	120	VAL	CA-CB	-5.80	1.42	1.54
2	C	120	VAL	CB-CG2	-5.79	1.40	1.52
3	U	249	SER	CB-OG	5.79	1.49	1.42
2	C	52	GLN	CD-NE2	5.78	1.47	1.32
3	S	235	LYS	CG-CD	-5.78	1.32	1.52
2	F	63	GLY	CA-C	-5.78	1.42	1.51
2	F	74	ARG	CZ-NH2	5.78	1.40	1.33
2	F	145	LYS	CB-CG	-5.78	1.36	1.52
2	C	153	ARG	CD-NE	5.78	1.56	1.46
1	E	145	ARG	CG-CD	-5.78	1.37	1.51
1	H	22	GLU	CD-OE2	5.78	1.32	1.25
1	K	6	ALA	CA-C	5.78	1.68	1.52
3	V	243	GLU	CB-CG	-5.78	1.41	1.52
1	B	47	GLN	C-O	5.77	1.34	1.23
1	B	75	PHE	C-O	5.77	1.34	1.23
3	T	246	ILE	C-O	-5.77	1.12	1.23
1	E	77	THR	N-CA	-5.77	1.34	1.46
1	E	124	PRO	C-O	5.77	1.34	1.23
1	E	156	ILE	CA-CB	5.77	1.68	1.54
2	I	142	TYR	CD1-CE1	5.77	1.48	1.39
2	L	84	ARG	CG-CD	5.77	1.66	1.51
1	E	99	TRP	C-O	5.77	1.34	1.23
1	K	137	GLU	CD-OE2	5.76	1.31	1.25
3	S	260	GLU	CA-C	-5.76	1.38	1.52
1	K	44	ALA	CA-C	5.76	1.68	1.52
3	S	294	PHE	CE1-CZ	5.76	1.48	1.37
2	I	37	LYS	CE-NZ	5.76	1.63	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	156	MET	CA-CB	-5.76	1.41	1.53
3	T	252	THR	N-CA	-5.75	1.34	1.46
2	F	124	ASN	C-O	5.75	1.34	1.23
1	K	151	TYR	CD1-CE1	5.75	1.48	1.39
1	B	6	ALA	C-O	-5.75	1.12	1.23
1	K	31	PRO	CA-C	-5.75	1.41	1.52
2	C	99	GLY	C-O	5.74	1.32	1.23
1	B	39	PHE	C-O	-5.74	1.12	1.23
2	L	62	TRP	CZ3-CH2	5.74	1.49	1.40
2	I	153	ARG	CG-CD	5.74	1.66	1.51
3	S	261	HIS	CA-CB	-5.74	1.41	1.53
1	B	75	PHE	CG-CD2	-5.74	1.30	1.38
1	H	22	GLU	CB-CG	5.73	1.63	1.52
3	T	239	GLU	CD-OE2	5.73	1.31	1.25
2	F	38	VAL	N-CA	5.72	1.57	1.46
3	S	238	PHE	CD2-CE2	5.72	1.50	1.39
2	C	67	ASP	CG-OD1	5.72	1.38	1.25
3	U	243	GLU	CB-CG	-5.72	1.41	1.52
2	L	137	LYS	CB-CG	5.72	1.68	1.52
1	K	95	LEU	C-O	-5.71	1.12	1.23
1	B	143	THR	N-CA	-5.71	1.34	1.46
1	H	30	GLU	C-O	-5.71	1.12	1.23
3	V	255	ARG	CZ-NH2	5.71	1.40	1.33
1	E	85	ASP	N-CA	-5.71	1.34	1.46
3	V	260	GLU	CD-OE1	5.71	1.31	1.25
1	E	75	PHE	CA-CB	-5.71	1.41	1.53
2	F	108	PHE	CE2-CZ	5.70	1.48	1.37
1	H	102	ALA	CA-CB	-5.70	1.40	1.52
3	U	242	ARG	CZ-NH2	5.70	1.40	1.33
1	E	112	ILE	CA-CB	-5.70	1.41	1.54
3	S	279	GLU	N-CA	5.70	1.57	1.46
1	E	89	ARG	C-O	5.69	1.34	1.23
2	F	74	ARG	CA-C	-5.69	1.38	1.52
1	E	37	ARG	CZ-NH1	5.69	1.40	1.33
1	E	135	THR	C-O	5.69	1.34	1.23
3	S	279	GLU	CB-CG	-5.69	1.41	1.52
2	C	110	ARG	CG-CD	-5.68	1.37	1.51
2	C	159	GLU	CD-OE2	5.68	1.31	1.25
2	F	88	GLU	CB-CG	-5.68	1.41	1.52
2	I	126	VAL	CB-CG2	-5.68	1.41	1.52
3	V	273	ARG	CZ-NH1	5.68	1.40	1.33
1	H	45	GLY	N-CA	5.68	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	280	GLN	CD-NE2	5.68	1.47	1.32
2	F	168	GLU	CB-CG	-5.67	1.41	1.52
2	F	131	ALA	CA-CB	-5.67	1.40	1.52
2	F	75	TRP	CG-CD1	5.67	1.44	1.36
3	U	234	GLY	C-O	5.67	1.32	1.23
2	F	171	CYS	CB-SG	5.67	1.91	1.82
3	S	300	TRP	CD2-CE2	5.67	1.48	1.41
2	C	168	GLU	CD-OE2	5.66	1.31	1.25
2	F	151	LEU	N-CA	-5.66	1.35	1.46
3	V	251	ILE	CA-CB	5.65	1.67	1.54
1	K	30	GLU	CD-OE2	5.65	1.31	1.25
1	B	128	ASP	C-O	5.64	1.34	1.23
2	F	92	TYR	CZ-OH	5.64	1.47	1.37
3	T	303	ASP	CA-C	5.64	1.67	1.52
3	S	279	GLU	CG-CD	5.64	1.60	1.51
1	E	151	TYR	CB-CG	5.64	1.60	1.51
2	I	59	THR	CA-C	5.64	1.67	1.52
2	L	76	THR	CB-CG2	5.64	1.71	1.52
1	B	74	ARG	C-O	-5.63	1.12	1.23
1	B	10	ARG	CB-CG	5.63	1.67	1.52
2	L	96	ILE	CB-CG2	-5.63	1.35	1.52
1	E	78	LYS	C-O	-5.62	1.12	1.23
1	H	95	LEU	CA-C	-5.62	1.38	1.52
2	C	96	ILE	CA-CB	-5.62	1.42	1.54
2	F	48	LEU	N-CA	-5.62	1.35	1.46
1	H	145	ARG	CZ-NH2	5.62	1.40	1.33
1	K	57	LYS	CD-CE	5.61	1.65	1.51
1	E	137	GLU	CB-CG	5.61	1.62	1.52
3	S	245	CYS	CA-CB	-5.61	1.41	1.53
2	I	52	GLN	CD-NE2	5.60	1.46	1.32
2	C	171	CYS	CB-SG	5.59	1.91	1.82
2	I	39	PRO	N-CA	5.59	1.56	1.47
1	B	64	GLU	CD-OE1	5.59	1.31	1.25
2	F	142	TYR	CE1-CZ	5.59	1.45	1.38
2	F	150	GLU	CB-CG	-5.59	1.41	1.52
1	H	68	MET	CG-SD	5.59	1.95	1.81
2	L	64	LEU	C-O	5.58	1.33	1.23
2	L	92	TYR	CE1-CZ	-5.58	1.31	1.38
2	C	165	GLN	CA-C	-5.58	1.38	1.52
3	U	242	ARG	CZ-NH1	5.58	1.40	1.33
1	B	155	ASN	CB-CG	5.58	1.63	1.51
1	H	135	THR	CA-CB	5.58	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	TYR	N-CA	-5.58	1.35	1.46
2	C	127	VAL	CB-CG1	-5.58	1.41	1.52
1	E	43	ILE	CA-CB	-5.58	1.42	1.54
3	V	229	PRO	C-O	5.57	1.34	1.23
2	L	174	ASN	C-O	5.57	1.33	1.23
1	K	36	ALA	CA-CB	5.57	1.64	1.52
2	L	55	VAL	CB-CG2	5.57	1.64	1.52
2	F	165	GLN	C-O	-5.57	1.12	1.23
1	K	100	SER	C-O	5.57	1.33	1.23
1	K	147	TRP	C-O	5.57	1.33	1.23
2	L	159	GLU	CD-OE1	5.57	1.31	1.25
1	E	84	VAL	CB-CG1	5.56	1.64	1.52
1	K	66	TYR	CE2-CZ	5.56	1.45	1.38
2	L	59	THR	CB-CG2	5.56	1.70	1.52
1	E	81	HIS	CA-CB	5.56	1.66	1.53
3	T	227	ASP	CB-CG	5.56	1.63	1.51
1	B	37	ARG	CG-CD	-5.56	1.38	1.51
2	L	50	GLU	CD-OE1	5.55	1.31	1.25
3	T	236	ILE	CA-CB	-5.55	1.42	1.54
2	I	142	TYR	CG-CD2	5.55	1.46	1.39
1	K	120	ASN	C-O	5.55	1.33	1.23
1	H	28	LYS	CB-CG	5.55	1.67	1.52
1	K	64	GLU	CB-CG	5.55	1.62	1.52
1	B	155	ASN	CA-C	5.54	1.67	1.52
1	B	68	MET	CA-CB	-5.54	1.41	1.53
1	B	84	VAL	CA-CB	-5.53	1.43	1.54
3	S	259	GLU	CG-CD	5.53	1.60	1.51
1	B	98	LYS	CE-NZ	5.53	1.62	1.49
1	E	132	GLN	CB-CG	-5.53	1.37	1.52
1	B	38	TYR	CE1-CZ	5.52	1.45	1.38
1	E	60	LEU	N-CA	5.52	1.57	1.46
3	S	248	PRO	C-O	-5.52	1.12	1.23
3	S	231	TYR	CE2-CZ	5.52	1.45	1.38
1	B	25	PRO	CA-C	5.52	1.63	1.52
2	C	143	SER	C-O	5.52	1.33	1.23
1	K	69	ALA	C-O	5.52	1.33	1.23
3	V	280	GLN	C-O	5.52	1.33	1.23
1	E	119	PRO	C-O	5.51	1.34	1.23
2	L	162	LYS	CE-NZ	5.51	1.62	1.49
3	V	268	PHE	CE1-CZ	-5.51	1.26	1.37
2	F	122	SER	CB-OG	-5.51	1.35	1.42
3	T	289	GLU	C-O	5.51	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	LYS	CA-C	-5.49	1.38	1.52
2	C	41	ASN	CA-CB	-5.48	1.38	1.53
1	B	3	ALA	C-N	5.47	1.43	1.33
1	B	63	PRO	C-O	-5.47	1.12	1.23
2	I	79	ILE	C-O	5.47	1.33	1.23
2	L	46	GLU	CD-OE2	5.47	1.31	1.25
3	S	276	LEU	C-O	-5.47	1.12	1.23
1	K	99	TRP	CD2-CE2	5.47	1.48	1.41
2	F	138	TRP	CB-CG	-5.47	1.40	1.50
3	U	260	GLU	CG-CD	5.47	1.60	1.51
1	E	129	VAL	N-CA	-5.47	1.35	1.46
1	K	42	VAL	C-O	5.46	1.33	1.23
1	B	24	VAL	C-O	-5.46	1.12	1.23
2	C	146	VAL	CB-CG1	-5.46	1.41	1.52
2	C	79	ILE	CA-CB	-5.45	1.42	1.54
3	V	240	LEU	CG-CD1	5.45	1.72	1.51
2	I	87	TYR	CG-CD2	5.45	1.46	1.39
1	E	35	ASN	C-O	5.45	1.33	1.23
3	U	295	ILE	CB-CG2	5.45	1.69	1.52
2	L	68	GLU	CD-OE1	5.44	1.31	1.25
1	K	110	LEU	C-O	5.44	1.33	1.23
1	B	3	ALA	C-O	5.44	1.33	1.23
3	V	259	GLU	CB-CG	5.44	1.62	1.52
1	H	119	PRO	CB-CG	5.43	1.77	1.50
2	L	163	LEU	N-CA	5.43	1.57	1.46
2	L	109	VAL	CB-CG2	-5.42	1.41	1.52
2	I	150	GLU	CA-C	5.42	1.67	1.52
1	B	93	ASP	CB-CG	5.42	1.63	1.51
3	S	227	ASP	CG-OD2	5.42	1.37	1.25
1	E	128	ASP	CG-OD1	5.42	1.37	1.25
1	H	124	PRO	CA-C	5.42	1.63	1.52
3	V	237	SER	CA-CB	5.42	1.61	1.52
2	I	56	GLY	C-O	5.41	1.32	1.23
2	L	37	LYS	CD-CE	5.41	1.64	1.51
1	B	98	LYS	N-CA	-5.41	1.35	1.46
1	E	102	ALA	CA-CB	5.40	1.63	1.52
2	F	57	ASP	CG-OD2	5.40	1.37	1.25
1	K	140	ALA	C-O	5.40	1.33	1.23
2	F	130	ARG	CG-CD	-5.40	1.38	1.51
1	B	88	GLY	CA-C	5.39	1.60	1.51
1	B	89	ARG	CZ-NH1	5.39	1.40	1.33
3	V	268	PHE	N-CA	5.39	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	145	ARG	CZ-NH1	5.39	1.40	1.33
2	L	66	ASP	C-O	5.39	1.33	1.23
2	F	40	ARG	N-CA	5.39	1.57	1.46
1	H	16	THR	CA-CB	5.39	1.67	1.53
1	H	34	SER	CA-CB	5.39	1.61	1.52
1	B	7	GLY	N-CA	-5.38	1.38	1.46
2	F	158	LYS	CA-C	-5.38	1.39	1.52
1	K	26	GLY	N-CA	5.38	1.54	1.46
1	K	143	THR	CB-CG2	5.38	1.70	1.52
2	F	169	GLY	C-O	-5.37	1.15	1.23
3	V	288	LYS	CD-CE	5.37	1.64	1.51
1	E	29	ALA	N-CA	5.37	1.57	1.46
2	F	111	PHE	CD2-CE2	5.37	1.50	1.39
2	C	48	LEU	N-CA	-5.37	1.35	1.46
1	H	10	ARG	N-CA	-5.37	1.35	1.46
1	K	100	SER	CA-CB	5.36	1.60	1.52
1	H	142	GLU	CB-CG	5.36	1.62	1.52
3	S	242	ARG	CD-NE	5.36	1.55	1.46
1	E	59	GLU	CD-OE1	5.36	1.31	1.25
2	C	74	ARG	NE-CZ	5.35	1.40	1.33
1	H	10	ARG	CZ-NH1	5.35	1.40	1.33
3	S	276	LEU	CA-C	-5.35	1.39	1.52
1	E	93	ASP	C-O	5.35	1.33	1.23
1	E	59	GLU	C-O	5.35	1.33	1.23
2	F	49	GLU	CD-OE1	5.35	1.31	1.25
3	T	303	ASP	CB-CG	5.35	1.62	1.51
3	V	263	GLN	CB-CG	5.35	1.67	1.52
1	B	22	GLU	C-O	5.35	1.33	1.23
1	H	35	ASN	C-O	5.34	1.33	1.23
2	I	68	GLU	CG-CD	5.34	1.59	1.51
3	T	238	PHE	CB-CG	5.34	1.60	1.51
3	T	271	VAL	C-O	-5.34	1.13	1.23
1	B	43	ILE	CB-CG2	-5.34	1.36	1.52
2	C	123	SER	CA-CB	-5.34	1.45	1.52
1	H	24	VAL	C-O	5.34	1.33	1.23
1	E	51	PHE	CB-CG	-5.33	1.42	1.51
1	K	28	LYS	CE-NZ	5.33	1.62	1.49
3	T	260	GLU	C-O	-5.33	1.13	1.23
2	I	39	PRO	CG-CD	5.33	1.68	1.50
1	B	51	PHE	CE2-CZ	5.33	1.47	1.37
3	V	260	GLU	CB-CG	5.33	1.62	1.52
2	C	158	LYS	CG-CD	5.33	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	97	GLU	C-O	-5.33	1.13	1.23
2	F	68	GLU	CD-OE1	5.33	1.31	1.25
1	K	156	ILE	N-CA	5.32	1.56	1.46
1	E	75	PHE	CE2-CZ	-5.32	1.27	1.37
3	U	229	PRO	CG-CD	5.32	1.68	1.50
2	F	153	ARG	N-CA	5.31	1.56	1.46
2	C	165	GLN	C-O	-5.31	1.13	1.23
1	H	138	ALA	N-CA	5.31	1.56	1.46
1	E	132	GLN	CA-CB	-5.30	1.42	1.53
2	C	49	GLU	CB-CG	5.30	1.62	1.52
1	K	155	ASN	CB-CG	5.30	1.63	1.51
2	C	80	LEU	CG-CD2	-5.30	1.32	1.51
2	C	137	LYS	CG-CD	-5.30	1.34	1.52
3	T	260	GLU	CG-CD	5.30	1.59	1.51
3	U	295	ILE	N-CA	5.30	1.56	1.46
1	B	124	PRO	CB-CG	5.29	1.76	1.50
1	K	81	HIS	CA-C	5.29	1.66	1.52
2	C	55	VAL	CA-CB	5.29	1.65	1.54
3	V	279	GLU	C-O	-5.29	1.13	1.23
3	U	276	LEU	CA-C	-5.28	1.39	1.52
2	F	65	GLU	CB-CG	-5.28	1.42	1.52
1	E	38	TYR	CZ-OH	5.28	1.46	1.37
2	F	56	GLY	CA-C	5.28	1.60	1.51
1	H	120	ASN	CG-OD1	5.27	1.35	1.24
3	T	300	TRP	CE2-CZ2	5.27	1.48	1.39
2	F	153	ARG	NE-CZ	5.27	1.39	1.33
1	B	29	ALA	C-O	-5.26	1.13	1.23
1	B	137	GLU	CG-CD	5.26	1.59	1.51
1	K	42	VAL	CA-CB	-5.26	1.43	1.54
2	F	111	PHE	N-CA	5.26	1.56	1.46
1	K	152	ALA	CA-CB	5.26	1.63	1.52
3	T	302	GLU	CD-OE1	5.26	1.31	1.25
1	H	141	ILE	CA-CB	5.26	1.67	1.54
1	K	67	PRO	CA-C	-5.26	1.42	1.52
3	U	235	LYS	CA-C	5.26	1.66	1.52
2	I	92	TYR	C-O	5.26	1.33	1.23
2	C	34	THR	CA-C	5.26	1.66	1.52
3	S	248	PRO	CA-CB	-5.26	1.43	1.53
1	E	30	GLU	CB-CG	-5.25	1.42	1.52
1	B	127	ASN	CB-CG	5.25	1.63	1.51
2	F	130	ARG	NE-CZ	5.25	1.39	1.33
2	L	130	ARG	CB-CG	-5.25	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	136	ALA	N-CA	-5.25	1.35	1.46
2	F	41	ASN	CG-ND2	5.25	1.46	1.32
1	E	39	PHE	CA-CB	-5.25	1.42	1.53
1	K	93	ASP	CG-OD1	5.25	1.37	1.25
1	B	28	LYS	C-O	-5.24	1.13	1.23
3	V	273	ARG	CB-CG	5.24	1.66	1.52
1	H	147	TRP	CZ3-CH2	5.24	1.48	1.40
2	L	132	ILE	N-CA	-5.24	1.35	1.46
3	S	242	ARG	CZ-NH1	5.24	1.39	1.33
3	S	257	ASP	CA-C	-5.23	1.39	1.52
1	B	117	SER	CA-CB	-5.23	1.45	1.52
3	V	260	GLU	CG-CD	5.23	1.59	1.51
3	V	274	SER	C-O	5.23	1.33	1.23
3	T	231	TYR	CG-CD1	5.23	1.46	1.39
1	E	78	LYS	CA-CB	5.23	1.65	1.53
2	F	129	PRO	C-O	-5.23	1.12	1.23
1	E	121	PRO	CA-C	5.22	1.63	1.52
2	I	168	GLU	N-CA	5.22	1.56	1.46
2	L	53	LYS	CE-NZ	5.22	1.62	1.49
3	T	282	ILE	C-O	-5.22	1.13	1.23
2	L	41	ASN	C-O	5.21	1.33	1.23
3	T	270	PRO	N-CA	-5.20	1.38	1.47
1	H	65	GLU	CD-OE1	5.20	1.31	1.25
2	I	47	GLU	CB-CG	-5.20	1.42	1.52
1	B	90	ILE	CA-CB	-5.20	1.42	1.54
2	C	128	ASP	N-CA	-5.20	1.35	1.46
3	U	251	ILE	C-O	5.20	1.33	1.23
3	T	259	GLU	CD-OE2	5.19	1.31	1.25
3	T	288	LYS	N-CA	5.19	1.56	1.46
2	C	172	TYR	CE2-CZ	-5.19	1.31	1.38
3	T	287	MET	CG-SD	5.19	1.94	1.81
1	H	19	LEU	CG-CD2	5.19	1.71	1.51
1	K	149	ARG	CZ-NH2	5.18	1.39	1.33
3	V	257	ASP	N-CA	5.18	1.56	1.46
2	C	42	PHE	CE2-CZ	-5.18	1.27	1.37
2	I	117	MET	CG-SD	5.18	1.94	1.81
1	K	105	ILE	CA-CB	-5.18	1.43	1.54
3	T	248	PRO	CA-C	-5.18	1.42	1.52
2	C	158	LYS	CA-CB	-5.18	1.42	1.53
2	L	112	VAL	CB-CG1	-5.18	1.42	1.52
1	B	111	SER	C-O	5.18	1.33	1.23
3	V	292	ASP	N-CA	5.18	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	50	GLU	CD-OE1	5.17	1.31	1.25
1	K	59	GLU	C-O	5.17	1.33	1.23
3	S	236	ILE	N-CA	-5.17	1.36	1.46
3	S	242	ARG	C-O	-5.17	1.13	1.23
1	K	25	PRO	CA-C	5.17	1.63	1.52
3	U	273	ARG	CD-NE	5.17	1.55	1.46
3	T	234	GLY	N-CA	5.16	1.53	1.46
2	L	43	ARG	CZ-NH2	5.16	1.39	1.33
1	H	24	VAL	CB-CG1	5.16	1.63	1.52
2	L	88	GLU	CB-CG	5.16	1.61	1.52
3	U	242	ARG	NE-CZ	5.16	1.39	1.33
1	B	32	ASP	CB-CG	5.16	1.62	1.51
1	H	106	ARG	CG-CD	5.16	1.64	1.51
2	L	46	GLU	CD-OE1	5.16	1.31	1.25
3	U	248	PRO	CA-C	-5.16	1.42	1.52
1	B	85	ASP	C-O	-5.16	1.13	1.23
1	B	67	PRO	N-CA	-5.16	1.38	1.47
1	E	120	ASN	C-N	5.16	1.44	1.34
3	T	282	ILE	CB-CG2	-5.16	1.36	1.52
1	K	150	LEU	CB-CG	5.15	1.67	1.52
1	B	149	ARG	CA-CB	-5.15	1.42	1.53
2	C	33	THR	CA-CB	5.15	1.66	1.53
2	I	73	THR	CA-CB	-5.15	1.40	1.53
1	E	61	PHE	C-O	5.14	1.33	1.23
2	F	113	THR	C-O	-5.14	1.13	1.23
3	T	279	GLU	CB-CG	-5.14	1.42	1.52
3	U	228	ILE	CA-C	5.13	1.66	1.52
3	V	251	ILE	CA-C	-5.13	1.39	1.52
2	I	74	ARG	CZ-NH1	5.13	1.39	1.33
1	B	108	VAL	CB-CG1	-5.13	1.42	1.52
2	I	120	VAL	C-O	5.13	1.33	1.23
3	U	253	TYR	CA-C	-5.13	1.39	1.52
1	E	21	ALA	CA-CB	5.13	1.63	1.52
3	T	256	LYS	CD-CE	5.13	1.64	1.51
2	I	172	TYR	CB-CG	-5.13	1.44	1.51
2	L	84	ARG	CZ-NH2	5.13	1.39	1.33
1	B	6	ALA	CA-C	5.12	1.66	1.52
1	E	89	ARG	CA-C	-5.12	1.39	1.52
1	H	6	ALA	CA-C	5.12	1.66	1.52
3	T	270	PRO	CG-CD	5.12	1.67	1.50
2	I	55	VAL	C-O	5.12	1.33	1.23
2	F	65	GLU	CD-OE2	5.11	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	59	THR	CB-CG2	5.11	1.69	1.52
1	B	44	ALA	CA-CB	-5.11	1.41	1.52
3	V	260	GLU	C-O	5.11	1.33	1.23
1	H	59	GLU	CG-CD	5.11	1.59	1.51
1	K	108	VAL	CB-CG2	-5.10	1.42	1.52
1	B	18	ARG	CZ-NH2	5.10	1.39	1.33
2	L	49	GLU	CD-OE2	5.10	1.31	1.25
3	V	285	LEU	CG-CD1	5.10	1.70	1.51
2	I	46	GLU	CG-CD	5.10	1.59	1.51
3	S	300	TRP	CE3-CZ3	5.10	1.47	1.38
2	C	46	GLU	CG-CD	5.09	1.59	1.51
2	C	152	ARG	C-O	-5.09	1.13	1.23
2	C	172	TYR	CD2-CE2	-5.09	1.31	1.39
2	L	169	GLY	CA-C	5.09	1.59	1.51
1	E	22	GLU	C-O	5.09	1.33	1.23
2	C	47	GLU	CG-CD	5.09	1.59	1.51
3	T	244	PRO	CB-CG	-5.09	1.24	1.50
2	L	65	GLU	CG-CD	5.08	1.59	1.51
1	E	6	ALA	N-CA	5.08	1.56	1.46
2	F	40	ARG	CZ-NH1	5.08	1.39	1.33
1	E	121	PRO	N-CA	5.08	1.55	1.47
2	C	126	VAL	CA-CB	-5.08	1.44	1.54
2	F	143	SER	C-O	5.08	1.32	1.23
3	V	262	LEU	C-O	5.08	1.32	1.23
3	S	266	GLY	CA-C	5.07	1.59	1.51
3	V	242	ARG	CZ-NH2	5.07	1.39	1.33
1	E	105	ILE	C-O	5.07	1.32	1.23
2	L	84	ARG	CA-CB	5.06	1.65	1.53
1	E	66	TYR	CZ-OH	5.05	1.46	1.37
1	K	48	ASP	N-CA	5.05	1.56	1.46
1	B	37	ARG	CA-CB	-5.05	1.42	1.53
1	E	18	ARG	CG-CD	5.05	1.64	1.51
2	F	146	VAL	C-O	5.04	1.32	1.23
2	I	84	ARG	CB-CG	5.04	1.66	1.52
1	K	110	LEU	CG-CD2	5.04	1.70	1.51
1	H	151	TYR	N-CA	5.04	1.56	1.46
2	C	112	VAL	CB-CG1	-5.03	1.42	1.52
1	H	6	ALA	C-N	5.03	1.42	1.33
3	T	252	THR	C-O	-5.03	1.13	1.23
2	F	37	LYS	CG-CD	5.03	1.69	1.52
3	U	244	PRO	CB-CG	5.03	1.75	1.50
2	C	170	GLN	CB-CG	-5.03	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	145	LYS	CB-CG	5.03	1.66	1.52
1	K	99	TRP	CG-CD1	5.03	1.43	1.36
1	E	10	ARG	CG-CD	5.03	1.64	1.51
2	F	47	GLU	CA-CB	-5.03	1.42	1.53
2	L	75	TRP	CD2-CE2	5.03	1.47	1.41
2	L	132	ILE	CB-CG1	-5.02	1.40	1.54
3	S	300	TRP	CE2-CZ2	5.02	1.48	1.39
1	B	107	THR	CA-CB	-5.02	1.40	1.53
1	B	124	PRO	CA-CB	5.01	1.63	1.53
1	E	61	PHE	CE2-CZ	-5.01	1.27	1.37
1	H	156	ILE	N-CA	5.01	1.56	1.46
1	H	32	ASP	N-CA	-5.01	1.36	1.46
1	K	96	LYS	CB-CG	5.01	1.66	1.52
2	C	152	ARG	N-CA	-5.01	1.36	1.46
3	U	252	THR	CA-C	-5.01	1.40	1.52

All (734) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	89	ARG	NE-CZ-NH2	-21.83	109.38	120.30
1	B	89	ARG	NE-CZ-NH1	20.31	130.45	120.30
2	I	43	ARG	NE-CZ-NH2	-19.23	110.69	120.30
1	B	74	ARG	NE-CZ-NH2	-18.82	110.89	120.30
1	B	74	ARG	NE-CZ-NH1	18.64	129.62	120.30
2	C	43	ARG	NE-CZ-NH2	-17.07	111.77	120.30
1	E	85	ASP	CB-CG-OD1	16.29	132.96	118.30
3	S	264	ARG	NE-CZ-NH2	-16.20	112.20	120.30
2	C	110	ARG	NE-CZ-NH1	16.02	128.31	120.30
2	C	67	ASP	CB-CG-OD2	-15.90	103.99	118.30
2	F	163	LEU	CB-CG-CD1	-15.75	84.23	111.00
1	K	106	ARG	NE-CZ-NH2	-15.44	112.58	120.30
3	T	264	ARG	NE-CZ-NH2	-15.14	112.73	120.30
2	C	90	ARG	NE-CZ-NH2	15.00	127.80	120.30
1	B	145	ARG	NE-CZ-NH2	-14.55	113.02	120.30
2	C	74	ARG	NE-CZ-NH2	14.02	127.31	120.30
2	C	130	ARG	NE-CZ-NH2	13.69	127.14	120.30
1	E	145	ARG	NE-CZ-NH1	-13.55	113.53	120.30
2	C	130	ARG	NE-CZ-NH1	-13.47	113.57	120.30
1	B	153	MET	CG-SD-CE	13.37	121.60	100.20
3	T	257	ASP	CB-CG-OD2	-13.23	106.40	118.30
2	C	90	ARG	NE-CZ-NH1	-13.16	113.72	120.30
1	E	106	ARG	NE-CZ-NH1	-13.13	113.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	153	ARG	NE-CZ-NH1	13.10	126.85	120.30
2	L	128	ASP	CB-CG-OD2	-12.42	107.12	118.30
3	V	262	LEU	CA-CB-CG	-12.40	86.77	115.30
2	F	161	MET	CG-SD-CE	12.10	119.56	100.20
1	K	149	ARG	NE-CZ-NH2	-11.99	114.31	120.30
3	S	246	ILE	CG1-CB-CG2	-11.94	85.14	111.40
2	I	43	ARG	NE-CZ-NH1	11.70	126.15	120.30
2	I	40	ARG	NE-CZ-NH1	11.65	126.13	120.30
3	S	273	ARG	NE-CZ-NH1	-11.59	114.50	120.30
1	K	150	LEU	CB-CG-CD2	11.47	130.50	111.00
1	H	43	ILE	CG1-CB-CG2	-11.36	86.40	111.40
2	F	80	LEU	CB-CG-CD1	-11.14	92.06	111.00
2	L	171	CYS	CA-CB-SG	-11.12	93.99	114.00
2	C	74	ARG	CG-CD-NE	-11.11	88.47	111.80
1	E	128	ASP	CB-CG-OD1	11.02	128.22	118.30
1	K	74	ARG	NE-CZ-NH2	-10.93	114.83	120.30
1	K	72	LYS	CD-CE-NZ	-10.88	86.68	111.70
2	C	67	ASP	CB-CG-OD1	10.88	128.09	118.30
1	H	95	LEU	CB-CG-CD1	-10.84	92.57	111.00
3	T	257	ASP	CB-CG-OD1	10.71	127.94	118.30
2	L	43	ARG	NE-CZ-NH2	-10.71	114.95	120.30
3	S	254	ASP	CB-CG-OD2	-10.64	108.72	118.30
2	C	154	LEU	CB-CG-CD1	-10.58	93.01	111.00
1	K	37	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	H	89	ARG	NE-CZ-NH1	-10.43	115.09	120.30
1	B	22	GLU	OE1-CD-OE2	-10.32	110.92	123.30
1	E	153	MET	CG-SD-CE	10.24	116.59	100.20
1	B	52	GLU	C-N-CA	-10.24	100.80	122.30
1	B	87	LEU	CB-CG-CD2	-10.18	93.70	111.00
1	B	150	LEU	CA-CB-CG	10.05	138.41	115.30
2	F	67	ASP	CB-CG-OD2	-9.99	109.31	118.30
2	L	74	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	E	73	VAL	CA-CB-CG2	-9.94	96.00	110.90
1	B	19	LEU	CB-CG-CD2	-9.91	94.14	111.00
2	C	163	LEU	CB-CG-CD1	-9.89	94.19	111.00
2	C	78	MET	CG-SD-CE	-9.86	84.42	100.20
3	S	228	ILE	N-CA-C	-9.85	84.41	111.00
1	B	106	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	H	72	LYS	CD-CE-NZ	-9.76	89.25	111.70
2	C	137	LYS	CD-CE-NZ	-9.65	89.50	111.70
3	T	264	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	K	115	LEU	CA-CB-CG	-9.61	93.20	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	40	ARG	NE-CZ-NH2	-9.56	115.52	120.30
2	F	67	ASP	CB-CG-OD1	9.50	126.85	118.30
1	B	145	ARG	NE-CZ-NH1	9.47	125.03	120.30
2	L	70	MET	CG-SD-CE	9.41	115.25	100.20
1	H	149	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	K	89	ARG	NE-CZ-NH2	9.38	124.99	120.30
3	V	262	LEU	CB-CG-CD1	-9.39	95.04	111.00
1	H	18	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	H	110	LEU	CB-CG-CD1	-9.32	95.16	111.00
3	S	257	ASP	CB-CG-OD2	-9.29	109.94	118.30
1	K	62	LEU	CA-CB-CG	-9.23	94.06	115.30
1	H	74	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	B	97	ASP	CB-CG-OD1	9.18	126.56	118.30
1	B	97	ASP	CB-CG-OD2	-9.17	110.05	118.30
2	L	156	MET	CG-SD-CE	9.12	114.79	100.20
2	I	40	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	B	151	TYR	CB-CA-C	-9.06	92.27	110.40
2	F	69	ASP	CB-CG-OD1	8.99	126.40	118.30
1	K	37	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	E	74	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	H	89	ARG	NE-CZ-NH2	8.89	124.74	120.30
1	E	104	GLN	CA-CB-CG	-8.89	93.85	113.40
2	L	110	ARG	NE-CZ-NH1	8.88	124.74	120.30
2	C	155	MET	CG-SD-CE	8.86	114.37	100.20
3	S	273	ARG	CG-CD-NE	-8.85	93.21	111.80
1	E	128	ASP	CB-CG-OD2	-8.84	110.34	118.30
3	V	252	THR	CA-CB-CG2	-8.82	100.06	112.40
1	B	53	GLY	O-C-N	-8.77	108.29	123.20
3	T	292	ASP	CB-CG-OD2	8.72	126.14	118.30
1	H	91	CYS	CA-CB-SG	-8.71	98.33	114.00
2	I	110	ARG	NE-CZ-NH1	8.70	124.65	120.30
3	U	279	GLU	C-N-CA	-8.69	99.96	121.70
2	C	128	ASP	CB-CG-OD1	8.66	126.09	118.30
1	H	98	LYS	O-C-N	-8.64	108.88	122.70
1	K	11	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	B	92	LEU	CB-CG-CD1	-8.60	96.37	111.00
2	C	142	TYR	CD1-CE1-CZ	-8.60	112.06	119.80
3	V	264	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	B	122	ASP	CB-CG-OD2	-8.58	110.58	118.30
2	C	152	ARG	NE-CZ-NH1	-8.57	116.01	120.30
1	H	85	ASP	CB-CG-OD1	-8.56	110.59	118.30
2	I	56	GLY	N-CA-C	-8.56	91.70	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	150	GLU	OE1-CD-OE2	8.53	133.54	123.30
1	E	37	ARG	NE-CZ-NH2	-8.49	116.05	120.30
2	L	153	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	E	115	LEU	CB-CG-CD2	-8.48	96.58	111.00
3	S	292	ASP	CB-CG-OD2	8.46	125.92	118.30
1	H	8	LEU	CB-CG-CD2	8.44	125.35	111.00
2	F	153	ARG	NE-CZ-NH1	8.40	124.50	120.30
2	F	74	ARG	NE-CZ-NH2	-8.36	116.12	120.30
2	F	65	GLU	OE1-CD-OE2	-8.32	113.32	123.30
3	T	253	TYR	CB-CA-C	-8.31	93.79	110.40
3	V	245	CYS	CA-CB-SG	-8.30	99.06	114.00
1	K	4	GLY	N-CA-C	8.29	133.82	113.10
2	L	128	ASP	CB-CG-OD1	8.25	125.72	118.30
1	B	22	GLU	CB-CA-C	8.23	126.87	110.40
3	S	292	ASP	CB-CG-OD1	-8.22	110.90	118.30
3	S	239	GLU	CG-CD-OE2	-8.20	101.90	118.30
3	V	242	ARG	CA-CB-CG	-8.20	95.36	113.40
1	K	91	CYS	CA-CB-SG	-8.18	99.28	114.00
1	H	106	ARG	NE-CZ-NH2	-8.17	116.22	120.30
2	L	36	VAL	CB-CA-C	-8.16	95.89	111.40
1	B	142	GLU	OE1-CD-OE2	8.12	133.05	123.30
1	B	110	LEU	CB-CG-CD1	-8.11	97.21	111.00
2	F	150	GLU	OE1-CD-OE2	8.10	133.03	123.30
2	C	84	ARG	NE-CZ-NH1	8.07	124.34	120.30
3	S	266	GLY	N-CA-C	8.03	133.16	113.10
1	H	97	ASP	CB-CG-OD2	-8.02	111.08	118.30
3	S	264	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	B	10	ARG	NE-CZ-NH1	-7.97	116.31	120.30
1	H	11	ARG	NE-CZ-NH1	7.97	124.29	120.30
3	U	274	SER	CB-CA-C	-7.97	94.96	110.10
3	T	292	ASP	CB-CG-OD1	-7.96	111.14	118.30
3	S	263	GLN	C-N-CA	-7.95	101.82	121.70
1	E	74	ARG	NE-CZ-NH1	7.88	124.24	120.30
2	F	140	ASN	N-CA-CB	-7.88	96.42	110.60
3	S	232	LEU	CA-CB-CG	7.86	133.38	115.30
2	F	78	MET	CG-SD-CE	7.85	112.76	100.20
2	L	115	ILE	CB-CA-C	-7.82	95.96	111.60
3	V	240	LEU	CB-CG-CD1	7.81	124.27	111.00
1	K	115	LEU	CB-CG-CD2	7.81	124.27	111.00
3	S	230	ASP	CB-CG-OD2	-7.79	111.29	118.30
2	L	152	ARG	CG-CD-NE	-7.79	95.45	111.80
1	K	19	LEU	CA-CB-CG	-7.77	97.43	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	76	THR	CB-CA-C	-7.76	90.64	111.60
1	B	68	MET	CG-SD-CE	-7.75	87.80	100.20
1	B	110	LEU	CB-CG-CD2	7.75	124.17	111.00
3	S	258	ILE	C-N-CA	-7.74	102.35	121.70
3	V	243	GLU	OE1-CD-OE2	7.74	132.58	123.30
3	U	298	ASN	CA-C-N	7.72	131.64	116.20
1	E	92	LEU	CB-CA-C	-7.72	95.53	110.20
3	U	246	ILE	CG1-CB-CG2	-7.72	94.42	111.40
2	C	45	LEU	CA-CB-CG	-7.71	97.56	115.30
2	F	66	ASP	CB-CG-OD2	7.71	125.24	118.30
2	F	171	CYS	CA-CB-SG	-7.71	100.13	114.00
2	C	174	ASN	CA-C-O	-7.70	103.93	120.10
2	I	70	MET	CG-SD-CE	7.70	112.52	100.20
1	E	18	ARG	NE-CZ-NH1	-7.69	116.45	120.30
2	F	74	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	B	62	LEU	C-N-CD	7.69	144.54	128.40
3	S	242	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	H	96	LYS	CB-CG-CD	-7.67	91.67	111.60
1	E	142	GLU	CG-CD-OE1	-7.64	103.01	118.30
1	H	90	ILE	CB-CA-C	-7.64	96.32	111.60
2	F	108	PHE	CD1-CE1-CZ	-7.63	110.94	120.10
1	K	92	LEU	CB-CG-CD2	-7.62	98.04	111.00
1	H	19	LEU	CB-CG-CD2	7.59	123.90	111.00
2	F	66	ASP	CB-CG-OD1	-7.57	111.49	118.30
3	U	298	ASN	CA-C-O	-7.53	104.30	120.10
1	H	20	LEU	CB-CG-CD2	7.51	123.76	111.00
2	L	130	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	H	98	LYS	CD-CE-NZ	7.50	128.95	111.70
2	C	153	ARG	CD-NE-CZ	7.50	134.10	123.60
1	H	60	LEU	CB-CG-CD1	-7.48	98.28	111.00
1	B	96	LYS	CD-CE-NZ	-7.47	94.51	111.70
2	I	152	ARG	NE-CZ-NH2	7.47	124.04	120.30
2	I	152	ARG	N-CA-C	-7.47	90.82	111.00
1	B	89	ARG	CG-CD-NE	-7.45	96.16	111.80
3	T	239	GLU	OE1-CD-OE2	7.43	132.22	123.30
1	K	58	LEU	CB-CG-CD2	7.42	123.61	111.00
2	L	132	ILE	CA-CB-CG2	7.41	125.71	110.90
3	S	274	SER	CA-CB-OG	-7.39	91.24	111.20
3	U	264	ARG	NE-CZ-NH1	7.39	124.00	120.30
2	C	158	LYS	CD-CE-NZ	-7.38	94.72	111.70
1	B	58	LEU	CB-CG-CD2	7.37	123.53	111.00
1	K	81	HIS	C-N-CD	7.36	143.86	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	65	GLU	C-N-CA	-7.36	103.30	121.70
1	B	104	GLN	CA-CB-CG	-7.36	97.22	113.40
2	F	47	GLU	OE1-CD-OE2	-7.35	114.48	123.30
2	L	101	LYS	CD-CE-NZ	-7.35	94.79	111.70
1	E	37	ARG	NE-CZ-NH1	7.33	123.96	120.30
2	F	135	LEU	CA-CB-CG	7.32	132.14	115.30
2	L	135	LEU	CB-CG-CD2	-7.32	98.56	111.00
3	U	257	ASP	CB-CG-OD1	7.32	124.88	118.30
1	H	41	VAL	CB-CA-C	-7.31	97.51	111.40
1	B	22	GLU	CG-CD-OE1	7.29	132.88	118.30
1	B	116	LEU	CB-CG-CD1	-7.29	98.61	111.00
3	S	278	GLN	N-CA-CB	-7.28	97.50	110.60
1	K	69	ALA	N-CA-C	-7.26	91.41	111.00
3	V	267	HIS	C-N-CA	-7.25	103.58	121.70
2	I	36	VAL	CB-CA-C	-7.24	97.65	111.40
2	F	38	VAL	C-N-CD	7.22	143.57	128.40
1	E	98	LYS	CD-CE-NZ	-7.21	95.13	111.70
2	F	170	GLN	N-CA-CB	-7.20	97.63	110.60
2	L	84	ARG	CA-CB-CG	7.20	129.25	113.40
2	I	135	LEU	CB-CG-CD2	-7.19	98.77	111.00
2	C	45	LEU	C-N-CA	-7.18	103.74	121.70
3	V	296	SER	N-CA-C	-7.17	91.64	111.00
2	F	162	LYS	C-N-CA	-7.17	103.78	121.70
3	S	228	ILE	CG1-CB-CG2	-7.17	95.63	111.40
2	I	139	GLN	CB-CA-C	-7.17	96.07	110.40
3	V	292	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	H	18	ARG	NE-CZ-NH2	-7.14	116.73	120.30
3	U	267	HIS	N-CA-C	-7.13	91.75	111.00
1	H	97	ASP	CB-CG-OD1	7.11	124.70	118.30
2	I	110	ARG	NE-CZ-NH2	-7.11	116.74	120.30
2	I	67	ASP	CB-CG-OD2	7.11	124.70	118.30
1	K	118	ALA	C-N-CD	7.11	143.32	128.40
2	C	153	ARG	CA-CB-CG	7.09	129.01	113.40
3	T	251	ILE	N-CA-C	-7.09	91.86	111.00
2	C	171	CYS	CB-CA-C	-7.09	96.23	110.40
2	L	66	ASP	CB-CG-OD2	7.08	124.68	118.30
2	C	151	LEU	CB-CG-CD1	7.07	123.02	111.00
1	H	74	ARG	CA-CB-CG	-7.07	97.85	113.40
1	B	7	GLY	N-CA-C	-7.06	95.45	113.10
2	F	142	TYR	CD1-CE1-CZ	-7.06	113.45	119.80
3	S	236	ILE	O-C-N	-7.05	111.42	122.70
3	T	230	ASP	CB-CG-OD2	-7.05	111.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S	245	CYS	CA-CB-SG	-7.04	101.33	114.00
3	S	279	GLU	O-C-N	-7.02	111.47	122.70
1	K	142	GLU	OE1-CD-OE2	-7.02	114.88	123.30
1	B	53	GLY	C-N-CA	-7.01	107.57	122.30
2	F	153	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	K	24	VAL	CB-CA-C	-7.01	98.08	111.40
3	V	282	ILE	CB-CA-C	-7.00	97.60	111.60
2	C	45	LEU	CB-CG-CD2	6.99	122.89	111.00
1	B	91	CYS	CA-CB-SG	-6.99	101.42	114.00
3	T	245	CYS	CA-CB-SG	-6.97	101.45	114.00
3	V	264	ARG	NE-CZ-NH2	-6.97	116.82	120.30
3	T	236	ILE	CG1-CB-CG2	-6.96	96.09	111.40
1	H	89	ARG	CA-CB-CG	-6.96	98.10	113.40
1	E	48	ASP	CB-CG-OD2	6.94	124.55	118.30
2	F	57	ASP	CB-CA-C	-6.94	96.51	110.40
2	L	120	VAL	CB-CA-C	-6.92	98.25	111.40
3	S	253	TYR	CZ-CE2-CD2	6.92	126.03	119.80
3	U	228	ILE	N-CA-C	6.92	129.68	111.00
1	B	90	ILE	CG1-CB-CG2	-6.92	96.19	111.40
1	B	69	ALA	N-CA-CB	-6.91	100.42	110.10
1	B	111	SER	CB-CA-C	-6.90	96.99	110.10
3	S	233	CYS	CA-CB-SG	-6.90	101.58	114.00
1	K	110	LEU	CB-CG-CD2	6.89	122.72	111.00
1	K	32	ASP	CB-CG-OD1	-6.88	112.11	118.30
2	C	48	LEU	CA-CB-CG	-6.88	99.47	115.30
3	V	277	THR	N-CA-C	-6.88	92.42	111.00
3	T	258	ILE	CG1-CB-CG2	6.86	126.50	111.40
3	V	292	ASP	CB-CG-OD1	6.86	124.48	118.30
3	S	255	ARG	NE-CZ-NH2	6.86	123.73	120.30
3	S	296	SER	N-CA-C	-6.83	92.55	111.00
3	S	287	MET	CG-SD-CE	-6.83	89.27	100.20
1	E	89	ARG	CA-CB-CG	-6.82	98.39	113.40
2	F	159	GLU	CA-CB-CG	6.82	128.40	113.40
1	E	39	PHE	N-CA-CB	-6.81	98.35	110.60
3	S	233	CYS	N-CA-CB	-6.80	98.36	110.60
1	E	42	VAL	CB-CA-C	-6.79	98.49	111.40
1	K	92	LEU	CB-CG-CD1	-6.79	99.45	111.00
1	H	98	LYS	N-CA-C	6.79	129.34	111.00
3	U	264	ARG	CA-CB-CG	-6.79	98.46	113.40
1	K	149	ARG	NE-CZ-NH1	6.79	123.69	120.30
2	I	74	ARG	CG-CD-NE	-6.79	97.55	111.80
2	L	117	MET	CG-SD-CE	6.79	111.06	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	228	ILE	C-N-CD	6.78	142.65	128.40
3	U	233	CYS	CA-CB-SG	-6.78	101.79	114.00
3	U	235	LYS	CA-CB-CG	-6.78	98.48	113.40
1	E	78	LYS	CB-CA-C	6.78	123.95	110.40
1	K	106	ARG	CG-CD-NE	-6.78	97.57	111.80
3	U	276	LEU	CB-CG-CD1	-6.78	99.48	111.00
2	C	140	ASN	N-CA-C	-6.77	92.72	111.00
2	C	112	VAL	CG1-CB-CG2	6.76	121.72	110.90
2	C	80	LEU	CB-CG-CD2	-6.74	99.54	111.00
3	U	251	ILE	CG1-CB-CG2	-6.73	96.59	111.40
1	B	117	SER	CA-CB-OG	-6.73	93.03	111.20
1	B	127	ASN	N-CA-C	6.73	129.17	111.00
1	H	100	SER	N-CA-CB	-6.73	100.41	110.50
3	V	235	LYS	CB-CG-CD	6.72	129.08	111.60
2	F	128	ASP	C-N-CD	6.72	142.51	128.40
1	B	73	VAL	CA-CB-CG2	-6.72	100.83	110.90
2	I	168	GLU	N-CA-CB	6.71	122.68	110.60
3	S	240	LEU	CA-CB-CG	-6.69	99.90	115.30
2	C	38	VAL	CA-CB-CG1	6.68	120.92	110.90
2	C	76	THR	N-CA-CB	-6.68	97.61	110.30
3	S	255	ARG	CG-CD-NE	6.67	125.82	111.80
1	B	65	GLU	CG-CD-OE2	-6.67	104.96	118.30
3	V	259	GLU	N-CA-C	-6.67	93.00	111.00
3	U	235	LYS	CD-CE-NZ	-6.64	96.42	111.70
1	E	149	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	K	74	ARG	NE-CZ-NH1	6.64	123.62	120.30
3	V	256	LYS	CD-CE-NZ	-6.62	96.47	111.70
3	V	230	ASP	N-CA-C	6.61	128.85	111.00
2	C	153	ARG	CB-CA-C	6.61	123.62	110.40
1	H	145	ARG	NE-CZ-NH2	-6.61	117.00	120.30
2	C	68	GLU	CG-CD-OE2	-6.59	105.11	118.30
1	H	76	MET	CG-SD-CE	-6.59	89.65	100.20
3	V	291	ILE	CG1-CB-CG2	-6.59	96.89	111.40
3	S	297	GLU	N-CA-C	-6.59	93.20	111.00
1	K	68	MET	CG-SD-CE	-6.59	89.66	100.20
1	B	9	PRO	CA-N-CD	-6.57	102.30	111.50
2	C	114	LYS	CA-CB-CG	6.57	127.85	113.40
2	L	153	ARG	NH1-CZ-NH2	6.56	126.62	119.40
2	I	152	ARG	CA-C-N	6.55	131.62	117.20
2	L	73	THR	C-N-CA	-6.55	105.33	121.70
2	C	131	ALA	C-N-CA	6.55	138.07	121.70
3	T	239	GLU	CA-CB-CG	-6.55	99.00	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	45	LEU	CA-CB-CG	-6.54	100.25	115.30
3	V	298	ASN	N-CA-C	-6.54	93.36	111.00
3	T	276	LEU	CB-CG-CD2	6.53	122.10	111.00
2	C	148	LEU	CB-CG-CD2	6.53	122.10	111.00
1	B	106	ARG	NE-CZ-NH1	6.53	123.56	120.30
2	C	125	GLY	N-CA-C	6.52	129.41	113.10
3	S	263	GLN	O-C-N	-6.52	112.26	122.70
3	U	240	LEU	CB-CA-C	-6.52	97.81	110.20
3	U	255	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	B	70	ALA	C-N-CD	6.52	142.09	128.40
1	H	81	HIS	N-CA-CB	6.50	122.30	110.60
2	F	96	ILE	CB-CA-C	-6.50	98.60	111.60
2	L	72	LEU	CB-CG-CD2	-6.50	99.96	111.00
1	E	59	GLU	N-CA-C	-6.49	93.48	111.00
3	T	288	LYS	N-CA-CB	6.48	122.27	110.60
2	C	112	VAL	CA-CB-CG2	-6.48	101.18	110.90
2	C	72	LEU	CB-CG-CD1	-6.48	99.98	111.00
3	T	236	ILE	CB-CA-C	-6.48	98.65	111.60
1	B	89	ARG	CD-NE-CZ	6.47	132.66	123.60
2	I	153	ARG	N-CA-CB	6.47	122.25	110.60
2	F	123	SER	N-CA-C	6.47	128.47	111.00
3	T	275	PRO	N-CA-C	-6.47	95.28	112.10
2	F	166	PRO	N-CD-CG	-6.47	93.50	103.20
2	L	38	VAL	N-CA-C	-6.46	93.56	111.00
3	T	254	ASP	CB-CG-OD1	-6.45	112.49	118.30
2	C	150	GLU	CG-CD-OE1	-6.44	105.41	118.30
1	E	90	ILE	C-N-CA	-6.44	105.59	121.70
2	I	67	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	H	20	LEU	CA-CB-CG	6.41	130.04	115.30
1	E	111	SER	CA-CB-OG	-6.40	93.92	111.20
2	L	110	ARG	N-CA-CB	-6.40	99.08	110.60
2	C	171	CYS	CA-CB-SG	-6.40	102.49	114.00
1	H	69	ALA	N-CA-CB	-6.39	101.15	110.10
3	S	242	ARG	O-C-N	-6.39	112.48	122.70
1	H	97	ASP	N-CA-C	-6.39	93.76	111.00
2	L	106	PRO	C-N-CD	6.38	141.80	128.40
2	L	94	LEU	CA-CB-CG	6.38	129.97	115.30
1	K	106	ARG	NH1-CZ-NH2	6.37	126.41	119.40
1	K	123	ASP	N-CA-C	6.36	128.17	111.00
3	T	290	VAL	CB-CA-C	-6.36	99.31	111.40
2	C	41	ASN	C-N-CA	-6.35	105.82	121.70
2	C	69	ASP	CB-CG-OD1	6.35	124.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	148	LEU	CB-CG-CD1	-6.34	100.21	111.00
2	C	127	VAL	CG1-CB-CG2	-6.34	100.75	110.90
1	B	151	TYR	N-CA-C	6.34	128.11	111.00
2	F	55	VAL	N-CA-CB	6.30	125.37	111.50
1	E	69	ALA	N-CA-CB	-6.28	101.31	110.10
2	L	110	ARG	CA-CB-CG	6.27	127.19	113.40
2	F	110	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B	134	LYS	CB-CG-CD	6.27	127.89	111.60
3	S	239	GLU	CG-CD-OE1	6.26	130.83	118.30
3	V	279	GLU	CB-CA-C	-6.26	97.87	110.40
1	B	72	LYS	C-N-CA	-6.25	106.07	121.70
1	E	106	ARG	NH1-CZ-NH2	6.25	126.27	119.40
1	E	153	MET	CB-CG-SD	-6.24	93.68	112.40
2	C	33	THR	N-CA-C	6.24	127.84	111.00
1	B	22	GLU	CA-CB-CG	6.23	127.11	113.40
1	E	86	LYS	CD-CE-NZ	6.23	126.03	111.70
2	I	90	ARG	NE-CZ-NH2	-6.23	117.19	120.30
2	L	161	MET	CG-SD-CE	6.23	110.17	100.20
3	S	239	GLU	N-CA-CB	-6.23	99.39	110.60
2	L	139	GLN	N-CA-CB	-6.21	99.41	110.60
3	T	255	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	C	76	THR	CB-CA-C	-6.20	94.85	111.60
2	C	49	GLU	OE1-CD-OE2	6.20	130.74	123.30
2	C	84	ARG	CG-CD-NE	-6.20	98.78	111.80
2	C	153	ARG	NH1-CZ-NH2	-6.19	112.59	119.40
3	U	250	GLY	C-N-CA	-6.19	106.23	121.70
3	T	254	ASP	CB-CG-OD2	6.18	123.86	118.30
3	U	285	LEU	CA-CB-CG	-6.18	101.09	115.30
1	E	151	TYR	CA-CB-CG	6.17	125.12	113.40
1	E	60	LEU	CB-CG-CD1	6.17	121.48	111.00
3	T	292	ASP	CB-CA-C	-6.17	98.07	110.40
1	B	34	SER	CB-CA-C	6.16	121.80	110.10
3	V	264	ARG	CG-CD-NE	-6.14	98.90	111.80
2	I	72	LEU	CA-CB-CG	6.14	129.42	115.30
2	F	90	ARG	NE-CZ-NH2	6.14	123.37	120.30
2	C	53	LYS	CA-CB-CG	6.13	126.89	113.40
3	T	265	VAL	CG1-CB-CG2	6.13	120.71	110.90
2	F	174	ASN	CB-CA-C	6.13	122.66	110.40
2	C	78	MET	N-CA-CB	-6.12	99.58	110.60
1	K	145	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	B	107	THR	CB-CA-C	-6.10	95.13	111.60
1	H	74	ARG	NH1-CZ-NH2	6.09	126.10	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	240	LEU	CA-CB-CG	-6.09	101.30	115.30
1	K	87	LEU	CA-CB-CG	-6.08	101.31	115.30
2	C	110	ARG	NH1-CZ-NH2	-6.08	112.71	119.40
2	C	38	VAL	C-N-CD	6.07	141.15	128.40
2	I	38	VAL	CB-CA-C	-6.07	99.86	111.40
1	H	64	GLU	OE1-CD-OE2	6.07	130.58	123.30
2	I	155	MET	CG-SD-CE	-6.07	90.49	100.20
3	U	272	THR	CA-CB-CG2	-6.07	103.91	112.40
1	K	15	GLU	N-CA-CB	6.06	121.51	110.60
1	K	57	LYS	CD-CE-NZ	6.06	125.64	111.70
2	C	134	VAL	CA-CB-CG1	6.06	119.99	110.90
3	S	248	PRO	O-C-N	-6.05	113.01	122.70
2	I	55	VAL	CG1-CB-CG2	6.04	120.56	110.90
1	H	104	GLN	CA-CB-CG	-6.03	100.13	113.40
2	C	44	LEU	CA-CB-CG	-6.03	101.43	115.30
3	T	279	GLU	CA-CB-CG	-6.02	100.15	113.40
2	C	132	ILE	CG1-CB-CG2	-6.02	98.16	111.40
2	F	57	ASP	C-N-CA	-6.01	109.67	122.30
3	T	235	LYS	CD-CE-NZ	-6.01	97.88	111.70
1	B	37	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	C	79	ILE	CB-CA-C	-6.00	99.59	111.60
3	T	249	SER	O-C-N	-6.00	113.00	123.20
2	F	139	GLN	N-CA-CB	-6.00	99.80	110.60
2	L	115	ILE	CA-CB-CG2	6.00	122.89	110.90
2	L	153	ARG	NE-CZ-NH1	-5.99	117.30	120.30
2	I	154	LEU	CB-CG-CD1	-5.99	100.82	111.00
3	S	236	ILE	CG1-CB-CG2	5.99	124.57	111.40
3	U	279	GLU	CB-CA-C	-5.98	98.43	110.40
3	T	249	SER	C-N-CA	-5.98	109.74	122.30
1	K	94	ILE	O-C-N	-5.97	113.14	122.70
2	L	65	GLU	OE1-CD-OE2	5.97	130.47	123.30
2	L	58	GLY	C-N-CA	-5.97	106.78	121.70
1	K	103	LEU	CA-CB-CG	-5.97	101.58	115.30
3	U	267	HIS	C-N-CA	-5.97	106.78	121.70
3	S	260	GLU	CA-CB-CG	-5.96	100.28	113.40
1	B	115	LEU	CB-CG-CD1	5.96	121.13	111.00
2	L	64	LEU	CA-CB-CG	-5.96	101.59	115.30
1	H	85	ASP	CB-CG-OD2	5.95	123.66	118.30
2	I	37	LYS	CD-CE-NZ	5.95	125.37	111.70
2	C	59	THR	N-CA-C	5.94	127.05	111.00
1	E	64	GLU	CB-CA-C	-5.94	98.52	110.40
3	T	246	ILE	CG1-CB-CG2	-5.94	98.34	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	271	VAL	C-N-CA	-5.94	106.86	121.70
1	K	98	LYS	N-CA-C	-5.93	94.98	111.00
2	F	87	TYR	CB-CG-CD1	5.93	124.56	121.00
3	U	261	HIS	C-N-CA	-5.93	106.88	121.70
3	S	265	VAL	CA-CB-CG2	-5.92	102.02	110.90
3	V	298	ASN	CA-C-O	5.92	132.53	120.10
1	E	24	VAL	CB-CA-C	-5.91	100.17	111.40
1	B	118	ALA	N-CA-C	-5.91	95.05	111.00
3	T	302	GLU	N-CA-C	5.90	126.92	111.00
1	H	116	LEU	CA-CB-CG	-5.87	101.79	115.30
2	F	43	ARG	CB-CA-C	-5.86	98.67	110.40
2	C	108	PHE	N-CA-CB	-5.86	100.05	110.60
3	U	274	SER	N-CA-C	5.86	126.82	111.00
1	K	84	VAL	N-CA-C	-5.85	95.19	111.00
2	C	109	VAL	CB-CA-C	-5.84	100.30	111.40
2	I	76	THR	CB-CA-C	-5.84	95.83	111.60
2	F	110	ARG	NH1-CZ-NH2	-5.83	112.98	119.40
2	L	133	SER	N-CA-CB	-5.83	101.75	110.50
3	S	274	SER	N-CA-CB	-5.83	101.75	110.50
1	H	118	ALA	C-N-CD	5.83	140.64	128.40
2	L	40	ARG	NH1-CZ-NH2	5.83	125.81	119.40
2	L	104	GLU	OE1-CD-OE2	-5.83	116.31	123.30
2	F	62	TRP	C-N-CA	-5.80	110.12	122.30
1	K	95	LEU	CB-CG-CD2	5.80	120.86	111.00
1	B	103	LEU	CB-CG-CD1	-5.79	101.15	111.00
2	L	109	VAL	CB-CA-C	-5.79	100.39	111.40
3	T	236	ILE	O-C-N	-5.79	113.44	122.70
3	T	271	VAL	O-C-N	-5.79	113.44	122.70
2	L	125	GLY	N-CA-C	5.78	127.54	113.10
3	U	262	LEU	CB-CG-CD1	-5.77	101.19	111.00
2	L	40	ARG	C-N-CA	-5.75	107.31	121.70
3	S	243	GLU	CB-CA-C	5.74	121.89	110.40
3	U	276	LEU	C-N-CA	-5.74	107.36	121.70
3	V	254	ASP	CB-CG-OD2	5.73	123.46	118.30
2	L	128	ASP	C-N-CD	5.72	140.42	128.40
1	E	87	LEU	N-CA-C	5.72	126.44	111.00
3	T	233	CYS	CA-CB-SG	-5.72	103.71	114.00
1	K	65	GLU	CG-CD-OE1	5.71	129.73	118.30
2	L	145	LYS	CD-CE-NZ	5.71	124.84	111.70
1	E	129	VAL	CG1-CB-CG2	-5.71	101.76	110.90
2	F	94	LEU	CB-CG-CD1	-5.71	101.29	111.00
1	H	116	LEU	CB-CG-CD1	5.71	120.71	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	106	ARG	CA-CB-CG	-5.70	100.85	113.40
3	U	262	LEU	N-CA-CB	5.70	121.80	110.40
1	E	148	THR	CA-CB-CG2	-5.70	104.43	112.40
3	S	242	ARG	NE-CZ-NH1	5.70	123.15	120.30
3	S	264	ARG	CB-CG-CD	-5.69	96.81	111.60
2	I	116	ASN	N-CA-C	-5.69	95.65	111.00
1	B	53	GLY	N-CA-C	5.68	127.31	113.10
1	H	65	GLU	OE1-CD-OE2	-5.68	116.48	123.30
2	F	47	GLU	CG-CD-OE1	5.68	129.66	118.30
3	U	232	LEU	CB-CG-CD2	5.68	120.66	111.00
2	F	172	TYR	N-CA-C	-5.67	95.69	111.00
1	E	96	LYS	CD-CE-NZ	5.67	124.73	111.70
1	H	47	GLN	CA-CB-CG	5.66	125.86	113.40
3	V	259	GLU	CA-CB-CG	5.66	125.84	113.40
1	H	87	LEU	CB-CG-CD1	5.65	120.60	111.00
2	I	94	LEU	CA-CB-CG	-5.65	102.31	115.30
1	B	72	LYS	CA-CB-CG	-5.64	100.99	113.40
1	E	12	ILE	CG1-CB-CG2	5.63	123.79	111.40
1	K	62	LEU	CB-CG-CD1	5.63	120.57	111.00
2	F	53	LYS	C-N-CA	5.63	134.12	122.30
1	K	155	ASN	N-CA-C	-5.62	95.81	111.00
1	E	15	GLU	OE1-CD-OE2	5.62	130.05	123.30
2	L	174	ASN	CA-C-O	-5.62	108.29	120.10
3	T	236	ILE	C-N-CA	-5.62	107.64	121.70
1	B	108	VAL	CG1-CB-CG2	-5.62	101.91	110.90
2	I	152	ARG	N-CA-CB	5.62	120.72	110.60
1	H	137	GLU	CA-CB-CG	5.62	125.75	113.40
1	B	27	ILE	CG1-CB-CG2	5.61	123.75	111.40
1	H	8	LEU	CB-CG-CD1	-5.61	101.46	111.00
1	B	26	GLY	N-CA-C	5.61	127.12	113.10
2	F	168	GLU	CB-CA-C	-5.60	99.19	110.40
1	B	52	GLU	CB-CA-C	-5.60	99.20	110.40
1	E	53	GLY	C-N-CA	-5.60	110.55	122.30
1	B	58	LEU	CA-CB-CG	5.60	128.17	115.30
2	F	93	SER	CB-CA-C	-5.59	99.47	110.10
2	L	93	SER	C-N-CA	-5.59	107.72	121.70
2	I	130	ARG	C-N-CA	-5.58	107.75	121.70
1	K	65	GLU	CG-CD-OE2	-5.58	107.14	118.30
1	E	123	ASP	C-N-CD	-5.57	108.34	120.60
3	S	283	PRO	N-CA-CB	-5.57	96.47	102.60
1	K	82	PRO	CA-C-N	-5.57	104.94	117.20
2	F	85	THR	CA-CB-CG2	-5.57	104.61	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	68	MET	CB-CA-C	-5.56	99.28	110.40
1	B	55	THR	CB-CA-C	-5.55	96.61	111.60
2	C	50	GLU	N-CA-C	-5.54	96.03	111.00
2	L	101	LYS	CB-CG-CD	-5.54	97.19	111.60
3	S	279	GLU	CG-CD-OE2	-5.54	107.22	118.30
3	S	227	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	K	61	PHE	CB-CA-C	-5.53	99.34	110.40
3	V	266	GLY	C-N-CA	-5.53	107.89	121.70
2	C	66	ASP	O-C-N	-5.52	113.86	122.70
2	C	172	TYR	N-CA-C	-5.52	96.09	111.00
2	F	133	SER	N-CA-CB	-5.52	102.22	110.50
1	K	73	VAL	C-N-CA	-5.52	107.90	121.70
3	S	239	GLU	CB-CA-C	-5.52	99.37	110.40
2	F	117	MET	CB-CG-SD	-5.51	95.86	112.40
1	K	11	ARG	CA-CB-CG	-5.51	101.27	113.40
3	S	258	ILE	CB-CG1-CD1	-5.51	98.48	113.90
2	F	43	ARG	NE-CZ-NH2	-5.51	117.55	120.30
3	S	270	PRO	C-N-CA	-5.51	107.93	121.70
1	H	16	THR	OG1-CB-CG2	-5.50	97.34	110.00
3	V	293	ALA	CB-CA-C	-5.50	101.84	110.10
2	I	75	TRP	CB-CA-C	-5.50	99.40	110.40
3	S	273	ARG	NH1-CZ-NH2	5.50	125.44	119.40
1	H	42	VAL	C-N-CA	-5.50	107.96	121.70
2	L	48	LEU	CB-CA-C	-5.50	99.76	110.20
2	I	48	LEU	CB-CG-CD1	5.49	120.34	111.00
2	C	120	VAL	CG1-CB-CG2	-5.49	102.11	110.90
3	T	277	THR	CB-CA-C	-5.49	96.78	111.60
2	F	44	LEU	CA-CB-CG	-5.48	102.69	115.30
1	B	38	TYR	CB-CG-CD2	5.48	124.29	121.00
2	L	102	TYR	CD1-CE1-CZ	5.48	124.73	119.80
3	T	248	PRO	CA-C-N	5.48	129.25	117.20
3	U	236	ILE	C-N-CA	-5.48	108.00	121.70
1	E	142	GLU	OE1-CD-OE2	5.47	129.87	123.30
1	H	122	ASP	N-CA-C	-5.47	96.24	111.00
1	E	75	PHE	CB-CA-C	-5.46	99.47	110.40
1	E	19	LEU	CA-CB-CG	-5.45	102.76	115.30
2	F	54	GLY	CA-C-O	-5.45	110.80	120.60
1	B	79	ILE	CG1-CB-CG2	-5.44	99.43	111.40
1	K	105	ILE	CB-CA-C	-5.44	100.73	111.60
1	E	89	ARG	NE-CZ-NH2	-5.44	117.58	120.30
3	U	284	ASN	C-N-CA	5.43	135.29	121.70
1	B	106	ARG	CG-CD-NE	-5.43	100.40	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	101	LYS	O-C-N	-5.43	114.02	122.70
1	K	118	ALA	C-N-CA	-5.42	99.24	122.00
1	B	8	LEU	N-CA-CB	-5.42	99.56	110.40
3	T	264	ARG	CD-NE-CZ	5.42	131.19	123.60
2	L	170	GLN	N-CA-C	-5.41	96.39	111.00
3	U	295	ILE	N-CA-CB	5.41	123.24	110.80
3	T	272	THR	OG1-CB-CG2	-5.41	97.56	110.00
2	F	87	TYR	OH-CZ-CE2	-5.40	105.51	120.10
3	S	282	ILE	CB-CA-C	-5.40	100.80	111.60
2	I	78	MET	CB-CG-SD	-5.40	96.20	112.40
1	H	62	LEU	CB-CA-C	-5.40	99.94	110.20
2	L	172	TYR	OH-CZ-CE2	-5.40	105.52	120.10
2	C	162	LYS	C-N-CA	-5.39	108.23	121.70
1	E	85	ASP	CB-CG-OD2	-5.39	113.45	118.30
3	V	252	THR	N-CA-C	5.39	125.54	111.00
2	L	145	LYS	CB-CG-CD	5.38	125.59	111.60
2	C	43	ARG	NH1-CZ-NH2	5.37	125.31	119.40
2	C	84	ARG	NE-CZ-NH2	-5.37	117.62	120.30
3	T	247	THR	CA-CB-CG2	-5.37	104.89	112.40
2	L	139	GLN	CB-CA-C	-5.36	99.67	110.40
1	K	74	ARG	CA-C-N	-5.36	105.41	117.20
2	F	123	SER	CA-C-N	5.36	128.98	117.20
3	V	280	GLN	C-N-CA	-5.35	108.32	121.70
3	U	246	ILE	N-CA-C	-5.35	96.55	111.00
2	F	102	TYR	CA-CB-CG	5.35	123.56	113.40
2	F	130	ARG	NE-CZ-NH1	5.35	122.97	120.30
2	L	51	GLY	N-CA-C	-5.35	99.73	113.10
3	U	284	ASN	CA-C-N	-5.34	105.44	117.20
1	B	6	ALA	N-CA-C	5.34	125.42	111.00
3	U	253	TYR	CG-CD1-CE1	-5.34	117.03	121.30
3	U	290	VAL	CA-CB-CG2	5.34	118.91	110.90
2	F	43	ARG	CG-CD-NE	-5.33	100.61	111.80
2	F	87	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	H	148	THR	CA-CB-CG2	-5.32	104.95	112.40
2	I	152	ARG	CA-C-O	-5.32	108.92	120.10
2	L	172	TYR	CB-CG-CD2	-5.32	117.81	121.00
3	T	242	ARG	CB-CA-C	-5.32	99.76	110.40
2	L	130	ARG	CB-CG-CD	-5.32	97.77	111.60
2	L	36	VAL	CG1-CB-CG2	5.32	119.41	110.90
1	B	87	LEU	N-CA-C	5.31	125.33	111.00
2	C	68	GLU	CG-CD-OE1	5.31	128.92	118.30
2	I	166	PRO	CA-CB-CG	-5.31	93.91	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	276	LEU	CD1-CG-CD2	-5.30	94.59	110.50
3	S	241	MET	CG-SD-CE	5.30	108.69	100.20
3	U	256	LYS	CD-CE-NZ	-5.29	99.52	111.70
2	C	103	PRO	C-N-CA	-5.29	108.47	121.70
2	L	99	GLY	C-N-CD	5.28	139.48	128.40
2	I	44	LEU	CB-CG-CD2	-5.28	102.03	111.00
2	F	153	ARG	CB-CA-C	-5.27	99.86	110.40
1	K	60	LEU	CB-CG-CD2	-5.27	102.04	111.00
3	V	257	ASP	CB-CG-OD2	5.26	123.04	118.30
1	K	85	ASP	CB-CG-OD1	5.26	123.03	118.30
1	E	96	LYS	CB-CG-CD	5.26	125.27	111.60
1	B	37	ARG	N-CA-C	5.26	125.20	111.00
3	V	250	GLY	N-CA-C	-5.26	99.95	113.10
3	V	275	PRO	N-CA-C	-5.26	98.43	112.10
1	H	66	TYR	CG-CD1-CE1	5.25	125.50	121.30
1	B	8	LEU	C-N-CD	5.25	139.42	128.40
1	E	73	VAL	N-CA-C	5.25	125.17	111.00
2	I	84	ARG	CD-NE-CZ	5.25	130.95	123.60
2	C	84	ARG	CA-CB-CG	5.24	124.93	113.40
1	E	78	LYS	CB-CG-CD	5.24	125.22	111.60
1	B	62	LEU	CB-CG-CD1	5.24	119.90	111.00
2	C	43	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	C	84	ARG	N-CA-CB	5.24	120.02	110.60
1	B	65	GLU	OE1-CD-OE2	5.23	129.58	123.30
1	H	90	ILE	N-CA-C	-5.23	96.88	111.00
2	I	46	GLU	N-CA-CB	5.23	120.01	110.60
1	B	132	GLN	N-CA-CB	-5.22	101.20	110.60
3	V	249	SER	C-N-CA	-5.22	111.33	122.30
1	H	17	GLN	CA-CB-CG	-5.22	101.92	113.40
2	F	146	VAL	CG1-CB-CG2	5.21	119.23	110.90
2	C	84	ARG	CD-NE-CZ	5.21	130.89	123.60
2	C	143	SER	N-CA-CB	5.20	118.30	110.50
2	C	44	LEU	CB-CG-CD1	5.19	119.83	111.00
2	C	92	TYR	O-C-N	-5.19	114.39	122.70
3	S	264	ARG	CB-CA-C	-5.19	100.02	110.40
3	U	284	ASN	N-CA-C	-5.19	96.99	111.00
2	F	43	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	99	TRP	CE3-CZ3-CH2	-5.18	115.50	121.20
2	F	60	VAL	CB-CA-C	-5.17	101.57	111.40
1	H	99	TRP	CG-CD1-NE1	5.17	115.27	110.10
1	H	48	ASP	CB-CG-OD2	-5.17	113.65	118.30
3	U	230	ASP	CB-CG-OD1	5.17	122.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	TYR	C-N-CD	5.17	139.25	128.40
2	F	50	GLU	CB-CA-C	5.17	120.74	110.40
2	F	132	ILE	CB-CG1-CD1	-5.17	99.43	113.90
2	C	97	GLU	OE1-CD-OE2	-5.17	117.10	123.30
3	S	265	VAL	CG1-CB-CG2	5.17	119.17	110.90
1	E	102	ALA	N-CA-CB	5.17	117.33	110.10
2	C	89	ASN	N-CA-C	5.16	124.94	111.00
1	H	52	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	E	66	TYR	CB-CA-C	-5.16	100.08	110.40
2	C	79	ILE	CG1-CB-CG2	-5.16	100.05	111.40
3	S	242	ARG	CA-C-N	5.16	128.55	117.20
1	E	85	ASP	OD1-CG-OD2	-5.16	113.50	123.30
1	E	100	SER	CA-CB-OG	-5.15	97.29	111.20
2	I	143	SER	CA-CB-OG	-5.15	97.29	111.20
1	B	128	ASP	CB-CG-OD1	-5.15	113.67	118.30
3	U	291	ILE	CG1-CB-CG2	-5.15	100.08	111.40
3	S	270	PRO	O-C-N	-5.14	114.47	122.70
1	E	76	MET	CB-CG-SD	-5.14	96.97	112.40
1	K	122	ASP	CB-CG-OD2	5.14	122.93	118.30
1	E	149	ARG	CA-CB-CG	5.14	124.70	113.40
2	C	122	SER	CA-CB-OG	-5.14	97.33	111.20
2	F	47	GLU	CB-CA-C	5.14	120.67	110.40
1	H	74	ARG	N-CA-C	5.14	124.87	111.00
2	F	38	VAL	CB-CA-C	-5.13	101.65	111.40
2	F	145	LYS	CD-CE-NZ	-5.13	99.89	111.70
2	F	110	ARG	NE-CZ-NH2	5.13	122.87	120.30
2	I	152	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	B	73	VAL	CB-CA-C	-5.13	101.65	111.40
1	E	14	LYS	CB-CA-C	5.13	120.66	110.40
1	B	82	PRO	C-N-CA	-5.13	108.89	121.70
2	L	77	GLY	N-CA-C	5.13	125.92	113.10
1	K	133	TRP	CA-CB-CG	-5.12	103.97	113.70
1	B	92	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	B	142	GLU	CA-CB-CG	-5.12	102.15	113.40
2	L	167	PRO	C-N-CA	-5.12	108.91	121.70
3	T	282	ILE	C-N-CD	5.11	139.13	128.40
1	E	8	LEU	CA-CB-CG	-5.11	103.55	115.30
3	S	295	ILE	C-N-CA	-5.11	108.92	121.70
1	B	53	GLY	CA-C-N	5.11	126.42	116.20
3	T	304	TYR	CD1-CE1-CZ	-5.09	115.22	119.80
1	K	134	LYS	CD-CE-NZ	-5.09	99.99	111.70
3	S	279	GLU	OE1-CD-OE2	5.09	129.41	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	282	ILE	N-CA-CB	-5.09	99.09	110.80
2	C	76	THR	CA-C-N	5.09	126.38	116.20
2	I	125	GLY	N-CA-C	5.09	125.82	113.10
1	K	111	SER	CB-CA-C	5.09	119.76	110.10
2	F	172	TYR	CZ-CE2-CD2	-5.08	115.22	119.80
1	K	18	ARG	CB-CA-C	5.08	120.57	110.40
2	F	140	ASN	CB-CA-C	5.07	120.55	110.40
1	H	90	ILE	C-N-CA	-5.07	109.02	121.70
2	I	69	ASP	CB-CG-OD2	-5.07	113.73	118.30
2	L	54	GLY	N-CA-C	-5.07	100.43	113.10
2	C	131	ALA	CB-CA-C	5.07	117.70	110.10
3	S	256	LYS	CA-CB-CG	-5.07	102.25	113.40
3	T	282	ILE	N-CA-CB	-5.07	99.15	110.80
1	E	57	LYS	CD-CE-NZ	-5.06	100.06	111.70
2	I	74	ARG	NE-CZ-NH2	-5.06	117.77	120.30
3	V	279	GLU	CA-C-N	5.06	128.33	117.20
3	U	242	ARG	NE-CZ-NH1	5.06	122.83	120.30
3	S	248	PRO	C-N-CA	-5.05	109.07	121.70
1	K	8	LEU	CB-CG-CD2	5.05	119.59	111.00
1	K	129	VAL	CB-CA-C	-5.05	101.81	111.40
3	U	248	PRO	N-CA-C	-5.05	98.97	112.10
2	F	159	GLU	CB-CA-C	-5.04	100.32	110.40
2	F	157	SER	C-N-CA	-5.04	109.11	121.70
2	F	47	GLU	CA-CB-CG	-5.04	102.32	113.40
1	E	14	LYS	CD-CE-NZ	-5.03	100.12	111.70
1	E	28	LYS	N-CA-CB	-5.03	101.54	110.60
1	E	46	PRO	N-CA-C	5.03	125.19	112.10
2	I	151	LEU	CA-CB-CG	5.03	126.88	115.30
1	K	57	LYS	CB-CG-CD	5.03	124.67	111.60
1	K	59	GLU	CG-CD-OE2	5.03	128.35	118.30
2	L	104	GLU	CG-CD-OE2	5.02	128.35	118.30
1	B	52	GLU	CA-C-N	5.02	126.24	116.20
2	C	89	ASN	C-N-CA	-5.02	109.15	121.70
1	H	142	GLU	CB-CA-C	5.02	120.44	110.40
2	I	84	ARG	CG-CD-NE	5.01	122.33	111.80
1	K	75	PHE	CA-C-N	-5.01	106.18	117.20
1	K	108	VAL	CG1-CB-CG2	-5.01	102.89	110.90
2	I	156	MET	CB-CG-SD	5.01	127.42	112.40
3	U	269	ASN	C-N-CD	5.00	138.90	128.40

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
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

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Mol	Chain	Res	Type	Group
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
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1202	0	1209	137	1
1	E	1187	0	1196	144	1
1	H	1187	0	1196	187	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1202	0	1209	219	1
2	C	1123	0	1121	124	1
2	F	1109	0	1114	134	0
2	I	1109	0	1114	162	0
2	L	1109	0	1114	128	1
3	S	598	0	584	87	0
3	T	634	0	612	91	0
3	U	577	0	569	136	0
3	V	564	0	557	108	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
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	1587	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 68.

All (1587) 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:CB	3:U:228:ILE:CG2	1.74	1.64
3:V:288:LYS:CG	3:V:288:LYS:CD	1.74	1.63
1:E:8:LEU:CD1	1:E:8:LEU:CG	1.75	1.63
1:H:110:LEU:CG	1:H:110:LEU:CD2	1.77	1.62
1:K:78:LYS:CD	1:K:78:LYS:CE	1.75	1.62
3:T:242:ARG:CG	3:T:242:ARG:CD	1.74	1.62
2:L:145:LYS:CD	2:L:145:LYS:CE	1.77	1.61
2:C:84:ARG:CB	2:C:84:ARG:CG	1.75	1.61
1:K:156:ILE:CA	1:K:156:ILE:CB	1.78	1.60
1:E:96:LYS:CD	1:E:96:LYS:CG	1.77	1.60
1:E:94:ILE:CB	1:E:94:ILE:CG2	1.75	1.60
3:S:256:LYS:CG	3:S:256:LYS:CD	1.74	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:ALA:CA	1:E:6:ALA:CB	1.75	1.60
2:I:37:LYS:CE	2:I:37:LYS:CD	1.79	1.60
1:K:142:GLU:CB	1:K:142:GLU:CG	1.75	1.59
1:E:149:ARG:CG	1:E:149:ARG:CD	1.76	1.59
2:F:144:ILE:CG1	2:F:144:ILE:CD1	1.77	1.59
2:F:53:LYS:CD	2:F:53:LYS:CE	1.75	1.59
1:H:96:LYS:CD	1:H:96:LYS:CE	1.75	1.59
1:K:150:LEU:CD2	1:K:150:LEU:CG	1.79	1.58
2:C:159:GLU:CG	2:C:159:GLU:CB	1.80	1.58
1:E:78:LYS:CB	1:E:78:LYS:CG	1.78	1.58
2:I:37:LYS:CG	2:I:37:LYS:CD	1.74	1.58
3:U:295:ILE:CD1	3:U:295:ILE:CG1	1.77	1.58
3:V:270:PRO:CB	3:V:270:PRO:CG	1.80	1.58
3:U:252:THR:CB	3:U:252:THR:CA	1.74	1.58
3:S:242:ARG:CG	3:S:242:ARG:CD	1.82	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:CG1	3:T:228:ILE:CD1	1.76	1.57
1:K:106:ARG:CD	1:K:106:ARG:CG	1.78	1.56
3:U:295:ILE:CA	3:U:295:ILE:CB	1.75	1.56
3:V:248:PRO:CD	3:V:248:PRO:CG	1.79	1.56
2:F:153:ARG:CD	2:F:153:ARG:CG	1.75	1.56
2:F:37:LYS:CE	2:F:37:LYS:NZ	1.67	1.55
1:K:57:LYS:CG	1:K:57:LYS:CB	1.78	1.55
2:C:53:LYS:CD	2:C:53:LYS:CG	1.78	1.55
2:L:101:LYS:NZ	2:L:101:LYS:CE	1.69	1.55
3:T:288:LYS:CD	3:T:288:LYS:CE	1.78	1.55
1:B:22:GLU:CG	1:B:22:GLU:CB	1.76	1.55
2:C:159:GLU:CG	2:C:159:GLU:CD	1.74	1.54
1:B:86:LYS:NZ	1:B:86:LYS:CE	1.70	1.54
2:F:55:VAL:CG1	2:F:55:VAL:CB	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:CE	3:U:256:LYS:NZ	1.70	1.53
2:C:101:LYS:NZ	2:C:101:LYS:CE	1.68	1.52
2:F:55:VAL:CA	2:F:55:VAL:CB	1.85	1.52
1:B:28:LYS:CE	1:B:28:LYS:NZ	1.72	1.52
3:V:235:LYS:CE	3:V:235:LYS:NZ	1.68	1.51
3:T:288:LYS:CG	3:T:288:LYS:CD	1.85	1.51
3:T:256:LYS:CE	3:T:256:LYS:NZ	1.70	1.51
1:E:86:LYS:CE	1:E:86:LYS:NZ	1.74	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:114:LYS:NZ	2:C:114:LYS:CE	1.70	1.50
1:E:78:LYS:CD	1:E:78:LYS:CG	1.87	1.49
2:I:152:ARG:CG	2:I:152:ARG:CD	1.88	1.49
2:C:145:LYS:NZ	2:C:145:LYS:CE	1.72	1.49
3:U:245:CYS:SG	3:U:245:CYS:CB	2.03	1.47
1:B:134:LYS:CE	1:B:134:LYS:NZ	1.76	1.46
3:U:244:PRO:CB	3:U:244:PRO:CG	1.75	1.46
1:H:98:LYS:CE	1:H:98:LYS:NZ	1.78	1.46
2:F:95:LYS:CE	2:F:95:LYS:NZ	1.77	1.46
2:C:34:THR:CA	2:C:34:THR:CB	1.93	1.45
1:H:65:GLU:CG	1:H:65:GLU:CD	1.83	1.43
1:E:78:LYS:NZ	1:E:78:LYS:CE	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:CE	2:C:78:MET:SD	2.13	1.36
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
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
1:B:35:ASN:C	1:B:35:ASN:HD22	1.47	1.15
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:HH11	2:L:153:ARG:HG3	1.13	1.12
2:C:132:ILE:HD13	2:C:132:ILE:C	1.70	1.11
1:K:43:ILE:HD12	1:K:58:LEU:HD21	1.28	1.11
1:H:54:GLY:CA	1:H:152:ALA:HB1	1.81	1.11
2:F:130:ARG:HH11	2:F:130:ARG:HG3	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:HB2	2:I:84:ARG:HH11	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
3:V:268:PHE:O	3:V:270:PRO:HD3	1.56	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:81:HIS:CD2	1:K:83:ASN:HB2	1.88	1.06
1:H:50:PRO:HG3	1:H:141:ILE:HG23	1.35	1.05
1:E:149:ARG:HH11	1:E:149:ARG:CG	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:HH21	2:L:40:ARG:HG2	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
3:U:228:ILE:O	3:U:228:ILE:HG13	1.54	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
1:H:124:PRO:HB3	1:H:130:ALA:HB1	1.06	1.02
3:T:277:THR:CG2	3:T:278:GLN:N	2.21	1.02
1:H:92:LEU:O	1:H:95:LEU:HB2	1.58	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:N	1:K:128:ASP:OD2	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:N	3:V:282:ILE:HD13	1.75	1.00
1:H:65:GLU:HG2	1:H:69:ALA:HB2	1.39	1.00
2:F:37:LYS:HA	2:F:37:LYS:NZ	1.76	0.99
1:H:53:GLY:HA3	1:H:153:MET:HE3	1.39	0.99
2:F:37:LYS:HA	2:F:37:LYS:HZ2	1.22	0.99
1:B:150:LEU:HD13	1:B:151:TYR:CZ	1.98	0.99
1:E:149:ARG:HG2	1:E:149:ARG:HH11	1.26	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:159:GLU:CA	2:I:159:GLU:OE1	2.12	0.97
2:I:82:PRO:HB2	2:I:85:THR:HG21	1.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:234:GLY:HA3	3:U:237:SER:HB3	1.47	0.96
2:L:40:ARG:HG2	2:L:40:ARG:NH2	1.73	0.96
2:L:118:ASN:HD22	2:L:160:ASN:HD21	0.99	0.96
2:L:161:MET:CE	2:L:162:LYS:HZ2	1.79	0.95
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:O	2:C:76:THR:HG22	1.66	0.94
2:I:79:ILE:HG21	2:I:155:MET:HE1	1.50	0.93
1:B:81:HIS:HD2	1:B:83:ASN:H	0.95	0.93
2:F:55:VAL:HA	2:F:55:VAL:CB	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
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
3:S:257:ASP:N	3:S:257:ASP:OD2	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:O	3:U:258:ILE:HG13	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:B:35:ASN:ND2	1:B:35:ASN:C	2.26	0.89
1:H:81:HIS:HD2	1:H:83:ASN:HD21	0.93	0.89
1:E:122:ASP:HB3	1:E:134:LYS:HZ2	1.35	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:K:76:MET:O	2:L:70:MET:HE2	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:84:ARG:CB	2:I:84:ARG:HH11	1.85	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:143:THR:O	1:K:147:TRP:HD1	1.53	0.88
1:K:60:LEU:HD12	1:K:73:VAL:CG1	2.03	0.88
3:U:227:ASP:HA	3:U:228:ILE:CG2	2.04	0.88
1:K:81:HIS:CD2	1:K:82:PRO:CD	2.56	0.88
1:E:149:ARG:NH1	1:E:149:ARG:CG	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:K:35:ASN:C	1:K:35:ASN:HD22	1.78	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
1:H:65:GLU:HG2	1:H:69:ALA:CB	2.05	0.86
1:H:28:LYS:O	1:H:41:VAL:HA	1.74	0.86
2:F:132:ILE:HG12	2:F:132:ILE:O	1.73	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:NH1	2:F:130:ARG:HG3	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
2:I:140:ASN:HD22	2:I:141:SER:N	1.74	0.85
1:K:146:ALA:O	1:K:149:ARG:N	2.08	0.85
2:F:56:GLY:O	2:F:57:ASP:O	1.93	0.84
2:C:132:ILE:C	2:C:132:ILE:CD1	2.45	0.84
2:I:93:SER:C	2:I:94:LEU:HD12	1.97	0.84
2:I:83:PRO:HA	2:I:88:GLU:OE1	1.78	0.84
2:L:132:ILE:HG13	2:L:132:ILE:O	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:L:153:ARG:HA	2:L:156:MET:HE3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:K:109:LEU:HD23	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:88:GLY:N	2:C:70:MET:HE3	1.94	0.83
3:U:227:ASP:HA	3:U:228:ILE:HG22	1.61	0.83
2:F:163:LEU:O	2:F:165:GLN:NE2	2.11	0.83
1:B:38:TYR:HE1	1:B:40:HIS:CE1	1.96	0.83
2:I:82:PRO:HB3	2:I:85:THR:HG21	1.58	0.82
1:H:103:LEU:HD22	1:H:107:THR:HG21	1.62	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:86:LYS:O	1:K:87:LEU:HD23	1.78	0.82
3:U:228:ILE:CG1	3:U:228:ILE:O	2.28	0.82
3:V:282:ILE:H	3:V:282:ILE:HD13	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
3:S:297:GLU:C	3:S:297:GLU:OE1	2.18	0.82
1:H:81:HIS:CD2	1:H:83:ASN:HD22	1.93	0.82
1:E:35:ASN:HD22	1:E:37:ARG:H	1.26	0.82
1:K:51:PHE:CD1	1:K:51:PHE:N	2.48	0.81
1:K:56:PHE:CD1	1:K:79:ILE:HD12	2.16	0.81
1:K:56:PHE:CE1	1:K:79:ILE:HD12	2.15	0.81
2:I:114:LYS:CD	2:I:171:CYS:HA	2.11	0.81
1:H:119:PRO:O	1:H:121:PRO:HD2	1.79	0.81
2:F:167:PRO:HG2	2:F:170:GLN:HE22	1.44	0.81
1:E:64:GLU:OE1	1:E:64:GLU:HA	1.77	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
2:I:152:ARG:NH1	2:I:152:ARG:CG	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:53:GLY:HA3	1:H:153:MET:CE	2.11	0.81
1:B:154:ASN:HB2	1:B:156:ILE:HG12	1.60	0.81
2:L:140:ASN:HD22	2:L:141:SER:N	1.77	0.81
2:L:161:MET:CE	2:L:162:LYS:NZ	2.43	0.80
2:I:140:ASN:HD22	2:I:140:ASN:C	1.81	0.80
2:I:40:ARG:HG2	2:I:40:ARG:HH21	1.43	0.80
1:K:106:ARG:CG	1:K:106:ARG:NE	2.44	0.80
1:E:150:LEU:HD13	1:E:151:TYR:CE1	2.16	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:141:ILE:O	1:H:144:ALA:HB3	1.82	0.79
3:U:287:MET:HE1	3:V:286:ALA:C	2.02	0.79
3:U:242:ARG:HH11	3:U:242:ARG:HG3	1.46	0.79
2:C:165:GLN:HB3	2:C:166:PRO:HD2	1.62	0.79
2:I:94:LEU:N	2:I:94:LEU:HD12	1.97	0.79
2:F:167:PRO:HB2	2:F:170:GLN:NE2	1.98	0.79
3:U:247:THR:C	3:U:249:SER:N	2.32	0.79
3:V:247:THR:CG2	3:V:249:SER:H	1.96	0.79
1:H:27:ILE:CG1	1:H:43:ILE:HG13	2.13	0.78
2:C:132:ILE:HD13	2:C:132:ILE:O	1.83	0.78
3:U:272:THR:O	3:U:273:ARG:HB2	1.83	0.78
1:E:64:GLU:OE1	1:E:64:GLU:CA	2.29	0.78
1:K:59:GLU:HB3	1:K:76:MET:CE	2.13	0.78
2:C:84:ARG:HE	2:C:84:ARG:HB3	1.49	0.78
2:F:44:LEU:HD21	2:F:102:TYR:HE2	1.48	0.78
1:H:38:TYR:OH	1:H:59:GLU:OE1	2.01	0.78
1:E:44:ALA:O	1:E:46:PRO:HD3	1.83	0.78
2:I:43:ARG:NH2	2:I:143:SER:HB3	1.98	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
3:S:259:GLU:C	3:S:263:GLN:HE21	1.87	0.78
2:F:168:GLU:CG	2:F:169:GLY:H	1.96	0.78
3:V:234:GLY:O	3:V:236:ILE:N	2.16	0.78
3:S:229:PRO:HD2	3:S:232:LEU:HD22	1.66	0.78
1:E:98:LYS:O	3:U:273:ARG:NH2	2.17	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
1:H:124:PRO:HG3	1:H:134:LYS:HE3	1.66	0.77
2:C:47:GLU:OE1	2:C:143:SER:HB2	1.83	0.77
2:C:53:LYS:CE	2:C:53:LYS:CG	2.62	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:246:ILE:HG13	3:S:247:THR:H	1.49	0.77
1:B:153:MET:O	1:B:154:ASN:ND2	2.18	0.77
2:F:37:LYS:NZ	2:F:37:LYS:CA	2.47	0.77
3:V:288:LYS:CB	3:V:288:LYS:CD	2.62	0.77
3:T:290:VAL:O	3:T:293:ALA:HB3	1.85	0.77
3:U:228:ILE:HB	3:U:228:ILE:CG2	2.08	0.77
2:F:57:ASP:OD1	2:F:59:THR:HB	1.85	0.77
3:U:233:CYS:HA	3:U:239:GLU:O	1.85	0.77
3:T:243:GLU:HG2	3:T:255:ARG:HB2	1.65	0.77
2:L:40:ARG:CG	2:L:40:ARG:NH2	2.45	0.77
1:E:24:VAL:HG13	1:E:25:PRO:HD2	1.67	0.76
1:E:149:ARG:CB	1:E:149:ARG:CD	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:CD	2:L:101:LYS:NZ	2.48	0.75
1:B:130:ALA:O	1:B:131:GLU:C	2.23	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
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
1:H:76:MET:C	2:I:70:MET:HE3	2.07	0.74
1:H:121:PRO:C	1:H:123:ASP:H	1.90	0.74
2:I:40:ARG:HG3	2:I:102:TYR:O	1.88	0.74
2:L:126:VAL:HG12	2:L:127:VAL:N	2.01	0.74
1:B:116:LEU:HD23	1:B:116:LEU:N	2.02	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
3:T:269:ASN:HD22	3:T:271:VAL:H	1.33	0.74
2:F:40:ARG:HB2	2:F:102:TYR:O	1.88	0.73
1:B:106:ARG:O	1:B:106:ARG:HG2	1.88	0.73
1:H:133:TRP:C	1:H:133:TRP:CD1	2.60	0.73
1:K:35:ASN:C	1:K:35:ASN:ND2	2.41	0.73
2:L:157:SER:O	2:L:158:LYS:C	2.26	0.73
3:V:247:THR:HG22	3:V:251:ILE:H	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:139:GLN:O	2:F:141:SER:N	2.21	0.73
1:K:11:ARG:HH22	1:K:67:PRO:HG2	1.52	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:CD1	3:V:282:ILE:N	2.51	0.73
1:H:76:MET:O	2:I:70:MET:CE	2.36	0.73
1:H:57:LYS:HB3	1:H:76:MET:HB2	1.71	0.73
2:I:152:ARG:N	2:I:155:MET:HG3	2.04	0.73
1:H:150:LEU:HD23	1:H:150:LEU:C	2.09	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
2:F:160:ASN:HB3	2:F:163:LEU:CD1	2.19	0.72
1:E:81:HIS:HD2	1:E:83:ASN:H	1.36	0.72
1:B:62:LEU:HD11	1:B:105:ILE:HD11	1.70	0.72
3:V:261:HIS:CD2	3:V:261:HIS:C	2.62	0.72
1:B:78:LYS:HD2	1:B:151:TYR:CZ	2.24	0.72
1:K:136:ASN:C	1:K:136:ASN:HD22	1.92	0.72
2:C:53:LYS:NZ	2:C:53:LYS:CG	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:L:111:PHE:CE1	2:L:115:ILE:HD12	2.23	0.72
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:CD1	1:E:51:PHE:N	2.56	0.71
3:U:268:PHE:HD1	3:U:273:ARG:HA	1.56	0.71
2:I:114:LYS:CG	2:I:171:CYS:HA	2.20	0.71
2:L:145:LYS:O	2:L:149:GLN:HG3	1.90	0.71
1:K:43:ILE:HD12	1:K:58:LEU:CD2	2.14	0.71
1:B:114:ALA:O	1:B:117:SER:N	2.21	0.71
2:L:126:VAL:CG1	2:L:127:VAL:N	2.53	0.71
2:L:53:LYS:HD3	2:L:53:LYS:N	2.05	0.71
2:L:59:THR:O	2:L:60:VAL:HG13	1.90	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:U:247:THR:C	3:U:249:SER:H	1.91	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
3:V:258:ILE:HG13	3:V:258:ILE:O	1.91	0.71
1:H:20:LEU:O	1:H:22:GLU:N	2.24	0.71
2:C:158:LYS:HG3	2:C:159:GLU:N	2.05	0.70
1:E:51:PHE:CD2	1:E:79:ILE:HD11	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:277:THR:N	3:U:280:GLN:HE21	1.89	0.70
2:L:153:ARG:NH1	2:L:153:ARG:CG	2.49	0.70
2:C:132:ILE:O	2:C:132:ILE:CD1	2.39	0.70
3:U:254:ASP:OD1	3:U:255:ARG:N	2.23	0.70
1:B:134:LYS:NZ	1:B:134:LYS:CG	2.54	0.70
3:T:277:THR:CG2	3:T:278:GLN:H	2.03	0.70
2:L:153:ARG:NH1	2:L:153:ARG:HG3	1.95	0.70
1:H:32:ASP:HB2	1:H:40:HIS:HE2	1.55	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: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
2:C:53:LYS:HZ2	2:C:53:LYS:HG2	1.57	0.70
1:B:119:PRO:O	1:B:121:PRO:HD3	1.90	0.70
2:I:62:TRP:CH2	2:I:145:LYS:HB3	2.26	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:H:76:MET:O	2:I:70:MET:HE2	1.92	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
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
3:S:236:ILE:HG22	3:S:237:SER:N	2.07	0.69
1:B:74:ARG:HG3	1:B:75:PHE:O	1.92	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
2:I:90:ARG:HH11	2:I:168:GLU:HA	1.57	0.69
1:B:21:ALA:O	1:B:23:PRO:HD3	1.92	0.69
2:C:84:ARG:HE	2:C:84:ARG:CB	2.03	0.69
2:I:129:PRO:O	2:I:136:ALA:HB2	1.92	0.69
3:S:267:HIS:CD2	3:S:267:HIS:N	2.49	0.69
2:L:114:LYS:HA	2:L:172:TYR:CE1	2.28	0.69
2:F:160:ASN:HB3	2:F:163:LEU:HD11	1.73	0.69
3:S:237:SER:O	3:S:238:PHE:HB2	1.91	0.69
2:L:140:ASN:HD22	2:L:140:ASN:C	1.96	0.69
1:K:51:PHE:HD1	1:K:51:PHE:H	1.38	0.69
1:H:96:LYS:CG	1:H:96:LYS:CE	2.69	0.69
1:H:121:PRO:O	1:H:123:ASP:N	2.25	0.69
1:K:28:LYS:O	1:K:41:VAL:HG13	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:246:ILE:HG13	3:T:247:THR:N	2.06	0.69
1:K:28:LYS:HB3	1:K:28:LYS:NZ	2.08	0.69
2:I:132:ILE:HG23	2:I:134:VAL:HG13	1.75	0.69
3:U:252:THR:CA	3:U:252:THR:CG2	2.71	0.69
2:F:114:LYS:HE3	2:F:170:GLN:OE1	1.92	0.69
3:T:274:SER:C	3:T:275:PRO:O	2.22	0.69
3:V:268:PHE:O	3:V:270:PRO:CD	2.39	0.68
2:C:150:GLU:OE2	2:C:153:ARG:HD2	1.93	0.68
2:L:153:ARG:HA	2:L:156:MET:HE2	1.74	0.68
3:U:277:THR:N	3:U:280:GLN:NE2	2.36	0.68
1:K:142:GLU:CG	1:K:142:GLU:CA	2.72	0.68
2:C:130:ARG:O	2:C:131:ALA:C	2.32	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
2:F:43:ARG:NH2	2:F:142:TYR:O	2.25	0.68
1:H:12:ILE:HD13	1:H:62:LEU:HD13	1.75	0.68
1:K:68:MET:HE3	3:V:265:VAL:HG23	1.76	0.68
3:T:237:SER:HB3	3:T:257:ASP:OD2	1.94	0.68
1:K:49:SER:O	1:K:51:PHE:N	2.27	0.67
2:C:130:ARG:NH2	2:F:121:ASN:HA	2.06	0.67
2:C:80:LEU:N	2:C:80:LEU:HD13	2.09	0.67
3:T:301:VAL:CB	3:T:301:VAL:HA	2.13	0.67
1:H:148:THR:O	1:H:152:ALA:HB3	1.95	0.67
3:T:242:ARG:CD	3:T:242:ARG:CB	2.72	0.67
1:H:83:ASN:N	1:H:83:ASN:ND2	2.42	0.67
2:L:111:PHE:CD1	2:L:115:ILE:HD12	2.29	0.67
1:K:82:PRO:CD	1:K:83:ASN:H	1.99	0.67
1:B:150:LEU:HD13	1:B:151:TYR:CE1	2.29	0.67
2:L:143:SER:OG	2:L:146:VAL:HG23	1.94	0.67
3:S:259:GLU:C	3:S:263:GLN:NE2	2.45	0.67
2:I:60:VAL:HG22	2:I:148:LEU:HB3	1.76	0.67
1:B:88:GLY:N	2:C:70:MET:CE	2.57	0.67
2:C:42:PHE:O	2:C:46:GLU:HG3	1.94	0.67
1:B:56:PHE:O	1:B:58:LEU:HD23	1.95	0.67
2:F:153:ARG:CD	2:F:153:ARG:CB	2.72	0.67
3:U:256:LYS:CD	3:U:256:LYS:NZ	2.57	0.67
3:T:277:THR:HG23	3:T:278:GLN:H	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:295:ILE:CB	3:U:295:ILE:C	2.62	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:E:29:ALA:C	1:E:30:GLU:HG3	2.14	0.67
2:L:161:MET:HE3	2:L:162:LYS:HZ2	1.58	0.66
2:L:82:PRO:CA	2:L:152:ARG:NH2	2.54	0.66
3:U:247:THR:HG22	3:U:249:SER:N	2.10	0.66
1:B:15:GLU:OE1	1:B:104:GLN:HB2	1.94	0.66
1:K:105:ILE:O	1:K:108:VAL:N	2.27	0.66
3:T:287:MET:O	3:T:289:GLU:N	2.29	0.66
2:I:132:ILE:CG2	2:I:134:VAL:HG13	2.25	0.66
2:L:37:LYS:HZ2	2:L:37:LYS:HB2	1.58	0.66
1:H:24:VAL:O	1:H:26:GLY:N	2.29	0.66
1:E:47:GLN:O	1:E:48:ASP:HB2	1.94	0.66
3:U:241:MET:HG2	3:U:254:ASP:HB2	1.77	0.66
2:F:128:ASP:OD1	2:F:128:ASP:C	2.33	0.66
2:F:36:VAL:HG23	2:F:36:VAL:O	1.96	0.66
1:H:97:ASP:O	1:H:99:TRP:N	2.28	0.66
3:U:227:ASP:HA	3:U:228:ILE:HG23	1.75	0.66
3:T:242:ARG:NE	3:T:242:ARG:CG	2.59	0.66
2:F:37:LYS:HZ3	2:F:37:LYS:CA	2.08	0.66
1:B:86:LYS:HD3	2:C:68:GLU:HG2	1.77	0.66
1:B:83:ASN:HB3	1:B:91:CYS:HB3	1.78	0.66
1:E:58:LEU:HD12	1:E:58:LEU:N	2.11	0.66
3:V:243:GLU:OE1	3:V:256:LYS:CE	2.44	0.66
2:C:37:LYS:HG3	2:C:37:LYS:O	1.96	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:121:PRO:C	1:H:123:ASP:N	2.48	0.66
1:E:127:ASN:HD22	1:E:127:ASN:C	1.98	0.66
2:I:87:TYR:CD1	2:I:155:MET:HB3	2.31	0.65
1:H:43:ILE:HG22	1:H:44:ALA:O	1.95	0.65
2:F:140:ASN:HD22	2:F:140:ASN:C	1.99	0.65
1:E:94:ILE:CG1	1:E:94:ILE:CG2	2.71	0.65
2:I:131:ALA:O	2:I:132:ILE:HG13	1.95	0.65
1:B:29:ALA:C	1:B:30:GLU:HG3	2.16	0.65
2:F:114:LYS:HE2	2:F:170:GLN:HG2	1.78	0.65
2:F:167:PRO:HB2	2:F:170:GLN:HE21	1.60	0.65
2:C:82:PRO:HG2	2:C:85:THR:HG21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:11:ARG:NH2	1:B:67:PRO:CG	2.60	0.65
3:T:231:TYR:HD1	3:T:232:LEU:HD13	1.60	0.65
3:U:252:THR:CB	3:U:252:THR:C	2.61	0.65
3:S:272:THR:C	3:S:274:SER:H	1.98	0.65
1:B:50:PRO:O	1:B:145:ARG:HG3	1.96	0.65
3:T:232:LEU:O	3:T:240:LEU:HA	1.97	0.65
2:C:127:VAL:HG12	2:C:128:ASP:N	2.10	0.65
2:F:114:LYS:CE	2:F:170:GLN:HG2	2.28	0.64
1:E:73:VAL:HG12	1:E:90:ILE:HD13	1.78	0.64
2:F:138:TRP:CG	2:F:139:GLN:N	2.63	0.64
1:H:131:GLU:O	1:H:132:GLN:C	2.36	0.64
2:L:61:SER:HB3	2:L:78:MET:HG3	1.77	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
2:I:114:LYS:HG3	2:I:172:TYR:H	1.63	0.64
1:E:35:ASN:HD22	1:E:37:ARG:N	1.95	0.64
1:B:96:LYS:HB3	1:B:97:ASP:OD1	1.97	0.64
1:E:8:LEU:CD1	1:E:8:LEU:CB	2.72	0.64
1:K:150:LEU:CD2	1:K:150:LEU:CD1	2.76	0.64
2:I:154:LEU:O	2:I:157:SER:HB3	1.97	0.64
2:F:132:ILE:O	2:F:133:SER:C	2.34	0.64
2:I:36:VAL:HG12	2:I:37:LYS:N	2.13	0.64
2:F:166:PRO:C	2:F:167:PRO:O	2.36	0.64
2:L:157:SER:O	2:L:159:GLU:N	2.31	0.64
2:F:140:ASN:ND2	2:F:140:ASN:C	2.50	0.64
2:I:114:LYS:HG3	2:I:171:CYS:HA	1.80	0.64
1:E:32:ASP:O	1:E:35:ASN:N	2.30	0.64
3:U:268:PHE:HB2	3:U:273:ARG:O	1.98	0.63
2:F:44:LEU:CD2	2:F:102:TYR:HE2	2.10	0.63
2:C:118:ASN:H	2:C:160:ASN:HD21	1.46	0.63
2:L:50:GLU:OE1	2:L:55:VAL:HG21	1.98	0.63
1:H:14:LYS:NZ	3:T:228:ILE:HD12	2.12	0.63
2:C:114:LYS:HA	2:C:172:TYR:CZ	2.32	0.63
3:U:247:THR:CG2	3:U:249:SER:HB2	2.26	0.63
1:K:139:GLN:O	1:K:140:ALA:C	2.37	0.63
2:C:101:LYS:O	2:C:104:GLU:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:ALA:O	1:H:149:ARG:HB3	1.98	0.63
1:H:84:VAL:HG12	1:H:88:GLY:HA2	1.80	0.63
3:T:277:THR:HG23	3:T:278:GLN:N	2.13	0.63
2:I:140:ASN:C	2:I:140:ASN:ND2	2.52	0.63
3:T:241:MET:CE	3:T:253:TYR:HA	2.29	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
2:L:40:ARG:HB2	2:L:102:TYR:O	1.99	0.63
1:H:93:ASP:OD1	1:H:94:ILE:N	2.31	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
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:78:LYS:NZ	1:K:147:TRP:CH2	2.60	0.63
1:K:28:LYS:HB3	1:K:28:LYS:HZ2	1.64	0.63
2:C:159:GLU:CA	2:C:159:GLU:CG	2.73	0.63
1:K:81:HIS:O	1:K:129:VAL:HG11	1.99	0.63
1:E:35:ASN:HD22	1:E:35:ASN:C	2.02	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:B:52:GLU:O	1:B:53:GLY:C	2.35	0.62
1:H:91:CYS:O	1:H:91:CYS:SG	2.54	0.62
1:H:58:LEU:CD2	1:H:58:LEU:N	2.62	0.62
1:K:144:ALA:O	1:K:147:TRP:CB	2.42	0.62
1:H:65:GLU:CG	1:H:69:ALA:CB	2.71	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
3:T:237:SER:O	3:T:238:PHE:HB2	1.97	0.62
2:I:79:ILE:CG2	2:I:155:MET:HE1	2.28	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
3:U:242:ARG:O	3:U:243:GLU:HB2	2.00	0.62
1:K:104:GLN:HG3	1:K:106:ARG:H	1.65	0.62
3:U:247:THR:O	3:U:250:GLY:N	2.32	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:289:GLU:OE1	3:V:231:TYR:HB3	1.99	0.62
2:F:144:ILE:CB	2:F:144:ILE:CD1	2.72	0.62
1:B:81:HIS:NE2	1:B:83:ASN:ND2	2.47	0.62
1:K:80:TYR:HB3	1:K:144:ALA:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:54:GLY:O	2:L:55:VAL:HG23	1.98	0.62
2:F:53:LYS:CG	2:F:53:LYS:CE	2.77	0.62
1:K:114:ALA:O	1:K:115:LEU:C	2.38	0.62
2:I:152:ARG:H	2:I:155:MET:HG3	1.65	0.62
1:B:127:ASN:HB2	1:B:128:ASP:OD2	1.99	0.62
3:T:269:ASN:HB3	3:T:273:ARG:H	1.63	0.62
2:F:95:LYS:N	2:F:110:ARG:O	2.29	0.62
2:F:47:GLU:OE1	2:F:143:SER:HB2	1.99	0.62
1:H:133:TRP:C	1:H:133:TRP:HD1	2.02	0.61
1:K:128:ASP:C	1:K:130:ALA:N	2.51	0.61
3:U:287:MET:HE1	3:V:286:ALA:O	1.99	0.61
1:K:78:LYS:NZ	1:K:78:LYS:CD	2.61	0.61
3:U:245:CYS:SG	3:U:245:CYS:CA	2.85	0.61
1:B:28:LYS:HE2	1:B:30:GLU:OE2	1.99	0.61
2:F:168:GLU:CG	2:F:169:GLY:N	2.45	0.61
1:E:104:GLN:O	1:E:107:THR:N	2.33	0.61
3:U:285:LEU:HB2	3:V:250:GLY:O	2.00	0.61
3:S:243:GLU:HG2	3:S:255:ARG:HB3	1.82	0.61
1:K:80:TYR:HD2	1:K:144:ALA:HB2	1.65	0.61
2:F:66:ASP:C	2:F:66:ASP:OD2	2.39	0.61
2:I:153:ARG:O	2:I:156:MET:HB2	2.01	0.61
2:F:80:LEU:O	2:F:81:GLY:C	2.33	0.61
2:L:53:LYS:CD	2:L:53:LYS:N	2.62	0.61
2:C:132:ILE:HD13	2:C:133:SER:N	2.16	0.61
1:H:127:ASN:OD1	1:H:128:ASP:N	2.34	0.61
1:H:24:VAL:O	1:H:25:PRO:C	2.38	0.61
2:C:53:LYS:CB	2:C:53:LYS:CD	2.76	0.61
1:B:127:ASN:HD22	1:B:127:ASN:C	2.04	0.61
1:E:141:ILE:HG22	1:E:142:GLU:N	2.16	0.61
1:E:150:LEU:HD13	1:E:151:TYR:CD1	2.36	0.61
2:I:114:LYS:HD3	2:I:171:CYS:HA	1.83	0.61
2:F:118:ASN:HD22	2:F:160:ASN:HD22	1.47	0.61
1:B:24:VAL:HG13	1:B:25:PRO:HD2	1.83	0.61
1:K:142:GLU:O	1:K:143:THR:C	2.39	0.61
1:E:6:ALA:CB	1:E:6:ALA:HA	2.18	0.61
2:I:79:ILE:CG2	2:I:155:MET:CE	2.79	0.61
1:H:9:PRO:HG2	1:H:12:ILE:HG13	1.82	0.61
2:I:130:ARG:HH11	2:I:130:ARG:HG3	1.66	0.60
3:T:241:MET:HE3	3:T:253:TYR:HA	1.82	0.60
1:H:66:TYR:CD1	1:H:67:PRO:HA	2.36	0.60
3:T:242:ARG:HG2	3:T:303:ASP:OD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:PRO:O	1:H:121:PRO:CD	2.48	0.60
2:F:50:GLU:OE2	2:F:145:LYS:NZ	2.34	0.60
3:U:295:ILE:HB	3:U:295:ILE:CA	2.16	0.60
1:B:147:TRP:O	1:B:151:TYR:HD1	1.82	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:C:140:ASN:C	2:C:140:ASN:ND2	2.54	0.60
2:L:111:PHE:CD1	2:L:115:ILE:CD1	2.84	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
3:U:247:THR:CG2	3:U:249:SER:H	2.13	0.60
3:S:231:TYR:CD1	3:S:232:LEU:HD13	2.37	0.60
3:U:289:GLU:O	3:U:292:ASP:N	2.34	0.60
2:L:67:ASP:O	2:L:68:GLU:CG	2.44	0.60
3:V:271:VAL:O	3:V:271:VAL:CG1	2.49	0.60
1:H:70:ALA:HB1	1:H:71:PRO:HD2	1.83	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
3:S:284:ASN:O	3:S:284:ASN:OD1	2.20	0.60
1:E:153:MET:O	1:E:154:ASN:C	2.40	0.60
3:U:228:ILE:CA	3:U:228:ILE:CG2	2.77	0.59
1:K:68:MET:HE3	1:K:68:MET:HA	1.84	0.59
3:U:252:THR:CB	3:U:252:THR:N	2.58	0.59
3:T:291:ILE:O	3:T:294:PHE:N	2.35	0.59
3:S:247:THR:HG21	3:S:269:ASN:HD21	1.67	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:E:8:LEU:CD1	1:E:8:LEU:HG	2.15	0.59
1:B:154:ASN:CB	1:B:156:ILE:HG12	2.32	0.59
3:T:241:MET:HE2	3:T:253:TYR:C	2.23	0.59
2:C:82:PRO:HG2	2:C:85:THR:CG2	2.32	0.59
3:T:299:GLY:O	3:T:300:TRP:HE3	1.81	0.59
1:E:70:ALA:HB1	1:E:71:PRO:HD2	1.83	0.59
1:B:59:GLU:HG3	1:B:59:GLU:O	2.02	0.59
2:F:65:GLU:OE2	2:F:95:LYS:CE	2.48	0.59
1:B:144:ALA:O	1:B:145:ARG:C	2.37	0.59
3:V:243:GLU:OE2	3:V:255:ARG:HD2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:LYS:HD3	1:H:18:ARG:NH2	2.16	0.59
2:I:152:ARG:O	2:I:153:ARG:C	2.41	0.59
1:E:24:VAL:CG1	1:E:25:PRO:HD2	2.32	0.59
3:T:243:GLU:HG2	3:T:255:ARG:CB	2.33	0.59
2:L:118:ASN:ND2	2:L:160:ASN:HD21	1.84	0.59
3:U:247:THR:O	3:U:248:PRO:C	2.42	0.59
1:E:28:LYS:HG3	1:E:29:ALA:N	2.18	0.59
3:U:233:CYS:CA	3:U:239:GLU:O	2.51	0.58
1:B:47:GLN:HA	1:B:52:GLU:HG3	1.85	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
3:T:246:ILE:HG13	3:T:247:THR:H	1.65	0.58
2:I:63:GLY:O	2:I:75:TRP:HE3	1.87	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:K:149:ARG:O	1:K:150:LEU:C	2.42	0.58
2:F:118:ASN:ND2	2:F:160:ASN:HD22	2.02	0.58
1:B:68:MET:HE1	3:S:261:HIS:HA	1.86	0.58
3:T:247:THR:O	3:T:250:GLY:HA2	2.03	0.58
1:B:27:ILE:HG21	1:B:109:LEU:HD13	1.86	0.58
1:B:4:GLY:O	1:B:5:SER:HB3	2.04	0.58
1:K:7:GLY:H	1:K:8:LEU:HB3	1.68	0.58
3:T:292:ASP:HA	3:T:295:ILE:HG13	1.86	0.58
1:H:141:ILE:O	1:H:142:GLU:O	2.22	0.58
1:K:58:LEU:CD2	1:K:58:LEU:N	2.66	0.58
1:E:99:TRP:C	3:U:273:ARG:HH22	2.07	0.58
3:S:261:HIS:CD2	3:S:261:HIS:C	2.75	0.58
3:T:297:GLU:O	3:T:298:ASN:C	2.39	0.58
2:C:123:SER:O	2:C:172:TYR:HD2	1.87	0.58
2:C:34:THR:CB	2:C:34:THR:HA	2.22	0.58
1:H:53:GLY:CA	1:H:153:MET:HE3	2.26	0.58
3:S:246:ILE:HG13	3:S:247:THR:N	2.19	0.58
3:S:229:PRO:HD2	3:S:232:LEU:CD2	2.33	0.58
1:B:155:ASN:N	1:B:155:ASN:OD1	2.19	0.58
3:S:271:VAL:O	3:S:271:VAL:HG12	2.04	0.58
1:K:136:ASN:C	1:K:136:ASN:ND2	2.57	0.58
2:L:43:ARG:HG2	2:L:103:PRO:HG3	1.85	0.58
2:C:94:LEU:HD12	2:C:94:LEU:N	2.18	0.58
2:C:78:MET:HB2	2:C:78:MET:CE	2.33	0.58
3:V:261:HIS:C	3:V:261:HIS:HD2	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:73:THR:HG22	2:F:73:THR:O	2.01	0.57
1:H:134:LYS:HG2	1:H:135:THR:H	1.67	0.57
1:B:104:GLN:O	1:B:105:ILE:C	2.40	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:V:234:GLY:C	3:V:236:ILE:H	2.08	0.57
1:H:76:MET:C	2:I:70:MET:CE	2.72	0.57
2:L:128:ASP:O	2:L:129:PRO:C	2.40	0.57
2:C:129:PRO:C	2:C:130:ARG:O	2.41	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
1:K:95:LEU:HD21	1:K:108:VAL:CG1	2.34	0.57
2:I:156:MET:O	2:I:157:SER:O	2.23	0.57
1:E:60:LEU:HA	1:E:73:VAL:CG2	2.34	0.57
2:L:48:LEU:O	2:L:52:GLN:HG3	2.05	0.57
1:E:67:PRO:O	1:E:101:PRO:HB3	2.04	0.57
1:B:98:LYS:CD	1:B:98:LYS:N	2.67	0.57
1:B:24:VAL:CG1	1:B:25:PRO:N	2.67	0.57
2:I:90:ARG:HH11	2:I:168:GLU:CA	2.17	0.57
2:F:158:LYS:HD2	2:F:159:GLU:OE1	2.05	0.57
1:B:68:MET:HE1	3:S:265:VAL:HG23	1.86	0.57
1:K:147:TRP:O	1:K:151:TYR:HB2	2.05	0.57
2:I:102:TYR:CD1	2:I:103:PRO:HA	2.40	0.57
1:H:24:VAL:HG13	1:H:25:PRO:HD2	1.87	0.57
1:K:120:ASN:OD1	1:K:122:ASP:CB	2.53	0.57
1:K:54:GLY:HA3	1:K:152:ALA:HB1	1.87	0.57
2:F:82:PRO:HG2	2:F:85:THR:HG21	1.87	0.57
3:S:227:ASP:O	3:S:228:ILE:HG13	2.05	0.57
2:I:46:GLU:O	2:I:48:LEU:N	2.37	0.57
1:K:80:TYR:HE2	1:K:140:ALA:HA	1.70	0.56
3:T:242:ARG:N	3:T:254:ASP:OD2	2.37	0.56
2:I:132:ILE:HG22	2:I:135:LEU:HB2	1.86	0.56
1:E:63:PRO:HG2	1:E:69:ALA:HB1	1.87	0.56
1:K:46:PRO:CD	1:K:116:LEU:HD13	2.31	0.56
3:V:237:SER:C	3:V:239:GLU:N	2.58	0.56
1:B:134:LYS:HB2	1:B:134:LYS:HZ2	1.69	0.56
1:B:134:LYS:CB	1:B:134:LYS:NZ	2.68	0.56
3:U:269:ASN:O	3:U:270:PRO:C	2.41	0.56
1:K:35:ASN:HD22	1:K:36:ALA:N	2.03	0.56
1:H:46:PRO:CG	1:H:116:LEU:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:276:LEU:HA	3:V:280:GLN:OE1	2.05	0.56
3:V:245:CYS:HB2	3:V:283:PRO:HA	1.88	0.56
3:U:278:GLN:HB3	3:U:279:GLU:OE2	2.06	0.56
1:H:81:HIS:HB3	1:H:84:VAL:HG23	1.88	0.56
3:U:269:ASN:CG	3:U:272:THR:HG1	2.08	0.56
2:I:43:ARG:HH22	2:I:143:SER:HB3	1.71	0.56
3:U:295:ILE:CB	3:U:295:ILE:HA	2.18	0.56
1:H:81:HIS:HE1	1:H:116:LEU:HA	1.69	0.56
2:F:43:ARG:HG3	2:F:103:PRO:HG2	1.88	0.56
3:V:231:TYR:HD1	3:V:232:LEU:N	2.03	0.56
1:H:81:HIS:CD2	1:H:82:PRO:CD	2.89	0.56
2:L:115:ILE:HD11	2:L:120:VAL:HG11	1.87	0.56
1:K:81:HIS:NE2	1:K:83:ASN:HB2	2.18	0.56
1:B:77:THR:CG2	1:B:78:LYS:N	2.64	0.56
3:S:272:THR:C	3:S:274:SER:N	2.58	0.56
1:K:93:ASP:N	1:K:93:ASP:OD1	2.39	0.56
1:E:8:LEU:HG	1:E:9:PRO:CD	2.33	0.56
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
1:B:137:GLU:O	1:B:138:ALA:C	2.42	0.56
2:F:118:ASN:ND2	2:F:160:ASN:ND2	2.52	0.56
1:K:120:ASN:OD1	1:K:122:ASP:CG	2.44	0.56
2:L:80:LEU:HD12	2:L:80:LEU:N	2.20	0.56
3:V:246:ILE:HA	3:V:252:THR:HG23	1.87	0.55
3:V:288:LYS:CG	3:V:288:LYS:CE	2.79	0.55
2:C:129:PRO:HG2	2:C:130:ARG:N	2.22	0.55
1:K:128:ASP:C	1:K:131:GLU:H	2.09	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
1:K:14:LYS:HE3	1:K:18:ARG:HH22	1.72	0.55
2:I:161:MET:CE	2:I:162:LYS:NZ	2.70	0.55
1:E:128:ASP:O	1:E:131:GLU:HB3	2.07	0.55
2:C:35:GLY:O	2:C:36:VAL:HB	2.07	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:HG	3:T:276:LEU:O	1.97	0.55
2:L:84:ARG:NE	2:L:84:ARG:HB3	2.22	0.55
1:H:76:MET:O	2:I:70:MET:HE3	2.02	0.55
3:V:232:LEU:O	3:V:241:MET:HE2	2.06	0.55
2:C:37:LYS:O	2:C:37:LYS:CG	2.54	0.55
1:K:50:PRO:CG	1:K:141:ILE:HD12	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:84:ARG:NE	2:C:84:ARG:CB	2.69	0.55
2:I:36:VAL:CG1	2:I:37:LYS:N	2.68	0.55
1:K:86:LYS:HD2	2:L:68:GLU:HG2	1.87	0.55
3:U:250:GLY:HA3	3:V:285:LEU:CD1	2.36	0.55
1:E:150:LEU:CD1	1:E:151:TYR:CE1	2.89	0.55
1:B:65:GLU:O	1:B:66:TYR:C	2.44	0.55
2:L:67:ASP:N	2:L:67:ASP:OD2	2.40	0.55
1:H:150:LEU:CD2	1:H:150:LEU:C	2.75	0.55
2:F:36:VAL:CG2	2:F:36:VAL:O	2.54	0.55
3:V:229:PRO:O	3:V:230:ASP:CB	2.55	0.55
1:E:123:ASP:H	1:E:124:PRO:HA	1.72	0.55
1:E:149:ARG:NE	1:E:149:ARG:CG	2.65	0.55
3:U:256:LYS:CG	3:U:256:LYS:NZ	2.70	0.55
2:I:94:LEU:N	2:I:94:LEU:CD1	2.65	0.55
1:K:104:GLN:O	1:K:107:THR:OG1	2.17	0.55
1:H:127:ASN:C	1:H:127:ASN:OD1	2.44	0.55
3:V:287:MET:O	3:V:290:VAL:N	2.40	0.55
2:L:140:ASN:C	2:L:140:ASN:ND2	2.61	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
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
3:U:266:GLY:C	3:U:268:PHE:H	2.08	0.54
3:U:266:GLY:C	3:U:268:PHE:N	2.61	0.54
1:E:150:LEU:HD13	1:E:151:TYR:CZ	2.42	0.54
3:V:237:SER:C	3:V:239:GLU:H	2.10	0.54
1:B:11:ARG:NH2	1:B:67:PRO:HG2	2.22	0.54
2:I:130:ARG:NH1	2:I:130:ARG:HG3	2.21	0.54
3:S:253:TYR:OH	3:S:271:VAL:HG23	2.07	0.54
2:L:145:LYS:CG	2:L:145:LYS:CE	2.75	0.54
1:K:65:GLU:O	1:K:68:MET:N	2.40	0.54
1:H:148:THR:HG22	1:H:152:ALA:CB	2.38	0.54
3:S:247:THR:HG21	3:S:251:ILE:HB	1.89	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:133:SER:OG	2:F:134:VAL:N	2.40	0.54
2:L:84:ARG:NE	2:L:84:ARG:CB	2.70	0.54
3:U:230:ASP:C	3:U:232:LEU:H	2.11	0.54
1:K:14:LYS:HE3	1:K:18:ARG:NH2	2.23	0.54
2:F:157:SER:O	2:F:161:MET:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:295:ILE:HD12	3:T:296:SER:OG	2.07	0.54
1:K:86:LYS:C	1:K:87:LEU:HD23	2.28	0.54
1:K:32:ASP:HB3	1:K:35:ASN:O	2.08	0.54
3:U:231:TYR:CD1	3:U:232:LEU:HD23	2.43	0.54
3:V:277:THR:HG23	3:V:280:GLN:OE1	2.08	0.54
1:H:58:LEU:HD13	1:H:75:PHE:CD2	2.42	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
3:S:292:ASP:O	3:S:293:ALA:C	2.45	0.54
1:B:154:ASN:O	1:B:154:ASN:ND2	2.41	0.54
3:V:236:ILE:O	3:V:238:PHE:N	2.41	0.54
2:F:53:LYS:NZ	2:F:53:LYS:CD	2.69	0.53
2:C:57:ASP:OD1	2:C:59:THR:HG21	2.07	0.53
2:C:45:LEU:O	2:C:49:GLU:HG3	2.08	0.53
1:K:74:ARG:NH1	2:L:41:ASN:HD22	2.06	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
3:S:297:GLU:OE1	3:S:298:ASN:OD1	2.25	0.53
3:S:229:PRO:CD	3:S:232:LEU:HD22	2.36	0.53
1:H:15:GLU:OE2	1:H:66:TYR:OH	2.25	0.53
2:I:161:MET:HE1	2:I:162:LYS:HZ3	1.73	0.53
1:K:27:ILE:HD11	1:K:113:GLN:CB	2.35	0.53
1:B:11:ARG:NH2	1:B:67:PRO:HG3	2.23	0.53
3:T:269:ASN:O	3:T:273:ARG:N	2.40	0.53
1:K:59:GLU:HB3	1:K:76:MET:HE1	1.87	0.53
2:I:132:ILE:O	2:I:136:ALA:N	2.41	0.53
2:F:81:GLY:CA	2:F:87:TYR:O	2.53	0.53
3:V:231:TYR:CD1	3:V:232:LEU:N	2.76	0.53
1:H:65:GLU:HG3	1:H:69:ALA:H	1.73	0.53
2:I:92:TYR:CZ	2:I:115:ILE:HD12	2.43	0.53
1:E:38:TYR:HE1	1:E:40:HIS:CE1	2.26	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
1:B:127:ASN:HD21	1:B:130:ALA:H	1.57	0.53
3:T:254:ASP:O	3:T:258:ILE:HG22	2.07	0.53
2:C:78:MET:CB	2:C:78:MET:CE	2.87	0.53
1:H:138:ALA:HA	1:H:141:ILE:HG13	1.91	0.53
2:F:160:ASN:HB3	2:F:163:LEU:HD12	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:GLU:HG3	1:H:65:GLU:N	2.22	0.53
1:E:81:HIS:CD2	1:E:83:ASN:H	2.21	0.53
2:L:143:SER:O	2:L:144:ILE:C	2.44	0.53
2:I:63:GLY:O	2:I:75:TRP:CE3	2.61	0.53
2:I:110:ARG:HB2	2:I:126:VAL:HA	1.91	0.53
1:B:154:ASN:HB2	1:B:156:ILE:CD1	2.38	0.53
2:L:66:ASP:O	2:L:69:ASP:HB3	2.09	0.53
3:T:303:ASP:CG	3:T:304:TYR:N	2.62	0.52
1:H:83:ASN:H	1:H:83:ASN:ND2	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
2:C:174:ASN:HB2	4:F:2002:HOH:O	2.09	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:62:LEU:O	1:B:63:PRO:C	2.41	0.52
2:C:80:LEU:CD1	2:C:80:LEU:N	2.72	0.52
1:H:65:GLU:O	1:H:68:MET:HB2	2.09	0.52
2:C:132:ILE:HD12	2:C:135:LEU:HB2	1.90	0.52
1:K:28:LYS:O	1:K:41:VAL:CG1	2.56	0.52
3:V:236:ILE:O	3:V:237:SER:C	2.48	0.52
1:K:145:ARG:HG2	1:K:149:ARG:NH1	2.25	0.52
1:E:89:ARG:HD3	2:F:45:LEU:CD2	2.39	0.52
3:T:287:MET:O	3:T:288:LYS:C	2.48	0.52
2:I:87:TYR:HD2	2:I:92:TYR:HH	1.57	0.52
1:K:59:GLU:HB3	1:K:76:MET:HE2	1.90	0.52
2:F:162:LYS:O	2:F:163:LEU:C	2.47	0.52
2:F:62:TRP:CH2	2:F:145:LYS:HB2	2.45	0.52
1:K:49:SER:O	1:K:50:PRO:C	2.47	0.52
1:K:51:PHE:CD2	1:K:79:ILE:HD11	2.45	0.52
1:E:70:ALA:HA	1:E:99:TRP:CE2	2.44	0.52
1:B:79:ILE:HG13	1:B:80:TYR:N	2.24	0.52
1:K:13:ILE:HG22	1:K:17:GLN:HE21	1.74	0.52
1:B:98:LYS:HD3	1:B:98:LYS:N	2.25	0.52
1:K:97:ASP:C	1:K:99:TRP:H	2.13	0.52
1:H:65:GLU:OE1	3:T:264:ARG:NH2	2.43	0.52
1:H:50:PRO:CB	1:H:141:ILE:HG23	2.39	0.52
3:U:286:ALA:O	3:U:290:VAL:HG23	2.10	0.52
2:I:152:ARG:CG	2:I:152:ARG:NE	2.70	0.52
2:C:51:GLY:HA2	2:C:62:TRP:CZ2	2.45	0.52
2:L:161:MET:HE2	2:L:162:LYS:NZ	2.25	0.52
1:H:128:ASP:CG	1:H:129:VAL:N	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:118:ASN:H	2:F:160:ASN:HD22	1.58	0.52
2:L:37:LYS:HE3	2:L:104:GLU:OE2	2.09	0.52
1:K:37:ARG:CG	1:K:62:LEU:HB2	2.38	0.52
3:V:243:GLU:OE1	3:V:256:LYS:HE3	2.09	0.52
3:S:254:ASP:O	3:S:255:ARG:C	2.46	0.52
1:E:94:ILE:CD1	1:E:94:ILE:CG2	2.87	0.52
1:E:149:ARG:CZ	1:E:149:ARG:CG	2.87	0.52
2:L:84:ARG:CD	2:L:84:ARG:CB	2.82	0.52
2:F:166:PRO:O	2:F:167:PRO:O	2.27	0.52
1:E:29:ALA:O	1:E:30:GLU:HG3	2.10	0.52
1:H:97:ASP:OD2	1:H:97:ASP:N	2.40	0.52
3:T:287:MET:C	3:T:289:GLU:N	2.63	0.52
2:C:156:MET:O	2:C:157:SER:C	2.45	0.52
2:I:79:ILE:HD13	2:I:151:LEU:O	2.10	0.52
2:C:144:ILE:O	2:C:145:LYS:C	2.46	0.52
2:I:67:ASP:O	2:I:68:GLU:HG3	2.10	0.52
3:U:246:ILE:HA	3:U:251:ILE:O	2.10	0.52
3:T:247:THR:O	3:T:248:PRO:C	2.47	0.52
1:E:29:ALA:O	1:E:30:GLU:CG	2.58	0.52
3:U:228:ILE:N	3:U:228:ILE:CG2	2.72	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:251:ILE:HG22	3:U:253:TYR:CZ	2.45	0.52
1:H:77:THR:C	2:I:70:MET:HE1	2.31	0.52
1:H:10:ARG:O	1:H:11:ARG:C	2.46	0.52
2:F:96:ILE:HG22	2:F:97:GLU:N	2.23	0.52
1:K:103:LEU:HD22	1:K:107:THR:HG21	1.92	0.51
2:C:50:GLU:OE1	2:C:145:LYS:HE2	2.10	0.51
1:K:82:PRO:CD	1:K:83:ASN:N	2.68	0.51
3:U:261:HIS:CD2	3:U:261:HIS:C	2.83	0.51
1:B:38:TYR:CE1	1:B:40:HIS:CE1	2.87	0.51
1:H:20:LEU:HD21	1:H:31:PRO:HD2	1.91	0.51
1:B:24:VAL:CG1	1:B:25:PRO:CD	2.88	0.51
3:V:282:ILE:HG22	3:V:283:PRO:O	2.10	0.51
2:I:43:ARG:NH1	2:I:140:ASN:O	2.42	0.51
2:C:49:GLU:C	2:C:51:GLY:N	2.60	0.51
2:F:167:PRO:CB	2:F:170:GLN:NE2	2.72	0.51
3:S:297:GLU:OE1	3:S:298:ASN:CG	2.49	0.51
2:I:87:TYR:HD1	2:I:155:MET:HB3	1.75	0.51
3:U:247:THR:HG21	3:U:269:ASN:ND2	2.26	0.51
3:S:257:ASP:C	3:S:259:GLU:N	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:39:PHE:N	1:K:60:LEU:O	2.42	0.51
1:K:81:HIS:HD2	1:K:83:ASN:CB	2.21	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:B:24:VAL:HG13	1:B:25:PRO:CD	2.41	0.51
1:K:61:PHE:CZ	2:L:38:VAL:HA	2.45	0.51
3:U:227:ASP:CA	3:U:228:ILE:HG23	2.39	0.51
2:I:85:THR:HA	2:I:161:MET:HB2	1.93	0.51
1:K:58:LEU:CD2	1:K:58:LEU:H	2.23	0.51
2:I:60:VAL:CG1	2:I:61:SER:N	2.71	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:L:116:ASN:O	2:L:117:MET:HB2	2.10	0.51
2:L:50:GLU:OE1	2:L:145:LYS:CE	2.58	0.51
3:U:234:GLY:C	3:U:237:SER:H	2.14	0.51
2:L:115:ILE:CG1	2:L:115:ILE:O	2.43	0.51
1:E:24:VAL:HG12	1:E:25:PRO:N	2.23	0.51
1:E:79:ILE:HG13	1:E:80:TYR:N	2.25	0.51
1:E:122:ASP:O	1:E:122:ASP:OD1	2.28	0.51
2:C:127:VAL:CG1	2:C:128:ASP:N	2.74	0.51
1:K:56:PHE:CE1	1:K:79:ILE:HD11	2.46	0.51
1:H:142:GLU:O	1:H:143:THR:C	2.48	0.51
2:L:113:THR:HG22	2:L:114:LYS:O	2.11	0.51
2:I:55:VAL:C	2:I:57:ASP:N	2.61	0.51
2:I:102:TYR:CG	2:I:103:PRO:HA	2.46	0.51
1:E:57:LYS:C	1:E:58:LEU:HD12	2.32	0.51
3:T:289:GLU:O	3:T:290:VAL:C	2.50	0.51
1:H:142:GLU:HG2	1:H:145:ARG:NH1	2.26	0.51
1:B:149:ARG:HA	1:B:153:MET:HG3	1.91	0.51
3:S:268:PHE:HD1	3:S:273:ARG:HA	1.75	0.51
1:E:127:ASN:HD21	1:E:130:ALA:H	1.57	0.51
2:L:62:TRP:CH2	2:L:145:LYS:HB2	2.46	0.50
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: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
3:V:284:ASN:CG	3:V:287:MET:HB2	2.32	0.50
3:V:258:ILE:CG1	3:V:258:ILE:O	2.59	0.50
3:T:300:TRP:O	3:T:301:VAL:O	2.29	0.50
2:I:162:LYS:O	2:I:163:LEU:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:37:LYS:CB	2:L:37:LYS:NZ	2.70	0.50
1:B:24:VAL:CG1	1:B:25:PRO:HD2	2.40	0.50
1:K:104:GLN:HG3	1:K:106:ARG:N	2.26	0.50
3:S:293:ALA:O	3:S:294:PHE:C	2.49	0.50
2:I:42:PHE:HA	2:I:45:LEU:HB2	1.94	0.50
1:E:79:ILE:CG2	1:E:84:VAL:HG11	2.42	0.50
2:I:55:VAL:O	2:I:56:GLY:C	2.43	0.50
1:B:65:GLU:O	1:B:68:MET:N	2.44	0.50
3:S:268:PHE:O	3:S:270:PRO:HD3	2.11	0.50
2:L:55:VAL:HG13	2:L:56:GLY:N	2.26	0.50
1:K:74:ARG:HG3	1:K:75:PHE:O	2.10	0.50
1:K:97:ASP:C	1:K:99:TRP:N	2.61	0.50
1:K:29:ALA:CB	1:K:41:VAL:HG13	2.35	0.50
1:H:132:GLN:O	1:H:133:TRP:C	2.49	0.50
3:U:284:ASN:O	3:U:287:MET:HB2	2.12	0.50
2:I:69:ASP:O	2:I:70:MET:C	2.46	0.50
1:B:50:PRO:HB3	1:B:141:ILE:HG23	1.94	0.50
3:U:230:ASP:C	3:U:232:LEU:N	2.63	0.50
1:B:135:THR:HG22	1:B:136:ASN:HB2	1.94	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
1:B:151:TYR:CD1	1:B:151:TYR:N	2.74	0.50
1:H:12:ILE:HD13	1:H:62:LEU:CD1	2.40	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
3:S:253:TYR:CD1	3:S:258:ILE:HD13	2.47	0.50
2:I:118:ASN:HD22	2:I:160:ASN:ND2	2.10	0.50
1:K:139:GLN:O	1:K:141:ILE:N	2.45	0.49
1:K:49:SER:HB3	1:K:117:SER:HB3	1.93	0.49
3:T:294:PHE:CD2	3:T:294:PHE:C	2.85	0.49
2:F:61:SER:O	2:F:62:TRP:HB3	2.12	0.49
2:I:81:GLY:HA3	2:I:87:TYR:O	2.12	0.49
1:K:29:ALA:HA	1:K:41:VAL:HA	1.94	0.49
3:U:287:MET:CE	3:V:286:ALA:C	2.78	0.49
2:I:143:SER:H	2:I:146:VAL:HB	1.76	0.49
2:F:166:PRO:O	2:F:167:PRO:C	2.50	0.49
1:K:48:ASP:N	1:K:48:ASP:OD1	2.45	0.49
1:H:141:ILE:O	1:H:142:GLU:C	2.48	0.49
1:K:81:HIS:CD2	1:K:83:ASN:CB	2.79	0.49
3:V:236:ILE:HG22	3:V:237:SER:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:272:THR:O	3:S:274:SER:N	2.46	0.49
1:B:123:ASP:HB2	1:B:124:PRO:C	2.33	0.49
1:H:53:GLY:CA	1:H:153:MET:CE	2.87	0.49
1:K:130:ALA:O	1:K:131:GLU:O	2.30	0.49
1:K:82:PRO:HB3	1:K:130:ALA:CA	2.42	0.49
2:L:106:PRO:HB3	2:L:135:LEU:HD23	1.95	0.49
1:K:82:PRO:HD2	1:K:83:ASN:H	1.73	0.49
2:F:128:ASP:OD1	2:F:129:PRO:N	2.45	0.49
3:S:256:LYS:CB	3:S:256:LYS:CD	2.81	0.49
2:C:167:PRO:O	2:C:168:GLU:C	2.51	0.49
1:B:121:PRO:O	1:B:130:ALA:HB1	2.12	0.49
1:E:130:ALA:O	1:E:131:GLU:C	2.49	0.49
1:E:14:LYS:HE2	3:U:238:PHE:O	2.13	0.49
2:F:61:SER:HB3	2:F:78:MET:HB3	1.95	0.49
1:E:66:TYR:CD1	1:E:67:PRO:HA	2.47	0.49
1:K:94:ILE:HA	1:K:98:LYS:O	2.12	0.49
1:H:14:LYS:HZ1	3:T:228:ILE:HD12	1.77	0.49
1:H:135:THR:C	1:H:136:ASN:OD1	2.51	0.49
1:B:8:LEU:HD12	1:B:9:PRO:CD	2.43	0.49
3:T:258:ILE:HG13	3:T:258:ILE:O	2.13	0.49
2:C:54:GLY:O	2:C:55:VAL:HB	2.13	0.49
3:S:297:GLU:O	3:S:297:GLU:OE1	2.31	0.49
3:T:236:ILE:O	3:T:236:ILE:HG22	2.07	0.49
1:K:78:LYS:HZ2	1:K:147:TRP:HH2	1.49	0.49
2:C:145:LYS:O	2:C:149:GLN:HG3	2.12	0.49
3:V:290:VAL:O	3:V:291:ILE:C	2.52	0.49
2:I:43:ARG:HH21	2:I:143:SER:HB3	1.74	0.49
1:K:9:PRO:HB2	1:K:12:ILE:HD12	1.95	0.49
2:F:145:LYS:O	2:F:146:VAL:C	2.49	0.49
2:F:73:THR:CG2	2:F:73:THR:O	2.60	0.49
1:K:95:LEU:HD21	1:K:108:VAL:HG13	1.95	0.49
1:H:93:ASP:C	1:H:95:LEU:H	2.15	0.49
3:U:261:HIS:O	3:U:261:HIS:CD2	2.66	0.49
1:E:122:ASP:O	1:E:122:ASP:CG	2.51	0.49
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:K:32:ASP:OD2	1:K:32:ASP:C	2.50	0.48
2:C:99:GLY:HA3	2:F:174:ASN:HD22	1.78	0.48
1:K:103:LEU:CD2	1:K:107:THR:HG21	2.43	0.48
2:F:37:LYS:N	2:F:37:LYS:HZ3	2.10	0.48
1:E:70:ALA:HB1	1:E:71:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:81:GLY:H	2:F:90:ARG:H	1.60	0.48
1:E:28:LYS:HG3	1:E:29:ALA:H	1.77	0.48
3:U:284:ASN:HD21	3:V:284:ASN:ND2	2.06	0.48
1:E:72:LYS:HB3	2:F:42:PHE:CE1	2.49	0.48
3:T:241:MET:HE3	3:T:253:TYR:CA	2.42	0.48
2:L:61:SER:HB3	2:L:78:MET:CG	2.43	0.48
1:K:53:GLY:HA2	1:K:153:MET:CE	2.44	0.48
3:T:303:ASP:CG	3:T:304:TYR:H	2.16	0.48
2:L:49:GLU:O	2:L:50:GLU:C	2.51	0.48
3:S:256:LYS:CE	3:S:256:LYS:CG	2.83	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:T:262:LEU:HD23	3:T:267:HIS:HA	1.96	0.48
1:K:58:LEU:HD13	1:K:75:PHE:CE2	2.49	0.48
3:U:277:THR:HG23	3:U:280:GLN:NE2	2.28	0.48
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
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
3:S:288:LYS:O	3:S:292:ASP:HB2	2.13	0.48
1:H:18:ARG:HG2	1:H:18:ARG:HH11	1.78	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:H:102:ALA:HB2	3:T:270:PRO:HB3	1.93	0.48
2:F:61:SER:CB	2:F:78:MET:HB3	2.44	0.48
3:U:295:ILE:CA	3:U:295:ILE:CG1	2.81	0.48
2:I:161:MET:HE3	2:I:162:LYS:NZ	2.29	0.48
1:K:128:ASP:O	1:K:129:VAL:C	2.52	0.48
1:B:74:ARG:CG	1:B:75:PHE:N	2.73	0.48
3:U:231:TYR:CD1	3:U:232:LEU:HD22	2.48	0.48
1:K:53:GLY:HA2	1:K:153:MET:HE3	1.95	0.48
1:H:22:GLU:O	1:H:22:GLU:HG2	2.13	0.48
3:T:243:GLU:N	3:T:244:PRO:HD3	2.29	0.48
2:C:45:LEU:O	2:C:46:GLU:C	2.48	0.48
1:B:127:ASN:ND2	1:B:129:VAL:H	2.12	0.48
2:I:171:CYS:O	2:I:171:CYS:SG	2.71	0.48
1:H:35:ASN:HB3	1:H:38:TYR:HB3	1.96	0.48
2:C:174:ASN:OXT	2:F:100:PRO:HG2	2.13	0.48
2:I:95:LYS:HD2	2:I:112:VAL:CG2	2.43	0.48
1:H:116:LEU:HD23	1:H:116:LEU:HA	1.49	0.48
1:H:84:VAL:CG1	1:H:88:GLY:HA2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:153:ARG:O	2:L:156:MET:N	2.35	0.48
1:H:92:LEU:HB3	1:H:95:LEU:HD12	1.96	0.48
3:T:241:MET:CE	3:T:253:TYR:C	2.81	0.48
1:K:120:ASN:OD1	1:K:122:ASP:HB2	2.13	0.48
1:B:136:ASN:C	1:B:136:ASN:HD22	2.05	0.48
1:E:39:PHE:CD1	1:E:39:PHE:N	2.82	0.48
1:E:96:LYS:O	1:E:97:ASP:C	2.52	0.47
1:K:82:PRO:HD2	1:K:83:ASN:N	2.29	0.47
3:U:248:PRO:HA	3:V:282:ILE:HG13	1.95	0.47
2:L:37:LYS:HE3	2:L:104:GLU:CD	2.34	0.47
2:C:81:GLY:HA3	2:C:87:TYR:O	2.14	0.47
2:F:96:ILE:CG2	2:F:97:GLU:N	2.77	0.47
1:K:75:PHE:HB2	1:K:88:GLY:CA	2.43	0.47
2:I:132:ILE:O	2:I:135:LEU:HB2	2.14	0.47
1:K:145:ARG:HG2	1:K:149:ARG:HH12	1.79	0.47
2:C:145:LYS:CD	2:C:145:LYS:NZ	2.71	0.47
2:I:40:ARG:HG2	2:I:44:LEU:HD12	1.96	0.47
1:H:6:ALA:N	1:H:8:LEU:HD23	2.29	0.47
1:H:64:GLU:HB3	2:I:36:VAL:HG21	1.96	0.47
2:C:153:ARG:CB	2:C:153:ARG:CD	2.86	0.47
2:C:129:PRO:HG2	2:C:130:ARG:H	1.78	0.47
3:V:267:HIS:HB3	3:V:276:LEU:O	2.14	0.47
3:S:295:ILE:HG22	3:S:296:SER:N	2.29	0.47
1:B:111:SER:O	1:B:114:ALA:N	2.44	0.47
1:E:127:ASN:ND2	1:E:129:VAL:H	2.11	0.47
3:T:282:ILE:HG22	3:T:283:PRO:O	2.13	0.47
2:L:86:ILE:O	2:L:86:ILE:HG12	2.14	0.47
1:B:134:LYS:CG	1:B:134:LYS:HZ3	2.24	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:B:74:ARG:HG3	1:B:75:PHE:N	2.29	0.47
1:E:94:ILE:CG2	1:E:94:ILE:CA	2.81	0.47
2:L:40:ARG:HD2	2:L:102:TYR:H	1.78	0.47
3:V:259:GLU:O	3:V:262:LEU:HB2	2.14	0.47
3:U:290:VAL:HG11	3:V:290:VAL:HG11	1.95	0.47
3:S:257:ASP:O	3:S:258:ILE:C	2.50	0.47
1:B:127:ASN:ND2	1:B:127:ASN:C	2.67	0.47
1:K:74:ARG:HH12	2:L:41:ASN:HD22	1.61	0.47
1:K:46:PRO:CD	1:K:116:LEU:CD1	2.83	0.47
1:B:131:GLU:OE1	1:B:131:GLU:HA	2.15	0.47
1:K:24:VAL:HG11	1:K:27:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:MET:HE1	3:S:265:VAL:CG2	2.44	0.47
1:B:52:GLU:O	1:B:54:GLY:N	2.47	0.47
1:K:120:ASN:CG	1:K:120:ASN:O	2.53	0.47
1:H:155:ASN:N	1:H:155:ASN:OD1	2.48	0.47
1:B:107:THR:HB	1:B:108:VAL:H	1.45	0.47
2:I:115:ILE:CG2	2:I:120:VAL:HG11	2.45	0.47
2:I:82:PRO:HB3	2:I:85:THR:CG2	2.38	0.47
1:H:145:ARG:O	1:H:146:ALA:C	2.53	0.47
3:U:277:THR:HG23	3:U:280:GLN:HE21	1.79	0.47
2:L:126:VAL:CG1	2:L:127:VAL:H	2.28	0.47
3:T:241:MET:HE2	3:T:253:TYR:CA	2.44	0.47
2:C:161:MET:HE3	2:C:161:MET:HB3	1.75	0.47
2:C:48:LEU:HD12	2:C:48:LEU:HA	1.69	0.47
3:S:237:SER:O	3:S:238:PHE:CB	2.52	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
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
3:U:235:LYS:O	3:U:238:PHE:HE1	1.97	0.47
2:L:80:LEU:CD1	2:L:80:LEU:N	2.78	0.47
3:U:284:ASN:ND2	3:V:284:ASN:ND2	2.63	0.46
3:S:258:ILE:HD12	3:S:258:ILE:HA	1.62	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
3:U:287:MET:HE2	3:V:287:MET:SD	2.55	0.46
3:U:242:ARG:O	3:U:243:GLU:CB	2.63	0.46
3:T:236:ILE:HB	4:T:2002:HOH:O	2.15	0.46
2:L:106:PRO:HB3	2:L:135:LEU:CD2	2.45	0.46
1:K:156:ILE:CB	1:K:156:ILE:C	2.75	0.46
1:B:130:ALA:O	1:B:131:GLU:O	2.33	0.46
1:K:77:THR:HG23	1:K:151:TYR:O	2.15	0.46
2:C:53:LYS:NZ	2:C:53:LYS:CD	2.73	0.46
3:S:258:ILE:CG2	3:S:259:GLU:N	2.76	0.46
3:V:234:GLY:C	3:V:236:ILE:N	2.68	0.46
3:T:234:GLY:HA3	3:T:237:SER:H	1.81	0.46
2:C:86:ILE:HB	2:C:161:MET:O	2.15	0.46
2:C:83:PRO:HB2	2:C:84:ARG:HG2	1.98	0.46
1:K:74:ARG:HB2	1:K:88:GLY:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:131:GLU:O	1:H:134:LYS:HG2	2.15	0.46
1:E:127:ASN:ND2	1:E:127:ASN:C	2.66	0.46
1:H:78:LYS:HB3	1:H:78:LYS:HE2	1.40	0.46
1:H:65:GLU:HB2	3:T:264:ARG:HH22	1.81	0.46
2:I:114:LYS:HA	2:I:172:TYR:CE1	2.51	0.46
2:F:137:LYS:O	2:F:138:TRP:C	2.53	0.46
1:H:128:ASP:C	1:H:130:ALA:N	2.68	0.46
1:B:87:LEU:C	2:C:70:MET:CE	2.84	0.46
1:B:41:VAL:HB	1:B:58:LEU:HB2	1.96	0.46
1:K:13:ILE:O	1:K:17:GLN:HB2	2.16	0.46
2:I:96:ILE:HG23	2:I:109:VAL:HG22	1.96	0.46
2:L:83:PRO:HA	2:L:88:GLU:HB3	1.97	0.46
3:T:235:LYS:HD2	3:T:235:LYS:HA	1.46	0.46
1:H:65:GLU:HG3	1:H:65:GLU:O	2.16	0.46
2:L:81:GLY:HA2	2:L:82:PRO:HD2	1.66	0.46
3:V:247:THR:CG2	3:V:269:ASN:ND2	2.78	0.46
2:C:97:GLU:HB3	2:C:108:PHE:HB2	1.97	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
3:T:303:ASP:OD1	3:T:304:TYR:N	2.44	0.46
1:H:81:HIS:CE1	1:H:116:LEU:HA	2.49	0.46
1:E:38:TYR:CE1	1:E:40:HIS:CE1	3.03	0.46
2:I:113:THR:HA	2:I:171:CYS:CB	2.45	0.46
2:C:165:GLN:CB	2:C:166:PRO:HD2	2.34	0.46
2:F:142:TYR:CD2	2:F:142:TYR:N	2.83	0.46
1:E:108:VAL:O	1:E:109:LEU:C	2.52	0.46
1:K:68:MET:CE	3:V:265:VAL:CG2	2.90	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:I:140:ASN:N	2:I:140:ASN:ND2	2.62	0.46
1:E:43:ILE:CG2	1:E:44:ALA:N	2.79	0.46
3:S:271:VAL:O	3:S:271:VAL:CG1	2.64	0.45
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
2:I:88:GLU:O	2:I:89:ASN:O	2.34	0.45
2:L:37:LYS:HB2	2:L:37:LYS:HZ3	1.81	0.45
1:B:97:ASP:N	1:B:97:ASP:OD1	2.48	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
2:F:168:GLU:O	2:F:169:GLY:C	2.54	0.45
1:B:4:GLY:O	1:B:5:SER:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:F:165:GLN:HB3	2:F:166:PRO:CD	2.47	0.45
2:C:80:LEU:O	2:C:81:GLY:C	2.55	0.45
1:H:24:VAL:CG1	1:H:25:PRO:HD2	2.46	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
3:T:298:ASN:ND2	3:T:300:TRP:CE3	2.85	0.45
3:T:291:ILE:O	3:T:292:ASP:C	2.55	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
1:E:29:ALA:C	1:E:30:GLU:CG	2.84	0.45
2:F:50:GLU:HG3	2:F:62:TRP:HZ2	1.81	0.45
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.71	0.45
1:H:81:HIS:HA	1:H:82:PRO:HD3	1.73	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:E:149:ARG:HG2	1:E:149:ARG:NH1	2.09	0.45
3:T:287:MET:C	3:T:289:GLU:H	2.20	0.45
3:V:235:LYS:CD	3:V:235:LYS:NZ	2.75	0.45
3:V:245:CYS:CB	3:V:283:PRO:HA	2.45	0.45
1:B:51:PHE:CE2	1:B:79:ILE:HD11	2.52	0.45
2:F:50:GLU:O	2:F:51:GLY:C	2.55	0.45
2:I:78:MET:C	2:I:78:MET:SD	2.94	0.45
1:K:73:VAL:O	1:K:74:ARG:CB	2.63	0.45
2:F:80:LEU:HD13	2:F:80:LEU:HA	1.36	0.45
1:B:96:LYS:CB	1:B:97:ASP:OD1	2.64	0.45
1:H:85:ASP:O	1:H:86:LYS:C	2.55	0.45
2:I:73:THR:HG22	2:I:74:ARG:HG2	1.99	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:V:237:SER:OG	3:V:239:GLU:HG2	2.17	0.45
1:B:98:LYS:HD2	1:B:98:LYS:HA	1.62	0.45
3:T:254:ASP:OD1	3:T:255:ARG:N	2.49	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
1:H:32:ASP:HB2	1:H:40:HIS:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:VAL:HG11	1:E:112:ILE:HD11	1.99	0.45
3:T:234:GLY:C	3:T:236:ILE:H	2.20	0.45
1:K:80:TYR:CB	1:K:144:ALA:HA	2.46	0.44
1:K:78:LYS:HG2	1:K:147:TRP:CZ3	2.53	0.44
1:K:68:MET:CE	3:V:261:HIS:HA	2.47	0.44
1:H:49:SER:O	1:H:50:PRO:C	2.55	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
1:H:109:LEU:HA	1:H:109:LEU:HD23	1.54	0.44
2:L:79:ILE:HG21	2:L:155:MET:CE	2.47	0.44
1:K:109:LEU:CD2	1:K:109:LEU:H	2.27	0.44
3:S:231:TYR:CD1	3:S:232:LEU:CD1	3.01	0.44
3:V:231:TYR:C	3:V:231:TYR:CD1	2.88	0.44
3:U:285:LEU:HB2	4:V:2003:HOH:O	2.16	0.44
1:H:78:LYS:HE2	1:H:147:TRP:CZ3	2.52	0.44
3:U:293:ALA:HB3	3:U:294:PHE:H	1.37	0.44
2:C:75:TRP:CD1	2:C:75:TRP:N	2.85	0.44
1:K:49:SER:CB	1:K:117:SER:HB3	2.48	0.44
1:E:15:GLU:C	1:E:17:GLN:N	2.65	0.44
2:C:44:LEU:HA	2:C:44:LEU:HD23	1.78	0.44
3:U:257:ASP:N	3:U:257:ASP:OD2	2.49	0.44
2:I:156:MET:O	2:I:157:SER:C	2.56	0.44
1:H:82:PRO:HD2	1:H:83:ASN:HD21	1.83	0.44
1:B:118:ALA:N	1:B:119:PRO:HD3	2.32	0.44
3:U:236:ILE:CG2	3:U:236:ILE:O	2.65	0.44
2:L:147:VAL:O	2:L:148:LEU:C	2.52	0.44
1:E:51:PHE:H	1:E:51:PHE:HD1	1.64	0.44
1:K:87:LEU:HD23	1:K:87:LEU:HA	1.71	0.44
1:H:115:LEU:HD12	1:H:115:LEU:HA	1.62	0.44
2:I:163:LEU:HA	2:I:164:PRO:HD2	1.74	0.44
2:I:82:PRO:HA	2:I:83:PRO:HD3	1.70	0.44
3:S:247:THR:CG2	3:S:251:ILE:HB	2.47	0.44
2:I:144:ILE:CG2	2:I:148:LEU:HD12	2.47	0.44
3:V:236:ILE:O	3:V:238:PHE:CD1	2.70	0.44
2:C:143:SER:O	2:C:146:VAL:N	2.50	0.44
3:V:241:MET:HE2	3:V:241:MET:HB2	1.63	0.44
1:E:123:ASP:H	1:E:124:PRO:CA	2.31	0.44
1:E:106:ARG:HD3	1:E:106:ARG:HH11	1.41	0.44
1:H:44:ALA:O	1:H:46:PRO:HD3	2.18	0.44
1:K:58:LEU:N	1:K:58:LEU:HD22	2.32	0.44
2:I:56:GLY:O	2:I:58:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:290:VAL:O	3:U:291:ILE:C	2.56	0.44
3:S:229:PRO:CG	3:S:232:LEU:HD22	2.47	0.44
2:C:174:ASN:O	2:F:101:LYS:N	2.51	0.44
2:L:55:VAL:CG1	2:L:56:GLY:N	2.76	0.43
1:B:29:ALA:O	1:B:30:GLU:HG3	2.17	0.43
1:E:24:VAL:CG1	1:E:25:PRO:CD	2.96	0.43
2:L:98:CYS:O	2:L:99:GLY:O	2.35	0.43
1:K:80:TYR:HB2	1:K:147:TRP:CD2	2.53	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:K:37:ARG:HG2	1:K:62:LEU:O	2.18	0.43
2:F:62:TRP:CZ3	2:F:145:LYS:HB2	2.53	0.43
1:K:123:ASP:HB2	1:K:124:PRO:O	2.18	0.43
2:I:88:GLU:O	2:I:89:ASN:C	2.56	0.43
2:I:135:LEU:HD23	2:I:135:LEU:HA	1.48	0.43
3:V:284:ASN:OD1	3:V:287:MET:HB2	2.18	0.43
2:I:168:GLU:HG2	2:I:169:GLY:N	2.33	0.43
1:E:12:ILE:HD11	1:E:66:TYR:HD2	1.82	0.43
3:V:268:PHE:N	3:V:268:PHE:CD2	2.86	0.43
1:H:117:SER:O	1:H:119:PRO:CD	2.66	0.43
3:U:266:GLY:HA3	3:U:268:PHE:CD2	2.54	0.43
3:U:284:ASN:OD1	3:U:284:ASN:C	2.56	0.43
2:I:113:THR:HA	2:I:171:CYS:HB2	2.00	0.43
1:H:32:ASP:CB	1:H:40:HIS:HE2	2.26	0.43
1:E:60:LEU:HG	1:E:73:VAL:HG21	2.00	0.43
1:K:12:ILE:O	1:K:13:ILE:C	2.56	0.43
1:K:150:LEU:HB3	1:K:151:TYR:CD1	2.54	0.43
1:H:18:ARG:CG	1:H:18:ARG:HH11	2.32	0.43
1:K:105:ILE:O	1:K:106:ARG:C	2.56	0.43
2:I:151:LEU:O	2:I:152:ARG:HB2	2.18	0.43
2:I:130:ARG:CG	2:I:130:ARG:HH11	2.30	0.43
1:H:95:LEU:HA	1:H:95:LEU:HD23	1.48	0.43
2:I:114:LYS:H	2:I:171:CYS:CB	2.32	0.43
1:B:154:ASN:CA	1:B:156:ILE:HG12	2.49	0.43
2:I:47:GLU:O	2:I:48:LEU:C	2.53	0.43
1:B:136:ASN:C	1:B:136:ASN:ND2	2.65	0.43
1:E:92:LEU:HD12	1:E:95:LEU:CD1	2.48	0.43
1:K:50:PRO:HG2	1:K:51:PHE:CE1	2.54	0.43
3:T:298:ASN:ND2	3:T:298:ASN:C	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:18:ARG:O	1:E:22:GLU:N	2.51	0.43
1:E:78:LYS:NZ	2:F:68:GLU:HB3	2.33	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
2:F:56:GLY:C	2:F:57:ASP:O	2.56	0.43
2:I:102:TYR:CD2	2:I:102:TYR:C	2.90	0.43
3:V:237:SER:CB	3:V:257:ASP:OD2	2.67	0.43
1:B:21:ALA:C	1:B:23:PRO:HD3	2.38	0.43
1:K:142:GLU:CB	1:K:142:GLU:CD	2.80	0.43
1:H:14:LYS:O	1:H:18:ARG:HD3	2.18	0.43
2:C:149:GLN:HG3	2:C:149:GLN:H	1.54	0.43
3:V:245:CYS:O	3:V:245:CYS:SG	2.76	0.43
2:I:142:TYR:O	2:I:143:SER:HB3	2.17	0.43
1:E:24:VAL:HG12	1:E:25:PRO:O	2.18	0.43
3:S:275:PRO:O	3:S:276:LEU:HB2	2.19	0.43
2:L:157:SER:C	2:L:159:GLU:N	2.71	0.43
1:H:47:GLN:O	1:H:48:ASP:HB2	2.18	0.43
2:I:145:LYS:HG3	2:I:146:VAL:N	2.33	0.43
1:B:68:MET:CE	3:S:261:HIS:HA	2.47	0.43
1:H:22:GLU:HA	1:H:23:PRO:HD3	1.65	0.43
3:S:267:HIS:N	3:S:267:HIS:HD2	2.12	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
2:F:132:ILE:HD12	2:F:132:ILE:HG21	1.49	0.43
3:S:240:LEU:HD12	3:S:240:LEU:HA	1.86	0.43
3:T:263:GLN:HG2	3:T:263:GLN:H	1.61	0.43
3:T:288:LYS:CD	3:T:288:LYS:NZ	2.76	0.42
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
2:F:134:VAL:HB	2:F:150:GLU:HG3	2.01	0.42
1:B:97:ASP:C	1:B:99:TRP:N	2.72	0.42
1:B:18:ARG:O	1:B:22:GLU:N	2.50	0.42
3:U:260:GLU:O	3:U:261:HIS:C	2.56	0.42
3:U:290:VAL:O	3:U:293:ALA:HB3	2.18	0.42
3:U:289:GLU:OE1	3:V:231:TYR:HB2	2.19	0.42
1:K:148:THR:O	1:K:152:ALA:HB3	2.19	0.42
1:E:22:GLU:HA	1:E:23:PRO:HD3	1.64	0.42
1:E:115:LEU:O	1:E:116:LEU:C	2.57	0.42
2:L:93:SER:O	2:L:94:LEU:HG	2.19	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:B:85:ASP:OD1	1:B:85:ASP:C	2.57	0.42
1:E:94:ILE:CD1	1:E:94:ILE:HG21	2.49	0.42
2:C:167:PRO:HG3	2:C:170:GLN:OE1	2.19	0.42
2:I:83:PRO:CA	2:I:88:GLU:OE1	2.61	0.42
2:C:129:PRO:CG	2:C:130:ARG:N	2.81	0.42
2:L:132:ILE:CG1	2:L:132:ILE:O	2.52	0.42
3:U:242:ARG:HG3	3:U:242:ARG:NH1	2.23	0.42
1:E:132:GLN:O	1:E:133:TRP:C	2.58	0.42
3:U:264:ARG:HB3	3:U:264:ARG:HE	1.57	0.42
2:L:50:GLU:O	2:L:50:GLU:HG2	2.19	0.42
2:L:44:LEU:O	2:L:47:GLU:N	2.52	0.42
1:K:116:LEU:C	1:K:118:ALA:H	2.22	0.42
1:K:62:LEU:HD23	1:K:62:LEU:HA	1.46	0.42
2:F:82:PRO:O	2:F:88:GLU:HA	2.20	0.42
3:T:230:ASP:O	3:T:233:CYS:N	2.51	0.42
3:T:277:THR:HG22	3:T:278:GLN:CA	2.47	0.42
1:K:43:ILE:HD13	1:K:58:LEU:HD11	2.01	0.42
1:K:59:GLU:OE2	1:K:74:ARG:NH1	2.46	0.42
2:F:132:ILE:HG23	2:F:132:ILE:HD13	1.53	0.42
1:B:66:TYR:CG	1:B:67:PRO:HA	2.55	0.42
3:S:265:VAL:O	3:S:265:VAL:HG12	2.19	0.42
1:B:116:LEU:H	1:B:116:LEU:HD23	1.81	0.42
2:C:115:ILE:HG13	2:C:116:ASN:N	2.35	0.42
3:V:230:ASP:O	3:V:233:CYS:N	2.52	0.42
3:S:284:ASN:ND2	3:S:287:MET:HG3	2.34	0.42
1:K:54:GLY:HA3	1:K:152:ALA:CB	2.48	0.42
2:F:151:LEU:HD23	2:F:151:LEU:HA	1.90	0.42
1:H:91:CYS:HB2	1:H:96:LYS:HZ1	1.77	0.42
2:I:161:MET:HE3	2:I:162:LYS:HZ2	1.84	0.42
1:K:128:ASP:O	1:K:130:ALA:N	2.52	0.42
2:I:114:LYS:HD3	2:I:170:GLN:OE1	2.20	0.42
2:I:60:VAL:HG13	2:I:61:SER:N	2.35	0.42
3:V:232:LEU:C	3:V:241:MET:HE2	2.39	0.42
3:S:282:ILE:HG23	3:S:283:PRO:HD2	2.01	0.42
1:K:19:LEU:HD23	1:K:19:LEU:HA	1.36	0.42
2:L:113:THR:HG22	2:L:114:LYS:N	2.34	0.42
1:E:70:ALA:HB2	1:E:99:TRP:CD2	2.55	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
1:B:100:SER:HA	1:B:101:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:137:LYS:C	2:F:138:TRP:O	2.57	0.42
3:T:229:PRO:HD2	3:T:232:LEU:HD22	2.01	0.42
1:E:149:ARG:HG3	1:E:149:ARG:NH1	2.27	0.42
2:I:85:THR:O	2:I:88:GLU:HG3	2.20	0.42
2:C:165:GLN:HG2	2:C:165:GLN:H	1.55	0.42
1:B:11:ARG:HD3	1:B:67:PRO:HG3	2.02	0.42
1:K:72:LYS:HG2	1:K:72:LYS:HZ2	1.63	0.42
2:C:114:LYS:HZ2	2:C:170:GLN:HE21	1.67	0.42
1:B:134:LYS:CB	1:B:134:LYS:HZ3	2.33	0.42
2:F:124:ASN:N	2:F:124:ASN:OD1	2.53	0.42
1:H:54:GLY:HA3	1:H:148:THR:HG22	2.02	0.42
2:F:80:LEU:N	2:F:80:LEU:HD22	2.35	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
1:E:128:ASP:O	1:E:131:GLU:N	2.52	0.42
3:U:274:SER:HA	3:U:275:PRO:HD3	1.85	0.42
1:K:134:LYS:CD	1:K:134:LYS:C	2.88	0.42
1:K:105:ILE:HB	1:K:106:ARG:H	1.68	0.42
2:L:132:ILE:HD13	2:L:132:ILE:HG21	1.64	0.42
1:E:15:GLU:OE1	1:E:104:GLN:HB2	2.20	0.42
2:I:46:GLU:C	2:I:48:LEU:N	2.73	0.42
1:E:61:PHE:CE1	2:F:39:PRO:HD3	2.55	0.42
2:L:139:GLN:HB3	2:L:142:TYR:CE1	2.54	0.42
2:F:153:ARG:N	2:F:153:ARG:HD2	2.35	0.41
2:C:78:MET:HE3	2:C:78:MET:CG	2.48	0.41
2:C:132:ILE:HD12	2:C:132:ILE:HG23	1.95	0.41
3:V:262:LEU:HD23	3:V:266:GLY:O	2.20	0.41
2:I:167:PRO:HG2	2:I:170:GLN:NE2	2.34	0.41
3:S:287:MET:HE2	3:S:287:MET:HB3	1.18	0.41
3:S:282:ILE:HG22	3:S:283:PRO:N	2.35	0.41
2:L:54:GLY:O	2:L:55:VAL:CG2	2.68	0.41
2:I:161:MET:HE1	2:I:162:LYS:NZ	2.34	0.41
2:L:153:ARG:NH1	2:L:153:ARG:CB	2.83	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:F:129:PRO:C	2:F:131:ALA:N	2.72	0.41
3:U:238:PHE:N	3:U:238:PHE:CD1	2.88	0.41
2:I:73:THR:HG22	2:I:74:ARG:CG	2.50	0.41
2:C:53:LYS:HZ3	2:C:53:LYS:CG	2.30	0.41
2:F:120:VAL:O	2:F:121:ASN:C	2.57	0.41
1:H:93:ASP:O	1:H:95:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:61:SER:C	2:I:62:TRP:HE3	2.23	0.41
1:B:6:ALA:HB1	1:B:8:LEU:H	1.85	0.41
1:H:20:LEU:O	1:H:21:ALA:C	2.58	0.41
1:K:93:ASP:O	1:K:94:ILE:C	2.58	0.41
1:K:142:GLU:C	1:K:144:ALA:N	2.73	0.41
3:T:293:ALA:HB3	3:T:294:PHE:H	1.62	0.41
2:F:44:LEU:CD2	2:F:102:TYR:CE2	2.87	0.41
3:V:255:ARG:O	3:V:256:LYS:C	2.58	0.41
1:H:73:VAL:O	1:H:90:ILE:HD12	2.21	0.41
1:E:14:LYS:O	1:E:17:GLN:HB2	2.20	0.41
1:H:80:TYR:CZ	1:H:129:VAL:HG13	2.56	0.41
1:B:66:TYR:CD1	1:B:67:PRO:HA	2.55	0.41
1:K:66:TYR:CD1	1:K:67:PRO:HA	2.55	0.41
1:H:27:ILE:HD12	1:H:113:GLN:OE1	2.20	0.41
1:E:59:GLU:O	1:E:59:GLU:HG3	2.19	0.41
2:I:39:PRO:O	2:I:40:ARG:C	2.58	0.41
3:V:236:ILE:HG21	3:V:236:ILE:HD13	1.84	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:76:MET:HB2	1:K:76:MET:HE2	1.81	0.41
3:S:297:GLU:CA	3:S:297:GLU:OE1	2.68	0.41
3:T:253:TYR:CE2	3:T:270:PRO:HG2	2.56	0.41
2:L:58:GLY:O	2:L:59:THR:HB	2.20	0.41
3:V:278:GLN:O	3:V:279:GLU:C	2.58	0.41
2:I:86:ILE:HG13	2:I:86:ILE:O	2.20	0.41
1:K:92:LEU:HD23	1:K:92:LEU:HA	1.56	0.41
3:U:245:CYS:O	3:U:252:THR:HA	2.20	0.41
2:I:161:MET:HE3	2:I:162:LYS:HD2	2.03	0.41
2:C:49:GLU:O	2:C:50:GLU:C	2.55	0.41
1:H:50:PRO:HB3	1:H:141:ILE:HG23	2.02	0.41
3:U:261:HIS:ND1	3:U:270:PRO:HG3	2.35	0.41
1:E:35:ASN:ND2	1:E:35:ASN:C	2.72	0.41
2:F:83:PRO:HA	2:F:88:GLU:OE1	2.21	0.41
1:E:74:ARG:NH2	2:F:41:ASN:ND2	2.69	0.41
3:U:227:ASP:CA	3:U:228:ILE:CG2	2.87	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:C:96:ILE:HG22	2:C:97:GLU:N	2.33	0.41
2:I:139:GLN:C	2:I:141:SER:H	2.23	0.41
2:L:104:GLU:HA	2:L:104:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:PRO:HG2	3:S:261:HIS:ND1	2.36	0.41
1:B:9:PRO:O	1:B:13:ILE:HD12	2.21	0.41
1:E:58:LEU:HG	1:E:75:PHE:HA	2.03	0.41
1:K:134:LYS:C	1:K:134:LYS:HD2	2.41	0.41
2:I:49:GLU:HA	2:I:52:GLN:HE21	1.85	0.41
1:K:100:SER:C	1:K:102:ALA:H	2.24	0.41
2:F:119:GLY:O	2:F:127:VAL:HA	2.20	0.41
1:H:50:PRO:HG3	1:H:141:ILE:HG21	1.93	0.41
1:K:43:ILE:CD1	1:K:58:LEU:HD11	2.51	0.41
3:S:268:PHE:HA	3:S:276:LEU:HB3	2.03	0.41
3:S:291:ILE:O	3:S:292:ASP:C	2.59	0.41
1:H:70:ALA:HB1	1:H:71:PRO:CD	2.50	0.41
1:K:93:ASP:HB2	1:K:98:LYS:HB2	2.03	0.41
1:H:17:GLN:HE21	1:H:17:GLN:HB3	1.70	0.41
1:K:84:VAL:HG13	1:K:88:GLY:HA2	2.03	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:I:114:LYS:N	2:I:171:CYS:HB2	2.37	0.40
2:F:80:LEU:N	2:F:80:LEU:CD2	2.85	0.40
3:S:293:ALA:HB2	3:T:231:TYR:CE2	2.57	0.40
1:K:115:LEU:HD12	1:K:115:LEU:HA	1.29	0.40
1:E:149:ARG:HB2	1:E:149:ARG:CD	2.48	0.40
2:C:114:LYS:NZ	2:C:170:GLN:NE2	2.69	0.40
1:H:50:PRO:HB3	1:H:144:ALA:HB1	2.03	0.40
1:K:85:ASP:OD2	1:K:89:ARG:HB2	2.21	0.40
3:V:262:LEU:HA	3:V:262:LEU:HD23	1.76	0.40
1:E:150:LEU:CD1	1:E:151:TYR:CZ	3.03	0.40
1:E:141:ILE:O	1:E:144:ALA:HB3	2.21	0.40
2:I:45:LEU:O	2:I:46:GLU:O	2.39	0.40
2:F:66:ASP:O	2:F:68:GLU:N	2.54	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
2:I:56:GLY:C	2:I:58:GLY:N	2.74	0.40
2:I:139:GLN:HB2	2:I:142:TYR:CD2	2.56	0.40
2:C:79:ILE:HD13	2:C:79:ILE:HG21	1.82	0.40
1:K:95:LEU:HD21	1:K:108:VAL:HG11	2.03	0.40
1:B:134:LYS:HZ3	1:B:134:LYS:HG2	1.87	0.40
2:C:132:ILE:O	2:C:132:ILE:HD12	2.17	0.40
3:U:286:ALA:CB	3:V:252:THR:OG1	2.70	0.40
1:K:27:ILE:HG13	1:K:113:GLN:OE1	2.22	0.40
2:L:37:LYS:CB	2:L:37:LYS:HZ3	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:LEU:HD21	1:H:105:ILE:HD11	2.04	0.40
1:E:131:GLU:HG3	1:E:132:GLN:N	2.37	0.40
2:C:86:ILE:HD12	2:C:86:ILE:HA	1.90	0.40
1:K:64:GLU:HG2	1:K:64:GLU:H	1.65	0.40
2:C:158:LYS:HZ2	2:C:158:LYS:CB	2.35	0.40
1:K:68:MET:HE3	3:V:265:VAL:CG2	2.49	0.40
3:T:301:VAL:CA	3:T:301:VAL:CG2	2.89	0.40
1:K:67:PRO:C	1:K:69:ALA:H	2.25	0.40
2:L:79:ILE:HG22	2:L:79:ILE:O	2.20	0.40
1:E:73:VAL:CG1	1:E:90:ILE:HD13	2.50	0.40
1:E:44:ALA:O	1:E:46:PRO:CD	2.62	0.40
1:H:73:VAL:HG12	1:H:74:ARG:N	2.37	0.40
1:H:11:ARG:O	1:H:11:ARG:HG2	2.21	0.40
1:B:122:ASP:N	1:B:122:ASP:OD2	2.55	0.40
3:V:240:LEU:HD12	3:V:240:LEU:HA	1.85	0.40
2:L:130:ARG:H	2:L:130:ARG:HG3	1.75	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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	3 14
1	E	145/154 (94%)	122 (84%)	13 (9%)	10 (7%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	145/154 (94%)	103 (71%)	23 (16%)	19 (13%)	0 1
1	K	148/154 (96%)	92 (62%)	27 (18%)	29 (20%)	0 0
2	C	140/142 (99%)	114 (81%)	12 (9%)	14 (10%)	1 2
2	F	137/142 (96%)	113 (82%)	12 (9%)	12 (9%)	1 2
2	I	137/142 (96%)	94 (69%)	20 (15%)	23 (17%)	0 0
2	L	137/142 (96%)	106 (77%)	17 (12%)	14 (10%)	1 2
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 1
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
2	I	57	ASP
2	I	78	MET
2	I	89	ASN

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Mol	Chain	Res	Type
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
3	U	278	GLN
3	V	230	ASP
3	V	235	LYS

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Mol	Chain	Res	Type
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
3	V	270	PRO
3	V	287	MET
3	V	291	ILE

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Mol	Chain	Res	Type
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
3	S	255	ARG
3	U	274	SER
1	E	18	ARG

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Mol	Chain	Res	Type
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 (i)

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%)	91 (71%)	37 (29%)	0	1
1	E	127/129 (98%)	94 (74%)	33 (26%)	0	2
1	H	127/129 (98%)	97 (76%)	30 (24%)	1	2
1	K	128/129 (99%)	90 (70%)	38 (30%)	0	1
2	C	125/127 (98%)	100 (80%)	25 (20%)	1	5
2	F	125/127 (98%)	98 (78%)	27 (22%)	1	3
2	I	125/127 (98%)	85 (68%)	40 (32%)	0	1
2	L	125/127 (98%)	92 (74%)	33 (26%)	0	2
3	S	68/72 (94%)	49 (72%)	19 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	T	72/72 (100%)	55 (76%)	17 (24%)	1 2
3	U	66/72 (92%)	56 (85%)	10 (15%)	3 10
3	V	65/72 (90%)	34 (52%)	31 (48%)	0 0
All	All	1281/1312 (98%)	941 (74%)	340 (26%)	0 2

All (340) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	9	PRO
1	B	10	ARG
1	B	20	LEU
1	B	22	GLU
1	B	34	SER
1	B	35	ASN
1	B	51	PHE
1	B	58	LEU
1	B	64	GLU
1	B	65	GLU
1	B	73	VAL
1	B	74	ARG
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	115	LEU
1	B	116	LEU
1	B	117	SER
1	B	122	ASP
1	B	124	PRO
1	B	127	ASN
1	B	128	ASP
1	B	133	TRP
1	B	134	LYS
1	B	136	ASN
1	B	142	GLU
1	B	148	THR

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Mol	Chain	Res	Type
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	78	MET
2	C	80	LEU
2	C	84	ARG
2	C	89	ASN
2	C	95	LYS
2	C	115	ILE
2	C	132	ILE
2	C	133	SER
2	C	134	VAL
2	C	137	LYS
2	C	141	SER
2	C	147	VAL
2	C	158	LYS
2	C	160	ASN
2	C	163	LEU
2	C	173	SER
1	E	10	ARG
1	E	14	LYS
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	74	ARG
1	E	76	MET

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Mol	Chain	Res	Type
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	117	SER
1	E	127	ASN
1	E	131	GLU
1	E	133	TRP
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	55	VAL
2	F	61	SER
2	F	64	LEU
2	F	67	ASP
2	F	71	THR
2	F	72	LEU
2	F	86	ILE
2	F	97	GLU
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

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Mol	Chain	Res	Type
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	13	ILE
1	H	16	THR
1	H	18	ARG
1	H	19	LEU
1	H	30	GLU
1	H	32	ASP
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	81	HIS
1	H	83	ASN
1	H	91	CYS
1	H	96	LYS
1	H	100	SER
1	H	108	VAL
1	H	110	LEU
1	H	111	SER
1	H	117	SER
1	H	128	ASP
1	H	131	GLU
1	H	134	LYS
1	H	143	THR
1	H	145	ARG
1	H	153	MET
1	H	155	ASN
2	I	37	LYS
2	I	38	VAL
2	I	47	GLU
2	I	53	LYS
2	I	55	VAL
2	I	64	LEU
2	I	66	ASP

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Mol	Chain	Res	Type
2	I	67	ASP
2	I	70	MET
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	103	PRO
2	I	110	ARG
2	I	111	PHE
2	I	130	ARG
2	I	132	ILE
2	I	134	VAL
2	I	140	ASN
2	I	141	SER
2	I	145	LYS
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	162	LYS
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

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Mol	Chain	Res	Type
1	K	33	GLU
1	K	35	ASN
1	K	37	ARG
1	K	48	ASP
1	K	51	PHE
1	K	58	LEU
1	K	60	LEU
1	K	64	GLU
1	K	66	TYR
1	K	74	ARG
1	K	76	MET
1	K	91	CYS
1	K	92	LEU
1	K	93	ASP
1	K	94	ILE
1	K	96	LYS
1	K	98	LYS
1	K	100	SER
1	K	106	ARG
1	K	107	THR
1	K	117	SER
1	K	127	ASN
1	K	128	ASP
1	K	134	LYS
1	K	136	ASN
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	53	LYS
2	L	59	THR
2	L	60	VAL
2	L	64	LEU
2	L	67	ASP
2	L	70	MET
2	L	74	ARG

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Mol	Chain	Res	Type
2	L	78	MET
2	L	80	LEU
2	L	84	ARG
2	L	115	ILE
2	L	130	ARG
2	L	132	ILE
2	L	134	VAL
2	L	140	ASN
2	L	141	SER
2	L	142	TYR
2	L	151	LEU
2	L	153	ARG
2	L	158	LYS
2	L	159	GLU
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	255	ARG
3	S	257	ASP
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	288	LYS
3	S	297	GLU
3	T	227	ASP
3	T	230	ASP
3	T	232	LEU

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Mol	Chain	Res	Type
3	T	235	LYS
3	T	241	MET
3	T	246	ILE
3	T	263	GLN
3	T	269	ASN
3	T	270	PRO
3	T	274	SER
3	T	277	THR
3	T	278	GLN
3	T	279	GLU
3	T	288	LYS
3	T	298	ASN
3	T	300	TRP
3	T	301	VAL
3	U	229	PRO
3	U	237	SER
3	U	242	ARG
3	U	243	GLU
3	U	249	SER
3	U	260	GLU
3	U	262	LEU
3	U	263	GLN
3	U	296	SER
3	U	297	GLU
3	V	229	PRO
3	V	231	TYR
3	V	232	LEU
3	V	235	LYS
3	V	237	SER
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	258	ILE
3	V	261	HIS
3	V	263	GLN
3	V	264	ARG
3	V	270	PRO
3	V	273	ARG

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Mol	Chain	Res	Type
3	V	277	THR
3	V	278	GLN
3	V	279	GLU
3	V	280	GLN
3	V	281	LEU
3	V	282	ILE
3	V	285	LEU
3	V	287	MET
3	V	288	LYS
3	V	291	ILE
3	V	292	ASP
3	V	294	PHE
3	V	295	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	GLN
1	B	35	ASN
1	B	83	ASN
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	81	HIS
1	E	127	ASN
1	E	136	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
2	I	52	GLN
2	I	89	ASN
2	I	140	ASN
2	I	160	ASN

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Mol	Chain	Res	Type
1	K	17	GLN
1	K	35	ASN
1	K	81	HIS
1	K	83	ASN
1	K	136	ASN
1	K	154	ASN
2	L	140	ASN
2	L	160	ASN
3	S	263	GLN
3	S	278	GLN
3	T	269	ASN
3	T	298	ASN
3	U	280	GLN
3	U	284	ASN
3	V	261	HIS
3	V	263	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.19	3 (1%) 68 64	2, 2, 12, 28	0
1	E	149/154 (96%)	-0.28	2 (1%) 79 78	2, 2, 18, 32	0
1	H	149/154 (96%)	-0.03	5 (3%) 49 41	2, 2, 20, 27	0
1	K	152/154 (98%)	0.46	17 (11%) 7 4	2, 3, 29, 38	0
2	C	142/142 (100%)	-0.00	2 (1%) 78 76	2, 2, 10, 28	0
2	F	139/142 (97%)	-0.26	1 (0%) 89 88	2, 2, 10, 20	0
2	I	139/142 (97%)	-0.01	2 (1%) 78 76	2, 2, 10, 17	0
2	L	139/142 (97%)	-0.27	0 100 100	2, 2, 10, 13	0
3	S	75/78 (96%)	-0.32	0 100 100	2, 2, 17, 21	0
3	T	78/78 (100%)	0.16	6 (7%) 16 11	2, 2, 50, 59	0
3	U	73/78 (93%)	-0.29	1 (1%) 78 76	2, 2, 11, 17	0
3	V	71/78 (91%)	-0.40	1 (1%) 78 76	2, 3, 14, 27	0
All	All	1458/1496 (97%)	-0.10	40 (2%) 58 52	2, 2, 18, 59	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	4	GLY	7.9
1	K	3	ALA	6.6
1	K	156	ILE	5.3
1	E	6	ALA	4.9
1	K	124	PRO	4.8
3	T	303	ASP	4.8
3	T	304	TYR	4.5
1	H	156	ILE	4.5
3	T	300	TRP	4.3
1	K	137	GLU	4.1
1	K	6	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	K	5	SER	3.9
1	H	6	ALA	3.7
1	K	133	TRP	3.6
1	B	124	PRO	3.6
1	K	130	ALA	3.4
3	T	302	GLU	3.3
1	K	134	LYS	3.3
1	H	138	ALA	3.2
1	B	3	ALA	3.2
1	K	154	ASN	3.0
1	K	132	GLN	2.8
2	C	58	GLY	2.7
1	B	156	ILE	2.6
1	H	124	PRO	2.6
1	K	47	GLN	2.6
3	T	227	ASP	2.6
2	I	84	ARG	2.5
1	E	156	ILE	2.4
2	C	34	THR	2.4
1	K	138	ALA	2.4
1	K	8	LEU	2.4
2	I	162	LYS	2.2
3	U	295	ILE	2.2
1	H	135	THR	2.2
2	F	55	VAL	2.2
1	K	20	LEU	2.1
3	T	301	VAL	2.1
3	V	298	ASN	2.1
1	K	117	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.