



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Feb 13, 2017 – 10:54 AM EST

PDB ID : 5TJT
EMDB ID: : EMD-8419
Title : T5 bacteriophage major capsid protein - one PB8 hexon
Authors : Conway, J.; Huet, A.
Deposited on : 2016-10-05
Resolution : 9.00 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

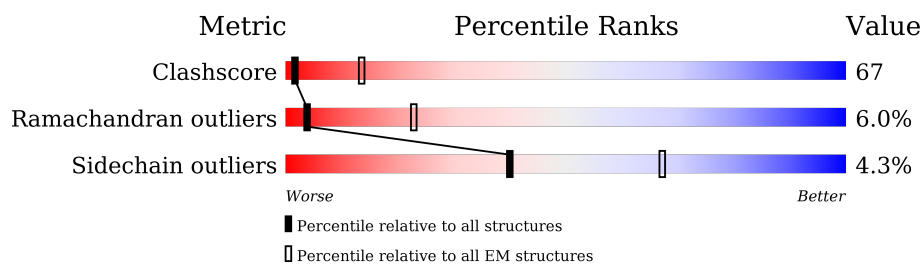
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	299	55% 31% 11% ..
1	B	299	53% 34% 11% ..
1	C	299	55% 32% 10% ..
1	D	299	51% 38% 8% .
1	E	299	56% 33% 8% ..
1	F	299	57% 31% 8% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27426 atoms, of which 13800 are hydrogens and 0 are deuteriums.

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

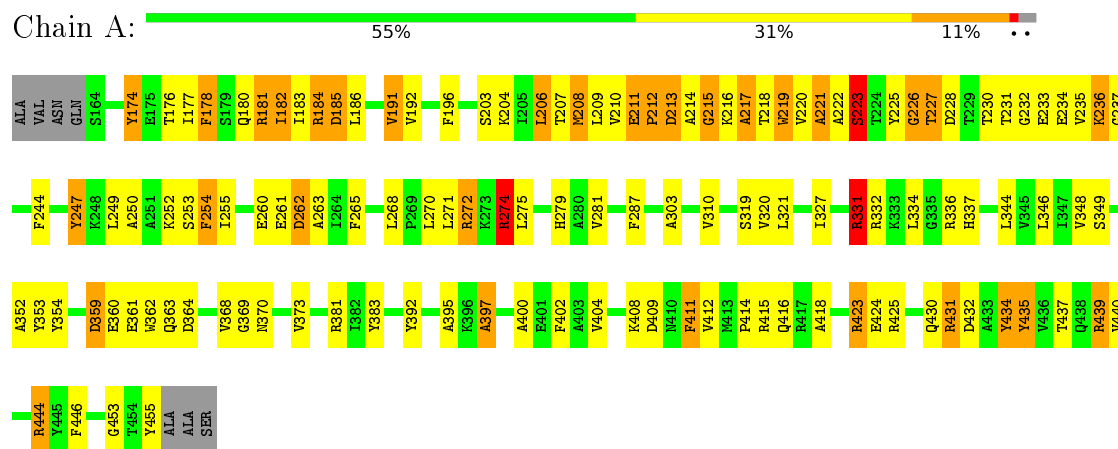
- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	292	Total	C	H	N	O	S	0	0
			4571	1440	2300	382	444	5		
1	B	292	Total	C	H	N	O	S	0	0
			4571	1440	2300	382	444	5		
1	C	292	Total	C	H	N	O	S	0	0
			4571	1440	2300	382	444	5		
1	D	292	Total	C	H	N	O	S	0	0
			4571	1440	2300	382	444	5		
1	E	292	Total	C	H	N	O	S	0	0
			4571	1440	2300	382	444	5		
1	F	292	Total	C	H	N	O	S	0	0
			4571	1440	2300	382	444	5		

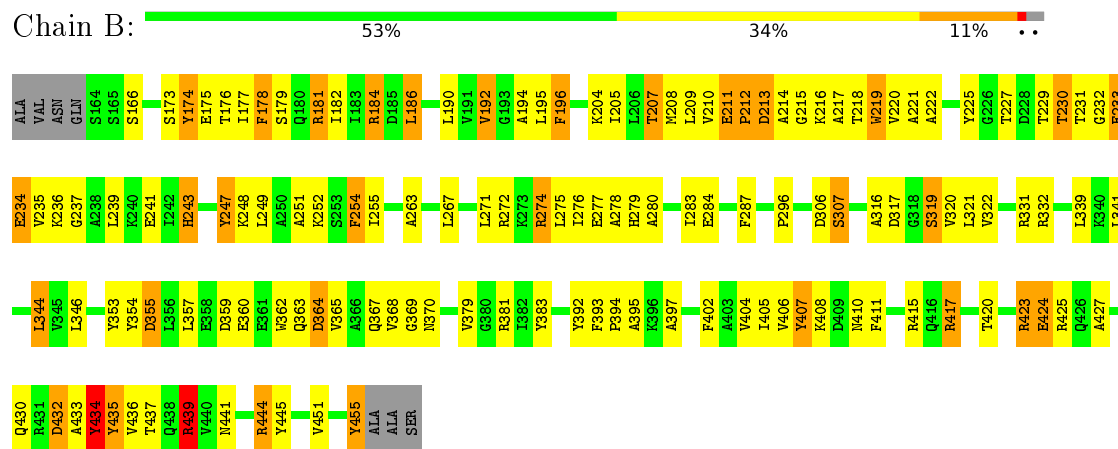
3 Residue-property plots

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. 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. 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.

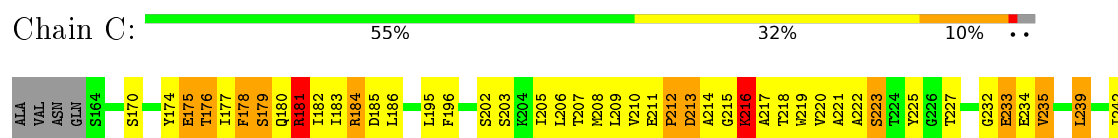
- Molecule 1: Major capsid protein

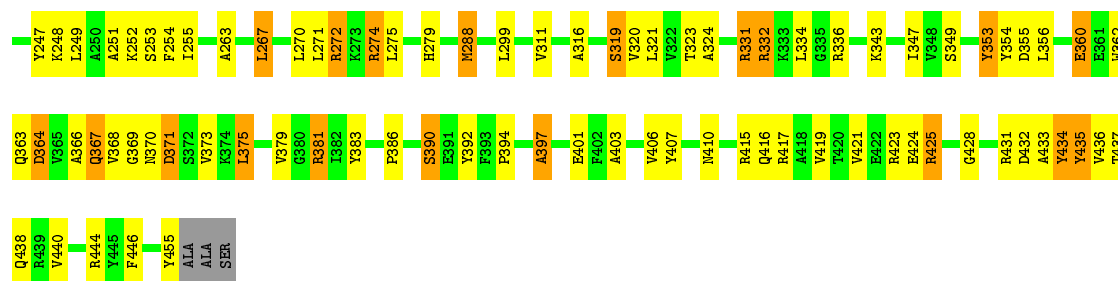


- Molecule 1: Major capsid protein



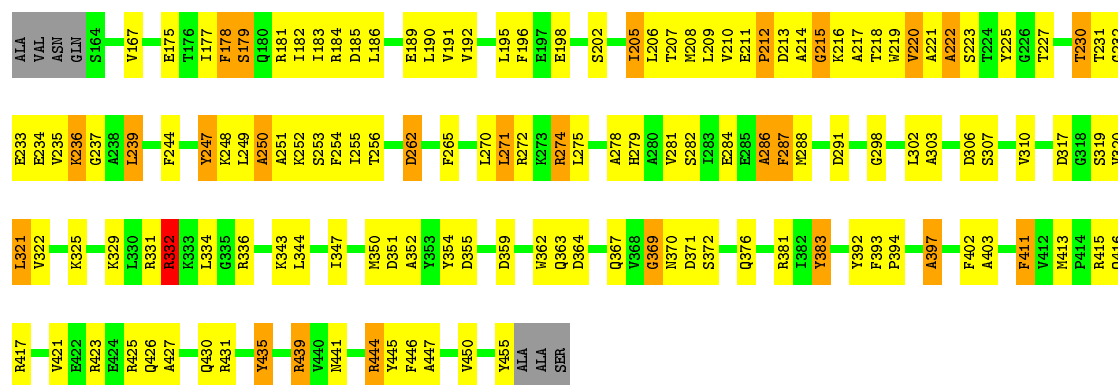
- Molecule 1: Major capsid protein





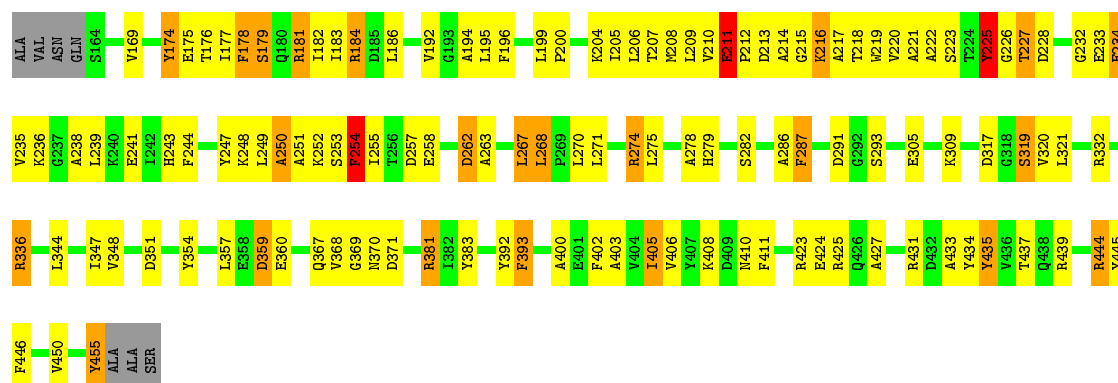
- Molecule 1: Major capsid protein

Chain D: 51% 38% 8%



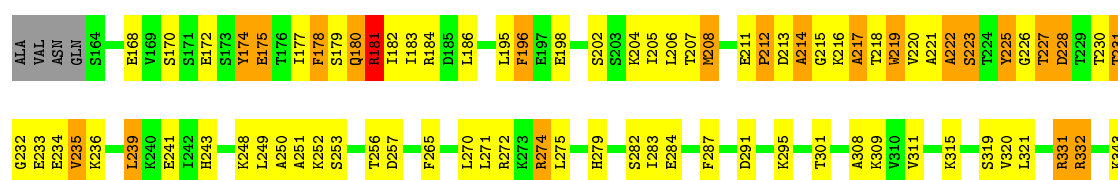
- Molecule 1: Major capsid protein

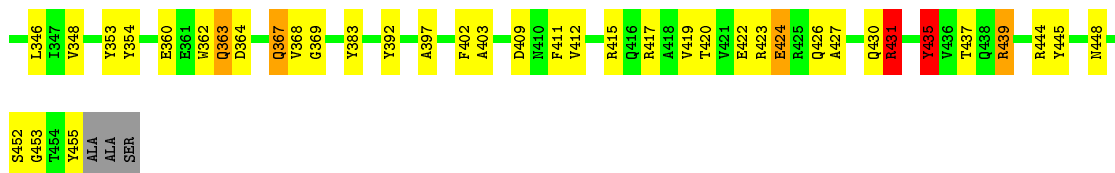
Chain E: 56% 33% 8%



- Molecule 1: Major capsid protein

Chain F: 57% 31% 8%





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	1856	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.72	24/2306 (1.0%)	2.00	64/3116 (2.1%)
1	B	1.80	25/2306 (1.1%)	2.02	65/3116 (2.1%)
1	C	1.71	14/2306 (0.6%)	1.97	49/3116 (1.6%)
1	D	1.76	28/2306 (1.2%)	1.95	54/3116 (1.7%)
1	E	1.74	17/2306 (0.7%)	1.88	48/3116 (1.5%)
1	F	1.70	18/2306 (0.8%)	1.97	54/3116 (1.7%)
All	All	1.74	126/13836 (0.9%)	1.97	334/18696 (1.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	B	0	10
1	C	0	7
1	D	0	7
1	E	0	14
1	F	0	6
All	All	0	54

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	TYR	CE1-CZ	10.12	1.51	1.38
1	B	407	TYR	CE1-CZ	9.15	1.50	1.38
1	C	184	ARG	CZ-NH2	8.85	1.44	1.33
1	A	453	GLY	N-CA	-8.01	1.34	1.46
1	B	445	TYR	CB-CG	-7.67	1.40	1.51
1	C	203	SER	CB-OG	-7.43	1.32	1.42
1	A	181	ARG	NE-CZ	7.41	1.42	1.33
1	A	272	ARG	CZ-NH1	7.25	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	307	SER	CA-CB	7.12	1.63	1.52
1	D	381	ARG	NE-CZ	7.08	1.42	1.33
1	D	331	ARG	CZ-NH1	7.06	1.42	1.33
1	A	337	HIS	CB-CG	7.06	1.62	1.50
1	A	431	ARG	CD-NE	7.02	1.58	1.46
1	F	198	GLU	CD-OE1	-6.93	1.18	1.25
1	E	293	SER	CA-CB	6.85	1.63	1.52
1	E	247	TYR	CE1-CZ	6.82	1.47	1.38
1	B	434	TYR	CG-CD1	6.72	1.47	1.39
1	D	181	ARG	NE-CZ	6.69	1.41	1.33
1	D	332	ARG	CD-NE	6.68	1.57	1.46
1	C	181	ARG	CZ-NH1	6.61	1.41	1.33
1	B	425	ARG	CZ-NH2	6.54	1.41	1.33
1	D	272	ARG	NE-CZ	6.52	1.41	1.33
1	B	173	SER	CA-CB	6.47	1.62	1.52
1	E	174	TYR	CE2-CZ	6.43	1.47	1.38
1	A	354	TYR	CG-CD2	6.37	1.47	1.39
1	B	332	ARG	CZ-NH1	6.37	1.41	1.33
1	E	445	TYR	CE1-CZ	6.34	1.46	1.38
1	F	332	ARG	NE-CZ	6.34	1.41	1.33
1	F	452	SER	CA-CB	6.31	1.62	1.52
1	D	372	SER	CA-CB	6.24	1.62	1.52
1	F	319	SER	CA-CB	6.18	1.62	1.52
1	D	415	ARG	NE-CZ	6.16	1.41	1.33
1	F	184	ARG	CD-NE	6.14	1.56	1.46
1	F	331	ARG	NE-CZ	6.09	1.41	1.33
1	D	310	VAL	N-CA	-6.06	1.34	1.46
1	A	354	TYR	CB-CG	6.06	1.60	1.51
1	B	332	ARG	CD-NE	6.01	1.56	1.46
1	A	383	TYR	CG-CD1	6.01	1.47	1.39
1	F	392	TYR	CG-CD2	5.99	1.47	1.39
1	C	407	TYR	CE1-CZ	5.96	1.46	1.38
1	D	392	TYR	CG-CD1	5.94	1.46	1.39
1	E	392	TYR	CE2-CZ	5.86	1.46	1.38
1	D	417	ARG	CZ-NH1	5.83	1.40	1.33
1	A	414	PRO	N-CD	-5.82	1.39	1.47
1	A	392	TYR	CZ-OH	5.79	1.47	1.37
1	C	417	ARG	CZ-NH1	5.79	1.40	1.33
1	A	381	ARG	CZ-NH1	5.78	1.40	1.33
1	B	190	LEU	CA-C	-5.78	1.38	1.52
1	A	274	ARG	NE-CZ	5.78	1.40	1.33
1	D	236	LYS	C-N	5.72	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	ARG	CZ-NH2	5.71	1.40	1.33
1	E	381	ARG	N-CA	-5.71	1.34	1.46
1	A	254	PHE	CG-CD2	5.71	1.47	1.38
1	C	386	PRO	N-CD	-5.70	1.39	1.47
1	B	455	TYR	CZ-OH	5.66	1.47	1.37
1	A	423	ARG	CZ-NH1	5.64	1.40	1.33
1	F	202	SER	CA-CB	5.62	1.61	1.52
1	D	444	ARG	NE-CZ	5.61	1.40	1.33
1	E	184	ARG	CZ-NH2	5.59	1.40	1.33
1	F	444	ARG	NE-CZ	5.59	1.40	1.33
1	A	395	ALA	CA-CB	5.59	1.64	1.52
1	C	272	ARG	NE-CZ	5.58	1.40	1.33
1	C	428	GLY	CA-C	5.56	1.60	1.51
1	D	439	ARG	NE-CZ	5.52	1.40	1.33
1	A	392	TYR	CG-CD2	5.51	1.46	1.39
1	B	455	TYR	CE2-CZ	5.46	1.45	1.38
1	A	353	TYR	CE2-CZ	5.46	1.45	1.38
1	E	225	TYR	CG-CD1	5.45	1.46	1.39
1	C	336	ARG	NE-CZ	5.45	1.40	1.33
1	E	354	TYR	CE2-CZ	5.44	1.45	1.38
1	B	274	ARG	NE-CZ	5.43	1.40	1.33
1	D	369	GLY	CA-C	-5.43	1.43	1.51
1	E	423	ARG	CZ-NH1	5.42	1.40	1.33
1	F	178	PHE	CG-CD1	5.42	1.46	1.38
1	C	434	TYR	CD1-CE1	-5.42	1.31	1.39
1	D	334	LEU	C-N	5.39	1.42	1.33
1	D	202	SER	CA-CB	5.38	1.61	1.52
1	B	455	TYR	CG-CD2	5.38	1.46	1.39
1	F	184	ARG	CZ-NH1	5.37	1.40	1.33
1	F	272	ARG	CZ-NH2	5.34	1.40	1.33
1	D	425	ARG	CD-NE	5.33	1.55	1.46
1	B	181	ARG	CZ-NH2	5.33	1.40	1.33
1	D	423	ARG	CZ-NH1	5.30	1.40	1.33
1	E	211	GLU	CG-CD	5.30	1.59	1.51
1	D	181	ARG	CD-NE	5.29	1.55	1.46
1	B	439	ARG	CZ-NH2	5.29	1.40	1.33
1	B	381	ARG	NE-CZ	5.29	1.40	1.33
1	D	298	GLY	N-CA	-5.28	1.38	1.46
1	A	274	ARG	CZ-NH1	5.28	1.40	1.33
1	C	242	ILE	CA-CB	-5.27	1.42	1.54
1	D	331	ARG	CD-NE	5.27	1.55	1.46
1	F	274	ARG	NE-CZ	5.26	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	TYR	CZ-OH	5.26	1.46	1.37
1	F	353	TYR	CE2-CZ	5.26	1.45	1.38
1	F	445	TYR	CZ-OH	5.26	1.46	1.37
1	B	284	GLU	CD-OE2	5.25	1.31	1.25
1	B	243	HIS	CB-CG	5.25	1.59	1.50
1	C	349	SER	CB-OG	5.24	1.49	1.42
1	E	405	ILE	N-CA	-5.24	1.35	1.46
1	C	332	ARG	NE-CZ	5.22	1.39	1.33
1	E	319	SER	CA-CB	5.22	1.60	1.52
1	E	431	ARG	CZ-NH2	5.20	1.39	1.33
1	D	383	TYR	CB-CG	-5.18	1.43	1.51
1	B	219	TRP	CE2-CZ2	-5.18	1.30	1.39
1	A	260	GLU	CD-OE2	5.17	1.31	1.25
1	E	181	ARG	NE-CZ	5.17	1.39	1.33
1	B	423	ARG	NE-CZ	5.17	1.39	1.33
1	F	184	ARG	CZ-NH2	5.17	1.39	1.33
1	A	439	ARG	NE-CZ	5.16	1.39	1.33
1	D	435	TYR	CG-CD2	5.14	1.45	1.39
1	F	435	TYR	CB-CG	5.14	1.59	1.51
1	C	423	ARG	CZ-NH1	5.12	1.39	1.33
1	A	260	GLU	CA-CB	5.11	1.65	1.53
1	B	392	TYR	CG-CD2	5.11	1.45	1.39
1	B	307	SER	CA-CB	5.10	1.60	1.52
1	A	211	GLU	CG-CD	5.09	1.59	1.51
1	F	409	ASP	CB-CG	5.08	1.62	1.51
1	B	353	TYR	CD1-CE1	5.07	1.47	1.39
1	B	272	ARG	NE-CZ	5.04	1.39	1.33
1	E	267	LEU	N-CA	-5.04	1.36	1.46
1	E	181	ARG	CZ-NH1	5.03	1.39	1.33
1	D	455	TYR	CE1-CZ	5.03	1.45	1.38
1	D	225	TYR	CD1-CE1	5.02	1.46	1.39
1	B	415	ARG	NE-CZ	5.01	1.39	1.33
1	D	286	ALA	CA-CB	5.01	1.62	1.52
1	D	381	ARG	CD-NE	5.00	1.54	1.46

All (334) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	381	ARG	NE-CZ-NH2	15.40	128.00	120.30
1	C	444	ARG	NE-CZ-NH1	-15.36	112.62	120.30
1	F	435	TYR	CB-CG-CD1	15.35	130.21	121.00
1	F	181	ARG	NE-CZ-NH2	15.24	127.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	PHE	CB-CG-CD1	-13.83	111.12	120.80
1	F	423	ARG	NE-CZ-NH1	-13.55	113.53	120.30
1	B	423	ARG	NE-CZ-NH2	-13.35	113.63	120.30
1	A	434	TYR	CB-CG-CD2	-13.23	113.06	121.00
1	A	383	TYR	CB-CG-CD1	-12.47	113.52	121.00
1	D	244	PHE	CB-CG-CD1	12.46	129.53	120.80
1	B	174	TYR	CB-CG-CD2	-12.45	113.53	121.00
1	E	174	TYR	CB-CG-CD1	-11.92	113.85	121.00
1	B	272	ARG	NE-CZ-NH1	-11.75	114.43	120.30
1	F	181	ARG	NE-CZ-NH1	-11.67	114.46	120.30
1	C	425	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	C	274	ARG	NE-CZ-NH1	-11.59	114.51	120.30
1	A	381	ARG	NE-CZ-NH2	11.57	126.09	120.30
1	D	444	ARG	NE-CZ-NH1	-11.08	114.76	120.30
1	A	446	PHE	CB-CG-CD1	-11.06	113.06	120.80
1	D	411	PHE	CB-CG-CD1	-10.79	113.25	120.80
1	B	455	TYR	CB-CG-CD1	-10.63	114.62	121.00
1	D	423	ARG	NE-CZ-NH2	10.44	125.52	120.30
1	B	444	ARG	NE-CZ-NH1	-10.39	115.10	120.30
1	D	393	PHE	CB-CG-CD2	-10.25	113.62	120.80
1	F	383	TYR	CB-CG-CD1	-10.12	114.92	121.00
1	C	174	TYR	CB-CG-CD1	-10.06	114.96	121.00
1	E	381	ARG	NE-CZ-NH2	10.00	125.30	120.30
1	F	435	TYR	CB-CG-CD2	-9.89	115.06	121.00
1	D	317	ASP	CB-CG-OD2	-9.89	109.40	118.30
1	B	178	PHE	CB-CG-CD2	-9.79	113.94	120.80
1	C	274	ARG	NE-CZ-NH2	9.70	125.15	120.30
1	A	444	ARG	NE-CZ-NH1	-9.60	115.50	120.30
1	E	354	TYR	CB-CG-CD1	-9.52	115.29	121.00
1	D	445	TYR	CB-CG-CD1	-9.48	115.31	121.00
1	F	354	TYR	CB-CG-CD2	-9.47	115.32	121.00
1	C	331	ARG	NE-CZ-NH2	9.46	125.03	120.30
1	D	411	PHE	CB-CG-CD2	9.34	127.34	120.80
1	C	423	ARG	NE-CZ-NH1	-9.33	115.63	120.30
1	C	423	ARG	NE-CZ-NH2	9.25	124.93	120.30
1	A	431	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	D	247	TYR	CB-CG-CD1	-9.22	115.47	121.00
1	F	178	PHE	CB-CG-CD2	9.16	127.21	120.80
1	A	381	ARG	NE-CZ-NH1	-9.14	115.73	120.30
1	A	332	ARG	NE-CZ-NH1	-9.10	115.75	120.30
1	A	336	ARG	NE-CZ-NH2	9.06	124.83	120.30
1	B	435	TYR	CB-CG-CD2	9.04	126.42	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	444	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	B	331	ARG	NE-CZ-NH1	-8.93	115.83	120.30
1	B	196	PHE	CB-CG-CD2	-8.90	114.57	120.80
1	B	331	ARG	NE-CZ-NH2	8.90	124.75	120.30
1	A	244	PHE	CB-CG-CD2	-8.88	114.58	120.80
1	A	331	ARG	NE-CZ-NH1	-8.87	115.86	120.30
1	B	417	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	E	425	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	C	174	TYR	CG-CD2-CE2	-8.74	114.31	121.30
1	B	247	TYR	CB-CG-CD1	-8.65	115.81	121.00
1	F	332	ARG	NE-CZ-NH1	-8.65	115.98	120.30
1	A	411	PHE	CB-CG-CD2	8.64	126.84	120.80
1	E	196	PHE	CB-CG-CD2	8.60	126.82	120.80
1	B	407	TYR	CB-CG-CD2	-8.46	115.92	121.00
1	B	353	TYR	CB-CG-CD1	-8.38	115.97	121.00
1	F	431	ARG	NE-CZ-NH2	8.31	124.46	120.30
1	F	402	PHE	CB-CG-CD2	-8.29	114.99	120.80
1	B	174	TYR	CB-CG-CD1	8.27	125.96	121.00
1	B	381	ARG	NE-CZ-NH1	-8.21	116.20	120.30
1	F	178	PHE	CB-CG-CD1	-8.21	115.06	120.80
1	F	354	TYR	CB-CG-CD1	8.09	125.85	121.00
1	A	223	SER	N-CA-CB	8.08	122.62	110.50
1	F	284	GLU	OE1-CD-OE2	8.04	132.94	123.30
1	C	299	LEU	CB-CG-CD1	8.01	124.61	111.00
1	E	403	ALA	N-CA-CB	7.98	121.28	110.10
1	A	196	PHE	CB-CG-CD2	-7.88	115.28	120.80
1	D	435	TYR	CB-CG-CD2	-7.76	116.34	121.00
1	D	336	ARG	NE-CZ-NH2	7.73	124.17	120.30
1	A	373	VAL	CG1-CB-CG2	-7.73	98.53	110.90
1	C	354	TYR	CB-CG-CD1	7.72	125.63	121.00
1	B	247	TYR	CB-CG-CD2	7.71	125.62	121.00
1	E	425	ARG	NE-CZ-NH1	-7.65	116.47	120.30
1	B	425	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	E	359	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	B	354	TYR	CB-CG-CD1	-7.56	116.47	121.00
1	C	288	MET	CG-SD-CE	-7.53	88.14	100.20
1	A	425	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	A	435	TYR	CB-CG-CD2	7.41	125.44	121.00
1	D	331	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	C	432	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	446	PHE	CB-CG-CD2	7.36	125.95	120.80
1	C	446	PHE	CB-CG-CD1	7.33	125.93	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	PHE	CB-CG-CD2	7.33	125.93	120.80
1	F	403	ALA	N-CA-CB	7.23	120.22	110.10
1	E	446	PHE	CB-CG-CD1	7.21	125.85	120.80
1	E	370	ASN	N-CA-C	-7.20	91.55	111.00
1	A	435	TYR	CB-CG-CD1	-7.20	116.68	121.00
1	E	179	SER	N-CA-CB	7.19	121.29	110.50
1	B	207	THR	CA-CB-CG2	-7.18	102.35	112.40
1	D	392	TYR	CB-CG-CD1	-7.15	116.71	121.00
1	C	373	VAL	CB-CA-C	-7.01	98.08	111.40
1	B	395	ALA	CB-CA-C	-7.01	99.59	110.10
1	E	257	ASP	CB-CG-OD1	6.97	124.58	118.30
1	B	178	PHE	CB-CG-CD1	6.97	125.68	120.80
1	C	381	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	E	450	VAL	CG1-CB-CG2	6.95	122.02	110.90
1	D	359	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	B	194	ALA	N-CA-CB	6.91	119.77	110.10
1	A	383	TYR	CG-CD1-CE1	-6.91	115.78	121.30
1	A	409	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	F	308	ALA	CB-CA-C	-6.90	99.75	110.10
1	C	444	ARG	CD-NE-CZ	-6.88	113.96	123.60
1	B	415	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	262	ASP	N-CA-CB	6.83	122.90	110.60
1	D	189	GLU	OE1-CD-OE2	6.83	131.49	123.30
1	E	435	TYR	CA-CB-CG	-6.82	100.44	113.40
1	C	319	SER	N-CA-CB	6.79	120.69	110.50
1	F	343	LYS	N-CA-CB	6.78	122.81	110.60
1	D	185	ASP	CB-CG-OD2	6.78	124.40	118.30
1	B	221	ALA	CB-CA-C	-6.72	100.02	110.10
1	F	178	PHE	CZ-CE2-CD2	6.69	128.13	120.10
1	B	435	TYR	CB-CG-CD1	-6.67	117.00	121.00
1	E	445	TYR	CB-CG-CD1	-6.66	117.00	121.00
1	D	402	PHE	CB-CG-CD2	-6.65	116.14	120.80
1	D	302	LEU	CB-CG-CD1	-6.64	99.71	111.00
1	B	407	TYR	CD1-CG-CD2	6.63	125.19	117.90
1	B	254	PHE	CB-CG-CD2	-6.62	116.16	120.80
1	C	431	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	C	379	VAL	CA-CB-CG2	6.61	120.82	110.90
1	B	317	ASP	CB-CG-OD1	6.60	124.24	118.30
1	E	393	PHE	CB-CA-C	-6.58	97.23	110.40
1	B	455	TYR	CB-CG-CD2	6.57	124.94	121.00
1	C	431	ARG	N-CA-CB	6.56	122.41	110.60
1	D	430	GLN	C-N-CA	6.55	138.08	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	VAL	CA-CB-CG1	-6.55	101.07	110.90
1	F	455	TYR	CB-CG-CD1	-6.52	117.08	121.00
1	F	223	SER	N-CA-CB	6.51	120.27	110.50
1	F	257	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	E	178	PHE	CB-CG-CD1	6.44	125.31	120.80
1	C	370	ASN	C-N-CA	6.44	137.80	121.70
1	D	220	VAL	CG1-CB-CG2	-6.43	100.61	110.90
1	A	411	PHE	N-CA-CB	6.42	122.16	110.60
1	D	392	TYR	CB-CG-CD2	6.42	124.85	121.00
1	D	288	MET	CG-SD-CE	-6.39	89.98	100.20
1	D	306	ASP	CB-CG-OD1	6.37	124.04	118.30
1	B	166	SER	N-CA-CB	6.36	120.04	110.50
1	E	402	PHE	CB-CG-CD2	6.36	125.25	120.80
1	A	319	SER	N-CA-CB	6.34	120.00	110.50
1	E	174	TYR	CB-CG-CD2	6.33	124.80	121.00
1	C	424	GLU	N-CA-C	-6.33	93.92	111.00
1	E	402	PHE	CB-CG-CD1	-6.32	116.38	120.80
1	D	265	PHE	CB-CG-CD1	6.31	125.22	120.80
1	E	354	TYR	CG-CD2-CE2	-6.30	116.26	121.30
1	C	362	TRP	N-CA-CB	6.29	121.93	110.60
1	F	430	GLN	C-N-CA	6.28	137.39	121.70
1	F	423	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	F	274	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	244	PHE	N-CA-CB	6.24	121.83	110.60
1	A	434	TYR	CB-CG-CD1	6.23	124.74	121.00
1	B	319	SER	N-CA-CB	6.23	119.84	110.50
1	D	271	LEU	CB-CG-CD2	6.22	121.58	111.00
1	B	184	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	B	451	VAL	CA-CB-CG2	-6.19	101.62	110.90
1	A	455	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	B	455	TYR	CD1-CE1-CZ	6.16	125.34	119.80
1	E	287	PHE	CB-CG-CD2	6.15	125.11	120.80
1	F	435	TYR	CZ-CE2-CD2	-6.11	114.30	119.80
1	D	415	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	B	355	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	F	225	TYR	CG-CD1-CE1	6.08	126.16	121.30
1	D	332	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	D	317	ASP	CB-CG-OD1	6.05	123.74	118.30
1	A	247	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	C	334	LEU	O-C-N	-6.02	112.97	123.20
1	E	348	VAL	CA-CB-CG2	6.01	119.92	110.90
1	C	397	ALA	N-CA-CB	6.01	118.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	174	TYR	C-N-CA	6.00	136.69	121.70
1	D	198	GLU	N-CA-CB	5.97	121.35	110.60
1	B	341	LEU	N-CA-C	-5.95	94.92	111.00
1	D	343	LYS	N-CA-CB	5.94	121.30	110.60
1	A	260	GLU	OE1-CD-OE2	5.94	130.43	123.30
1	C	407	TYR	CB-CG-CD2	-5.92	117.44	121.00
1	E	336	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	C	371	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	A	185	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	306	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	B	344	LEU	N-CA-CB	5.86	122.12	110.40
1	F	417	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	B	402	PHE	CG-CD1-CE1	-5.85	114.37	120.80
1	C	178	PHE	CB-CG-CD1	-5.84	116.71	120.80
1	A	221	ALA	N-CA-CB	5.84	118.28	110.10
1	C	421	VAL	CG1-CB-CG2	-5.84	101.56	110.90
1	B	225	TYR	CB-CG-CD1	5.82	124.49	121.00
1	E	411	PHE	CB-CG-CD2	5.82	124.87	120.80
1	A	418	ALA	CB-CA-C	-5.80	101.40	110.10
1	B	353	TYR	CZ-CE2-CD2	5.80	125.02	119.80
1	D	274	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	F	412	VAL	CG1-CB-CG2	-5.80	101.62	110.90
1	D	244	PHE	CG-CD1-CE1	5.80	127.18	120.80
1	B	211	GLU	N-CA-C	-5.79	95.35	111.00
1	E	234	GLU	N-CA-CB	5.78	121.01	110.60
1	F	214	ALA	N-CA-CB	5.78	118.19	110.10
1	C	185	ASP	N-CA-C	-5.77	95.41	111.00
1	B	354	TYR	CZ-CE2-CD2	-5.76	114.61	119.80
1	E	347	ILE	C-N-CA	5.75	136.08	121.70
1	B	415	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	181	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	287	PHE	CB-CG-CD2	-5.74	116.78	120.80
1	F	367	GLN	N-CA-CB	5.72	120.90	110.60
1	A	359	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	D	239	LEU	C-N-CA	5.70	135.96	121.70
1	D	423	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	A	226	GLY	N-CA-C	-5.67	98.92	113.10
1	D	281	VAL	CA-CB-CG1	-5.67	102.39	110.90
1	A	434	TYR	CG-CD2-CE2	-5.67	116.77	121.30
1	F	180	GLN	C-N-CA	5.66	135.85	121.70
1	A	444	ARG	NE-CZ-NH2	5.65	123.13	120.30
1	A	353	TYR	CB-CG-CD2	-5.64	117.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	444	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	C	213	ASP	CB-CG-OD1	5.64	123.37	118.30
1	A	265	PHE	CB-CG-CD2	5.63	124.74	120.80
1	C	176	THR	O-C-N	-5.63	113.69	122.70
1	E	291	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	E	250	ALA	CB-CA-C	-5.62	101.67	110.10
1	E	344	LEU	CB-CG-CD2	-5.60	101.49	111.00
1	C	332	ARG	CD-NE-CZ	-5.59	115.77	123.60
1	A	435	TYR	CZ-CE2-CD2	-5.58	114.78	119.80
1	D	186	LEU	C-N-CA	5.58	135.66	121.70
1	B	274	ARG	NE-CZ-NH2	5.57	123.09	120.30
1	F	415	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	A	402	PHE	CB-CG-CD2	-5.57	116.91	120.80
1	F	419	VAL	CA-CB-CG1	5.57	119.25	110.90
1	C	403	ALA	N-CA-CB	5.56	117.88	110.10
1	A	397	ALA	N-CA-CB	5.55	117.86	110.10
1	D	247	TYR	CG-CD1-CE1	-5.54	116.87	121.30
1	F	309	LYS	N-CA-CB	5.53	120.55	110.60
1	F	455	TYR	CB-CG-CD2	5.52	124.31	121.00
1	E	367	GLN	C-N-CA	5.51	135.48	121.70
1	D	167	VAL	C-N-CA	5.50	135.46	121.70
1	F	420	THR	CA-CB-CG2	-5.50	104.69	112.40
1	A	336	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	424	GLU	N-CA-CB	5.49	120.49	110.60
1	D	435	TYR	CB-CG-CD1	5.49	124.29	121.00
1	A	217	ALA	N-CA-CB	5.47	117.76	110.10
1	C	336	ARG	NE-CZ-NH1	-5.47	117.57	120.30
1	C	247	TYR	N-CA-C	-5.46	96.25	111.00
1	B	370	ASN	N-CA-C	-5.44	96.30	111.00
1	F	219	TRP	CB-CA-C	-5.44	99.51	110.40
1	D	417	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	310	VAL	CG1-CB-CG2	-5.44	102.20	110.90
1	B	225	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	C	324	ALA	CB-CA-C	-5.43	101.96	110.10
1	B	353	TYR	CG-CD1-CE1	-5.42	116.96	121.30
1	E	268	LEU	CB-CG-CD2	5.42	120.22	111.00
1	C	415	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	E	392	TYR	CG-CD1-CE1	5.40	125.62	121.30
1	D	250	ALA	N-CA-CB	5.40	117.66	110.10
1	E	174	TYR	C-N-CA	5.39	135.18	121.70
1	C	375	LEU	CB-CA-C	-5.38	99.97	110.20
1	A	400	ALA	N-CA-CB	5.37	117.61	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	196	PHE	CB-CG-CD1	-5.35	117.06	120.80
1	D	421	VAL	CG1-CB-CG2	5.35	119.45	110.90
1	B	404	VAL	CA-CB-CG2	5.34	118.92	110.90
1	B	213	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	D	287	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	E	257	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	D	350	MET	CA-CB-CG	5.32	122.34	113.30
1	F	383	TYR	CG-CD1-CE1	-5.32	117.05	121.30
1	F	346	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	D	344	LEU	CB-CG-CD1	5.29	120.00	111.00
1	E	317	ASP	CB-CG-OD2	5.29	123.06	118.30
1	E	227	THR	N-CA-CB	5.29	120.36	110.30
1	B	296	PRO	N-CA-CB	5.27	109.63	103.30
1	E	383	TYR	CG-CD2-CE2	-5.27	117.08	121.30
1	E	332	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	C	223	SER	N-CA-CB	5.26	118.39	110.50
1	A	206	LEU	N-CA-CB	5.26	120.92	110.40
1	B	230	THR	N-CA-CB	5.26	120.29	110.30
1	F	362	TRP	CA-CB-CG	5.26	123.69	113.70
1	F	272	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	A	431	ARG	N-CA-CB	5.26	120.06	110.60
1	D	383	TYR	CB-CG-CD2	5.26	124.15	121.00
1	F	239	LEU	CB-CG-CD2	5.25	119.93	111.00
1	E	411	PHE	CB-CG-CD1	-5.25	117.13	120.80
1	A	178	PHE	CA-CB-CG	-5.25	101.31	113.90
1	A	321	LEU	CB-CA-C	5.24	120.15	110.20
1	E	431	ARG	N-CA-CB	5.24	120.02	110.60
1	F	431	ARG	N-CA-CB	5.22	120.01	110.60
1	D	205	ILE	N-CA-C	-5.22	96.90	111.00
1	F	265	PHE	CZ-CE2-CD2	-5.21	113.85	120.10
1	F	186	LEU	CB-CG-CD2	-5.21	102.15	111.00
1	F	424	GLU	CA-CB-CG	5.21	124.86	113.40
1	B	383	TYR	CB-CG-CD2	5.21	124.12	121.00
1	D	359	ASP	C-N-CA	5.21	134.71	121.70
1	E	262	ASP	N-CA-CB	5.21	119.97	110.60
1	A	281	VAL	CB-CA-C	-5.20	101.51	111.40
1	B	194	ALA	N-CA-C	-5.20	96.95	111.00
1	D	364	ASP	N-CA-CB	5.20	119.96	110.60
1	A	412	VAL	N-CA-C	-5.20	96.97	111.00
1	F	308	ALA	N-CA-CB	5.18	117.36	110.10
1	A	423	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	F	196	PHE	CB-CG-CD2	-5.17	117.18	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	453	GLY	O-C-N	5.17	130.97	122.70
1	A	411	PHE	CB-CA-C	-5.16	100.08	110.40
1	A	354	TYR	CB-CG-CD1	5.16	124.09	121.00
1	E	194	ALA	N-CA-C	-5.16	97.08	111.00
1	B	181	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	D	403	ALA	N-CA-CB	5.15	117.31	110.10
1	A	219	TRP	CH2-CZ2-CE2	5.14	122.54	117.40
1	B	424	GLU	O-C-N	-5.14	114.47	122.70
1	E	424	GLU	CB-CG-CD	-5.14	100.33	114.20
1	A	191	VAL	CA-CB-CG2	5.13	118.60	110.90
1	F	448	ASN	CA-CB-CG	-5.13	102.11	113.40
1	C	247	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	D	426	GLN	CA-CB-CG	5.13	124.68	113.40
1	A	383	TYR	CB-CG-CD2	5.12	124.07	121.00
1	B	234	GLU	C-N-CA	5.12	134.49	121.70
1	A	303	ALA	CB-CA-C	-5.11	102.43	110.10
1	F	217	ALA	CB-CA-C	5.11	117.76	110.10
1	D	397	ALA	N-CA-CB	5.10	117.24	110.10
1	E	455	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	C	390	SER	N-CA-CB	5.10	118.15	110.50
1	F	411	PHE	N-CA-CB	5.08	119.75	110.60
1	A	254	PHE	CB-CG-CD2	5.08	124.36	120.80
1	C	323	THR	CA-CB-CG2	-5.08	105.29	112.40
1	A	174	TYR	CZ-CE2-CD2	-5.07	115.23	119.80
1	C	235	VAL	CA-CB-CG2	5.07	118.50	110.90
1	E	408	LYS	O-C-N	5.06	130.80	122.70
1	B	393	PHE	CB-CA-C	-5.06	100.28	110.40
1	C	239	LEU	N-CA-C	-5.05	97.37	111.00
1	B	186	LEU	N-CA-CB	5.05	120.50	110.40
1	D	350	MET	C-N-CA	5.05	134.32	121.70
1	B	430	GLN	C-N-CA	5.04	134.31	121.70
1	E	244	PHE	CB-CG-CD1	-5.04	117.27	120.80
1	F	348	VAL	CG1-CB-CG2	5.04	118.96	110.90
1	D	230	THR	CA-CB-CG2	-5.03	105.36	112.40
1	A	402	PHE	CB-CG-CD1	5.02	124.32	120.80
1	C	343	LYS	N-CA-CB	5.02	119.63	110.60

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	247	TYR	Sidechain
1	A	261	GLU	Peptide
1	A	272	ARG	Sidechain
1	A	274	ARG	Sidechain
1	A	331	ARG	Sidechain
1	A	415	ARG	Sidechain
1	A	423	ARG	Sidechain
1	A	430	GLN	Peptide
1	A	444	ARG	Sidechain
1	B	196	PHE	Sidechain
1	B	247	TYR	Sidechain
1	B	407	TYR	Sidechain
1	B	411	PHE	Sidechain
1	B	417	ARG	Sidechain
1	B	423	ARG	Sidechain
1	B	434	TYR	Sidechain
1	B	439	ARG	Sidechain
1	B	444	ARG	Sidechain
1	B	455	TYR	Sidechain
1	C	272	ARG	Sidechain
1	C	353	TYR	Sidechain
1	C	381	ARG	Sidechain
1	C	392	TYR	Sidechain
1	C	425	ARG	Sidechain
1	C	435	TYR	Sidechain
1	C	455	TYR	Sidechain
1	D	178	PHE	Sidechain
1	D	196	PHE	Sidechain
1	D	215	GLY	Peptide
1	D	247	TYR	Sidechain
1	D	332	ARG	Sidechain
1	D	354	TYR	Sidechain
1	D	411	PHE	Sidechain
1	E	174	TYR	Sidechain
1	E	211	GLU	Peptide
1	E	225	TYR	Sidechain
1	E	236	LYS	Peptide
1	E	238	ALA	Peptide
1	E	239	LEU	Peptide
1	E	243	HIS	Sidechain
1	E	254	PHE	Peptide
1	E	274	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	287	PHE	Sidechain
1	E	336	ARG	Sidechain
1	E	381	ARG	Sidechain
1	E	393	PHE	Peptide
1	E	435	TYR	Sidechain
1	F	174	TYR	Sidechain
1	F	196	PHE	Sidechain
1	F	225	TYR	Sidechain
1	F	239	LEU	Peptide
1	F	435	TYR	Sidechain
1	F	439	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2271	2300	2281	558	0
1	B	2271	2300	2282	597	0
1	C	2271	2300	2279	624	0
1	D	2271	2300	2291	659	0
1	E	2271	2300	2287	618	0
1	F	2271	2300	2289	552	0
All	All	13626	13800	13709	1822	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 67.

All (1822) 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:D:216:LYS:CG	1:E:278:ALA:HB2	1.21	1.67
1:A:178:PHE:CD2	1:F:207:THR:CG2	1.74	1.64
1:C:217:ALA:CB	1:D:279:HIS:HB2	1.16	1.64
1:D:207:THR:H	1:E:177:ILE:CB	1.02	1.62
1:C:235:VAL:CG2	1:D:271:LEU:HD11	1.23	1.61
1:A:235:VAL:HG23	1:B:271:LEU:CD2	1.20	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:LYS:HG3	1:E:278:ALA:CB	1.17	1.59
1:C:216:LYS:HE3	1:D:278:ALA:CB	1.33	1.58
1:B:220:VAL:CG2	1:C:437:THR:HG22	1.23	1.58
1:C:220:VAL:HB	1:D:250:ALA:CB	1.30	1.57
1:C:221:ALA:HA	1:D:248:LYS:CB	1.24	1.57
1:E:211:GLU:CG	1:F:182:ILE:HD12	1.30	1.56
1:A:362:TRP:HH2	1:B:362:TRP:CD1	1.24	1.55
1:A:178:PHE:CD2	1:F:207:THR:HG22	1.30	1.55
1:A:215:GLY:CA	1:B:271:LEU:HD12	1.27	1.54
1:E:211:GLU:HG2	1:F:182:ILE:CD1	1.24	1.54
1:E:213:ASP:HA	1:F:274:ARG:CD	1.11	1.54
1:C:217:ALA:HB3	1:D:279:HIS:CB	1.37	1.53
1:E:214:ALA:CB	1:F:271:LEU:HA	1.09	1.53
1:A:178:PHE:CE2	1:F:207:THR:HG21	1.42	1.52
1:A:275:LEU:CD2	1:F:216:LYS:N	1.70	1.52
1:B:217:ALA:H	1:C:275:LEU:CD2	1.17	1.52
1:A:220:VAL:CG2	1:B:252:LYS:HG2	1.40	1.51
1:A:250:ALA:H	1:F:219:TRP:CB	1.04	1.51
1:E:241:GLU:CG	1:F:179:SER:HB3	1.36	1.50
1:A:271:LEU:CD1	1:F:236:LYS:H	1.18	1.50
1:D:217:ALA:H	1:E:278:ALA:CB	1.24	1.49
1:E:213:ASP:CG	1:F:274:ARG:HD3	1.29	1.49
1:D:217:ALA:N	1:E:278:ALA:HB3	1.17	1.48
1:D:211:GLU:C	1:E:182:ILE:HG12	1.13	1.48
1:C:219:TRP:CZ2	1:D:282:SER:O	1.67	1.48
1:E:210:VAL:CA	1:F:182:ILE:HA	1.38	1.47
1:D:235:VAL:HG21	1:E:255:ILE:CG1	1.44	1.47
1:E:232:GLY:CA	1:F:252:LYS:HB2	1.45	1.47
1:E:220:VAL:HG11	1:F:435:TYR:CE1	1.50	1.47
1:C:220:VAL:CB	1:D:250:ALA:HB3	1.41	1.47
1:D:212:PRO:CA	1:E:182:ILE:HD13	1.42	1.47
1:E:214:ALA:H	1:F:274:ARG:CB	1.28	1.47
1:E:217:ALA:CB	1:F:279:HIS:HB2	1.38	1.46
1:D:211:GLU:C	1:E:182:ILE:CG1	1.83	1.46
1:C:213:ASP:CA	1:D:274:ARG:HD3	1.20	1.46
1:E:234:GLU:N	1:F:253:SER:CA	1.72	1.45
1:A:271:LEU:CD1	1:F:236:LYS:N	1.72	1.45
1:B:212:PRO:CB	1:C:183:ILE:O	1.63	1.44
1:A:215:GLY:N	1:B:271:LEU:CD1	1.80	1.44
1:E:213:ASP:C	1:F:274:ARG:HG3	1.22	1.44
1:B:220:VAL:HG21	1:C:437:THR:CG2	1.46	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:GLU:OE1	1:E:433:ALA:CA	1.65	1.44
1:E:214:ALA:N	1:F:274:ARG:HG3	1.24	1.43
1:A:220:VAL:HG22	1:B:252:LYS:CG	1.43	1.43
1:D:233:GLU:OE1	1:E:433:ALA:CB	1.64	1.43
1:E:232:GLY:C	1:F:252:LYS:HB2	1.36	1.43
1:E:210:VAL:HA	1:F:182:ILE:CA	1.46	1.42
1:A:215:GLY:CA	1:B:271:LEU:CD1	1.95	1.42
1:E:233:GLU:N	1:F:252:LYS:CB	1.81	1.42
1:C:214:ALA:CB	1:D:271:LEU:HA	1.46	1.42
1:E:241:GLU:HG3	1:F:179:SER:CB	1.47	1.42
1:C:331:ARG:CZ	1:D:376:GLN:NE2	1.83	1.42
1:A:233:GLU:HG2	1:B:434:TYR:N	1.10	1.41
1:C:216:LYS:N	1:D:275:LEU:HA	1.26	1.41
1:D:217:ALA:N	1:E:278:ALA:CB	1.79	1.41
1:D:211:GLU:CA	1:E:182:ILE:HG12	1.20	1.41
1:E:232:GLY:C	1:F:252:LYS:CB	1.89	1.40
1:A:331:ARG:NH1	1:B:355:ASP:HB3	1.29	1.40
1:A:220:VAL:HG23	1:B:251:ALA:C	1.36	1.39
1:E:214:ALA:N	1:F:274:ARG:CG	1.85	1.39
1:C:233:GLU:OE1	1:D:252:LYS:CB	1.71	1.39
1:B:210:VAL:HG12	1:C:182:ILE:CA	1.53	1.38
1:D:235:VAL:CA	1:E:271:LEU:HD11	1.51	1.38
1:E:213:ASP:OD1	1:F:274:ARG:CD	1.66	1.38
1:C:221:ALA:CA	1:D:248:LYS:HB2	1.53	1.38
1:A:331:ARG:HH12	1:B:355:ASP:CB	1.36	1.37
1:E:213:ASP:CA	1:F:274:ARG:CD	2.00	1.37
1:E:214:ALA:CB	1:F:271:LEU:CA	2.00	1.37
1:A:362:TRP:CH2	1:B:362:TRP:CD1	2.11	1.36
1:A:361:GLU:HG2	1:B:363:GLN:CD	1.43	1.36
1:A:235:VAL:CG2	1:B:271:LEU:HD22	1.54	1.36
1:D:214:ALA:H	1:E:274:ARG:CG	1.37	1.36
1:A:183:ILE:N	1:F:211:GLU:O	1.58	1.35
1:D:237:GLY:HA2	1:E:267:LEU:CD1	1.57	1.35
1:C:220:VAL:CG2	1:D:250:ALA:O	1.73	1.34
1:D:207:THR:OG1	1:E:177:ILE:N	1.60	1.34
1:A:176:THR:HA	1:F:205:ILE:CG2	1.55	1.34
1:B:233:GLU:OE1	1:C:433:ALA:CB	1.72	1.34
1:A:235:VAL:CG2	1:B:271:LEU:CD2	2.04	1.34
1:C:235:VAL:HG23	1:D:271:LEU:CD1	1.56	1.34
1:A:217:ALA:CA	1:B:275:LEU:HB3	1.45	1.34
1:A:217:ALA:CB	1:B:275:LEU:HB3	1.56	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ASP:O	1:C:274:ARG:NH2	1.59	1.33
1:C:218:THR:HG22	1:D:251:ALA:CB	1.55	1.33
1:D:216:LYS:O	1:E:275:LEU:HA	1.27	1.33
1:A:216:LYS:H	1:B:275:LEU:CD2	1.41	1.33
1:A:219:TRP:CD1	1:B:279:HIS:HE1	1.47	1.33
1:E:228:ASP:HB3	1:F:252:LYS:NZ	1.39	1.33
1:A:221:ALA:O	1:B:439:ARG:NH1	1.57	1.33
1:C:216:LYS:CE	1:D:278:ALA:CB	2.05	1.33
1:B:220:VAL:CG2	1:C:437:THR:CG2	2.01	1.32
1:D:235:VAL:HG21	1:E:255:ILE:CB	1.58	1.32
1:B:217:ALA:N	1:C:275:LEU:CD2	1.91	1.32
1:A:220:VAL:CG2	1:B:252:LYS:CG	2.00	1.32
1:C:227:THR:OG1	1:D:435:TYR:CZ	1.78	1.32
1:D:212:PRO:CB	1:E:183:ILE:O	1.78	1.32
1:C:218:THR:CG2	1:D:251:ALA:HB2	1.59	1.31
1:C:216:LYS:CA	1:D:278:ALA:HB3	1.60	1.31
1:D:235:VAL:CG2	1:E:255:ILE:HD12	1.59	1.31
1:E:213:ASP:CA	1:F:274:ARG:HD2	1.55	1.31
1:B:217:ALA:CB	1:C:436:VAL:HG21	1.59	1.31
1:E:234:GLU:N	1:F:253:SER:CB	1.93	1.31
1:E:217:ALA:HB1	1:F:279:HIS:CB	1.60	1.30
1:A:210:VAL:CG1	1:B:182:ILE:HA	1.60	1.30
1:B:217:ALA:HB1	1:C:436:VAL:CG2	1.62	1.30
1:C:220:VAL:N	1:D:250:ALA:N	1.79	1.30
1:D:233:GLU:CD	1:E:434:TYR:N	1.86	1.30
1:D:237:GLY:CA	1:E:267:LEU:HD11	1.62	1.29
1:A:271:LEU:HD12	1:F:215:GLY:N	1.45	1.29
1:C:211:GLU:OE2	1:D:270:LEU:HD23	1.18	1.29
1:E:211:GLU:HG3	1:F:182:ILE:CB	1.61	1.29
1:C:233:GLU:OE1	1:D:252:LYS:HB2	1.27	1.29
1:D:235:VAL:CG2	1:E:255:ILE:HB	1.61	1.29
1:A:352:ALA:HB1	1:F:332:ARG:NE	1.47	1.29
1:C:221:ALA:CA	1:D:248:LYS:CB	2.07	1.28
1:D:212:PRO:HB3	1:E:183:ILE:O	1.28	1.28
1:D:212:PRO:HA	1:E:182:ILE:CD1	1.63	1.28
1:B:210:VAL:CG1	1:C:182:ILE:HA	1.62	1.28
1:D:235:VAL:HA	1:E:271:LEU:CD1	1.60	1.28
1:B:233:GLU:OE2	1:C:435:TYR:CE2	1.86	1.28
1:B:212:PRO:CG	1:C:183:ILE:O	1.80	1.28
1:D:235:VAL:HG11	1:E:255:ILE:CA	1.64	1.28
1:E:220:VAL:HG23	1:F:250:ALA:C	1.49	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ASP:CA	1:D:274:ARG:CD	1.79	1.27
1:D:235:VAL:HG21	1:E:255:ILE:CD1	1.62	1.27
1:D:214:ALA:N	1:E:274:ARG:HG3	1.48	1.27
1:A:362:TRP:C	1:F:360:GLU:OE1	1.72	1.27
1:D:207:THR:N	1:E:177:ILE:HB	0.94	1.27
1:D:212:PRO:CA	1:E:182:ILE:CD1	2.12	1.26
1:A:212:PRO:O	1:B:184:ARG:HG2	1.17	1.26
1:A:361:GLU:CG	1:B:363:GLN:OE1	1.83	1.26
1:A:216:LYS:N	1:B:275:LEU:HD23	1.47	1.26
1:A:214:ALA:O	1:B:274:ARG:HB2	1.11	1.26
1:D:235:VAL:CG1	1:E:255:ILE:HA	1.63	1.26
1:D:208:MET:HA	1:E:178:PHE:O	1.35	1.26
1:E:232:GLY:CA	1:F:252:LYS:CB	2.13	1.26
1:A:279:HIS:HE1	1:F:219:TRP:CD1	1.53	1.26
1:A:217:ALA:HB3	1:B:275:LEU:C	1.53	1.25
1:C:209:LEU:O	1:D:179:SER:CB	1.82	1.25
1:E:213:ASP:HA	1:F:274:ARG:CG	1.65	1.25
1:A:210:VAL:HA	1:B:181:ARG:O	1.37	1.25
1:D:216:LYS:C	1:E:275:LEU:HA	1.57	1.25
1:A:178:PHE:O	1:F:208:MET:HA	1.37	1.24
1:A:182:ILE:CA	1:F:211:GLU:O	1.85	1.24
1:A:215:GLY:H	1:B:271:LEU:CD1	1.45	1.24
1:E:214:ALA:N	1:F:274:ARG:CB	1.97	1.24
1:D:233:GLU:OE2	1:E:434:TYR:N	1.67	1.24
1:A:178:PHE:CG	1:F:207:THR:HG22	1.71	1.24
1:A:271:LEU:HD12	1:F:214:ALA:C	1.58	1.24
1:A:275:LEU:HD11	1:F:234:GLU:O	1.37	1.24
1:A:275:LEU:HD22	1:F:217:ALA:N	1.53	1.23
1:C:235:VAL:CG2	1:D:271:LEU:CD1	2.10	1.23
1:B:227:THR:HB	1:C:252:LYS:CD	1.52	1.23
1:E:217:ALA:HB3	1:F:279:HIS:N	1.52	1.23
1:A:217:ALA:H	1:B:275:LEU:CD2	1.51	1.23
1:C:208:MET:HA	1:D:179:SER:N	1.53	1.23
1:E:233:GLU:OE2	1:F:252:LYS:HE2	1.33	1.23
1:A:178:PHE:C	1:F:208:MET:CA	1.92	1.23
1:A:214:ALA:O	1:B:274:ARG:CB	1.86	1.22
1:D:232:GLY:O	1:E:252:LYS:O	1.54	1.22
1:A:275:LEU:HD23	1:F:216:LYS:CA	1.67	1.22
1:E:227:THR:O	1:F:252:LYS:CD	1.88	1.22
1:A:233:GLU:HG3	1:B:434:TYR:O	1.38	1.22
1:A:362:TRP:CH2	1:B:362:TRP:CG	2.27	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:H	1:D:275:LEU:CD1	1.53	1.22
1:A:352:ALA:HB1	1:F:332:ARG:CD	1.68	1.22
1:C:219:TRP:HZ2	1:D:282:SER:O	0.86	1.21
1:D:215:GLY:CA	1:E:275:LEU:HD23	1.69	1.21
1:E:232:GLY:C	1:F:252:LYS:CA	1.93	1.21
1:C:216:LYS:HA	1:D:278:ALA:CB	1.70	1.21
1:C:216:LYS:HE3	1:D:278:ALA:CA	1.70	1.21
1:E:233:GLU:N	1:F:252:LYS:HB2	1.42	1.21
1:A:233:GLU:OE1	1:B:433:ALA:HB1	1.05	1.21
1:B:234:GLU:O	1:C:275:LEU:HD11	1.39	1.21
1:B:210:VAL:CG1	1:C:182:ILE:CA	2.18	1.21
1:E:211:GLU:CG	1:F:182:ILE:CD1	1.95	1.21
1:A:235:VAL:CB	1:B:271:LEU:HD21	1.70	1.20
1:A:220:VAL:HG23	1:B:251:ALA:O	1.35	1.20
1:C:214:ALA:HB3	1:D:271:LEU:HA	1.22	1.20
1:A:250:ALA:N	1:F:219:TRP:HB3	1.35	1.20
1:C:213:ASP:HA	1:D:274:ARG:CD	1.05	1.20
1:C:216:LYS:N	1:D:275:LEU:HD12	1.55	1.20
1:B:227:THR:OG1	1:C:252:LYS:HE2	1.39	1.20
1:C:221:ALA:O	1:D:248:LYS:HG2	1.03	1.20
1:E:213:ASP:CA	1:F:274:ARG:HG3	1.70	1.20
1:D:214:ALA:N	1:E:274:ARG:CG	1.99	1.20
1:A:233:GLU:CG	1:B:434:TYR:N	2.03	1.20
1:B:217:ALA:CA	1:C:275:LEU:HD22	1.71	1.19
1:D:232:GLY:O	1:E:252:LYS:HG3	1.40	1.19
1:C:209:LEU:O	1:D:179:SER:HB3	1.42	1.19
1:D:216:LYS:O	1:E:275:LEU:CA	1.89	1.19
1:A:254:PHE:CD1	1:F:233:GLU:OE1	1.94	1.19
1:A:215:GLY:N	1:B:271:LEU:HD12	0.87	1.19
1:A:215:GLY:O	1:B:274:ARG:HB3	1.37	1.19
1:D:211:GLU:C	1:E:182:ILE:CD1	2.11	1.19
1:E:232:GLY:O	1:F:252:LYS:N	1.59	1.18
1:A:271:LEU:O	1:F:214:ALA:O	1.61	1.18
1:A:275:LEU:HD23	1:F:216:LYS:N	0.87	1.18
1:B:212:PRO:CB	1:C:183:ILE:C	2.10	1.18
1:C:227:THR:O	1:D:252:LYS:HD2	1.44	1.18
1:B:233:GLU:OE1	1:C:433:ALA:HB1	1.05	1.18
1:A:216:LYS:NZ	1:B:278:ALA:N	1.81	1.18
1:E:217:ALA:CB	1:F:279:HIS:CB	2.18	1.17
1:E:221:ALA:HA	1:F:248:LYS:CB	1.74	1.17
1:A:178:PHE:C	1:F:208:MET:HA	1.22	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:O	1:D:279:HIS:N	1.76	1.17
1:D:219:TRP:CZ2	1:E:286:ALA:HB2	1.79	1.17
1:C:227:THR:OG1	1:D:435:TYR:CE2	1.96	1.17
1:D:223:SER:N	1:E:439:ARG:NH1	1.93	1.16
1:E:207:THR:OG1	1:F:177:ILE:O	1.62	1.16
1:B:232:GLY:O	1:C:253:SER:HA	1.38	1.16
1:C:216:LYS:HE3	1:D:278:ALA:HB1	1.20	1.16
1:C:221:ALA:O	1:D:248:LYS:CG	1.92	1.16
1:E:208:MET:C	1:F:180:GLN:H	1.47	1.16
1:D:233:GLU:OE2	1:E:434:TYR:C	1.85	1.16
1:E:205:ILE:CG2	1:F:177:ILE:HG12	1.75	1.16
1:A:233:GLU:OE1	1:B:433:ALA:CB	1.92	1.16
1:B:214:ALA:C	1:C:271:LEU:HA	1.66	1.16
1:E:227:THR:O	1:F:252:LYS:HD2	1.00	1.16
1:A:220:VAL:HG12	1:B:437:THR:CG2	1.74	1.15
1:D:212:PRO:CB	1:E:182:ILE:HD13	1.74	1.15
1:C:215:GLY:HA3	1:D:275:LEU:N	1.60	1.15
1:E:225:TYR:HA	1:F:422:GLU:OE2	1.47	1.15
1:A:231:THR:O	1:B:252:LYS:HB2	1.46	1.15
1:A:215:GLY:HA2	1:B:271:LEU:CD1	1.75	1.15
1:A:234:GLU:HB2	1:B:275:LEU:HD22	1.18	1.15
1:D:206:LEU:HA	1:E:177:ILE:CG1	1.76	1.15
1:D:232:GLY:O	1:E:252:LYS:C	1.83	1.15
1:D:235:VAL:CB	1:E:255:ILE:HB	1.76	1.15
1:A:217:ALA:CB	1:B:275:LEU:CB	2.25	1.15
1:D:233:GLU:OE1	1:E:433:ALA:HB1	1.21	1.15
1:A:226:GLY:HA3	1:B:424:GLU:OE1	1.45	1.14
1:E:228:ASP:CB	1:F:252:LYS:HZ3	1.57	1.14
1:A:271:LEU:HD13	1:F:236:LYS:N	1.36	1.14
1:E:232:GLY:C	1:F:252:LYS:N	1.97	1.14
1:C:220:VAL:H	1:D:250:ALA:N	1.37	1.14
1:A:184:ARG:HA	1:F:212:PRO:O	1.46	1.14
1:B:235:VAL:HG11	1:C:255:ILE:HG12	1.30	1.14
1:A:271:LEU:HA	1:F:214:ALA:CB	1.78	1.13
1:B:233:GLU:OE2	1:C:435:TYR:CD2	2.01	1.13
1:A:219:TRP:CD1	1:B:279:HIS:CE1	2.37	1.13
1:A:362:TRP:HH2	1:B:362:TRP:CG	1.64	1.13
1:E:211:GLU:HG2	1:F:182:ILE:HD13	1.26	1.13
1:E:219:TRP:HB3	1:F:249:LEU:HA	1.27	1.13
1:B:217:ALA:N	1:C:275:LEU:HD23	1.54	1.13
1:B:209:LEU:O	1:C:180:GLN:C	1.86	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:TYR:O	1:F:233:GLU:HG3	1.45	1.13
1:D:235:VAL:HB	1:E:254:PHE:O	1.45	1.12
1:A:352:ALA:CB	1:F:332:ARG:CD	2.27	1.12
1:B:207:THR:OG1	1:C:177:ILE:HB	1.49	1.12
1:A:217:ALA:HB2	1:B:275:LEU:HB3	1.28	1.12
1:E:220:VAL:HG23	1:F:251:ALA:N	1.64	1.12
1:C:234:GLU:HB2	1:D:275:LEU:HD11	1.15	1.12
1:A:362:TRP:CA	1:F:360:GLU:OE1	1.94	1.12
1:C:219:TRP:CD1	1:D:249:LEU:HD13	1.84	1.12
1:C:216:LYS:CE	1:D:278:ALA:HB1	1.71	1.12
1:A:178:PHE:CG	1:F:207:THR:CG2	2.28	1.12
1:A:352:ALA:CB	1:F:332:ARG:HD2	1.79	1.12
1:D:236:LYS:N	1:E:271:LEU:HD12	1.65	1.12
1:B:220:VAL:HG21	1:C:437:THR:HG23	1.27	1.12
1:A:217:ALA:CA	1:B:275:LEU:CB	2.25	1.12
1:D:216:LYS:C	1:E:278:ALA:HB3	1.70	1.12
1:E:214:ALA:H	1:F:274:ARG:HB3	1.09	1.11
1:A:178:PHE:CD2	1:F:207:THR:HG21	1.58	1.11
1:B:209:LEU:O	1:C:180:GLN:O	1.66	1.11
1:C:217:ALA:CB	1:D:279:HIS:CB	2.09	1.11
1:E:214:ALA:O	1:F:274:ARG:CB	1.98	1.11
1:D:233:GLU:OE2	1:E:434:TYR:CA	1.99	1.11
1:B:217:ALA:CB	1:C:275:LEU:HB3	1.80	1.11
1:C:234:GLU:HB2	1:D:275:LEU:CD1	1.80	1.11
1:B:220:VAL:CG1	1:C:251:ALA:O	1.98	1.11
1:D:235:VAL:HG23	1:E:271:LEU:HD13	1.20	1.11
1:E:205:ILE:HG22	1:F:177:ILE:HG12	1.25	1.11
1:A:236:LYS:H	1:B:271:LEU:HD13	1.13	1.11
1:B:227:THR:CB	1:C:252:LYS:HD3	1.81	1.10
1:A:217:ALA:HB2	1:B:275:LEU:CB	1.79	1.10
1:A:236:LYS:H	1:B:271:LEU:CD1	1.65	1.10
1:C:209:LEU:O	1:D:179:SER:OG	1.68	1.10
1:E:220:VAL:CG1	1:F:435:TYR:HE1	1.64	1.10
1:E:214:ALA:HB1	1:F:271:LEU:HG	1.31	1.10
1:E:214:ALA:H	1:F:274:ARG:CG	1.54	1.10
1:D:214:ALA:H	1:E:274:ARG:HG2	0.95	1.10
1:A:182:ILE:CB	1:F:211:GLU:O	2.00	1.10
1:D:215:GLY:HA3	1:E:275:LEU:HD23	1.32	1.09
1:A:271:LEU:HD11	1:F:236:LYS:N	1.66	1.09
1:A:219:TRP:HD1	1:B:279:HIS:CE1	1.70	1.09
1:B:209:LEU:N	1:C:180:GLN:H	1.50	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:VAL:HG13	1:D:182:ILE:HA	1.12	1.09
1:D:232:GLY:HA2	1:E:252:LYS:HE2	1.23	1.09
1:B:217:ALA:HA	1:C:275:LEU:HD22	1.26	1.09
1:C:214:ALA:HB1	1:D:271:LEU:HA	1.25	1.09
1:A:250:ALA:N	1:F:219:TRP:CB	1.78	1.09
1:C:235:VAL:HG23	1:D:271:LEU:CD2	1.83	1.09
1:D:232:GLY:O	1:E:252:LYS:CG	2.01	1.09
1:C:215:GLY:CA	1:D:275:LEU:HB2	1.82	1.09
1:A:206:LEU:HA	1:B:177:ILE:CG1	1.81	1.09
1:B:215:GLY:N	1:C:271:LEU:HA	1.66	1.09
1:C:211:GLU:OE2	1:D:270:LEU:CD2	1.99	1.09
1:C:207:THR:O	1:D:177:ILE:HG22	1.53	1.09
1:B:217:ALA:HB2	1:C:275:LEU:HB3	1.29	1.09
1:B:212:PRO:HG3	1:C:183:ILE:O	1.48	1.08
1:D:215:GLY:N	1:E:271:LEU:HG	1.68	1.08
1:A:214:ALA:C	1:B:271:LEU:HA	1.73	1.08
1:C:221:ALA:HA	1:D:248:LYS:HB3	1.21	1.08
1:D:206:LEU:C	1:E:177:ILE:HB	1.73	1.08
1:C:220:VAL:N	1:D:250:ALA:H	1.46	1.08
1:A:207:THR:CB	1:B:177:ILE:N	2.16	1.08
1:C:210:VAL:CG1	1:D:182:ILE:HA	1.84	1.08
1:A:271:LEU:HA	1:F:214:ALA:C	1.73	1.08
1:B:210:VAL:HG12	1:C:182:ILE:C	1.74	1.08
1:D:211:GLU:CA	1:E:182:ILE:CG1	2.13	1.08
1:E:234:GLU:O	1:F:253:SER:HB3	1.53	1.08
1:A:233:GLU:HG2	1:B:434:TYR:CA	1.84	1.08
1:A:216:LYS:NZ	1:B:277:GLU:C	2.07	1.08
1:A:271:LEU:HA	1:F:214:ALA:O	1.53	1.08
1:A:222:ALA:C	1:B:439:ARG:NH1	2.08	1.07
1:E:234:GLU:O	1:F:253:SER:CB	2.02	1.07
1:A:210:VAL:HG12	1:B:182:ILE:HA	1.32	1.07
1:A:233:GLU:HG3	1:B:434:TYR:C	1.74	1.07
1:D:237:GLY:HA2	1:E:267:LEU:HD11	1.11	1.07
1:C:219:TRP:HB3	1:D:249:LEU:CD2	1.85	1.07
1:C:214:ALA:CB	1:D:271:LEU:CA	2.31	1.07
1:A:362:TRP:CH2	1:B:362:TRP:CB	2.37	1.07
1:C:227:THR:CB	1:D:435:TYR:CZ	2.38	1.07
1:E:206:LEU:HA	1:F:177:ILE:HG21	1.34	1.07
1:A:254:PHE:CG	1:F:233:GLU:OE1	2.07	1.07
1:A:275:LEU:CD2	1:F:217:ALA:N	2.18	1.07
1:A:212:PRO:O	1:B:184:ARG:CG	2.01	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:N	1:D:275:LEU:CA	2.18	1.07
1:A:271:LEU:CA	1:F:214:ALA:HB3	1.84	1.07
1:A:279:HIS:CE1	1:F:219:TRP:CD1	2.43	1.07
1:A:216:LYS:H	1:B:275:LEU:CG	1.66	1.07
1:B:235:VAL:CG1	1:C:255:ILE:HG12	1.84	1.07
1:A:222:ALA:C	1:B:439:ARG:HH12	1.55	1.07
1:C:216:LYS:CD	1:D:278:ALA:CB	2.32	1.07
1:E:213:ASP:OD1	1:F:274:ARG:HD3	0.89	1.07
1:B:234:GLU:C	1:C:275:LEU:HD21	1.75	1.06
1:A:176:THR:HG23	1:F:205:ILE:HG21	1.35	1.06
1:A:271:LEU:CA	1:F:214:ALA:CB	2.33	1.06
1:B:233:GLU:OE1	1:C:433:ALA:CA	2.02	1.06
1:A:275:LEU:HA	1:F:216:LYS:CA	1.86	1.06
1:D:235:VAL:CB	1:E:254:PHE:O	2.02	1.06
1:D:208:MET:HA	1:E:178:PHE:C	1.57	1.06
1:A:176:THR:HA	1:F:205:ILE:HG23	1.34	1.06
1:D:206:LEU:HA	1:E:177:ILE:HG13	1.34	1.06
1:B:232:GLY:O	1:C:253:SER:CA	2.01	1.06
1:B:209:LEU:H	1:C:180:GLN:N	1.53	1.05
1:C:213:ASP:CA	1:D:274:ARG:HD2	1.74	1.05
1:D:211:GLU:O	1:E:182:ILE:HD11	1.54	1.05
1:C:219:TRP:C	1:D:250:ALA:H	1.60	1.05
1:D:207:THR:CB	1:E:177:ILE:N	2.09	1.05
1:D:232:GLY:C	1:E:252:LYS:HG3	1.56	1.05
1:E:214:ALA:HB2	1:F:271:LEU:HA	1.09	1.05
1:A:212:PRO:HB2	1:B:184:ARG:HA	1.34	1.05
1:E:211:GLU:CG	1:F:182:ILE:HB	1.86	1.05
1:A:178:PHE:O	1:F:208:MET:CA	2.00	1.05
1:A:206:LEU:HA	1:B:177:ILE:HG13	1.34	1.05
1:C:216:LYS:H	1:D:275:LEU:HD12	0.92	1.05
1:D:210:VAL:HG13	1:E:182:ILE:CB	1.84	1.05
1:A:215:GLY:HA2	1:B:271:LEU:HD11	1.38	1.05
1:E:219:TRP:C	1:F:250:ALA:O	1.94	1.05
1:A:220:VAL:HG12	1:B:437:THR:HG21	1.33	1.05
1:E:228:ASP:CB	1:F:252:LYS:NZ	2.15	1.05
1:A:271:LEU:N	1:F:214:ALA:HB3	1.71	1.05
1:D:210:VAL:CG1	1:E:182:ILE:CB	2.35	1.04
1:E:214:ALA:HB3	1:F:271:LEU:HA	1.12	1.04
1:A:361:GLU:CG	1:B:363:GLN:CD	2.23	1.04
1:D:211:GLU:O	1:E:182:ILE:CD1	2.05	1.04
1:D:235:VAL:CG2	1:E:255:ILE:CD1	2.27	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:PRO:HA	1:E:182:ILE:HD11	1.37	1.04
1:E:234:GLU:N	1:F:253:SER:HB3	1.71	1.04
1:B:215:GLY:N	1:C:271:LEU:HD12	1.72	1.04
1:C:220:VAL:CG2	1:D:250:ALA:C	2.26	1.04
1:C:219:TRP:CA	1:D:250:ALA:H	1.70	1.04
1:C:220:VAL:HG23	1:D:250:ALA:O	0.88	1.04
1:D:215:GLY:HA3	1:E:275:LEU:CD2	1.86	1.04
1:A:217:ALA:H	1:B:275:LEU:HD22	1.21	1.04
1:A:253:SER:H	1:F:233:GLU:HG3	1.20	1.04
1:C:217:ALA:H	1:D:275:LEU:CD1	1.71	1.04
1:D:217:ALA:H	1:E:278:ALA:HB1	0.92	1.04
1:E:227:THR:C	1:F:252:LYS:HD2	1.77	1.04
1:A:361:GLU:HG2	1:B:363:GLN:CG	1.88	1.04
1:D:232:GLY:CA	1:E:252:LYS:HE2	1.82	1.04
1:A:234:GLU:HB2	1:B:275:LEU:CD2	1.88	1.04
1:B:232:GLY:HA3	1:C:254:PHE:CD1	1.92	1.03
1:D:216:LYS:HG3	1:E:278:ALA:HB1	1.38	1.03
1:D:233:GLU:OE1	1:E:433:ALA:HA	1.58	1.03
1:D:236:LYS:H	1:E:271:LEU:CD1	1.72	1.03
1:B:210:VAL:HG12	1:C:182:ILE:HA	1.08	1.03
1:E:214:ALA:HB1	1:F:271:LEU:HA	1.37	1.03
1:C:217:ALA:N	1:D:275:LEU:HD12	1.74	1.03
1:A:439:ARG:NH1	1:F:221:ALA:O	1.89	1.03
1:B:235:VAL:CG1	1:C:255:ILE:HG21	1.87	1.03
1:E:221:ALA:HA	1:F:248:LYS:HB2	1.35	1.03
1:C:235:VAL:HG22	1:D:271:LEU:HD11	1.08	1.03
1:E:217:ALA:HB3	1:F:279:HIS:CA	1.88	1.03
1:C:219:TRP:CB	1:D:249:LEU:HD22	1.87	1.03
1:B:212:PRO:HB3	1:C:183:ILE:C	1.75	1.03
1:A:233:GLU:CG	1:B:434:TYR:C	2.27	1.03
1:D:235:VAL:CG2	1:E:271:LEU:HD13	1.88	1.02
1:E:227:THR:OG1	1:F:435:TYR:CZ	2.13	1.02
1:C:207:THR:HB	1:D:177:ILE:O	1.58	1.02
1:D:208:MET:CA	1:E:179:SER:HA	1.90	1.02
1:D:210:VAL:HG13	1:E:182:ILE:CA	1.88	1.02
1:C:215:GLY:HA3	1:D:275:LEU:CA	1.88	1.02
1:A:220:VAL:CG2	1:B:251:ALA:O	2.07	1.02
1:C:232:GLY:HA2	1:D:251:ALA:HA	1.39	1.02
1:B:220:VAL:HG13	1:C:436:VAL:O	1.57	1.02
1:B:212:PRO:HB3	1:C:183:ILE:N	1.74	1.02
1:B:210:VAL:CG1	1:C:182:ILE:C	2.26	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:CA	1:B:271:LEU:HD21	1.90	1.02
1:B:241:GLU:OE2	1:C:178:PHE:HB3	1.57	1.02
1:E:211:GLU:HG3	1:F:182:ILE:CG1	1.89	1.02
1:A:233:GLU:CG	1:B:434:TYR:H	1.66	1.01
1:B:212:PRO:HB2	1:C:183:ILE:C	1.80	1.01
1:C:216:LYS:CG	1:D:278:ALA:HB1	1.90	1.01
1:D:216:LYS:CA	1:E:275:LEU:HA	1.90	1.01
1:A:331:ARG:CZ	1:B:355:ASP:HB3	1.90	1.01
1:A:217:ALA:N	1:B:275:LEU:CD2	2.22	1.01
1:A:434:TYR:H	1:F:233:GLU:HG2	1.18	1.01
1:E:222:ALA:HB3	1:F:439:ARG:NH2	1.75	1.01
1:E:225:TYR:CA	1:F:422:GLU:OE2	2.07	1.01
1:A:210:VAL:HG13	1:B:182:ILE:HA	1.38	1.01
1:A:220:VAL:HG13	1:B:252:LYS:HE3	1.37	1.01
1:A:362:TRP:CZ2	1:B:362:TRP:CB	2.44	1.01
1:D:211:GLU:O	1:E:182:ILE:CG1	2.08	1.01
1:A:182:ILE:HB	1:F:211:GLU:O	1.59	1.01
1:A:217:ALA:CB	1:B:275:LEU:C	2.27	1.01
1:B:234:GLU:O	1:C:275:LEU:HD21	1.61	1.01
1:E:223:SER:OG	1:F:439:ARG:NH1	1.94	1.01
1:A:181:ARG:N	1:F:211:GLU:OE2	1.93	1.01
1:E:221:ALA:O	1:F:248:LYS:HG2	1.59	1.01
1:B:214:ALA:HB3	1:C:270:LEU:C	1.80	1.01
1:A:362:TRP:CZ2	1:B:362:TRP:CG	2.49	1.01
1:C:216:LYS:CD	1:D:278:ALA:HB1	1.91	1.01
1:A:362:TRP:CH2	1:B:362:TRP:HB2	1.95	1.00
1:D:215:GLY:CA	1:E:275:LEU:CD2	2.39	1.00
1:C:234:GLU:O	1:D:253:SER:HB3	1.61	1.00
1:C:216:LYS:CE	1:D:278:ALA:HB2	1.86	1.00
1:E:213:ASP:CB	1:F:274:ARG:HD3	1.89	1.00
1:A:216:LYS:HZ1	1:B:277:GLU:C	1.64	1.00
1:D:235:VAL:CG2	1:E:255:ILE:CG1	2.39	1.00
1:E:220:VAL:CG2	1:F:250:ALA:C	2.26	1.00
1:C:331:ARG:NH1	1:D:376:GLN:NE2	2.09	1.00
1:E:205:ILE:CG2	1:F:177:ILE:CG1	2.39	1.00
1:A:178:PHE:CZ	1:F:207:THR:HG21	1.96	1.00
1:B:235:VAL:HG12	1:C:255:ILE:HG21	1.44	1.00
1:D:221:ALA:HA	1:E:248:LYS:HB3	1.42	1.00
1:E:205:ILE:HG23	1:F:177:ILE:CG1	1.90	1.00
1:D:208:MET:CA	1:E:178:PHE:C	2.29	1.00
1:A:220:VAL:CG1	1:B:437:THR:CG2	2.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ALA:HB2	1:F:332:ARG:HD2	1.41	1.00
1:A:222:ALA:HB2	1:B:437:THR:HG21	1.44	0.99
1:C:235:VAL:HG23	1:D:271:LEU:HD21	1.42	0.99
1:B:220:VAL:HG22	1:C:436:VAL:O	1.61	0.99
1:A:178:PHE:CE2	1:F:207:THR:CG2	2.19	0.99
1:B:231:THR:O	1:C:252:LYS:HB2	1.62	0.99
1:A:207:THR:HB	1:B:177:ILE:N	1.49	0.99
1:B:212:PRO:HB3	1:C:183:ILE:O	1.55	0.99
1:C:214:ALA:HB1	1:D:271:LEU:CA	1.91	0.99
1:A:220:VAL:CG2	1:B:251:ALA:C	2.29	0.99
1:B:217:ALA:HB1	1:C:436:VAL:HG21	1.17	0.99
1:A:249:LEU:HB3	1:F:219:TRP:CD1	1.98	0.99
1:C:217:ALA:HB1	1:D:279:HIS:HB2	1.42	0.99
1:C:220:VAL:HG23	1:D:250:ALA:C	1.81	0.99
1:B:220:VAL:HG23	1:C:437:THR:HG22	0.99	0.99
1:C:233:GLU:HB3	1:D:254:PHE:N	1.78	0.99
1:C:235:VAL:HG23	1:D:271:LEU:HD11	1.00	0.99
1:E:222:ALA:CB	1:F:439:ARG:HH22	1.76	0.99
1:A:216:LYS:H	1:B:275:LEU:HD23	1.04	0.98
1:C:215:GLY:HA3	1:D:275:LEU:CB	1.92	0.98
1:E:220:VAL:CG2	1:F:251:ALA:N	2.25	0.98
1:E:205:ILE:O	1:F:177:ILE:HG13	1.62	0.98
1:A:271:LEU:HD13	1:F:236:LYS:CA	1.92	0.98
1:C:219:TRP:HB3	1:D:249:LEU:HD22	1.38	0.98
1:A:217:ALA:O	1:B:279:HIS:HB2	1.62	0.98
1:E:220:VAL:HG23	1:F:251:ALA:CA	1.92	0.98
1:A:362:TRP:HH2	1:B:362:TRP:HD1	1.03	0.98
1:B:234:GLU:O	1:C:275:LEU:CD1	2.10	0.98
1:C:218:THR:O	1:D:279:HIS:CE1	2.15	0.98
1:E:207:THR:HG22	1:F:179:SER:HA	1.44	0.98
1:A:271:LEU:CD1	1:F:215:GLY:N	2.25	0.98
1:A:214:ALA:O	1:B:271:LEU:HA	1.62	0.98
1:E:232:GLY:HA3	1:F:252:LYS:HB2	1.45	0.98
1:E:227:THR:OG1	1:F:435:TYR:CE2	2.17	0.98
1:A:235:VAL:HA	1:B:271:LEU:HD21	1.43	0.98
1:C:223:SER:H	1:D:439:ARG:NH1	1.60	0.98
1:C:220:VAL:HB	1:D:250:ALA:CA	1.94	0.97
1:D:236:LYS:H	1:E:271:LEU:HD12	0.83	0.97
1:A:233:GLU:CG	1:B:434:TYR:O	2.12	0.97
1:B:210:VAL:CG1	1:C:183:ILE:N	2.28	0.97
1:C:331:ARG:CZ	1:D:376:GLN:HE22	1.56	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:VAL:HG23	1:F:250:ALA:O	1.65	0.97
1:A:275:LEU:CD2	1:F:217:ALA:H	1.74	0.97
1:A:361:GLU:HG2	1:B:363:GLN:OE1	1.48	0.97
1:E:233:GLU:N	1:F:252:LYS:HB3	1.79	0.97
1:B:220:VAL:HG13	1:C:251:ALA:O	1.65	0.97
1:A:434:TYR:O	1:F:233:GLU:CG	2.11	0.97
1:B:215:GLY:H	1:C:271:LEU:HD12	1.20	0.97
1:A:218:THR:HG23	1:B:251:ALA:HA	1.46	0.97
1:A:252:LYS:N	1:F:218:THR:H	1.48	0.97
1:A:216:LYS:HA	1:B:274:ARG:C	1.82	0.96
1:E:211:GLU:HG3	1:F:182:ILE:HB	0.98	0.96
1:E:213:ASP:C	1:F:274:ARG:CG	2.17	0.96
1:E:241:GLU:CD	1:F:179:SER:HB3	1.85	0.96
1:C:220:VAL:H	1:D:249:LEU:C	1.66	0.96
1:C:213:ASP:HA	1:D:274:ARG:HD2	1.34	0.96
1:D:215:GLY:O	1:E:274:ARG:HB2	1.62	0.96
1:A:182:ILE:C	1:F:211:GLU:O	2.04	0.96
1:A:271:LEU:HD13	1:F:236:LYS:H	0.83	0.96
1:B:232:GLY:HA2	1:C:252:LYS:HB3	1.44	0.96
1:E:211:GLU:CD	1:F:182:ILE:HD12	1.86	0.96
1:B:207:THR:OG1	1:C:177:ILE:CB	2.12	0.96
1:C:232:GLY:HA3	1:D:252:LYS:HG3	1.43	0.96
1:D:210:VAL:CG1	1:E:182:ILE:HB	1.94	0.96
1:C:215:GLY:C	1:D:275:LEU:HA	1.86	0.96
1:E:220:VAL:CG2	1:F:251:ALA:HA	1.95	0.96
1:C:212:PRO:HB2	1:D:184:ARG:CA	1.96	0.96
1:C:208:MET:HB2	1:D:179:SER:HA	1.44	0.96
1:C:216:LYS:HA	1:D:278:ALA:HB3	0.98	0.96
1:D:233:GLU:CD	1:E:434:TYR:H	1.57	0.96
1:A:176:THR:HG22	1:F:207:THR:OG1	1.64	0.95
1:D:212:PRO:N	1:E:182:ILE:HD13	1.79	0.95
1:A:218:THR:CG2	1:B:252:LYS:H	1.78	0.95
1:A:250:ALA:H	1:F:219:TRP:HB3	0.96	0.95
1:B:233:GLU:HB3	1:C:434:TYR:HB2	1.44	0.95
1:A:184:ARG:CA	1:F:212:PRO:O	2.12	0.95
1:B:216:LYS:CA	1:C:274:ARG:O	2.14	0.95
1:D:223:SER:N	1:E:439:ARG:HH11	1.63	0.95
1:A:331:ARG:HH22	1:B:355:ASP:CG	1.70	0.95
1:C:211:GLU:HB3	1:D:182:ILE:HG12	1.46	0.95
1:C:214:ALA:HB3	1:D:271:LEU:CA	1.95	0.95
1:A:235:VAL:HG23	1:B:271:LEU:HD21	1.42	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ASP:CA	1:F:274:ARG:CG	2.21	0.95
1:D:209:LEU:HB2	1:E:178:PHE:HB2	1.46	0.95
1:E:227:THR:OG1	1:F:435:TYR:OH	1.85	0.95
1:A:275:LEU:HD22	1:F:217:ALA:H	1.21	0.95
1:E:227:THR:CB	1:F:435:TYR:CZ	2.50	0.95
1:A:235:VAL:HG12	1:B:254:PHE:O	1.66	0.94
1:D:233:GLU:OE1	1:E:433:ALA:C	2.05	0.94
1:C:233:GLU:C	1:D:253:SER:HA	1.84	0.94
1:A:254:PHE:CE1	1:F:233:GLU:OE1	2.18	0.94
1:C:219:TRP:CD1	1:D:249:LEU:HB3	2.02	0.94
1:E:232:GLY:HA2	1:F:252:LYS:HG3	1.49	0.94
1:A:252:LYS:O	1:F:217:ALA:HA	1.66	0.94
1:D:215:GLY:O	1:E:274:ARG:CB	2.15	0.94
1:B:220:VAL:CG1	1:C:436:VAL:O	2.16	0.94
1:C:233:GLU:HB3	1:D:253:SER:CA	1.97	0.94
1:E:211:GLU:CG	1:F:182:ILE:CB	2.45	0.94
1:A:176:THR:HA	1:F:205:ILE:HG22	1.48	0.94
1:A:216:LYS:CA	1:B:275:LEU:HD23	1.97	0.94
1:A:220:VAL:HG21	1:B:252:LYS:HG2	0.96	0.94
1:A:220:VAL:HG22	1:B:252:LYS:HG3	0.97	0.94
1:E:206:LEU:CA	1:F:177:ILE:HG21	1.96	0.94
1:E:220:VAL:CG1	1:F:435:TYR:CE1	2.43	0.94
1:E:219:TRP:HB3	1:F:249:LEU:CA	1.97	0.94
1:D:233:GLU:HG2	1:E:434:TYR:O	1.68	0.94
1:A:250:ALA:N	1:F:219:TRP:CD1	2.36	0.94
1:B:207:THR:CB	1:C:177:ILE:CB	2.46	0.94
1:A:271:LEU:HB2	1:F:214:ALA:HB1	1.50	0.94
1:A:216:LYS:N	1:B:275:LEU:CD2	2.16	0.94
1:A:361:GLU:CB	1:B:363:GLN:OE1	2.15	0.93
1:C:215:GLY:HA3	1:D:275:LEU:HB2	1.45	0.93
1:D:232:GLY:C	1:E:252:LYS:CG	2.37	0.93
1:A:217:ALA:HB3	1:B:275:LEU:O	1.67	0.93
1:C:234:GLU:O	1:D:253:SER:CB	2.16	0.93
1:E:220:VAL:CG2	1:F:251:ALA:CA	2.46	0.93
1:E:234:GLU:C	1:F:253:SER:CB	2.36	0.93
1:B:210:VAL:C	1:C:182:ILE:HA	1.86	0.93
1:C:216:LYS:CA	1:D:278:ALA:CB	2.39	0.93
1:E:220:VAL:O	1:F:250:ALA:HB2	1.67	0.93
1:E:214:ALA:O	1:F:274:ARG:HB3	1.68	0.93
1:B:215:GLY:CA	1:C:275:LEU:HG	1.98	0.93
1:D:207:THR:H	1:E:177:ILE:CA	1.78	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:ARG:HD3	1:D:355:ASP:OD2	1.68	0.93
1:C:207:THR:O	1:D:177:ILE:CG2	2.15	0.93
1:B:210:VAL:HG12	1:C:183:ILE:N	1.83	0.92
1:E:233:GLU:OE2	1:F:252:LYS:CE	2.18	0.92
1:A:216:LYS:H	1:B:275:LEU:HG	1.34	0.92
1:C:235:VAL:HG21	1:D:255:ILE:HD12	1.49	0.92
1:A:271:LEU:CG	1:F:236:LYS:H	1.70	0.92
1:E:221:ALA:HA	1:F:248:LYS:HB3	1.47	0.92
1:D:210:VAL:HG13	1:E:182:ILE:HA	1.48	0.92
1:D:210:VAL:HG12	1:E:182:ILE:HB	1.47	0.92
1:E:214:ALA:O	1:F:274:ARG:HB2	1.67	0.92
1:E:228:ASP:HB3	1:F:252:LYS:HZ3	0.76	0.92
1:D:235:VAL:HB	1:E:255:ILE:HB	1.50	0.92
1:B:220:VAL:CG2	1:C:436:VAL:O	2.17	0.92
1:A:271:LEU:CB	1:F:214:ALA:HB1	2.00	0.92
1:E:232:GLY:HA2	1:F:252:LYS:CB	2.00	0.92
1:D:216:LYS:CD	1:E:278:ALA:HB2	2.00	0.92
1:E:207:THR:N	1:F:177:ILE:CG2	2.33	0.92
1:A:434:TYR:N	1:F:233:GLU:HG2	1.83	0.92
1:B:233:GLU:HB3	1:C:434:TYR:CB	1.95	0.91
1:E:213:ASP:CB	1:F:274:ARG:CD	2.46	0.91
1:A:216:LYS:HZ2	1:B:278:ALA:N	1.56	0.91
1:C:216:LYS:CD	1:D:278:ALA:HB2	1.97	0.91
1:C:217:ALA:N	1:D:275:LEU:CD1	2.30	0.91
1:E:219:TRP:HE1	1:F:282:SER:C	1.72	0.91
1:E:232:GLY:HA2	1:F:252:LYS:CG	1.99	0.91
1:B:216:LYS:H	1:C:275:LEU:HD23	1.36	0.91
1:C:233:GLU:OE1	1:D:252:LYS:HB3	1.71	0.91
1:A:182:ILE:HA	1:F:211:GLU:O	1.68	0.91
1:A:275:LEU:HA	1:F:216:LYS:HA	1.50	0.91
1:A:220:VAL:CB	1:B:437:THR:HG22	1.99	0.91
1:A:236:LYS:N	1:B:271:LEU:CD1	2.34	0.91
1:A:271:LEU:CA	1:F:214:ALA:O	2.17	0.90
1:A:234:GLU:O	1:B:275:LEU:HD11	1.72	0.90
1:B:212:PRO:HB2	1:C:183:ILE:O	1.71	0.90
1:B:227:THR:CB	1:C:252:LYS:CD	2.29	0.90
1:E:214:ALA:HB1	1:F:271:LEU:CA	1.96	0.90
1:C:235:VAL:HG23	1:D:271:LEU:CG	2.01	0.90
1:D:235:VAL:HG23	1:E:271:LEU:CD1	2.01	0.90
1:C:219:TRP:HA	1:D:250:ALA:N	1.86	0.90
1:B:237:GLY:N	1:C:267:LEU:HD21	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:GLU:HB3	1:D:253:SER:HA	1.51	0.90
1:D:235:VAL:CG1	1:E:254:PHE:O	2.19	0.90
1:E:220:VAL:O	1:F:250:ALA:CB	2.18	0.90
1:A:275:LEU:CD1	1:F:234:GLU:O	2.20	0.90
1:A:178:PHE:HA	1:F:207:THR:HG22	1.51	0.90
1:B:214:ALA:C	1:C:274:ARG:HB2	1.92	0.90
1:C:215:GLY:HA3	1:D:275:LEU:H	1.28	0.90
1:C:227:THR:OG1	1:D:435:TYR:OH	1.61	0.90
1:E:234:GLU:C	1:F:253:SER:HB3	1.92	0.90
1:E:216:LYS:H	1:F:275:LEU:HD12	1.37	0.90
1:D:212:PRO:HB2	1:E:183:ILE:O	1.73	0.89
1:A:183:ILE:HG13	1:F:212:PRO:HB3	1.53	0.89
1:A:226:GLY:CA	1:B:424:GLU:OE1	2.19	0.89
1:B:212:PRO:C	1:C:182:ILE:HD11	1.71	0.89
1:A:218:THR:HG23	1:B:251:ALA:CA	2.02	0.89
1:C:215:GLY:CA	1:D:275:LEU:N	2.34	0.89
1:A:215:GLY:O	1:B:274:ARG:CB	2.19	0.89
1:A:233:GLU:HG2	1:B:434:TYR:H	1.06	0.89
1:C:207:THR:CG2	1:D:177:ILE:O	2.20	0.89
1:D:209:LEU:HB3	1:E:178:PHE:HD1	1.35	0.89
1:C:223:SER:H	1:D:439:ARG:HH12	0.92	0.89
1:E:205:ILE:C	1:F:177:ILE:HG13	1.92	0.89
1:D:216:LYS:CG	1:E:278:ALA:CB	2.02	0.89
1:E:217:ALA:HB3	1:F:279:HIS:H	1.30	0.89
1:A:217:ALA:HA	1:B:275:LEU:HB3	1.55	0.89
1:B:214:ALA:CB	1:C:270:LEU:HG	2.02	0.89
1:C:208:MET:CA	1:D:179:SER:N	2.35	0.89
1:A:362:TRP:CZ2	1:B:362:TRP:HB3	2.08	0.89
1:B:212:PRO:C	1:C:182:ILE:CD1	1.77	0.89
1:E:214:ALA:HB3	1:F:271:LEU:CA	1.79	0.89
1:E:207:THR:CG2	1:F:178:PHE:C	2.41	0.89
1:B:210:VAL:CA	1:C:182:ILE:HA	2.02	0.88
1:C:219:TRP:CH2	1:D:286:ALA:HB2	2.07	0.88
1:E:211:GLU:CG	1:F:182:ILE:CG1	2.50	0.88
1:E:207:THR:HG21	1:F:178:PHE:C	1.92	0.88
1:E:211:GLU:HG3	1:F:182:ILE:CD1	2.02	0.88
1:D:212:PRO:N	1:E:182:ILE:CD1	2.33	0.88
1:A:279:HIS:HE1	1:F:219:TRP:HD1	1.14	0.88
1:A:221:ALA:O	1:B:439:ARG:CZ	2.21	0.88
1:B:235:VAL:HG12	1:C:255:ILE:CG2	2.02	0.88
1:D:214:ALA:N	1:E:274:ARG:HG2	1.76	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:TRP:CH2	1:E:286:ALA:HB2	2.08	0.88
1:A:216:LYS:HA	1:B:274:ARG:O	1.74	0.88
1:B:232:GLY:HA3	1:C:254:PHE:CE1	2.09	0.88
1:B:234:GLU:HB2	1:C:275:LEU:CD2	2.04	0.88
1:C:210:VAL:CG1	1:D:183:ILE:H	1.86	0.88
1:A:176:THR:CA	1:F:205:ILE:CG2	2.47	0.88
1:B:217:ALA:H	1:C:275:LEU:HD23	0.73	0.88
1:D:235:VAL:CG2	1:E:271:LEU:CD1	2.52	0.88
1:A:178:PHE:HD2	1:F:207:THR:HG22	1.37	0.88
1:D:233:GLU:OE2	1:E:434:TYR:O	1.91	0.88
1:C:233:GLU:OE1	1:D:252:LYS:HD3	1.74	0.87
1:A:235:VAL:CG1	1:B:254:PHE:O	2.22	0.87
1:D:209:LEU:HB3	1:E:178:PHE:CD1	2.09	0.87
1:C:216:LYS:HE3	1:D:278:ALA:HA	1.54	0.87
1:D:219:TRP:NE1	1:E:249:LEU:HD13	1.89	0.87
1:C:234:GLU:H	1:D:253:SER:HB3	1.39	0.87
1:B:215:GLY:N	1:C:274:ARG:HB2	1.88	0.87
1:D:212:PRO:HB3	1:E:182:ILE:HD13	1.54	0.87
1:B:214:ALA:C	1:C:271:LEU:CA	2.43	0.87
1:C:208:MET:CB	1:D:179:SER:HA	2.04	0.87
1:C:215:GLY:HA2	1:D:275:LEU:HB2	1.54	0.87
1:C:223:SER:N	1:D:439:ARG:HH12	1.71	0.87
1:C:219:TRP:CA	1:D:250:ALA:N	2.38	0.87
1:A:207:THR:C	1:B:177:ILE:HG22	1.94	0.87
1:E:222:ALA:HB2	1:F:437:THR:OG1	1.74	0.87
1:B:207:THR:HB	1:C:177:ILE:HG22	1.57	0.87
1:C:233:GLU:CB	1:D:253:SER:HA	2.05	0.87
1:A:217:ALA:O	1:B:275:LEU:O	1.91	0.86
1:B:216:LYS:HA	1:C:274:ARG:O	1.48	0.86
1:A:235:VAL:CG2	1:B:271:LEU:HD21	1.84	0.86
1:E:220:VAL:HG23	1:F:251:ALA:HA	1.53	0.86
1:E:227:THR:HB	1:F:435:TYR:CZ	2.10	0.86
1:E:233:GLU:C	1:F:252:LYS:O	1.99	0.86
1:C:233:GLU:N	1:D:252:LYS:HB2	1.88	0.86
1:D:216:LYS:CB	1:E:278:ALA:HB2	2.05	0.86
1:D:235:VAL:CA	1:E:271:LEU:CD1	2.35	0.86
1:A:214:ALA:O	1:B:274:ARG:CG	2.18	0.86
1:B:236:LYS:O	1:C:274:ARG:NH1	2.08	0.86
1:C:217:ALA:H	1:D:275:LEU:HD12	1.32	0.86
1:C:215:GLY:CA	1:D:275:LEU:CA	2.53	0.86
1:C:215:GLY:CA	1:D:275:LEU:CB	2.51	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:LYS:HA	1:E:274:ARG:O	1.76	0.86
1:B:217:ALA:HB1	1:C:436:VAL:HG23	1.56	0.86
1:B:227:THR:HB	1:C:252:LYS:HD3	0.86	0.86
1:C:227:THR:HB	1:D:435:TYR:CZ	2.11	0.86
1:A:271:LEU:HA	1:F:214:ALA:HB3	1.49	0.86
1:A:233:GLU:CD	1:B:433:ALA:HB1	1.95	0.86
1:E:233:GLU:H	1:F:252:LYS:CB	1.87	0.86
1:D:235:VAL:HG12	1:E:254:PHE:O	1.76	0.85
1:B:213:ASP:O	1:C:274:ARG:CZ	2.12	0.85
1:D:209:LEU:CB	1:E:178:PHE:HB2	2.05	0.85
1:E:207:THR:N	1:F:177:ILE:HG21	1.91	0.85
1:E:214:ALA:CA	1:F:274:ARG:HB2	2.05	0.85
1:C:216:LYS:HE3	1:D:278:ALA:HB2	1.48	0.85
1:C:220:VAL:CB	1:D:250:ALA:C	2.45	0.85
1:A:275:LEU:HA	1:F:216:LYS:C	1.97	0.85
1:B:220:VAL:HG12	1:C:251:ALA:O	1.75	0.85
1:C:207:THR:CB	1:D:177:ILE:O	2.25	0.85
1:C:218:THR:O	1:D:279:HIS:ND1	2.08	0.85
1:A:182:ILE:HB	1:F:211:GLU:C	1.97	0.85
1:A:275:LEU:HD23	1:F:215:GLY:C	1.95	0.85
1:A:235:VAL:HA	1:B:271:LEU:HD11	1.58	0.85
1:D:216:LYS:CB	1:E:278:ALA:CB	2.55	0.85
1:C:210:VAL:HG12	1:D:183:ILE:H	1.42	0.85
1:C:216:LYS:C	1:D:278:ALA:HB3	1.96	0.85
1:D:222:ALA:C	1:E:439:ARG:HH11	1.80	0.84
1:C:233:GLU:OE1	1:D:252:LYS:CD	2.26	0.84
1:A:210:VAL:HG12	1:B:182:ILE:CA	2.07	0.84
1:A:252:LYS:N	1:F:218:THR:N	2.25	0.84
1:B:214:ALA:HB3	1:C:270:LEU:HG	1.57	0.84
1:B:217:ALA:CB	1:C:436:VAL:CG2	2.35	0.84
1:A:215:GLY:HA3	1:B:271:LEU:CD1	2.06	0.84
1:B:207:THR:CB	1:C:177:ILE:HB	2.05	0.84
1:A:214:ALA:C	1:B:274:ARG:HB2	1.96	0.84
1:B:241:GLU:OE2	1:C:178:PHE:CB	2.24	0.84
1:B:217:ALA:HB3	1:C:436:VAL:HG21	1.59	0.84
1:E:234:GLU:C	1:F:253:SER:HB2	1.97	0.84
1:A:220:VAL:HB	1:B:437:THR:HG22	1.60	0.84
1:E:214:ALA:N	1:F:274:ARG:HB2	1.91	0.84
1:E:232:GLY:CA	1:F:252:LYS:N	2.40	0.84
1:C:221:ALA:CB	1:D:248:LYS:HB2	2.06	0.84
1:C:216:LYS:HD2	1:D:278:ALA:HB2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:ALA:HB1	1:F:271:LEU:CG	2.08	0.83
1:C:221:ALA:CA	1:D:248:LYS:HB3	1.90	0.83
1:A:271:LEU:HD12	1:F:214:ALA:CA	2.08	0.83
1:B:237:GLY:CA	1:C:267:LEU:HD21	2.09	0.83
1:D:216:LYS:HA	1:E:274:ARG:C	1.98	0.83
1:A:435:TYR:CE2	1:F:233:GLU:OE2	2.32	0.83
1:A:212:PRO:HB2	1:B:184:ARG:CA	2.07	0.83
1:B:241:GLU:OE1	1:C:178:PHE:HD2	1.62	0.83
1:A:233:GLU:CB	1:B:434:TYR:H	1.90	0.83
1:B:207:THR:HB	1:C:177:ILE:CG2	2.08	0.83
1:C:214:ALA:HB1	1:D:271:LEU:CB	2.09	0.83
1:C:220:VAL:CG1	1:D:250:ALA:HB3	2.09	0.83
1:E:241:GLU:CG	1:F:179:SER:CB	2.28	0.83
1:B:215:GLY:HA2	1:C:275:LEU:HG	1.59	0.83
1:A:250:ALA:N	1:F:219:TRP:CG	2.25	0.82
1:C:234:GLU:CB	1:D:275:LEU:CD1	2.57	0.82
1:E:214:ALA:C	1:F:274:ARG:HB2	1.99	0.82
1:C:221:ALA:HA	1:D:248:LYS:HB2	0.83	0.82
1:D:211:GLU:CB	1:E:182:ILE:HG12	2.09	0.82
1:E:207:THR:H	1:F:177:ILE:CG2	1.92	0.82
1:A:210:VAL:CG1	1:B:182:ILE:CA	2.51	0.82
1:B:220:VAL:HG22	1:C:437:THR:HA	1.58	0.82
1:A:220:VAL:CG2	1:B:252:LYS:HG3	1.86	0.82
1:C:210:VAL:HG13	1:D:182:ILE:CA	2.04	0.82
1:B:215:GLY:CA	1:C:271:LEU:HD12	2.08	0.82
1:E:222:ALA:HB3	1:F:439:ARG:HH22	1.37	0.82
1:A:207:THR:CB	1:B:177:ILE:H	1.91	0.82
1:C:216:LYS:HG3	1:D:278:ALA:HB1	1.60	0.82
1:A:219:TRP:CG	1:B:279:HIS:HE1	1.97	0.82
1:E:217:ALA:CB	1:F:279:HIS:CA	2.54	0.82
1:A:213:ASP:C	1:B:274:ARG:HH21	1.80	0.82
1:A:218:THR:CB	1:B:251:ALA:HB1	1.62	0.82
1:D:220:VAL:CG2	1:E:251:ALA:N	2.43	0.82
1:E:207:THR:HB	1:F:178:PHE:O	1.79	0.82
1:A:271:LEU:HA	1:F:214:ALA:CA	2.08	0.82
1:B:230:THR:OG1	1:C:252:LYS:HD2	1.80	0.82
1:C:219:TRP:CG	1:D:249:LEU:HD22	2.15	0.82
1:D:216:LYS:N	1:E:275:LEU:HD23	1.95	0.82
1:A:204:LYS:HB2	1:B:174:TYR:HE2	1.45	0.81
1:C:212:PRO:HB2	1:D:184:ARG:HA	1.62	0.81
1:C:219:TRP:HB3	1:D:249:LEU:HA	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLU:O	1:C:275:LEU:CD2	2.27	0.81
1:C:208:MET:HA	1:D:178:PHE:C	2.01	0.81
1:C:233:GLU:OE1	1:D:252:LYS:CG	2.27	0.81
1:D:208:MET:CB	1:E:179:SER:HA	2.10	0.81
1:A:271:LEU:C	1:F:214:ALA:O	2.17	0.81
1:A:250:ALA:HB2	1:F:220:VAL:O	1.81	0.81
1:B:219:TRP:CD2	1:C:249:LEU:HD23	2.14	0.81
1:E:214:ALA:HB3	1:F:271:LEU:C	2.01	0.81
1:E:208:MET:HE3	1:F:181:ARG:HB2	1.62	0.81
1:A:435:TYR:CD2	1:F:233:GLU:OE2	2.33	0.81
1:B:316:ALA:O	1:C:353:TYR:OH	1.98	0.81
1:A:253:SER:N	1:F:233:GLU:HG3	1.95	0.81
1:B:217:ALA:H	1:C:275:LEU:CG	1.92	0.81
1:B:232:GLY:CA	1:C:252:LYS:HB3	2.10	0.81
1:D:219:TRP:CG	1:E:249:LEU:HD22	2.16	0.81
1:A:221:ALA:C	1:B:439:ARG:NH1	2.34	0.81
1:C:234:GLU:N	1:D:253:SER:HA	1.94	0.81
1:D:233:GLU:CG	1:E:434:TYR:O	2.29	0.81
1:E:207:THR:CB	1:F:177:ILE:HG22	2.11	0.81
1:A:185:ASP:OD1	1:F:213:ASP:CB	2.29	0.81
1:A:219:TRP:HH2	1:B:248:LYS:HB2	1.46	0.81
1:C:213:ASP:CB	1:D:274:ARG:HD3	2.11	0.81
1:B:216:LYS:H	1:C:275:LEU:CD2	1.94	0.81
1:A:219:TRP:CG	1:B:249:LEU:HB3	1.84	0.80
1:C:233:GLU:HG2	1:D:254:PHE:HB2	1.63	0.80
1:C:220:VAL:H	1:D:249:LEU:CA	1.94	0.80
1:E:205:ILE:HG23	1:F:177:ILE:CB	2.10	0.80
1:A:207:THR:HG21	1:B:176:THR:HG22	1.61	0.80
1:A:252:LYS:HD2	1:F:231:THR:O	1.80	0.80
1:A:218:THR:HG22	1:B:252:LYS:H	1.45	0.80
1:B:207:THR:HB	1:C:177:ILE:CB	1.96	0.80
1:D:207:THR:N	1:E:177:ILE:CB	1.83	0.80
1:D:232:GLY:HA2	1:E:252:LYS:CE	2.09	0.80
1:D:233:GLU:CD	1:E:433:ALA:C	2.40	0.80
1:A:275:LEU:HD23	1:F:216:LYS:C	2.02	0.80
1:A:216:LYS:CA	1:B:274:ARG:C	2.47	0.80
1:D:219:TRP:CZ2	1:E:282:SER:O	2.34	0.80
1:C:360:GLU:HB2	1:D:362:TRP:O	1.80	0.80
1:C:217:ALA:H	1:D:275:LEU:HD11	1.47	0.80
1:C:233:GLU:CB	1:D:253:SER:CA	2.54	0.80
1:C:219:TRP:HB3	1:D:249:LEU:CB	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LYS:N	1:B:271:LEU:HD11	1.94	0.80
1:D:215:GLY:C	1:E:275:LEU:HD23	2.01	0.80
1:E:233:GLU:H	1:F:252:LYS:HB2	1.40	0.80
1:A:352:ALA:CB	1:F:332:ARG:NE	2.40	0.80
1:B:235:VAL:HG13	1:C:255:ILE:HG21	1.63	0.80
1:C:219:TRP:CD1	1:D:249:LEU:CD1	2.64	0.80
1:D:206:LEU:CA	1:E:177:ILE:HB	2.12	0.80
1:B:209:LEU:O	1:C:181:ARG:O	1.88	0.80
1:C:212:PRO:HA	1:D:182:ILE:HD13	1.63	0.80
1:C:232:GLY:O	1:D:251:ALA:HB1	1.82	0.80
1:B:216:LYS:CB	1:C:274:ARG:O	2.30	0.80
1:A:279:HIS:CE1	1:F:219:TRP:HD1	1.93	0.79
1:A:231:THR:O	1:B:252:LYS:CB	2.29	0.79
1:A:217:ALA:HB1	1:B:436:VAL:CG2	2.12	0.79
1:C:219:TRP:CZ2	1:D:282:SER:C	2.54	0.79
1:A:217:ALA:O	1:B:279:HIS:CB	2.30	0.79
1:D:206:LEU:HA	1:E:177:ILE:CB	2.12	0.79
1:D:231:THR:OG1	1:E:252:LYS:HG2	1.81	0.79
1:E:234:GLU:CA	1:F:253:SER:HB3	2.12	0.79
1:D:235:VAL:CB	1:E:255:ILE:CB	2.60	0.79
1:E:208:MET:C	1:F:180:GLN:N	2.31	0.79
1:C:232:GLY:HA2	1:D:251:ALA:CA	2.11	0.79
1:C:233:GLU:HB3	1:D:254:PHE:H	1.45	0.79
1:A:217:ALA:HB3	1:B:276:ILE:N	1.98	0.79
1:A:233:GLU:HG2	1:B:434:TYR:C	1.98	0.79
1:E:225:TYR:CB	1:F:422:GLU:OE2	2.31	0.79
1:A:216:LYS:N	1:B:275:LEU:CG	2.45	0.79
1:A:235:VAL:HA	1:B:271:LEU:CD2	2.12	0.79
1:E:241:GLU:HG3	1:F:179:SER:HB3	0.79	0.79
1:C:233:GLU:CD	1:D:252:LYS:HB2	2.03	0.78
1:A:206:LEU:CA	1:B:177:ILE:CG1	2.62	0.78
1:A:219:TRP:HA	1:B:279:HIS:ND1	1.97	0.78
1:B:210:VAL:CB	1:C:182:ILE:HA	2.14	0.78
1:D:233:GLU:OE1	1:E:434:TYR:N	2.13	0.78
1:A:219:TRP:CA	1:B:279:HIS:ND1	2.46	0.78
1:E:207:THR:OG1	1:F:177:ILE:C	2.20	0.78
1:A:252:LYS:HD3	1:F:233:GLU:OE2	1.82	0.78
1:A:206:LEU:CA	1:B:177:ILE:HG13	2.13	0.78
1:D:232:GLY:O	1:E:252:LYS:CA	2.31	0.78
1:D:235:VAL:HG22	1:E:255:ILE:HD12	1.63	0.78
1:A:216:LYS:N	1:B:275:LEU:HG	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:THR:OG1	1:C:177:ILE:CA	2.24	0.78
1:A:207:THR:O	1:B:177:ILE:CG2	2.21	0.78
1:A:222:ALA:CA	1:B:439:ARG:NH1	2.46	0.78
1:A:252:LYS:HE2	1:F:230:THR:OG1	1.82	0.78
1:A:274:ARG:HB2	1:F:214:ALA:O	1.83	0.78
1:A:212:PRO:CB	1:B:184:ARG:HA	2.12	0.78
1:E:232:GLY:CA	1:F:252:LYS:CG	2.61	0.78
1:E:219:TRP:CB	1:F:249:LEU:HA	2.09	0.78
1:A:218:THR:CG2	1:B:252:LYS:N	2.47	0.77
1:A:349:SER:OG	1:F:315:LYS:O	2.00	0.77
1:A:182:ILE:CB	1:F:211:GLU:C	2.50	0.77
1:B:214:ALA:HB3	1:C:270:LEU:CB	2.13	0.77
1:E:222:ALA:CB	1:F:439:ARG:NH2	2.40	0.77
1:E:207:THR:N	1:F:177:ILE:HG22	1.99	0.77
1:B:214:ALA:C	1:C:274:ARG:CG	2.50	0.77
1:E:214:ALA:HB3	1:F:271:LEU:O	1.85	0.77
1:A:271:LEU:HD11	1:F:235:VAL:C	1.99	0.77
1:B:210:VAL:HG13	1:C:182:ILE:CA	2.14	0.77
1:C:216:LYS:CA	1:D:275:LEU:HA	2.15	0.77
1:E:205:ILE:HG23	1:F:177:ILE:HB	1.65	0.77
1:D:236:LYS:N	1:E:271:LEU:CD1	2.41	0.77
1:A:274:ARG:NH1	1:F:212:PRO:CD	2.39	0.77
1:A:215:GLY:H	1:B:271:LEU:HD13	1.50	0.77
1:C:220:VAL:HB	1:D:250:ALA:C	2.04	0.77
1:D:222:ALA:HB3	1:E:437:THR:OG1	1.85	0.77
1:C:216:LYS:CA	1:D:275:LEU:HD12	2.14	0.77
1:E:207:THR:HG22	1:F:179:SER:CA	2.14	0.77
1:E:219:TRP:CZ2	1:F:282:SER:O	2.37	0.77
1:C:234:GLU:N	1:D:253:SER:CA	2.47	0.77
1:C:316:ALA:CB	1:D:352:ALA:HB1	2.15	0.77
1:A:174:TYR:CZ	1:F:204:LYS:HB2	2.11	0.76
1:A:210:VAL:CA	1:B:181:ARG:O	2.28	0.76
1:C:233:GLU:HB3	1:D:253:SER:C	2.06	0.76
1:A:207:THR:O	1:B:177:ILE:HG22	1.81	0.76
1:B:214:ALA:HB3	1:C:270:LEU:CG	2.14	0.76
1:A:217:ALA:HB1	1:B:436:VAL:HG21	1.66	0.76
1:A:361:GLU:CD	1:B:363:GLN:OE1	2.23	0.76
1:A:181:ARG:CA	1:F:211:GLU:OE2	2.33	0.76
1:A:331:ARG:HH12	1:B:355:ASP:HB2	1.44	0.76
1:B:231:THR:O	1:C:252:LYS:CB	2.34	0.76
1:C:383:TYR:HA	1:D:371:ASP:HB3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:THR:CG2	1:F:205:ILE:HG21	2.14	0.76
1:A:217:ALA:HB2	1:B:275:LEU:HB2	1.66	0.76
1:B:212:PRO:HB3	1:C:183:ILE:CA	2.15	0.76
1:A:185:ASP:OD1	1:F:213:ASP:HB2	1.85	0.76
1:E:221:ALA:CA	1:F:248:LYS:CB	2.61	0.76
1:D:233:GLU:CD	1:E:433:ALA:HB1	2.07	0.76
1:C:232:GLY:HA3	1:D:252:LYS:CG	2.16	0.76
1:D:237:GLY:HA2	1:E:267:LEU:HD13	1.65	0.76
1:E:219:TRP:CG	1:F:249:LEU:HD22	2.21	0.76
1:A:275:LEU:HD21	1:F:216:LYS:N	1.94	0.76
1:A:268:LEU:HG	1:F:235:VAL:HG21	1.68	0.75
1:A:235:VAL:HB	1:B:271:LEU:HD21	1.64	0.75
1:C:220:VAL:HG21	1:D:251:ALA:HA	1.68	0.75
1:B:204:LYS:HB2	1:C:175:GLU:OE1	1.86	0.75
1:C:219:TRP:CG	1:D:249:LEU:HD13	2.21	0.75
1:C:216:LYS:N	1:D:275:LEU:CD1	2.28	0.75
1:D:211:GLU:O	1:E:182:ILE:HG12	1.72	0.75
1:A:275:LEU:HD21	1:F:234:GLU:HB2	1.69	0.75
1:D:232:GLY:O	1:E:252:LYS:CB	2.35	0.75
1:C:223:SER:N	1:D:439:ARG:NH1	2.29	0.75
1:E:207:THR:OG1	1:F:177:ILE:HB	1.87	0.75
1:A:211:GLU:H	1:B:181:ARG:C	1.88	0.75
1:D:220:VAL:CB	1:E:251:ALA:N	2.47	0.75
1:E:233:GLU:HG3	1:F:252:LYS:HB3	1.67	0.75
1:B:209:LEU:N	1:C:180:GLN:N	2.23	0.75
1:C:221:ALA:C	1:D:248:LYS:CB	2.56	0.75
1:E:219:TRP:HZ2	1:F:282:SER:O	1.69	0.75
1:D:219:TRP:HZ2	1:E:286:ALA:HB2	1.43	0.75
1:E:228:ASP:OD1	1:F:252:LYS:NZ	2.19	0.75
1:C:331:ARG:NH1	1:D:376:GLN:HE21	1.83	0.74
1:C:212:PRO:O	1:D:274:ARG:NH2	2.19	0.74
1:E:221:ALA:CA	1:F:248:LYS:HB3	2.15	0.74
1:B:232:GLY:HA3	1:C:254:PHE:HD1	1.50	0.74
1:C:234:GLU:H	1:D:253:SER:CB	2.00	0.74
1:E:234:GLU:N	1:F:253:SER:HA	1.14	0.74
1:A:252:LYS:HB2	1:F:232:GLY:O	1.88	0.74
1:A:215:GLY:H	1:B:271:LEU:HD12	0.91	0.74
1:C:235:VAL:CG2	1:D:271:LEU:HD21	2.16	0.74
1:E:227:THR:HB	1:F:435:TYR:CE1	2.22	0.74
1:E:207:THR:HB	1:F:177:ILE:HG22	1.68	0.74
1:A:222:ALA:O	1:B:439:ARG:NH1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:VAL:HG23	1:C:437:THR:CG2	1.96	0.74
1:D:208:MET:HB3	1:E:179:SER:HA	1.67	0.74
1:A:275:LEU:CD2	1:F:215:GLY:C	2.53	0.74
1:A:218:THR:HG23	1:B:252:LYS:H	1.51	0.74
1:A:220:VAL:HB	1:B:437:THR:CG2	2.17	0.74
1:C:219:TRP:CB	1:D:249:LEU:HB3	2.18	0.74
1:C:208:MET:HB2	1:D:179:SER:CA	2.18	0.74
1:D:446:PHE:HZ	1:E:183:ILE:HD11	1.51	0.74
1:D:235:VAL:HG23	1:E:255:ILE:HD12	1.69	0.74
1:B:210:VAL:CG1	1:C:183:ILE:H	2.01	0.74
1:A:176:THR:CA	1:F:205:ILE:HG23	2.12	0.74
1:B:214:ALA:C	1:C:274:ARG:CB	2.55	0.74
1:E:213:ASP:OD1	1:F:274:ARG:NE	2.21	0.74
1:B:280:ALA:HA	1:B:283:ILE:HD12	1.69	0.73
1:B:234:GLU:HG2	1:C:252:LYS:O	1.87	0.73
1:C:208:MET:CA	1:D:179:SER:CA	2.65	0.73
1:C:331:ARG:CZ	1:D:376:GLN:HE21	1.99	0.73
1:C:227:THR:CB	1:D:435:TYR:OH	2.34	0.73
1:C:383:TYR:HD2	1:D:371:ASP:HB2	1.53	0.73
1:D:215:GLY:H	1:E:271:LEU:HG	1.49	0.73
1:C:234:GLU:N	1:D:253:SER:HB3	2.03	0.73
1:D:237:GLY:CA	1:E:267:LEU:CD1	2.37	0.73
1:A:227:THR:N	1:B:435:TYR:CE1	2.55	0.73
1:D:332:ARG:NH1	1:E:351:ASP:OD2	2.21	0.73
1:E:210:VAL:CB	1:F:182:ILE:HA	2.16	0.73
1:A:252:LYS:HE3	1:F:227:THR:OG1	1.88	0.73
1:A:218:THR:HG22	1:B:252:LYS:N	2.04	0.73
1:A:220:VAL:HG13	1:B:252:LYS:CE	2.17	0.73
1:E:219:TRP:HB3	1:F:249:LEU:CB	2.19	0.73
1:B:214:ALA:HB3	1:C:271:LEU:N	2.03	0.73
1:E:217:ALA:HB1	1:F:279:HIS:HB2	0.73	0.73
1:A:217:ALA:CB	1:B:275:LEU:O	2.36	0.73
1:A:220:VAL:CB	1:B:437:THR:CG2	2.65	0.73
1:A:352:ALA:HB1	1:F:332:ARG:HE	1.52	0.73
1:E:234:GLU:O	1:F:253:SER:HB2	1.88	0.73
1:E:235:VAL:HG12	1:F:271:LEU:HD21	1.70	0.73
1:D:446:PHE:HZ	1:E:183:ILE:CD1	2.02	0.73
1:E:211:GLU:HG2	1:F:182:ILE:HD12	0.87	0.73
1:A:331:ARG:NH1	1:B:355:ASP:CB	2.13	0.72
1:B:216:LYS:N	1:C:275:LEU:CG	2.52	0.72
1:C:216:LYS:CG	1:D:278:ALA:CB	2.62	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:MET:HA	1:D:179:SER:CA	2.19	0.72
1:C:234:GLU:N	1:D:253:SER:CB	2.52	0.72
1:C:216:LYS:O	1:D:278:ALA:C	2.27	0.72
1:A:233:GLU:HG2	1:B:433:ALA:C	2.05	0.72
1:D:237:GLY:C	1:E:267:LEU:HD11	2.10	0.72
1:D:235:VAL:CG1	1:E:255:ILE:CA	2.42	0.72
1:E:234:GLU:CA	1:F:253:SER:CB	2.67	0.72
1:C:219:TRP:CG	1:D:249:LEU:HB3	2.23	0.72
1:C:360:GLU:CB	1:D:362:TRP:O	2.37	0.72
1:C:212:PRO:HB2	1:D:184:ARG:C	2.09	0.72
1:E:228:ASP:CB	1:F:252:LYS:HZ2	2.03	0.72
1:C:215:GLY:C	1:D:275:LEU:CA	2.54	0.72
1:A:271:LEU:CD1	1:F:214:ALA:C	2.51	0.72
1:A:203:SER:OG	1:B:175:GLU:OE1	2.05	0.72
1:E:210:VAL:HB	1:F:183:ILE:H	1.54	0.72
1:C:383:TYR:CB	1:D:371:ASP:HB3	2.19	0.72
1:C:234:GLU:CB	1:D:275:LEU:HD11	2.09	0.72
1:E:217:ALA:HB3	1:F:279:HIS:CB	2.05	0.71
1:A:219:TRP:CH2	1:B:248:LYS:CB	2.73	0.71
1:C:219:TRP:HA	1:D:249:LEU:CA	2.20	0.71
1:C:383:TYR:HB3	1:D:371:ASP:HB3	1.71	0.71
1:A:215:GLY:HA3	1:B:271:LEU:CG	2.21	0.71
1:C:205:ILE:O	1:D:177:ILE:HG12	1.90	0.71
1:C:220:VAL:CB	1:D:250:ALA:CB	2.24	0.71
1:E:213:ASP:HA	1:F:274:ARG:HD2	0.72	0.71
1:A:275:LEU:CD2	1:F:216:LYS:C	2.56	0.71
1:A:275:LEU:HD21	1:F:234:GLU:CB	2.21	0.71
1:A:218:THR:CG2	1:B:251:ALA:HB1	2.20	0.71
1:B:214:ALA:CB	1:C:270:LEU:CG	2.68	0.71
1:A:230:THR:OG1	1:B:252:LYS:HD2	1.89	0.71
1:E:228:ASP:CG	1:F:252:LYS:NZ	2.43	0.71
1:A:215:GLY:C	1:B:274:ARG:HB3	2.11	0.71
1:E:214:ALA:CA	1:F:274:ARG:CB	2.67	0.71
1:A:185:ASP:OD1	1:F:213:ASP:HB3	1.91	0.71
1:C:219:TRP:HB3	1:D:249:LEU:CA	2.20	0.71
1:C:212:PRO:CA	1:D:182:ILE:HD13	2.17	0.71
1:D:232:GLY:C	1:E:252:LYS:C	2.39	0.71
1:A:227:THR:H	1:B:435:TYR:HE1	1.38	0.71
1:A:237:GLY:HA2	1:B:267:LEU:HD13	1.71	0.71
1:B:212:PRO:HB3	1:C:182:ILE:C	2.11	0.71
1:C:219:TRP:HA	1:D:249:LEU:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:LEU:CA	1:E:177:ILE:CB	2.68	0.70
1:A:275:LEU:CD2	1:F:234:GLU:HB2	2.21	0.70
1:A:226:GLY:HA3	1:B:424:GLU:CD	2.10	0.70
1:B:215:GLY:HA2	1:C:271:LEU:HD12	1.72	0.70
1:B:214:ALA:CB	1:C:271:LEU:N	2.55	0.70
1:D:216:LYS:O	1:E:275:LEU:C	2.30	0.70
1:C:217:ALA:HB1	1:D:279:HIS:CG	2.27	0.70
1:C:219:TRP:CB	1:D:249:LEU:CB	2.69	0.70
1:E:227:THR:CB	1:F:435:TYR:OH	2.39	0.70
1:D:215:GLY:O	1:E:274:ARG:HB3	1.91	0.70
1:C:316:ALA:HB2	1:D:352:ALA:HB1	1.73	0.70
1:E:208:MET:CE	1:F:181:ARG:HB2	2.22	0.70
1:E:207:THR:CG2	1:F:178:PHE:O	2.40	0.70
1:D:219:TRP:HB3	1:E:249:LEU:HD22	1.73	0.70
1:A:215:GLY:C	1:B:274:ARG:CB	2.60	0.70
1:A:220:VAL:C	1:B:437:THR:HG22	2.13	0.70
1:C:220:VAL:CA	1:D:250:ALA:HB3	2.19	0.70
1:A:234:GLU:O	1:B:275:LEU:CD1	2.40	0.69
1:C:219:TRP:HA	1:D:249:LEU:C	2.12	0.69
1:D:219:TRP:CZ2	1:E:286:ALA:CB	2.68	0.69
1:E:220:VAL:HG11	1:F:435:TYR:CZ	2.24	0.69
1:A:176:THR:HG23	1:F:205:ILE:HD13	1.73	0.69
1:B:212:PRO:HB2	1:C:184:ARG:N	2.08	0.69
1:A:222:ALA:HB2	1:B:437:THR:CG2	2.20	0.69
1:A:178:PHE:CA	1:F:207:THR:HG22	2.21	0.69
1:A:217:ALA:CB	1:B:275:LEU:CA	2.69	0.69
1:A:217:ALA:H	1:B:275:LEU:HD23	1.53	0.69
1:C:227:THR:HB	1:D:435:TYR:CE1	2.26	0.69
1:A:235:VAL:CA	1:B:271:LEU:HD11	2.22	0.69
1:A:178:PHE:HA	1:F:207:THR:CG2	2.22	0.69
1:A:220:VAL:CG1	1:B:252:LYS:HE3	2.19	0.69
1:B:217:ALA:CA	1:C:275:LEU:CD2	2.44	0.69
1:A:213:ASP:O	1:B:274:ARG:NH2	2.16	0.69
1:A:178:PHE:O	1:F:208:MET:CB	2.41	0.69
1:B:216:LYS:HB2	1:C:274:ARG:O	1.93	0.69
1:D:207:THR:N	1:E:177:ILE:CA	2.45	0.69
1:D:235:VAL:HG11	1:E:255:ILE:CB	2.23	0.69
1:A:252:LYS:H	1:F:218:THR:N	1.87	0.68
1:A:252:LYS:HG3	1:F:220:VAL:CG2	2.23	0.68
1:A:271:LEU:HD12	1:F:215:GLY:H	1.55	0.68
1:B:214:ALA:O	1:C:274:ARG:HG3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:VAL:CG2	1:E:255:ILE:CB	2.32	0.68
1:C:331:ARG:NH2	1:D:376:GLN:NE2	2.40	0.68
1:D:234:GLU:HG3	1:E:253:SER:HB3	1.74	0.68
1:A:220:VAL:HG23	1:B:251:ALA:CA	2.24	0.68
1:D:219:TRP:HZ2	1:E:282:SER:O	1.72	0.68
1:A:219:TRP:HH2	1:B:248:LYS:CB	2.06	0.68
1:B:316:ALA:HB1	1:C:353:TYR:CE1	2.28	0.68
1:C:210:VAL:CG1	1:D:182:ILE:CA	2.67	0.68
1:C:216:LYS:O	1:D:278:ALA:HB3	1.92	0.68
1:E:220:VAL:HG21	1:F:251:ALA:CA	2.23	0.68
1:A:216:LYS:HZ2	1:B:277:GLU:C	1.87	0.68
1:A:252:LYS:CG	1:F:220:VAL:CG2	2.72	0.68
1:D:233:GLU:OE2	1:E:433:ALA:C	2.31	0.68
1:C:216:LYS:C	1:D:275:LEU:HD12	2.12	0.68
1:A:219:TRP:HA	1:B:279:HIS:CE1	2.29	0.68
1:A:222:ALA:CA	1:B:439:ARG:HH12	2.04	0.68
1:A:252:LYS:N	1:F:217:ALA:HB1	2.09	0.68
1:C:205:ILE:O	1:D:177:ILE:CG1	2.42	0.68
1:C:219:TRP:NE1	1:D:249:LEU:HD13	2.07	0.68
1:D:214:ALA:C	1:E:274:ARG:HB2	2.14	0.68
1:E:214:ALA:HB1	1:F:271:LEU:CB	2.24	0.68
1:B:216:LYS:H	1:C:275:LEU:CG	2.06	0.67
1:C:235:VAL:HG22	1:D:271:LEU:CD1	1.97	0.67
1:B:207:THR:HG21	1:C:178:PHE:HA	1.75	0.67
1:A:222:ALA:CB	1:B:437:THR:HG21	2.22	0.67
1:E:209:LEU:HB2	1:F:180:GLN:N	2.10	0.67
1:A:210:VAL:HG13	1:B:182:ILE:CA	2.17	0.67
1:D:234:GLU:CG	1:E:253:SER:HB3	1.99	0.67
1:B:216:LYS:N	1:C:275:LEU:HG	2.09	0.67
1:A:234:GLU:CB	1:B:275:LEU:CD2	2.70	0.67
1:B:236:LYS:C	1:C:267:LEU:HD21	2.15	0.67
1:D:206:LEU:CA	1:E:177:ILE:CG1	2.65	0.67
1:E:207:THR:H	1:F:177:ILE:HG21	1.55	0.67
1:E:241:GLU:HG3	1:F:179:SER:CA	2.22	0.67
1:E:235:VAL:HG13	1:F:253:SER:HB2	1.76	0.67
1:D:207:THR:OG1	1:E:176:THR:C	2.30	0.67
1:C:219:TRP:HD1	1:D:249:LEU:HB3	1.58	0.66
1:E:217:ALA:HB2	1:F:275:LEU:O	1.95	0.66
1:C:218:THR:HG22	1:D:251:ALA:HB2	0.74	0.66
1:D:215:GLY:HA2	1:E:275:LEU:CD2	2.24	0.66
1:A:217:ALA:CB	1:B:436:VAL:HG21	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:HA	1:B:271:LEU:CD1	2.25	0.66
1:E:225:TYR:HB3	1:F:422:GLU:OE2	1.94	0.66
1:E:222:ALA:HB1	1:F:439:ARG:HH22	1.58	0.66
1:A:236:LYS:N	1:B:271:LEU:HD13	1.97	0.66
1:C:220:VAL:HB	1:D:250:ALA:HB3	0.67	0.66
1:A:218:THR:HG23	1:B:252:LYS:N	2.10	0.66
1:D:213:ASP:C	1:E:274:ARG:HG3	2.14	0.66
1:E:227:THR:O	1:F:252:LYS:CG	2.43	0.66
1:E:218:THR:HG23	1:F:250:ALA:O	1.96	0.66
1:B:210:VAL:HG13	1:C:182:ILE:C	2.14	0.66
1:D:216:LYS:HD2	1:E:274:ARG:O	1.96	0.66
1:C:221:ALA:C	1:D:248:LYS:HG2	2.06	0.66
1:A:275:LEU:O	1:F:216:LYS:O	2.13	0.66
1:C:232:GLY:O	1:D:251:ALA:CB	2.40	0.66
1:D:235:VAL:HG11	1:E:255:ILE:HA	0.75	0.66
1:C:220:VAL:CB	1:D:250:ALA:O	2.42	0.66
1:A:362:TRP:O	1:F:360:GLU:OE1	2.13	0.66
1:B:214:ALA:N	1:C:270:LEU:HG	2.09	0.66
1:D:213:ASP:HB2	1:E:274:ARG:NH2	2.11	0.66
1:A:176:THR:HG23	1:F:205:ILE:CG2	2.21	0.65
1:E:205:ILE:HG22	1:F:177:ILE:CG1	2.09	0.65
1:A:204:LYS:CB	1:B:174:TYR:HE2	2.09	0.65
1:B:233:GLU:OE1	1:C:433:ALA:C	2.32	0.65
1:A:217:ALA:CA	1:B:275:LEU:O	2.44	0.65
1:A:362:TRP:CH2	1:B:362:TRP:HD1	1.85	0.65
1:C:207:THR:HB	1:D:177:ILE:C	2.16	0.65
1:C:220:VAL:CB	1:D:250:ALA:CA	2.68	0.65
1:B:212:PRO:O	1:C:182:ILE:HD11	1.95	0.65
1:A:254:PHE:CD2	1:F:233:GLU:OE1	2.50	0.65
1:E:228:ASP:HB3	1:F:252:LYS:CE	2.23	0.65
1:A:331:ARG:NH2	1:B:355:ASP:CG	2.46	0.65
1:B:406:VAL:HG13	1:B:410:ASN:HB2	1.79	0.65
1:C:219:TRP:CZ2	1:D:286:ALA:HB2	2.30	0.65
1:C:232:GLY:O	1:D:252:LYS:O	2.05	0.65
1:E:207:THR:CB	1:F:178:PHE:O	2.45	0.65
1:C:219:TRP:CB	1:D:249:LEU:HA	2.27	0.65
1:C:331:ARG:NE	1:D:376:GLN:HE22	1.93	0.65
1:B:212:PRO:O	1:C:182:ILE:CD1	2.40	0.65
1:D:216:LYS:C	1:E:275:LEU:CA	2.46	0.65
1:D:216:LYS:HG3	1:E:278:ALA:CA	2.19	0.65
1:D:220:VAL:HG23	1:E:251:ALA:N	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:LYS:O	1:E:275:LEU:O	2.14	0.64
1:D:232:GLY:C	1:E:252:LYS:O	2.32	0.64
1:A:232:GLY:O	1:B:252:LYS:C	2.36	0.64
1:C:214:ALA:HB3	1:D:271:LEU:N	2.12	0.64
1:C:332:ARG:NH1	1:D:351:ASP:OD2	2.30	0.64
1:D:232:GLY:C	1:E:252:LYS:CB	2.65	0.64
1:E:214:ALA:C	1:F:274:ARG:CB	2.61	0.64
1:E:228:ASP:CG	1:F:252:LYS:HZ2	2.00	0.64
1:B:210:VAL:HG12	1:C:183:ILE:H	1.56	0.64
1:C:221:ALA:C	1:D:248:LYS:HB3	2.16	0.64
1:B:241:GLU:CD	1:C:178:PHE:HD2	2.00	0.64
1:A:215:GLY:CA	1:B:271:LEU:CG	2.72	0.64
1:A:252:LYS:HB3	1:F:233:GLU:OE2	1.98	0.64
1:A:215:GLY:HA3	1:B:271:LEU:HG	1.78	0.64
1:C:219:TRP:CA	1:D:249:LEU:CA	2.75	0.64
1:A:213:ASP:H	1:B:182:ILE:HD11	1.62	0.64
1:D:235:VAL:HG21	1:E:255:ILE:HG13	1.68	0.64
1:A:230:THR:OG1	1:B:252:LYS:CD	2.47	0.63
1:D:212:PRO:HB2	1:E:184:ARG:HA	1.81	0.63
1:A:216:LYS:HD2	1:B:274:ARG:O	1.98	0.63
1:D:215:GLY:C	1:E:274:ARG:HB2	2.19	0.63
1:C:383:TYR:CA	1:D:371:ASP:HB3	2.27	0.63
1:E:214:ALA:O	1:F:274:ARG:C	2.37	0.63
1:A:274:ARG:CB	1:F:215:GLY:O	2.46	0.63
1:A:235:VAL:CB	1:B:271:LEU:CD2	2.51	0.63
1:A:215:GLY:HA3	1:B:271:LEU:HD12	1.61	0.63
1:D:237:GLY:HA2	1:E:267:LEU:CG	2.27	0.63
1:A:206:LEU:HA	1:B:177:ILE:HG12	1.78	0.63
1:E:225:TYR:HA	1:F:422:GLU:CD	2.18	0.63
1:A:254:PHE:CB	1:F:233:GLU:H	2.05	0.63
1:A:220:VAL:CG1	1:B:437:THR:HG22	2.21	0.63
1:E:214:ALA:HB2	1:F:271:LEU:CA	1.98	0.63
1:A:220:VAL:HG12	1:B:437:THR:HG22	1.75	0.63
1:C:232:GLY:CA	1:D:251:ALA:CA	2.75	0.63
1:A:218:THR:HG22	1:B:252:LYS:O	1.99	0.63
1:B:235:VAL:CG1	1:C:255:ILE:CG1	2.70	0.63
1:D:214:ALA:O	1:E:274:ARG:HB2	1.98	0.63
1:E:250:ALA:HA	1:E:279:HIS:HE1	1.64	0.63
1:A:213:ASP:H	1:B:182:ILE:CD1	2.11	0.62
1:D:220:VAL:HB	1:E:251:ALA:N	1.95	0.62
1:E:207:THR:OG1	1:F:177:ILE:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:THR:O	1:D:252:LYS:CD	2.34	0.62
1:D:216:LYS:HG3	1:E:278:ALA:HB2	0.64	0.62
1:E:210:VAL:HA	1:F:182:ILE:N	2.09	0.62
1:D:207:THR:H	1:E:177:ILE:CG2	2.02	0.62
1:D:210:VAL:HG12	1:E:182:ILE:CB	2.13	0.62
1:A:220:VAL:CG1	1:B:252:LYS:CE	2.77	0.62
1:C:219:TRP:CA	1:D:249:LEU:HA	2.30	0.62
1:A:180:GLN:H	1:F:208:MET:HE3	1.64	0.62
1:B:220:VAL:HG12	1:C:252:LYS:HG3	1.81	0.62
1:C:216:LYS:O	1:D:275:LEU:O	2.16	0.62
1:D:220:VAL:HG23	1:E:251:ALA:CA	2.29	0.62
1:A:219:TRP:CB	1:B:279:HIS:CE1	2.83	0.62
1:C:216:LYS:H	1:D:275:LEU:CA	1.99	0.62
1:B:237:GLY:CA	1:C:267:LEU:HD11	2.29	0.62
1:D:446:PHE:CZ	1:E:183:ILE:HD11	2.33	0.62
1:D:215:GLY:CA	1:E:271:LEU:HG	2.28	0.62
1:D:216:LYS:CA	1:E:278:ALA:CB	2.77	0.62
1:B:235:VAL:HG12	1:C:255:ILE:HG12	1.80	0.62
1:B:237:GLY:HA2	1:C:267:LEU:HD11	1.80	0.62
1:D:213:ASP:C	1:E:274:ARG:CG	2.68	0.62
1:D:235:VAL:N	1:E:254:PHE:O	2.33	0.62
1:E:219:TRP:NE1	1:F:282:SER:C	2.50	0.62
1:A:222:ALA:HB3	1:B:439:ARG:NH1	2.15	0.61
1:A:204:LYS:HB2	1:B:174:TYR:CE2	2.32	0.61
1:B:210:VAL:HG11	1:C:183:ILE:N	2.13	0.61
1:C:213:ASP:N	1:D:274:ARG:HD2	2.14	0.61
1:A:274:ARG:NH1	1:F:212:PRO:HD2	2.15	0.61
1:B:214:ALA:C	1:C:274:ARG:HG3	2.20	0.61
1:C:208:MET:CB	1:D:179:SER:CA	2.78	0.61
1:D:216:LYS:CA	1:E:278:ALA:HB3	2.30	0.61
1:E:219:TRP:CD1	1:F:249:LEU:HB3	2.35	0.61
1:A:215:GLY:N	1:B:271:LEU:HA	2.15	0.61
1:C:216:LYS:HD2	1:D:278:ALA:CB	2.21	0.61
1:E:220:VAL:N	1:F:250:ALA:O	2.34	0.61
1:D:213:ASP:CA	1:E:274:ARG:NH2	2.63	0.61
1:D:219:TRP:CB	1:E:249:LEU:HD22	2.30	0.61
1:A:235:VAL:C	1:B:271:LEU:HD11	2.20	0.61
1:C:210:VAL:HG12	1:D:183:ILE:N	2.14	0.61
1:D:210:VAL:HG23	1:E:179:SER:OG	2.00	0.61
1:C:227:THR:CB	1:D:435:TYR:HH	2.08	0.61
1:D:383:TYR:O	1:E:371:ASP:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:TRP:N	1:F:250:ALA:O	2.33	0.61
1:E:219:TRP:O	1:F:250:ALA:O	2.19	0.61
1:E:241:GLU:OE1	1:F:179:SER:HB3	2.01	0.61
1:A:216:LYS:N	1:B:275:LEU:N	2.38	0.61
1:E:207:THR:CB	1:F:177:ILE:O	2.48	0.61
1:C:220:VAL:N	1:D:249:LEU:HA	2.16	0.60
1:C:219:TRP:CZ2	1:D:286:ALA:CB	2.84	0.60
1:A:274:ARG:HB2	1:F:214:ALA:C	2.20	0.60
1:B:214:ALA:CB	1:C:270:LEU:C	2.63	0.60
1:E:214:ALA:CB	1:F:271:LEU:CB	2.79	0.60
1:E:209:LEU:N	1:F:180:GLN:H	1.92	0.60
1:A:331:ARG:HH22	1:B:355:ASP:CB	2.13	0.60
1:A:221:ALA:O	1:B:439:ARG:NE	2.34	0.60
1:C:221:ALA:O	1:D:248:LYS:CB	2.50	0.60
1:C:331:ARG:NE	1:D:376:GLN:NE2	2.45	0.60
1:E:209:LEU:CB	1:F:180:GLN:C	2.69	0.60
1:A:184:ARG:C	1:F:212:PRO:O	2.40	0.60
1:A:362:TRP:CB	1:F:360:GLU:OE1	2.50	0.60
1:B:220:VAL:HG12	1:C:252:LYS:CG	2.32	0.60
1:D:237:GLY:HA2	1:E:267:LEU:CD2	2.31	0.60
1:A:271:LEU:N	1:F:214:ALA:CB	2.55	0.60
1:D:220:VAL:HG23	1:E:250:ALA:C	2.22	0.60
1:B:217:ALA:HB2	1:C:275:LEU:CB	2.19	0.60
1:A:331:ARG:NH2	1:B:355:ASP:HB3	2.15	0.60
1:E:234:GLU:N	1:F:252:LYS:O	2.33	0.60
1:C:232:GLY:CA	1:D:252:LYS:CB	2.78	0.60
1:D:217:ALA:N	1:E:278:ALA:HB1	1.77	0.60
1:B:209:LEU:H	1:C:180:GLN:H	0.74	0.60
1:A:217:ALA:CA	1:B:275:LEU:C	2.69	0.60
1:C:234:GLU:C	1:D:253:SER:HB3	2.22	0.59
1:C:234:GLU:H	1:D:253:SER:CA	2.13	0.59
1:D:213:ASP:HA	1:E:274:ARG:NH2	2.16	0.59
1:A:227:THR:O	1:B:252:LYS:NZ	2.21	0.59
1:C:207:THR:HG22	1:D:177:ILE:O	2.00	0.59
1:C:383:TYR:HD2	1:D:371:ASP:CB	2.15	0.59
1:C:227:THR:HG21	1:D:435:TYR:OH	2.02	0.59
1:A:275:LEU:HD22	1:F:217:ALA:CA	2.31	0.59
1:C:218:THR:HG23	1:D:250:ALA:O	2.02	0.59
1:B:207:THR:CG2	1:C:178:PHE:CA	2.80	0.59
1:A:177:ILE:H	1:F:205:ILE:HG23	1.67	0.59
1:A:249:LEU:CB	1:F:219:TRP:CD1	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:GLU:N	1:C:181:ARG:C	2.56	0.59
1:C:316:ALA:HB1	1:D:352:ALA:HB1	1.84	0.59
1:D:213:ASP:C	1:E:270:LEU:HG	2.22	0.59
1:C:234:GLU:C	1:D:253:SER:CB	2.71	0.59
1:D:218:THR:O	1:E:279:HIS:ND1	2.36	0.59
1:A:220:VAL:CA	1:B:437:THR:HG22	2.33	0.59
1:B:232:GLY:C	1:C:252:LYS:HB3	2.22	0.59
1:B:214:ALA:HB2	1:C:270:LEU:HD23	1.83	0.59
1:C:210:VAL:CG1	1:D:183:ILE:N	2.61	0.58
1:E:214:ALA:N	1:F:274:ARG:HB3	1.91	0.58
1:E:217:ALA:CB	1:F:275:LEU:O	2.51	0.58
1:A:227:THR:N	1:B:435:TYR:HE1	1.99	0.58
1:B:207:THR:OG1	1:C:177:ILE:N	2.35	0.58
1:B:209:LEU:CA	1:C:180:GLN:H	2.16	0.58
1:D:221:ALA:HA	1:E:248:LYS:CB	2.27	0.58
1:A:270:LEU:C	1:F:214:ALA:HB3	2.23	0.58
1:B:243:HIS:CE1	1:C:176:THR:HG23	2.38	0.58
1:C:219:TRP:HB3	1:D:249:LEU:CG	2.33	0.58
1:C:321:LEU:H	1:C:321:LEU:HD23	1.67	0.58
1:D:219:TRP:CE2	1:E:249:LEU:HD13	2.38	0.58
1:D:233:GLU:CD	1:E:434:TYR:O	2.42	0.58
1:A:222:ALA:CB	1:B:439:ARG:HH12	2.16	0.58
1:C:219:TRP:HA	1:D:249:LEU:CB	2.33	0.58
1:C:232:GLY:CA	1:D:251:ALA:HA	2.24	0.58
1:C:216:LYS:O	1:D:278:ALA:CB	2.51	0.58
1:E:213:ASP:CG	1:F:274:ARG:CD	2.19	0.58
1:B:212:PRO:HB2	1:C:184:ARG:HA	1.85	0.58
1:B:207:THR:CG2	1:C:178:PHE:HA	2.32	0.58
1:B:234:GLU:CB	1:C:275:LEU:HD21	2.34	0.58
1:D:213:ASP:CA	1:E:274:ARG:CG	2.81	0.58
1:A:361:GLU:HG2	1:B:363:GLN:HG2	1.82	0.58
1:C:227:THR:CG2	1:D:435:TYR:OH	2.51	0.58
1:D:237:GLY:N	1:E:267:LEU:HD11	2.16	0.58
1:A:235:VAL:HG11	1:B:254:PHE:O	2.02	0.57
1:A:274:ARG:HB3	1:F:215:GLY:O	2.04	0.57
1:A:331:ARG:CZ	1:B:355:ASP:CB	2.76	0.57
1:A:236:LYS:O	1:B:271:LEU:HD13	2.03	0.57
1:A:361:GLU:HB3	1:B:363:GLN:OE1	2.00	0.57
1:A:435:TYR:HD2	1:F:233:GLU:OE2	1.82	0.57
1:B:215:GLY:H	1:C:271:LEU:CD1	2.05	0.57
1:D:222:ALA:CB	1:E:437:THR:OG1	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:ALA:CB	1:F:274:ARG:HB2	2.34	0.57
1:E:241:GLU:OE1	1:F:179:SER:N	2.37	0.57
1:B:205:ILE:HG23	1:C:177:ILE:CG1	2.34	0.57
1:B:234:GLU:HB2	1:C:275:LEU:HD21	1.83	0.57
1:C:220:VAL:N	1:D:249:LEU:CA	2.66	0.57
1:C:222:ALA:HB3	1:D:439:ARG:HH12	1.68	0.57
1:B:212:PRO:HB2	1:C:184:ARG:CA	2.35	0.57
1:B:207:THR:CB	1:C:177:ILE:HG22	2.33	0.57
1:A:232:GLY:O	1:B:252:LYS:O	2.22	0.57
1:A:271:LEU:CD1	1:F:236:LYS:CA	2.68	0.57
1:B:233:GLU:HA	1:C:434:TYR:O	2.04	0.57
1:A:185:ASP:N	1:F:212:PRO:O	2.37	0.57
1:B:233:GLU:OE1	1:C:433:ALA:HA	2.01	0.57
1:D:383:TYR:C	1:E:371:ASP:HB3	2.25	0.57
1:E:241:GLU:HG3	1:F:179:SER:HB2	1.70	0.57
1:E:209:LEU:HB3	1:F:180:GLN:C	2.25	0.57
1:A:252:LYS:HG3	1:F:220:VAL:HG22	1.85	0.57
1:A:362:TRP:HZ2	1:B:362:TRP:CG	2.16	0.57
1:C:207:THR:HB	1:D:177:ILE:CA	2.35	0.57
1:C:232:GLY:CA	1:D:252:LYS:HG3	2.27	0.57
1:E:205:ILE:HG23	1:F:177:ILE:HG13	1.84	0.57
1:E:207:THR:CG2	1:F:179:SER:N	2.66	0.57
1:A:217:ALA:C	1:B:275:LEU:O	2.43	0.56
1:C:222:ALA:HB3	1:D:439:ARG:NH1	2.20	0.56
1:C:383:TYR:HA	1:D:371:ASP:CB	2.35	0.56
1:E:219:TRP:HE1	1:F:283:ILE:N	2.02	0.56
1:E:221:ALA:O	1:F:248:LYS:CG	2.44	0.56
1:A:220:VAL:O	1:B:437:THR:HG22	2.05	0.56
1:A:235:VAL:HG23	1:B:271:LEU:HD22	0.59	0.56
1:E:208:MET:HE3	1:F:181:ARG:HD2	1.86	0.56
1:E:207:THR:HG21	1:F:179:SER:N	2.19	0.56
1:C:234:GLU:O	1:D:253:SER:HB2	2.05	0.56
1:A:212:PRO:O	1:B:184:ARG:CA	2.54	0.56
1:B:209:LEU:CA	1:C:180:GLN:N	2.63	0.56
1:B:207:THR:H	1:C:177:ILE:CG2	2.18	0.56
1:C:316:ALA:HB2	1:D:352:ALA:CB	2.35	0.56
1:D:220:VAL:O	1:E:249:LEU:C	2.43	0.56
1:B:218:THR:OG1	1:C:251:ALA:HA	1.91	0.56
1:A:222:ALA:CB	1:B:439:ARG:NH1	2.69	0.56
1:C:215:GLY:H	1:D:271:LEU:HG	1.69	0.56
1:C:216:LYS:H	1:D:275:LEU:CG	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:THR:N	1:F:435:TYR:CD2	2.73	0.56
1:A:331:ARG:NH2	1:B:355:ASP:CB	2.69	0.56
1:A:214:ALA:C	1:B:274:ARG:CB	2.62	0.56
1:E:207:THR:H	1:F:177:ILE:HG22	1.63	0.56
1:A:235:VAL:HA	1:B:271:LEU:CG	2.36	0.56
1:D:446:PHE:CZ	1:E:183:ILE:CD1	2.87	0.56
1:A:434:TYR:H	1:F:233:GLU:CG	2.06	0.56
1:C:218:THR:O	1:D:279:HIS:HE1	1.83	0.56
1:B:233:GLU:CB	1:C:434:TYR:HB2	2.28	0.56
1:E:217:ALA:HB1	1:F:279:HIS:CG	2.39	0.56
1:D:235:VAL:HG12	1:E:254:PHE:C	2.26	0.56
1:A:435:TYR:CE1	1:F:226:GLY:HA2	2.40	0.56
1:A:254:PHE:CZ	1:F:233:GLU:OE1	2.58	0.56
1:B:316:ALA:HB1	1:C:353:TYR:CZ	2.41	0.55
1:D:209:LEU:HB3	1:E:178:PHE:HB2	1.88	0.55
1:E:210:VAL:CA	1:F:182:ILE:CA	2.33	0.55
1:B:233:GLU:CA	1:C:434:TYR:O	2.49	0.55
1:D:211:GLU:CB	1:E:182:ILE:CG1	2.79	0.55
1:E:204:LYS:NZ	1:F:175:GLU:HB3	2.21	0.55
1:A:252:LYS:CA	1:F:217:ALA:HB1	2.36	0.55
1:B:220:VAL:HG11	1:C:436:VAL:H	1.72	0.55
1:B:230:THR:OG1	1:C:252:LYS:CD	2.54	0.55
1:A:215:GLY:C	1:B:274:ARG:HB2	2.27	0.55
1:C:217:ALA:HB3	1:D:279:HIS:HB2	0.55	0.55
1:C:220:VAL:HG11	1:D:435:TYR:HE1	1.71	0.55
1:E:207:THR:CA	1:F:177:ILE:HG22	2.36	0.55
1:B:241:GLU:OE2	1:C:178:PHE:CA	2.55	0.55
1:C:212:PRO:CB	1:D:184:ARG:HA	2.35	0.55
1:D:215:GLY:CA	1:E:275:LEU:HD21	2.33	0.55
1:A:434:TYR:O	1:F:233:GLU:HG2	2.02	0.55
1:B:232:GLY:O	1:C:252:LYS:C	2.37	0.55
1:A:219:TRP:CA	1:B:279:HIS:CE1	2.90	0.55
1:C:207:THR:O	1:D:177:ILE:CB	2.55	0.55
1:D:220:VAL:CG2	1:E:250:ALA:C	2.68	0.55
1:C:219:TRP:CA	1:D:249:LEU:HB3	2.36	0.55
1:E:211:GLU:OE2	1:F:182:ILE:HD12	2.07	0.55
1:E:206:LEU:C	1:F:177:ILE:HG21	2.26	0.55
1:E:228:ASP:HA	1:F:252:LYS:HD3	1.88	0.55
1:E:232:GLY:HA2	1:F:252:LYS:N	2.19	0.55
1:B:235:VAL:CG1	1:C:255:ILE:CG2	2.67	0.54
1:B:237:GLY:O	1:C:274:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:THR:CB	1:F:177:ILE:C	2.75	0.54
1:A:252:LYS:CB	1:F:232:GLY:O	2.55	0.54
1:B:216:LYS:N	1:C:275:LEU:HD23	2.16	0.54
1:D:182:ILE:O	1:D:182:ILE:HD12	2.06	0.54
1:C:234:GLU:CB	1:D:275:LEU:HD13	2.36	0.54
1:E:241:GLU:OE1	1:F:179:SER:CB	2.56	0.54
1:A:219:TRP:CH2	1:B:248:LYS:HB2	2.32	0.54
1:C:208:MET:CA	1:D:179:SER:HA	2.35	0.54
1:B:215:GLY:C	1:C:275:LEU:HG	2.28	0.54
1:D:235:VAL:CA	1:E:254:PHE:O	2.54	0.54
1:A:361:GLU:CD	1:B:363:GLN:CD	2.64	0.54
1:D:216:LYS:O	1:E:275:LEU:CB	2.53	0.54
1:C:332:ARG:CD	1:D:355:ASP:OD2	2.51	0.54
1:C:331:ARG:NH2	1:D:376:GLN:HE22	2.03	0.54
1:D:235:VAL:HA	1:E:271:LEU:HD11	0.66	0.54
1:C:217:ALA:CA	1:D:279:HIS:HB2	2.21	0.54
1:E:214:ALA:HB3	1:F:274:ARG:HB2	1.88	0.54
1:B:205:ILE:CG2	1:C:177:ILE:HG12	2.37	0.54
1:B:232:GLY:CA	1:C:254:PHE:HD1	2.20	0.54
1:C:209:LEU:C	1:D:179:SER:OG	2.32	0.54
1:D:219:TRP:HZ2	1:E:286:ALA:CB	2.14	0.54
1:A:249:LEU:C	1:F:219:TRP:HB3	2.20	0.54
1:B:241:GLU:OE1	1:C:178:PHE:CD2	2.52	0.54
1:B:220:VAL:CG2	1:C:437:THR:HA	2.35	0.54
1:E:210:VAL:HB	1:F:183:ILE:N	2.23	0.54
1:A:435:TYR:HE2	1:F:233:GLU:OE2	1.87	0.54
1:C:216:LYS:C	1:D:275:LEU:O	2.46	0.54
1:D:220:VAL:HG21	1:E:251:ALA:C	2.28	0.54
1:E:208:MET:CA	1:F:180:GLN:H	2.20	0.53
1:C:219:TRP:C	1:D:250:ALA:O	2.46	0.53
1:A:178:PHE:CG	1:F:207:THR:HG21	2.21	0.53
1:A:214:ALA:O	1:B:271:LEU:CA	2.47	0.53
1:D:235:VAL:CG1	1:E:254:PHE:C	2.76	0.53
1:B:207:THR:O	1:C:177:ILE:HG22	2.09	0.53
1:A:220:VAL:CG1	1:B:437:THR:HG23	2.36	0.53
1:A:204:LYS:CB	1:B:174:TYR:CE2	2.92	0.53
1:F:256:THR:HG22	1:F:431:ARG:HA	1.91	0.53
1:D:216:LYS:CA	1:E:275:LEU:CA	2.78	0.53
1:D:220:VAL:CG2	1:E:251:ALA:CA	2.86	0.53
1:A:213:ASP:C	1:B:274:ARG:NH2	2.48	0.53
1:B:236:LYS:HE2	1:C:274:ARG:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ALA:HB3	1:D:279:HIS:HB3	1.67	0.53
1:C:233:GLU:CD	1:D:252:LYS:CB	2.67	0.53
1:A:212:PRO:O	1:B:184:ARG:HA	2.09	0.53
1:D:220:VAL:O	1:E:250:ALA:N	2.41	0.53
1:A:249:LEU:C	1:F:219:TRP:CD1	2.83	0.53
1:C:207:THR:N	1:D:177:ILE:HB	2.24	0.53
1:D:218:THR:HG21	1:E:252:LYS:H	1.73	0.53
1:A:177:ILE:N	1:F:205:ILE:HG23	2.23	0.53
1:A:233:GLU:HB3	1:B:434:TYR:H	1.74	0.52
1:D:213:ASP:CB	1:E:274:ARG:NH2	2.71	0.52
1:A:271:LEU:CA	1:F:214:ALA:HB1	2.18	0.52
1:C:234:GLU:HB2	1:D:275:LEU:HD13	1.84	0.52
1:E:213:ASP:CG	1:F:274:ARG:CG	2.76	0.52
1:A:360:GLU:OE1	1:B:364:ASP:N	2.41	0.52
1:D:214:ALA:O	1:E:274:ARG:CB	2.57	0.52
1:E:220:VAL:HG21	1:F:251:ALA:N	2.21	0.52
1:A:213:ASP:N	1:B:182:ILE:CD1	2.72	0.52
1:E:214:ALA:CB	1:F:271:LEU:C	2.67	0.52
1:E:207:THR:HG22	1:F:178:PHE:C	2.28	0.52
1:E:214:ALA:CB	1:F:271:LEU:O	2.58	0.52
1:C:235:VAL:CG2	1:D:255:ILE:HD12	2.30	0.52
1:E:219:TRP:CB	1:F:249:LEU:HB3	2.40	0.52
1:E:220:VAL:CG1	1:F:435:TYR:CZ	2.90	0.52
1:C:216:LYS:CB	1:D:278:ALA:CB	2.87	0.52
1:E:207:THR:CG2	1:F:179:SER:HA	2.28	0.52
1:A:361:GLU:N	1:B:363:GLN:HG2	2.25	0.52
1:B:215:GLY:N	1:C:271:LEU:CA	2.48	0.52
1:E:219:TRP:CB	1:F:249:LEU:CA	2.77	0.52
1:E:360:GLU:HB2	1:F:363:GLN:HA	1.92	0.52
1:E:216:LYS:N	1:F:275:LEU:HD12	2.16	0.51
1:A:212:PRO:O	1:B:184:ARG:CB	2.57	0.51
1:B:205:ILE:HG23	1:C:177:ILE:HG12	1.92	0.51
1:A:226:GLY:CA	1:B:424:GLU:CD	2.75	0.51
1:C:220:VAL:N	1:D:250:ALA:CA	2.70	0.51
1:B:237:GLY:HA2	1:C:267:LEU:HD21	1.90	0.51
1:A:252:LYS:CE	1:F:227:THR:OG1	2.56	0.51
1:E:222:ALA:HA	1:F:435:TYR:OH	2.10	0.51
1:A:216:LYS:CB	1:B:275:LEU:HD23	2.41	0.51
1:C:235:VAL:CB	1:D:271:LEU:HD21	2.40	0.51
1:D:212:PRO:CG	1:E:183:ILE:O	2.55	0.51
1:D:216:LYS:N	1:E:275:LEU:HA	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:TRP:CE3	1:C:249:LEU:HD23	2.45	0.51
1:B:214:ALA:O	1:C:271:LEU:CA	2.58	0.51
1:E:204:LYS:HD2	1:F:175:GLU:HB3	1.92	0.51
1:C:217:ALA:HB2	1:D:275:LEU:HG	1.92	0.51
1:E:219:TRP:NE1	1:F:282:SER:O	2.44	0.51
1:D:303:ALA:HB2	1:D:450:VAL:HG13	1.92	0.51
1:B:219:TRP:HA	1:C:279:HIS:CE1	2.45	0.51
1:C:232:GLY:HA3	1:D:252:LYS:CB	2.39	0.51
1:C:222:ALA:CB	1:D:439:ARG:HH12	2.24	0.51
1:E:209:LEU:HB2	1:F:180:GLN:CA	2.40	0.51
1:E:213:ASP:CG	1:F:274:ARG:HB3	2.32	0.51
1:A:252:LYS:CE	1:F:230:THR:OG1	2.57	0.51
1:E:215:GLY:HA3	1:F:275:LEU:HB2	1.92	0.51
1:C:216:LYS:H	1:D:275:LEU:CB	2.22	0.51
1:B:220:VAL:CB	1:C:436:VAL:O	2.58	0.51
1:D:235:VAL:CG1	1:E:255:ILE:CB	2.83	0.51
1:E:219:TRP:CE2	1:F:282:SER:O	2.64	0.51
1:B:234:GLU:O	1:C:275:LEU:CG	2.59	0.50
1:E:233:GLU:CG	1:F:252:LYS:HB3	2.39	0.50
1:C:383:TYR:CD2	1:D:371:ASP:CB	2.94	0.50
1:B:220:VAL:CG1	1:C:436:VAL:H	2.24	0.50
1:C:360:GLU:HB3	1:D:362:TRP:O	2.12	0.50
1:A:275:LEU:CA	1:F:216:LYS:HA	2.31	0.50
1:E:223:SER:N	1:F:439:ARG:HH22	2.10	0.50
1:C:219:TRP:CD1	1:D:249:LEU:CB	2.85	0.50
1:D:218:THR:O	1:E:251:ALA:CB	2.45	0.50
1:E:211:GLU:HB3	1:F:270:LEU:HD11	1.93	0.50
1:E:228:ASP:HB3	1:F:252:LYS:CD	2.40	0.50
1:A:252:LYS:CG	1:F:220:VAL:HG22	2.40	0.50
1:B:235:VAL:HG12	1:C:255:ILE:CG1	2.41	0.50
1:C:217:ALA:N	1:D:275:LEU:HD11	2.15	0.50
1:C:234:GLU:C	1:D:253:SER:HB2	2.32	0.50
1:E:219:TRP:CA	1:F:250:ALA:O	2.58	0.50
1:A:223:SER:N	1:B:439:ARG:HH12	2.08	0.50
1:A:271:LEU:HD13	1:F:236:LYS:CB	2.41	0.50
1:D:205:ILE:O	1:E:177:ILE:HG12	2.12	0.50
1:D:232:GLY:CA	1:E:252:LYS:CE	2.61	0.50
1:A:271:LEU:HD11	1:F:236:LYS:HG3	1.94	0.50
1:A:219:TRP:CB	1:B:279:HIS:ND1	2.75	0.49
1:A:219:TRP:N	1:B:279:HIS:ND1	2.60	0.49
1:B:214:ALA:HB3	1:C:270:LEU:CA	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:PRO:HA	1:D:182:ILE:CD1	2.36	0.49
1:C:233:GLU:N	1:D:252:LYS:CB	2.48	0.49
1:B:214:ALA:CA	1:C:271:LEU:HA	2.39	0.49
1:D:221:ALA:CA	1:E:248:LYS:HB3	2.29	0.49
1:D:236:LYS:O	1:E:267:LEU:HD11	2.13	0.49
1:E:228:ASP:HA	1:F:252:LYS:CD	2.42	0.49
1:A:252:LYS:O	1:F:217:ALA:CA	2.51	0.49
1:A:212:PRO:C	1:B:184:ARG:HA	2.32	0.49
1:C:368:VAL:HG23	1:C:375:LEU:HD13	1.95	0.49
1:D:234:GLU:CA	1:E:254:PHE:H	2.22	0.49
1:C:216:LYS:CE	1:D:278:ALA:HA	2.34	0.49
1:A:212:PRO:CB	1:B:184:ARG:CA	2.83	0.49
1:B:210:VAL:HG11	1:C:183:ILE:H	1.76	0.49
1:D:237:GLY:HA2	1:E:267:LEU:HD21	1.94	0.49
1:A:207:THR:HG21	1:B:176:THR:CG2	2.36	0.49
1:A:206:LEU:HB3	1:B:177:ILE:HG21	1.95	0.49
1:B:208:MET:C	1:C:179:SER:HA	2.08	0.49
1:B:214:ALA:HB2	1:C:270:LEU:CD2	2.43	0.49
1:A:214:ALA:HB3	1:B:271:LEU:N	2.27	0.49
1:C:207:THR:O	1:D:177:ILE:HB	2.13	0.49
1:C:215:GLY:C	1:D:275:LEU:N	2.65	0.49
1:D:235:VAL:HB	1:E:254:PHE:C	2.27	0.49
1:C:220:VAL:O	1:D:249:LEU:N	2.46	0.49
1:E:213:ASP:OD1	1:F:274:ARG:NH2	2.45	0.49
1:A:178:PHE:CD1	1:F:207:THR:CG2	2.93	0.49
1:C:220:VAL:HG21	1:D:251:ALA:CA	2.40	0.49
1:D:236:LYS:O	1:E:267:LEU:HG	2.12	0.49
1:E:207:THR:CG2	1:F:179:SER:CA	2.89	0.49
1:A:331:ARG:NH2	1:B:355:ASP:OD2	2.45	0.49
1:C:219:TRP:CG	1:D:249:LEU:CD2	2.93	0.49
1:C:225:TYR:O	1:D:435:TYR:CD2	2.66	0.49
1:E:213:ASP:OD1	1:F:274:ARG:CG	2.55	0.49
1:B:215:GLY:HA2	1:C:271:LEU:CD1	2.42	0.48
1:D:237:GLY:C	1:E:267:LEU:CD1	2.77	0.48
1:D:235:VAL:C	1:E:271:LEU:CD1	2.82	0.48
1:B:220:VAL:HG22	1:C:437:THR:CA	2.35	0.48
1:D:236:LYS:C	1:E:267:LEU:HD11	2.33	0.48
1:E:219:TRP:CG	1:F:249:LEU:HB3	2.48	0.48
1:A:182:ILE:HA	1:F:211:GLU:CA	2.33	0.48
1:A:271:LEU:CA	1:F:214:ALA:C	2.63	0.48
1:D:207:THR:OG1	1:E:176:THR:CA	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:LYS:C	1:E:275:LEU:O	2.51	0.48
1:E:223:SER:H	1:F:439:ARG:HH22	1.59	0.48
1:A:435:TYR:CE2	1:F:233:GLU:CD	2.87	0.48
1:A:219:TRP:CG	1:B:279:HIS:CE1	2.83	0.48
1:C:211:GLU:CB	1:D:182:ILE:HG12	2.26	0.48
1:E:207:THR:HG21	1:F:178:PHE:CA	2.43	0.48
1:B:279:HIS:CD2	1:B:283:ILE:HD11	2.49	0.48
1:C:219:TRP:CE2	1:D:249:LEU:HD13	2.48	0.48
1:C:220:VAL:CG2	1:D:251:ALA:HA	2.41	0.48
1:D:235:VAL:CB	1:E:271:LEU:CD1	2.92	0.48
1:A:274:ARG:HB2	1:F:215:GLY:O	2.12	0.48
1:E:212:PRO:O	1:F:274:ARG:HD2	2.14	0.48
1:A:252:LYS:C	1:F:217:ALA:HB1	2.34	0.48
1:B:220:VAL:HG13	1:C:251:ALA:N	2.29	0.48
1:C:356:LEU:HD11	1:C:367:GLN:HE22	1.78	0.48
1:D:233:GLU:HG2	1:E:252:LYS:HB2	1.96	0.48
1:E:214:ALA:O	1:F:275:LEU:N	2.47	0.48
1:A:216:LYS:CA	1:B:274:ARG:O	2.55	0.48
1:D:209:LEU:CB	1:E:178:PHE:CB	2.87	0.48
1:E:226:GLY:HA2	1:F:435:TYR:HD2	1.78	0.48
1:D:218:THR:O	1:E:251:ALA:HB2	1.59	0.48
1:D:215:GLY:HA3	1:E:271:LEU:O	2.14	0.48
1:B:216:LYS:CD	1:C:274:ARG:O	2.62	0.48
1:D:219:TRP:CD2	1:E:249:LEU:HD22	2.49	0.48
1:A:177:ILE:N	1:F:207:THR:OG1	2.47	0.48
1:A:220:VAL:HG23	1:B:251:ALA:N	2.28	0.48
1:C:205:ILE:O	1:D:177:ILE:HG13	2.11	0.48
1:D:212:PRO:HB3	1:E:182:ILE:CD1	2.35	0.48
1:C:233:GLU:CB	1:D:253:SER:C	2.79	0.48
1:D:218:THR:C	1:E:251:ALA:CA	2.67	0.48
1:A:254:PHE:CG	1:F:233:GLU:N	2.82	0.47
1:A:216:LYS:NZ	1:B:277:GLU:O	2.19	0.47
1:A:181:ARG:HA	1:F:211:GLU:OE2	2.13	0.47
1:A:437:THR:HG22	1:F:220:VAL:HB	1.96	0.47
1:A:182:ILE:HA	1:F:211:GLU:C	2.32	0.47
1:B:214:ALA:HB3	1:C:270:LEU:HB3	1.96	0.47
1:E:219:TRP:CB	1:F:249:LEU:CB	2.90	0.47
1:A:271:LEU:HB3	1:F:235:VAL:HG23	1.86	0.47
1:B:214:ALA:O	1:C:274:ARG:CG	2.58	0.47
1:B:243:HIS:CE1	1:C:176:THR:CG2	2.97	0.47
1:F:424:GLU:HG2	1:F:426:GLN:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLU:HB2	1:C:275:LEU:HD22	1.93	0.47
1:E:234:GLU:O	1:F:275:LEU:HD13	2.14	0.47
1:B:212:PRO:HA	1:C:182:ILE:HD12	0.51	0.47
1:C:219:TRP:CG	1:D:249:LEU:CB	2.97	0.47
1:E:223:SER:N	1:F:439:ARG:HH12	2.13	0.47
1:A:361:GLU:CA	1:B:363:GLN:HG2	2.45	0.47
1:A:360:GLU:O	1:B:362:TRP:HB2	2.15	0.47
1:D:234:GLU:O	1:E:253:SER:CB	2.61	0.47
1:C:233:GLU:CB	1:D:254:PHE:N	2.64	0.47
1:D:237:GLY:CA	1:E:267:LEU:HD21	2.45	0.47
1:E:209:LEU:N	1:F:180:GLN:N	2.56	0.47
1:A:271:LEU:CD1	1:F:214:ALA:HB1	2.45	0.47
1:A:253:SER:H	1:F:233:GLU:CG	1.89	0.47
1:B:207:THR:CB	1:C:177:ILE:CG2	2.83	0.47
1:E:220:VAL:HG11	1:F:435:TYR:HE1	0.68	0.47
1:A:211:GLU:N	1:B:181:ARG:O	2.48	0.47
1:A:218:THR:CG2	1:B:251:ALA:CB	2.87	0.47
1:C:208:MET:HB2	1:D:179:SER:CB	2.44	0.47
1:D:234:GLU:C	1:E:254:PHE:O	2.52	0.47
1:B:237:GLY:HA3	1:C:267:LEU:HD11	1.97	0.47
1:C:347:ILE:HD11	1:C:401:GLU:H	1.79	0.47
1:E:207:THR:HG22	1:F:178:PHE:O	2.13	0.47
1:E:219:TRP:HB3	1:F:249:LEU:CD2	2.45	0.47
1:A:176:THR:HA	1:F:205:ILE:HG21	1.78	0.46
1:D:215:GLY:HA2	1:E:275:LEU:HD21	1.92	0.46
1:A:177:ILE:HG21	1:F:206:LEU:HB3	1.07	0.46
1:A:253:SER:N	1:F:233:GLU:CG	2.53	0.46
1:A:271:LEU:HD13	1:F:236:LYS:C	2.36	0.46
1:A:226:GLY:HA2	1:B:435:TYR:HE1	1.79	0.46
1:B:219:TRP:CG	1:C:249:LEU:CD2	2.98	0.46
1:A:222:ALA:N	1:B:439:ARG:NH1	2.64	0.46
1:D:236:LYS:O	1:E:267:LEU:CD1	2.64	0.46
1:E:406:VAL:O	1:E:410:ASN:HB2	2.16	0.46
1:D:222:ALA:C	1:E:439:ARG:NH1	2.50	0.46
1:A:218:THR:CB	1:B:251:ALA:CB	2.49	0.46
1:A:360:GLU:OE1	1:B:363:GLN:C	2.53	0.46
1:B:365:VAL:HB	1:C:369:GLY:HA3	1.97	0.46
1:B:234:GLU:CB	1:C:275:LEU:CD2	2.83	0.46
1:D:235:VAL:HB	1:E:255:ILE:CB	2.35	0.46
1:E:207:THR:HG22	1:F:179:SER:N	2.30	0.46
1:A:176:THR:CB	1:F:205:ILE:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:VAL:HG12	1:F:222:ALA:H	1.81	0.46
1:B:220:VAL:HG11	1:C:436:VAL:N	2.31	0.46
1:A:362:TRP:HB2	1:F:360:GLU:OE1	2.16	0.46
1:A:274:ARG:O	1:F:216:LYS:HD2	2.16	0.45
1:A:361:GLU:HB3	1:F:360:GLU:HG2	1.97	0.45
1:B:214:ALA:O	1:C:271:LEU:C	2.55	0.45
1:D:205:ILE:O	1:E:177:ILE:CG1	2.63	0.45
1:E:199:LEU:HD12	1:E:200:PRO:HD2	1.99	0.45
1:A:252:LYS:C	1:F:217:ALA:CB	2.84	0.45
1:A:234:GLU:C	1:B:275:LEU:HD21	2.37	0.45
1:A:275:LEU:HD21	1:F:234:GLU:HB3	1.95	0.45
1:B:211:GLU:N	1:C:182:ILE:N	2.40	0.45
1:B:219:TRP:CG	1:C:249:LEU:HD23	2.52	0.45
1:B:214:ALA:CA	1:C:270:LEU:HG	2.47	0.45
1:A:180:GLN:O	1:F:208:MET:CE	2.65	0.45
1:A:250:ALA:N	1:F:219:TRP:HD1	2.04	0.45
1:A:352:ALA:CB	1:F:332:ARG:HD3	2.37	0.45
1:A:217:ALA:N	1:B:275:LEU:HD23	2.09	0.45
1:A:275:LEU:HD22	1:F:234:GLU:HB2	1.98	0.45
1:E:221:ALA:C	1:F:248:LYS:HB3	2.36	0.45
1:A:233:GLU:CG	1:B:434:TYR:CA	2.63	0.45
1:A:275:LEU:HD21	1:F:215:GLY:CA	2.47	0.45
1:B:255:ILE:HD11	1:B:432:ASP:HB3	1.99	0.45
1:D:217:ALA:HA	1:E:275:LEU:O	2.15	0.45
1:C:213:ASP:HA	1:D:274:ARG:HD3	0.45	0.45
1:E:241:GLU:CD	1:F:179:SER:CB	2.72	0.45
1:E:210:VAL:HA	1:F:182:ILE:HA	0.55	0.45
1:C:217:ALA:CB	1:D:279:HIS:CG	2.83	0.45
1:D:219:TRP:HB3	1:E:249:LEU:CD2	2.46	0.45
1:D:234:GLU:O	1:E:253:SER:HB2	1.89	0.45
1:A:352:ALA:CA	1:F:332:ARG:CD	2.94	0.45
1:A:217:ALA:HB1	1:B:436:VAL:HG23	1.94	0.45
1:A:213:ASP:N	1:B:182:ILE:HD11	2.29	0.45
1:D:444:ARG:HH11	1:D:447:ALA:HB2	1.82	0.45
1:E:209:LEU:CB	1:F:180:GLN:CA	2.94	0.45
1:C:406:VAL:HG13	1:C:410:ASN:HB2	1.99	0.44
1:A:178:PHE:CE1	1:F:207:THR:HG21	2.48	0.44
1:E:233:GLU:H	1:F:252:LYS:HB3	1.64	0.44
1:A:178:PHE:HE2	1:F:241:GLU:OE1	2.01	0.44
1:B:209:LEU:C	1:C:180:GLN:O	2.49	0.44
1:B:222:ALA:HB3	1:C:248:LYS:CD	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:GLU:OE1	1:B:362:TRP:C	2.53	0.44
1:C:219:TRP:CB	1:D:249:LEU:CA	2.85	0.44
1:D:321:LEU:HD13	1:D:329:LYS:NZ	2.32	0.44
1:D:208:MET:HA	1:E:179:SER:HA	1.90	0.44
1:A:439:ARG:HH12	1:F:222:ALA:HB3	1.82	0.44
1:B:207:THR:N	1:C:177:ILE:HB	2.32	0.44
1:A:209:LEU:HD12	1:B:178:PHE:HB2	2.00	0.44
1:A:220:VAL:HG11	1:B:252:LYS:HE2	1.99	0.44
1:A:348:VAL:HG13	1:A:349:SER:N	2.33	0.44
1:B:227:THR:HG22	1:B:229:THR:H	1.82	0.44
1:C:220:VAL:N	1:D:250:ALA:O	2.51	0.44
1:D:347:ILE:H	1:D:347:ILE:HG13	1.66	0.44
1:E:215:GLY:HA3	1:F:275:LEU:CB	2.46	0.44
1:D:216:LYS:CG	1:E:278:ALA:HB1	2.16	0.44
1:E:213:ASP:OD1	1:F:274:ARG:CZ	2.66	0.44
1:A:252:LYS:HG2	1:F:220:VAL:HG21	1.99	0.44
1:A:176:THR:HG22	1:F:207:THR:HG1	1.78	0.44
1:D:216:LYS:HA	1:E:275:LEU:HA	1.91	0.44
1:F:249:LEU:HD21	1:F:295:LYS:HA	2.00	0.44
1:A:219:TRP:HB2	1:B:279:HIS:ND1	2.33	0.44
1:B:339:LEU:HD13	1:B:405:ILE:HD11	1.99	0.44
1:B:234:GLU:CA	1:C:275:LEU:HD21	2.44	0.44
1:D:190:LEU:HB3	1:D:284:GLU:HG3	2.00	0.44
1:D:219:TRP:CD1	1:E:249:LEU:HD13	2.53	0.44
1:E:208:MET:CA	1:F:180:GLN:N	2.79	0.44
1:E:226:GLY:HA2	1:F:435:TYR:CD2	2.53	0.44
1:A:216:LYS:C	1:B:275:LEU:HD23	2.36	0.43
1:D:235:VAL:CB	1:E:255:ILE:CA	2.93	0.43
1:E:220:VAL:HG12	1:F:435:TYR:OH	2.19	0.43
1:B:220:VAL:CG2	1:C:437:THR:CA	2.94	0.43
1:A:216:LYS:HD2	1:B:278:ALA:H	1.58	0.43
1:B:234:GLU:OE2	1:C:253:SER:HA	2.19	0.43
1:B:211:GLU:O	1:C:182:ILE:N	2.41	0.43
1:B:433:ALA:HB1	1:B:435:TYR:CE2	2.54	0.43
1:A:275:LEU:CD2	1:F:215:GLY:CA	2.95	0.43
1:A:219:TRP:HB2	1:B:279:HIS:CE1	2.53	0.43
1:A:255:ILE:HG12	1:F:235:VAL:HG11	1.33	0.43
1:A:178:PHE:CG	1:F:207:THR:CB	3.00	0.43
1:B:218:THR:N	1:C:251:ALA:C	2.68	0.43
1:A:271:LEU:CD1	1:F:214:ALA:CA	2.89	0.43
1:B:316:ALA:HB1	1:C:353:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:TRP:HA	1:F:279:HIS:HE1	1.83	0.43
1:A:208:MET:HB3	1:B:177:ILE:HG22	2.01	0.43
1:A:219:TRP:CG	1:B:249:LEU:CB	2.52	0.42
1:A:268:LEU:HD21	1:A:434:TYR:CE1	2.54	0.42
1:D:209:LEU:HB3	1:E:178:PHE:CB	2.49	0.42
1:D:218:THR:C	1:E:250:ALA:C	2.75	0.42
1:C:216:LYS:H	1:D:275:LEU:HA	1.30	0.42
1:A:249:LEU:CA	1:F:219:TRP:CD1	3.02	0.42
1:A:207:THR:C	1:B:177:ILE:CG2	2.63	0.42
1:B:360:GLU:OE1	1:C:364:ASP:OD2	2.36	0.42
1:A:217:ALA:CB	1:B:436:VAL:CG2	2.89	0.42
1:D:215:GLY:HA3	1:E:275:LEU:CG	2.48	0.42
1:D:211:GLU:HB3	1:E:182:ILE:CG1	2.49	0.42
1:D:235:VAL:CB	1:E:271:LEU:HD11	2.35	0.42
1:D:215:GLY:N	1:E:271:LEU:CG	2.60	0.42
1:C:212:PRO:O	1:D:274:ARG:CZ	2.68	0.42
1:D:216:LYS:HA	1:E:275:LEU:N	2.33	0.42
1:B:241:GLU:CD	1:C:178:PHE:CD2	2.86	0.42
1:E:211:GLU:CB	1:F:182:ILE:HB	2.47	0.42
1:C:214:ALA:HB1	1:D:271:LEU:HG	2.01	0.42
1:D:220:VAL:HG23	1:E:251:ALA:HA	2.01	0.42
1:E:305:GLU:HA	1:E:309:LYS:HA	2.02	0.42
1:B:219:TRP:CD2	1:C:249:LEU:CD2	2.95	0.42
1:A:271:LEU:CD1	1:F:215:GLY:H	2.21	0.42
1:D:222:ALA:CB	1:E:437:THR:CB	2.97	0.42
1:E:219:TRP:CD2	1:F:249:LEU:HD22	2.55	0.42
1:E:226:GLY:CA	1:F:435:TYR:HD2	2.33	0.42
1:C:332:ARG:HD3	1:D:355:ASP:CG	2.39	0.42
1:C:234:GLU:C	1:D:275:LEU:HD13	2.40	0.42
1:C:219:TRP:CG	1:D:249:LEU:CD1	2.97	0.41
1:B:207:THR:H	1:C:177:ILE:HG21	1.84	0.41
1:A:215:GLY:HA3	1:B:275:LEU:HG	2.03	0.41
1:C:233:GLU:HG2	1:D:254:PHE:CB	2.41	0.41
1:E:400:ALA:H	1:E:455:TYR:HB3	1.85	0.41
1:A:207:THR:CG2	1:B:176:THR:HG22	2.42	0.41
1:C:214:ALA:HB1	1:D:271:LEU:CG	2.51	0.41
1:C:219:TRP:CG	1:D:249:LEU:CG	3.03	0.41
1:B:237:GLY:C	1:C:274:ARG:HH22	2.22	0.41
1:D:256:THR:HG22	1:D:431:ARG:HG2	2.01	0.41
1:E:218:THR:HA	1:F:282:SER:OG	2.20	0.41
1:A:178:PHE:CD1	1:F:207:THR:HG21	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:HIS:NE2	1:B:283:ILE:HD11	2.34	0.41
1:B:215:GLY:HA3	1:C:275:LEU:HG	1.97	0.41
1:D:383:TYR:C	1:E:371:ASP:CB	2.88	0.41
1:E:220:VAL:CG1	1:F:435:TYR:OH	2.68	0.41
1:A:435:TYR:HE2	1:F:233:GLU:CD	2.23	0.41
1:A:252:LYS:CG	1:F:220:VAL:HG21	2.51	0.41
1:C:207:THR:HB	1:D:177:ILE:N	2.35	0.41
1:E:214:ALA:O	1:F:274:ARG:CA	2.63	0.41
1:E:209:LEU:O	1:F:180:GLN:O	2.33	0.41
1:A:352:ALA:CA	1:F:332:ARG:HD3	2.50	0.41
1:A:254:PHE:HA	1:F:233:GLU:HB2	1.66	0.41
1:B:212:PRO:CB	1:C:182:ILE:HD12	1.95	0.41
1:C:220:VAL:O	1:D:249:LEU:C	2.58	0.41
1:C:207:THR:H	1:D:177:ILE:HB	1.82	0.41
1:E:228:ASP:CA	1:F:252:LYS:CD	2.98	0.41
1:D:232:GLY:C	1:E:252:LYS:HB2	2.39	0.41
1:A:177:ILE:HG13	1:F:206:LEU:HG	1.52	0.41
1:D:322:VAL:HG22	1:D:325:LYS:HB2	2.03	0.41
1:D:217:ALA:CA	1:E:275:LEU:O	2.69	0.41
1:A:183:ILE:N	1:F:212:PRO:HA	2.33	0.41
1:B:241:GLU:OE2	1:C:179:SER:N	2.49	0.41
1:B:243:HIS:HE1	1:C:176:THR:CG2	2.33	0.41
1:B:232:GLY:CA	1:C:254:PHE:CD1	2.82	0.41
1:B:214:ALA:CB	1:C:270:LEU:CB	2.94	0.41
1:C:419:VAL:HB	1:C:438:GLN:HE21	1.86	0.41
1:C:210:VAL:HG12	1:D:182:ILE:CA	2.48	0.41
1:C:234:GLU:CA	1:D:253:SER:HB3	2.51	0.41
1:E:210:VAL:HA	1:F:181:ARG:C	2.35	0.41
1:E:211:GLU:CG	1:F:182:ILE:CG2	2.99	0.41
1:A:360:GLU:OE1	1:B:363:GLN:CA	2.68	0.41
1:B:207:THR:HG22	1:C:178:PHE:CA	2.49	0.41
1:A:216:LYS:O	1:B:274:ARG:O	2.39	0.41
1:A:217:ALA:N	1:B:275:LEU:HD22	2.04	0.41
1:E:228:ASP:HB3	1:F:252:LYS:HD3	2.02	0.41
1:A:207:THR:OG1	1:B:177:ILE:N	2.40	0.40
1:B:230:THR:HG1	1:C:252:LYS:HD2	1.83	0.40
1:D:287:PHE:CZ	1:D:413:MET:HG3	2.56	0.40
1:E:219:TRP:CA	1:F:249:LEU:CA	2.98	0.40
1:E:211:GLU:O	1:F:270:LEU:CD2	2.69	0.40
1:A:360:GLU:HG2	1:B:362:TRP:HA	1.76	0.40
1:B:192:VAL:HA	1:B:195:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:TRP:CZ2	1:D:286:ALA:HB3	2.56	0.40
1:C:316:ALA:CB	1:D:352:ALA:CB	2.93	0.40
1:E:213:ASP:CG	1:F:274:ARG:CB	2.90	0.40
1:A:275:LEU:HG	1:F:215:GLY:HA3	2.04	0.40
1:A:331:ARG:HA	1:A:334:LEU:HD12	2.04	0.40
1:A:208:MET:HB2	1:B:179:SER:HA	1.12	0.40
1:A:435:TYR:HE1	1:F:226:GLY:HA2	1.86	0.40
1:B:222:ALA:HB3	1:C:248:LYS:HD2	2.04	0.40
1:C:207:THR:HB	1:D:177:ILE:H	1.87	0.40
1:D:209:LEU:HB3	1:E:178:PHE:CG	2.55	0.40
1:D:220:VAL:HB	1:E:251:ALA:H	1.81	0.40
1:E:232:GLY:CA	1:F:252:LYS:CA	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	290/299 (97%)	246 (85%)	26 (9%)	18 (6%)	2	26
1	B	290/299 (97%)	230 (79%)	44 (15%)	16 (6%)	2	29
1	C	290/299 (97%)	233 (80%)	38 (13%)	19 (7%)	1	24
1	D	290/299 (97%)	242 (83%)	32 (11%)	16 (6%)	2	29
1	E	290/299 (97%)	238 (82%)	36 (12%)	16 (6%)	2	29
1	F	290/299 (97%)	237 (82%)	33 (11%)	20 (7%)	1	23
All	All	1740/1794 (97%)	1426 (82%)	209 (12%)	105 (6%)	4	26

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	VAL

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Mol	Chain	Res	Type
1	A	223	SER
1	A	262	ASP
1	A	370	ASN
1	A	411	PHE
1	B	192	VAL
1	B	263	ALA
1	B	319	SER
1	B	357	LEU
1	B	427	ALA
1	C	263	ALA
1	C	319	SER
1	C	371	ASP
1	D	192	VAL
1	D	394	PRO
1	D	397	ALA
1	E	192	VAL
1	E	195	LEU
1	E	319	SER
1	F	212	PRO
1	F	222	ALA
1	F	223	SER
1	F	231	THR
1	F	320	VAL
1	F	397	ALA
1	A	368	VAL
1	A	397	ALA
1	A	431	ARG
1	B	186	LEU
1	B	212	PRO
1	B	397	ALA
1	B	408	LYS
1	C	170	SER
1	C	186	LEU
1	C	320	VAL
1	C	363	GLN
1	C	364	ASP
1	C	367	GLN
1	D	175	GLU
1	D	319	SER
1	E	175	GLU
1	E	216	LYS
1	E	405	ILE

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Mol	Chain	Res	Type
1	F	175	GLU
1	F	195	LEU
1	A	213	ASP
1	A	363	GLN
1	A	369	GLY
1	A	408	LYS
1	C	175	GLU
1	C	181	ARG
1	C	216	LYS
1	D	212	PRO
1	D	369	GLY
1	E	320	VAL
1	E	357	LEU
1	E	369	GLY
1	F	228	ASP
1	F	363	GLN
1	F	431	ARG
1	A	186	LEU
1	A	212	PRO
1	A	364	ASP
1	B	233	GLU
1	B	307	SER
1	B	320	VAL
1	B	364	ASP
1	C	179	SER
1	C	397	ALA
1	D	195	LEU
1	D	262	ASP
1	D	320	VAL
1	D	363	GLN
1	D	367	GLN
1	D	370	ASN
1	E	427	ALA
1	F	168	GLU
1	F	181	ARG
1	F	369	GLY
1	F	427	ALA
1	B	369	GLY
1	C	195	LEU
1	C	212	PRO
1	C	366	ALA
1	C	394	PRO

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Mol	Chain	Res	Type
1	D	230	THR
1	E	181	ARG
1	E	258	GLU
1	E	263	ALA
1	E	368	VAL
1	F	170	SER
1	F	364	ASP
1	A	263	ALA
1	D	222	ALA
1	D	427	ALA
1	E	186	LEU
1	A	320	VAL
1	F	235	VAL
1	F	311	VAL
1	A	215	GLY
1	B	394	PRO
1	E	169	VAL
1	F	368	VAL
1	C	311	VAL
1	B	368	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/250 (98%)	232 (94%)	14 (6%)	25	62
1	B	246/250 (98%)	235 (96%)	11 (4%)	34	69
1	C	246/250 (98%)	234 (95%)	12 (5%)	31	67
1	D	246/250 (98%)	237 (96%)	9 (4%)	41	73
1	E	246/250 (98%)	240 (98%)	6 (2%)	57	82
1	F	246/250 (98%)	235 (96%)	11 (4%)	34	69
All	All	1476/1500 (98%)	1413 (96%)	63 (4%)	40	70

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	ILE
1	A	191	VAL
1	A	208	MET
1	A	227	THR
1	A	228	ASP
1	A	236	LYS
1	A	327	ILE
1	A	344	LEU
1	A	346	LEU
1	A	359	ASP
1	A	404	VAL
1	A	416	GLN
1	A	432	ASP
1	A	440	VAL
1	B	239	LEU
1	B	287	PHE
1	B	321	LEU
1	B	344	LEU
1	B	346	LEU
1	B	359	ASP
1	B	367	GLN
1	B	379	VAL
1	B	420	THR
1	B	432	ASP
1	B	441	ASN
1	C	202	SER
1	C	206	LEU
1	C	216	LYS
1	C	233	GLU
1	C	239	LEU
1	C	267	LEU
1	C	288	MET
1	C	355	ASP
1	C	360	GLU
1	C	390	SER
1	C	416	GLN
1	C	440	VAL
1	D	179	SER
1	D	191	VAL
1	D	227	THR
1	D	239	LEU
1	D	262	ASP
1	D	291	ASP

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Mol	Chain	Res	Type
1	D	321	LEU
1	D	416	GLN
1	D	441	ASN
1	E	254	PHE
1	E	262	ASP
1	E	268	LEU
1	E	321	LEU
1	E	359	ASP
1	E	444	ARG
1	F	172	GLU
1	F	208	MET
1	F	227	THR
1	F	228	ASP
1	F	243	HIS
1	F	287	PHE
1	F	291	ASP
1	F	301	THR
1	F	321	LEU
1	F	331	ARG
1	F	367	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	HIS
1	A	337	HIS
1	A	416	GLN
1	B	180	GLN
1	B	243	HIS
1	B	279	HIS
1	B	367	GLN
1	C	416	GLN
1	C	426	GLN
1	D	187	GLN
1	D	376	GLN
1	E	363	GLN
1	E	367	GLN
1	F	243	HIS

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.