



## wwPDB EM Map/Model Validation Report ⓘ

Jun 27, 2016 – 04:58 AM EDT

PDB ID : 5JB1  
EMDB ID: : EMD-8147  
Title : Pseudo-atomic structure of Human Papillomavirus Type 59 L1 Virus-like Particle  
Authors : Li, Z.H.; Yan, X.D.; Yu, H.; Zheng, Q.B.; Gu, Y.; Li, S.W.  
Deposited on : 2016-04-13  
Resolution : 6.00 Å(reported)  
Based on PDB ID : ?

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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-20027790

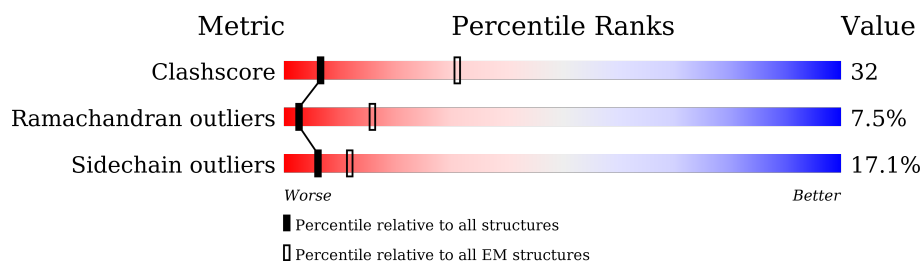
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.00 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  $\geq 3$ , 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	500	 32% 38% 13% 7% 9%
1	B	500	 33% 37% 16% 7% 7%
1	C	500	 33% 37% 15% 6% 9%
1	D	500	 31% 38% 14% 8% 9%
1	E	500	 30% 38% 16% 6% 9%
1	F	500	 33% 38% 15% 6% 7%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21696 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Major capsid protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	456	Total	C	N	O	S	0	0
			3598	2289	604	686	19		
1	B	464	Total	C	N	O	S	0	0
			3661	2333	613	696	19		
1	C	457	Total	C	N	O	S	0	0
			3604	2292	605	688	19		
1	D	454	Total	C	N	O	S	0	0
			3586	2281	602	684	19		
1	E	454	Total	C	N	O	S	0	0
			3586	2281	602	684	19		
1	F	464	Total	C	N	O	S	0	0
			3661	2333	613	696	19		

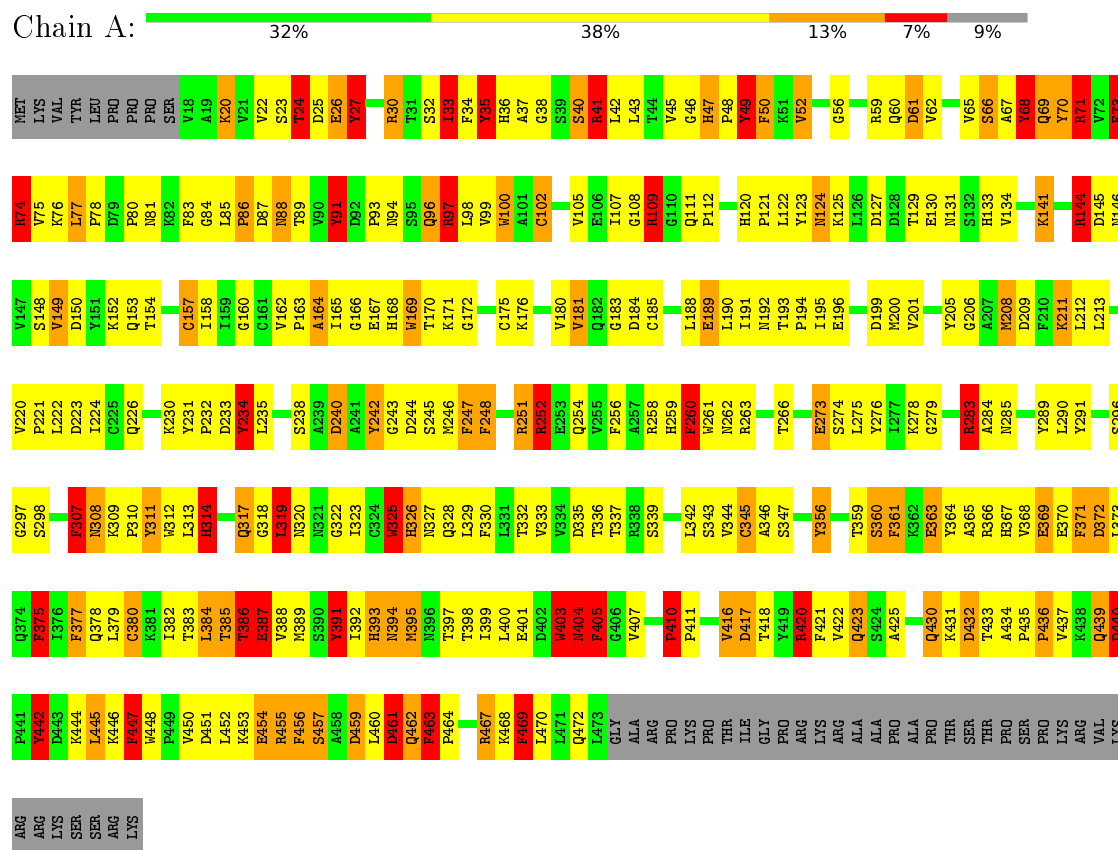
There are 6 discrepancies between the modelled and reference sequences:

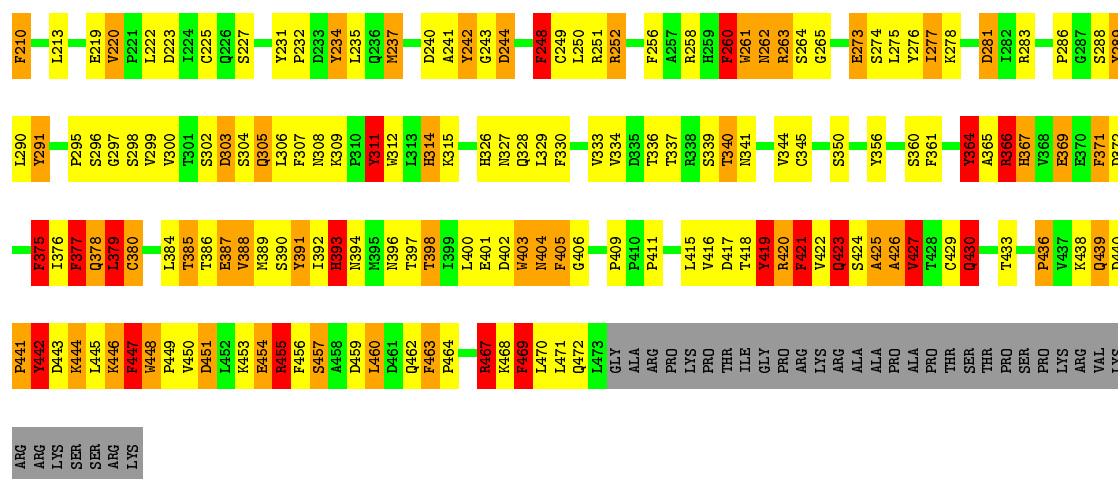
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP Q81971
B	9	MET	-	initiating methionine	UNP Q81971
C	9	MET	-	initiating methionine	UNP Q81971
D	9	MET	-	initiating methionine	UNP Q81971
E	9	MET	-	initiating methionine	UNP Q81971
F	9	MET	-	initiating methionine	UNP Q81971

### 3 Residue-property plots

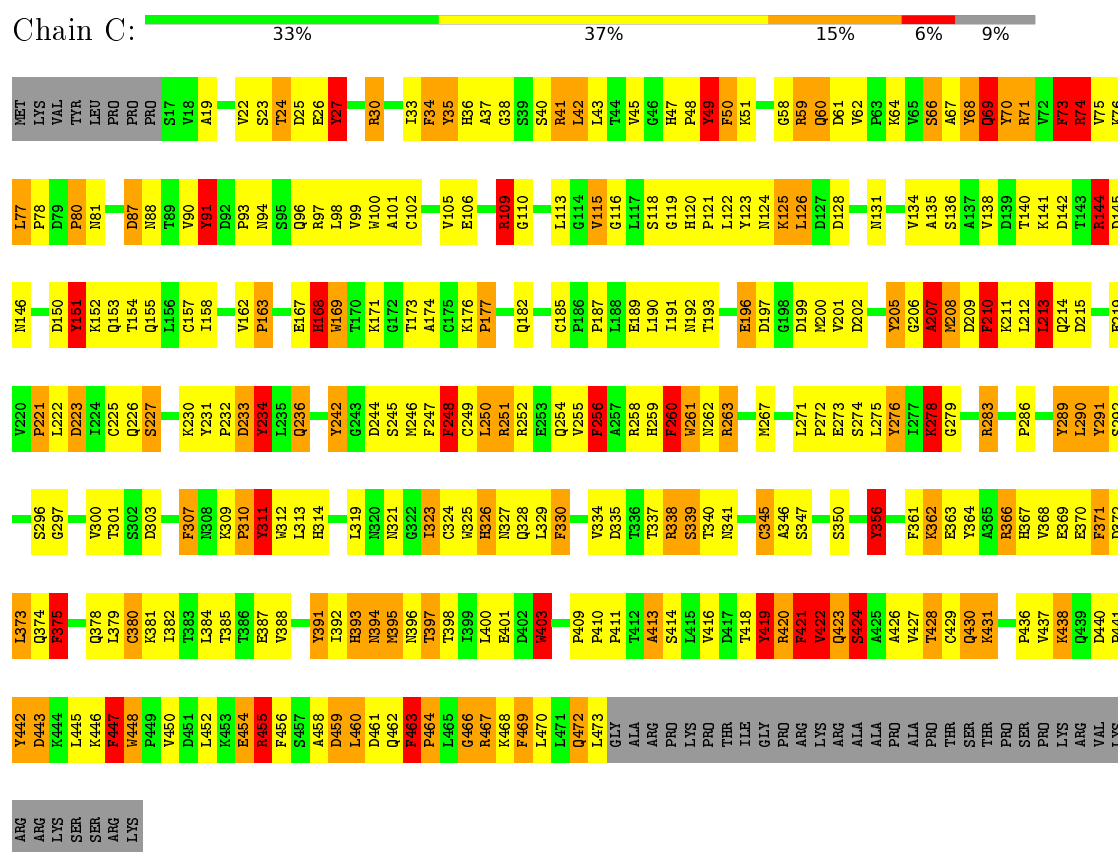
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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 L1

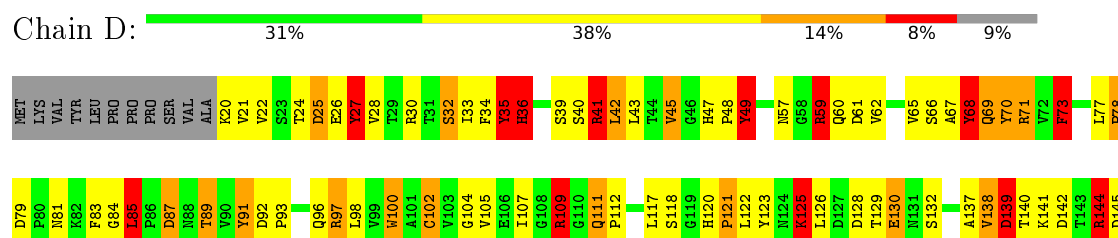


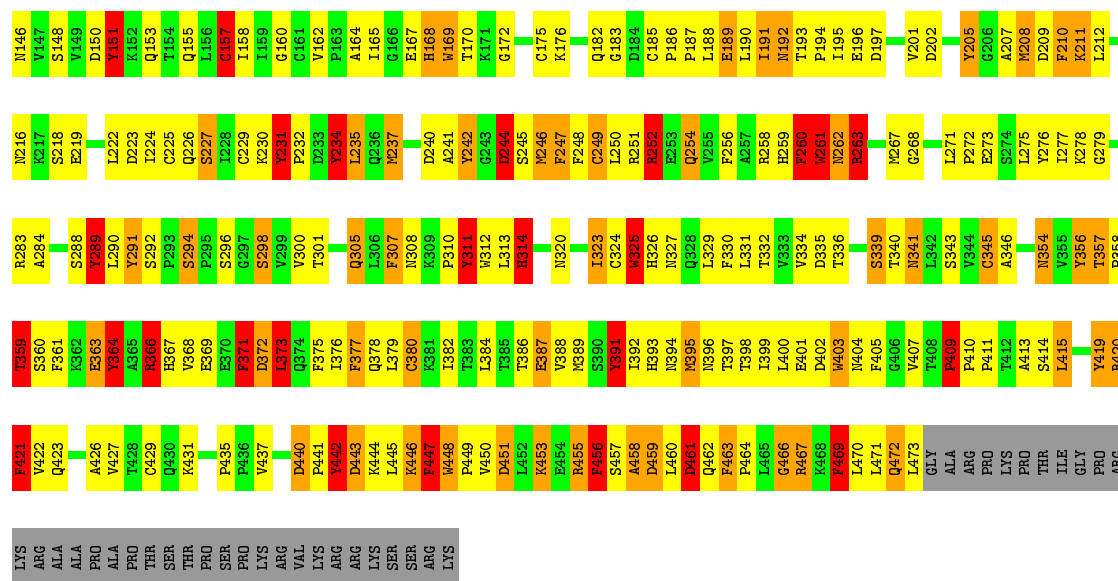


### • Molecule 1: Major capsid protein L1



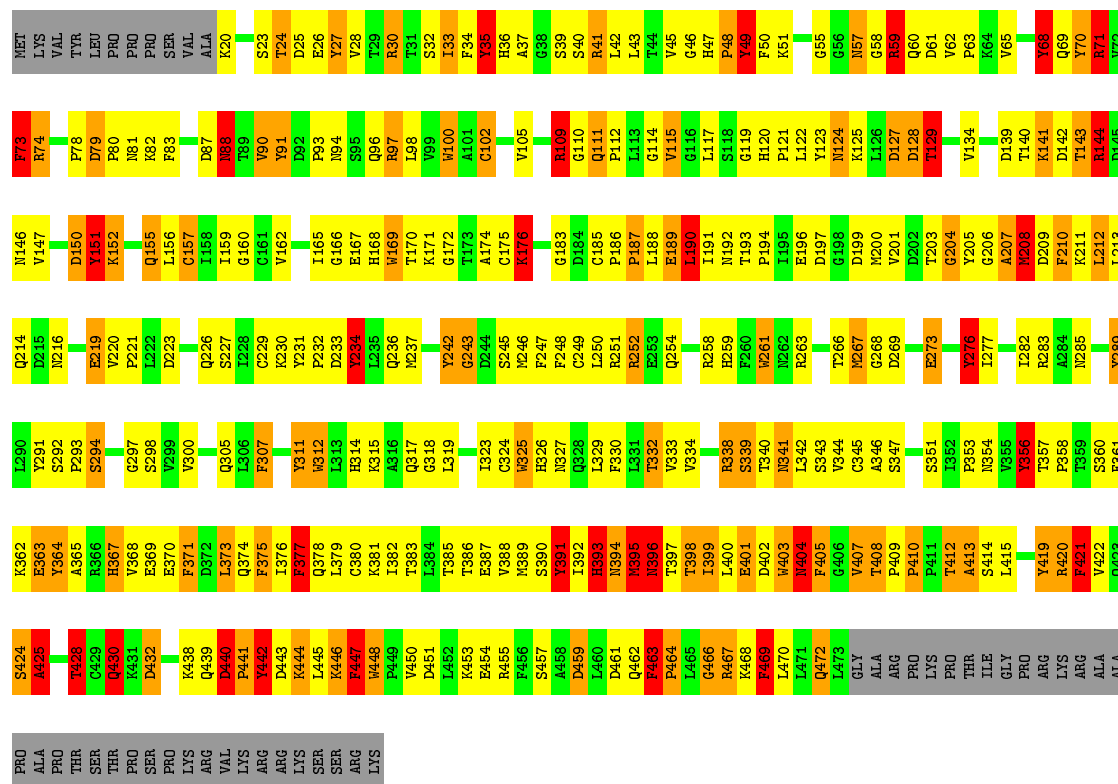
### • Molecule 1: Major capsid protein L1





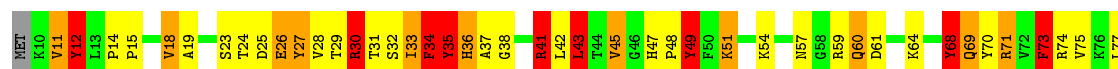
• Molecule 1: Major capsid protein L1

Chain E: 30% 38% 16% 6% 9%



• Molecule 1: Major capsid protein L1

Chain F: 33% 38% 15% 6% 7%



VAL	D440	C380	R307	S227	L156	P78
LYS	P441	K381	N308	I228	C157	D79
ARG	Y442	T382	K309	C229	I158	P80
ARG	D443	T383	P310	K230	I159	N81
LYS	K444	L384	W311	Y231	G160	K82
LYS	L445	T385	W312	P232	G161	K83
SER	K446	T386	I313	D233	G162	G84
SER	F447	R387	H314	Y234	I165	L85
ARG	W448	V388	Q317	L235	G166	P86
LYS	W449	K389	G318	Y236	E167	D87
	V450	S390	H319	K237	H168	N88
	D451	Y391	N320	D240	W169	T89
	L452	T392	I321	A241	T170	V90
	K453	R393	I323	I242	K171	N91
	E454	T394	C324	Y243	G172	D92
	R455	K395	W325	G243	T173	P93
	F456	N396	H326	D244	A174	N94
	S457	T397	N327	S245	C175	S95
	A458	T398	K246	F247	D184	O96
	D459	I399	Q328	F249	C185	A97
	L460	L400	L329	R251	G186	L98
	D461	E401	V333	R252	P187	V99
	F463	N403	W334	E253	L188	W100
	P464	N404	D335	F256	P189	A101
	L465	F405	S339	A257	E189	C102
	G466	G406	T340	R258	L190	V103
	R467	Y407	N341	H259	I191	E106
	K468	P409	C345	F260	T193	I107
	F469	P410	K346	N261	P194	G108
	L470	P411	S347	R262	I195	R109
	Q472	A413	I352	S264	E196	G110
	L473	S414	P353	N267	D199	Q111
	ALA	L415	N354	Y276	M200	P112
	ARG	V416	V355	I277	V201	H120
	PRO	D417	K356	K278	D202	P121
	LYS	T418	S360	D281	T203	L122
	PRO	Y419	K362	R283	G204	Y123
	THR	R420	F361	Y289	Y205	H124
	ILE	F421	R364	Y291	M208	K125
	GLY	V422	A365	P295	F209	L126
	PRO	Q423	R366	S296	F210	D127
	ARG	S424	H367	G297	K211	D128
	LYS	A425	V368	I373	L212	S132
	ARG	V427	E369	Q374	G214	V134
	ALA	T428	E370	F375	D215	H133
	PRO	Q429	F371	I376	N216	L134
	ALA	K430	D372	Q303	K217	D142
	PRO	R431	T373	S304	R218	T143
	THR	D432	Q374	Q305	E219	R144
	SER	T433	P375	L306	V220	D145
	THR	A434	F376		P221	N146
	PRO	P435	I377		L222	D150
	SER	P436	F378		D223	Y151
	PRO	Y437	L379		L224	K152
	LYS	K438			C225	Q153
	ARG	Q439			Q226	

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	3100	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	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	1.47	8/3694 (0.2%)	1.88	94/5036 (1.9%)
1	B	1.45	7/3761 (0.2%)	1.89	110/5130 (2.1%)
1	C	1.48	5/3700 (0.1%)	1.91	107/5044 (2.1%)
1	D	1.49	11/3682 (0.3%)	1.87	97/5019 (1.9%)
1	E	1.94	8/3682 (0.2%)	1.89	100/5019 (2.0%)
1	F	1.49	11/3761 (0.3%)	1.88	88/5130 (1.7%)
All	All	1.56	50/22280 (0.2%)	1.89	596/30378 (2.0%)

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	35
1	B	0	45
1	C	0	46
1	D	0	43
1	E	0	37
1	F	0	47
All	All	0	253

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	405	PHE	N-CA	77.19	3.00	1.46
1	B	35	TYR	CB-CG	-7.31	1.40	1.51
1	E	469	PHE	CB-CG	-6.46	1.40	1.51
1	F	392	ILE	N-CA	-6.36	1.33	1.46
1	A	447	PHE	CA-C	-6.18	1.36	1.52
1	A	440	ASP	C-N	-6.10	1.22	1.34
1	E	405	PHE	CA-CB	6.06	1.67	1.53
1	D	78	PRO	CA-C	-6.03	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	448	TRP	N-CA	-5.84	1.34	1.46
1	F	463	PHE	CA-C	-5.83	1.37	1.52
1	A	375	PHE	CB-CG	-5.77	1.41	1.51
1	A	69	GLN	N-CA	-5.75	1.34	1.46
1	F	469	PHE	N-CA	-5.70	1.34	1.46
1	B	49	TYR	CB-CG	-5.66	1.43	1.51
1	B	469	PHE	CB-CG	-5.66	1.41	1.51
1	A	310	PRO	CA-C	-5.64	1.41	1.52
1	A	377	PHE	CB-CG	-5.61	1.41	1.51
1	D	310	PRO	CA-C	-5.59	1.41	1.52
1	D	447	PHE	CA-C	-5.58	1.38	1.52
1	D	469	PHE	CB-CG	-5.55	1.42	1.51
1	B	398	THR	CA-C	-5.54	1.38	1.52
1	E	49	TYR	CB-CG	-5.54	1.43	1.51
1	E	466	GLY	CA-C	-5.47	1.43	1.51
1	D	442	TYR	CB-CG	-5.44	1.43	1.51
1	A	52	VAL	C-N	-5.41	1.24	1.34
1	C	466	GLY	CA-C	-5.38	1.43	1.51
1	D	311	TYR	CA-C	-5.38	1.39	1.52
1	C	310	PRO	CA-C	-5.36	1.42	1.52
1	D	325	TRP	CA-C	-5.33	1.39	1.52
1	E	469	PHE	N-CA	-5.31	1.35	1.46
1	F	466	GLY	CA-C	-5.30	1.43	1.51
1	F	231	TYR	C-N	-5.29	1.24	1.34
1	C	356	TYR	CB-CG	-5.26	1.43	1.51
1	F	469	PHE	CB-CG	-5.25	1.42	1.51
1	E	35	TYR	CB-CG	-5.23	1.43	1.51
1	A	93	PRO	CA-C	-5.23	1.42	1.52
1	D	403	TRP	CA-C	-5.20	1.39	1.52
1	F	447	PHE	CB-CG	-5.18	1.42	1.51
1	D	466	GLY	CA-C	-5.14	1.43	1.51
1	D	469	PHE	N-CA	-5.12	1.36	1.46
1	B	463	PHE	N-CA	-5.11	1.36	1.46
1	F	391	TYR	CA-C	-5.11	1.39	1.52
1	E	311	TYR	CB-CG	-5.11	1.44	1.51
1	C	125	LYS	N-CA	-5.08	1.36	1.46
1	B	311	TYR	CA-C	-5.08	1.39	1.52
1	F	172	GLY	CA-C	-5.07	1.43	1.51
1	B	168	HIS	CB-CG	-5.06	1.41	1.50
1	F	311	TYR	CB-CG	-5.05	1.44	1.51
1	C	61	ASP	N-CA	-5.02	1.36	1.46
1	F	392	ILE	CA-CB	-5.02	1.43	1.54

All (596) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	455	ARG	NE-CZ-NH1	13.91	127.26	120.30
1	B	91	TYR	CB-CG-CD2	-13.52	112.89	121.00
1	C	91	TYR	CB-CG-CD2	-13.48	112.91	121.00
1	C	420	ARG	NE-CZ-NH2	13.26	126.93	120.30
1	A	386	THR	N-CA-C	13.11	146.38	111.00
1	B	41	ARG	NE-CZ-NH1	13.08	126.84	120.30
1	B	91	TYR	CB-CG-CD1	12.30	128.38	121.00
1	A	91	TYR	CB-CG-CD2	-12.28	113.63	121.00
1	B	35	TYR	CB-CG-CD1	-12.21	113.67	121.00
1	C	330	PHE	CB-CG-CD1	-11.74	112.58	120.80
1	F	49	TYR	CB-CG-CD2	-11.63	114.02	121.00
1	C	356	TYR	CB-CG-CD1	-11.62	114.03	121.00
1	F	307	PHE	CB-CG-CD2	-11.56	112.71	120.80
1	C	91	TYR	CB-CG-CD1	11.37	127.82	121.00
1	F	389	MET	CG-SD-CE	11.25	118.20	100.20
1	E	144	ARG	NE-CZ-NH2	-11.23	114.69	120.30
1	F	144	ARG	NE-CZ-NH2	-11.19	114.71	120.30
1	A	307	PHE	CB-CG-CD1	-11.09	113.04	120.80
1	E	169	TRP	CB-CG-CD2	-10.93	112.40	126.60
1	E	311	TYR	CB-CG-CD1	-10.88	114.47	121.00
1	F	311	TYR	CB-CG-CD1	-10.74	114.56	121.00
1	E	405	PHE	N-CA-CB	10.51	129.51	110.60
1	D	311	TYR	CB-CG-CD1	-10.43	114.74	121.00
1	A	387	GLU	N-CA-CB	-10.39	91.89	110.60
1	A	391	TYR	CB-CG-CD1	-10.29	114.83	121.00
1	A	420	ARG	NE-CZ-NH2	10.01	125.31	120.30
1	F	307	PHE	CB-CG-CD1	-10.01	113.80	120.80
1	E	276	TYR	CB-CG-CD2	-9.97	115.02	121.00
1	B	311	TYR	CB-CG-CD1	-9.88	115.07	121.00
1	D	260	PHE	CB-CG-CD2	-9.86	113.90	120.80
1	D	144	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	C	455	ARG	NE-CZ-NH2	-9.75	115.42	120.30
1	E	404	ASN	C-N-CA	9.74	146.05	121.70
1	F	71	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	D	260	PHE	CB-CG-CD1	9.67	127.57	120.80
1	D	27	TYR	CB-CG-CD2	-9.64	115.22	121.00
1	F	41	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	E	405	PHE	CB-CA-C	-9.62	91.16	110.40
1	C	74	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	F	144	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	C	144	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	C	420	ARG	NE-CZ-NH1	-9.32	115.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	144	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	A	252	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	325	TRP	CB-CG-CD2	-9.09	114.79	126.60
1	B	311	TYR	CA-CB-CG	-9.04	96.23	113.40
1	F	49	TYR	CB-CG-CD1	9.01	126.41	121.00
1	B	364	TYR	CB-CG-CD2	-8.97	115.62	121.00
1	F	364	TYR	CB-CG-CD2	-8.96	115.62	121.00
1	E	311	TYR	CB-CG-CD2	-8.96	115.62	121.00
1	B	68	TYR	CB-CG-CD2	-8.89	115.67	121.00
1	E	356	TYR	CB-CG-CD1	-8.88	115.67	121.00
1	D	68	TYR	CB-CG-CD1	-8.84	115.69	121.00
1	D	263	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	375	PHE	CB-CG-CD1	-8.82	114.62	120.80
1	E	469	PHE	CB-CG-CD2	-8.79	114.65	120.80
1	E	459	ASP	CB-CG-OD2	8.77	126.19	118.30
1	A	68	TYR	CB-CG-CD2	-8.77	115.74	121.00
1	B	469	PHE	CB-CG-CD2	-8.76	114.67	120.80
1	D	443	ASP	CB-CG-OD2	8.74	126.17	118.30
1	F	102	CYS	N-CA-CB	8.67	126.21	110.60
1	A	144	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	C	109	ARG	CD-NE-CZ	-8.59	111.57	123.60
1	B	448	TRP	CB-CG-CD2	-8.57	115.45	126.60
1	D	421	PHE	CB-CG-CD2	8.43	126.70	120.80
1	E	364	TYR	CB-CG-CD2	-8.41	115.95	121.00
1	A	252	ARG	NE-CZ-NH2	-8.39	116.10	120.30
1	A	469	PHE	CB-CG-CD2	-8.39	114.93	120.80
1	B	469	PHE	CB-CG-CD1	-8.32	114.98	120.80
1	C	27	TYR	CB-CG-CD2	-8.28	116.03	121.00
1	A	144	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	205	TYR	CB-CG-CD2	-8.27	116.04	121.00
1	C	151	TYR	CB-CG-CD1	-8.25	116.05	121.00
1	C	49	TYR	CA-CB-CG	-8.23	97.76	113.40
1	D	263	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	F	456	PHE	N-CA-CB	-8.15	95.94	110.60
1	C	395	MET	N-CA-CB	-8.14	95.94	110.60
1	A	447	PHE	CB-CG-CD1	-8.13	115.11	120.80
1	B	74	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	D	311	TYR	CA-CB-CG	-8.12	97.98	113.40
1	E	234	TYR	CB-CG-CD1	-8.09	116.15	121.00
1	A	109	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	A	307	PHE	CB-CG-CD2	-8.06	115.16	120.80
1	B	314	HIS	CA-CB-CG	-8.05	99.91	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	TRP	CB-CG-CD2	-8.05	116.13	126.60
1	F	311	TYR	CB-CG-CD2	-7.96	116.22	121.00
1	F	314	HIS	CA-CB-CG	-7.90	100.17	113.60
1	C	74	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	D	41	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	59	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	E	391	TYR	CB-CG-CD1	-7.85	116.29	121.00
1	D	440	ASP	CA-C-N	7.84	139.06	117.10
1	D	448	TRP	CB-CG-CD2	-7.83	116.42	126.60
1	C	375	PHE	CB-CG-CD2	-7.80	115.34	120.80
1	B	169	TRP	CB-CG-CD2	-7.80	116.46	126.60
1	A	455	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	C	283	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	C	421	PHE	N-CA-CB	-7.77	96.61	110.60
1	A	356	TYR	CB-CG-CD1	-7.77	116.34	121.00
1	E	425	ALA	N-CA-CB	7.75	120.95	110.10
1	D	446	LYS	CB-CA-C	-7.74	94.92	110.40
1	E	373	LEU	CB-CA-C	7.74	124.90	110.20
1	F	366	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	D	40	SER	N-CA-C	7.74	131.89	111.00
1	B	68	TYR	CB-CG-CD1	-7.73	116.36	121.00
1	C	144	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	C	70	TYR	CB-CG-CD2	7.70	125.62	121.00
1	F	381	LYS	N-CA-CB	7.64	124.35	110.60
1	D	261	TRP	CB-CG-CD2	-7.63	116.68	126.60
1	E	210	PHE	CB-CG-CD1	-7.63	115.46	120.80
1	E	74	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	251	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	F	364	TYR	CB-CG-CD1	7.59	125.55	121.00
1	B	443	ASP	N-CA-CB	-7.58	96.96	110.60
1	F	380	CYS	CA-CB-SG	-7.55	100.41	114.00
1	D	91	TYR	CB-CG-CD1	-7.54	116.47	121.00
1	E	373	LEU	N-CA-CB	-7.47	95.45	110.40
1	A	27	TYR	CB-CG-CD1	-7.43	116.54	121.00
1	B	467	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	F	83	PHE	CB-CG-CD2	7.42	125.99	120.80
1	D	395	MET	CG-SD-CE	-7.39	88.38	100.20
1	F	391	TYR	CB-CG-CD2	-7.39	116.57	121.00
1	D	252	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	59	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	B	419	TYR	CB-CG-CD1	-7.35	116.59	121.00
1	C	419	TYR	C-N-CA	7.34	140.05	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	27	TYR	CB-CG-CD1	7.34	125.40	121.00
1	F	169	TRP	CB-CG-CD2	-7.33	117.07	126.60
1	E	311	TYR	CA-C-N	-7.33	101.07	117.20
1	E	208	MET	CG-SD-CE	-7.32	88.49	100.20
1	B	258	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	E	144	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	F	68	TYR	CA-CB-CG	-7.30	99.54	113.40
1	C	431	LYS	N-CA-C	-7.29	91.32	111.00
1	E	102	CYS	N-CA-CB	7.28	123.71	110.60
1	F	356	TYR	CB-CG-CD2	-7.28	116.63	121.00
1	F	463	PHE	CA-CB-CG	-7.28	96.44	113.90
1	D	442	TYR	CB-CG-CD2	-7.27	116.64	121.00
1	E	448	TRP	N-CA-CB	7.26	123.67	110.60
1	A	169	TRP	CB-CG-CD2	-7.25	117.18	126.60
1	F	258	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	B	35	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	D	125	LYS	N-CA-C	-7.22	91.49	111.00
1	D	68	TYR	CA-CB-CG	-7.22	99.68	113.40
1	A	102	CYS	N-CA-CB	7.22	123.59	110.60
1	C	247	PHE	CB-CG-CD2	7.21	125.85	120.80
1	B	18	VAL	C-N-CA	7.19	139.67	121.70
1	B	405	PHE	CB-CG-CD2	7.15	125.81	120.80
1	C	169	TRP	CB-CG-CD2	-7.15	117.31	126.60
1	E	463	PHE	CB-CG-CD2	-7.13	115.81	120.80
1	B	70	TYR	CB-CG-CD2	7.10	125.26	121.00
1	B	40	SER	N-CA-C	7.09	130.15	111.00
1	E	442	TYR	CB-CG-CD2	-7.08	116.75	121.00
1	F	311	TYR	CA-CB-CG	-7.03	100.05	113.40
1	F	356	TYR	CB-CG-CD1	7.03	125.22	121.00
1	F	430	GLN	N-CA-C	-7.03	92.03	111.00
1	C	430	GLN	N-CA-CB	7.02	123.24	110.60
1	E	203	THR	N-CA-CB	7.02	123.65	110.30
1	E	405	PHE	N-CA-C	7.01	129.92	111.00
1	F	192	ASN	N-CA-CB	7.01	123.21	110.60
1	B	377	PHE	CB-CA-C	-6.95	96.50	110.40
1	A	74	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	D	176	LYS	N-CA-C	-6.93	92.30	111.00
1	A	260	PHE	CB-CG-CD2	-6.89	115.98	120.80
1	E	97	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	447	PHE	CA-CB-CG	-6.87	97.42	113.90
1	E	252	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	C	443	ASP	N-CA-CB	-6.84	98.28	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	248	PHE	CB-CG-CD1	-6.84	116.01	120.80
1	E	35	TYR	CA-CB-CG	-6.83	100.43	113.40
1	D	459	ASP	CA-CB-CG	-6.82	98.40	113.40
1	C	87	ASP	CA-CB-CG	-6.81	98.42	113.40
1	B	41	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	375	PHE	CB-CA-C	-6.79	96.81	110.40
1	C	460	LEU	C-N-CA	6.78	138.66	121.70
1	D	447	PHE	CA-CB-CG	-6.78	97.63	113.90
1	D	455	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	192	ASN	CA-CB-CG	-6.76	98.52	113.40
1	E	39	SER	N-CA-CB	6.76	120.63	110.50
1	B	446	LYS	CB-CA-C	-6.75	96.91	110.40
1	B	102	CYS	N-CA-CB	6.75	122.74	110.60
1	A	385	THR	CA-CB-CG2	-6.74	102.96	112.40
1	C	279	GLY	N-CA-C	-6.74	96.26	113.10
1	F	34	PHE	CB-CG-CD1	-6.73	116.09	120.80
1	F	91	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	D	87	ASP	CA-CB-CG	-6.71	98.63	113.40
1	C	248	PHE	CB-CG-CD1	-6.71	116.10	120.80
1	B	447	PHE	CA-CB-CG	-6.71	97.80	113.90
1	A	405	PHE	CB-CG-CD1	-6.70	116.11	120.80
1	F	391	TYR	CB-CG-CD1	6.70	125.02	121.00
1	B	260	PHE	CB-CG-CD2	-6.70	116.11	120.80
1	F	12	TYR	CA-CB-CG	-6.69	100.68	113.40
1	C	256	PHE	CB-CG-CD2	-6.69	116.12	120.80
1	D	49	TYR	CB-CG-CD2	-6.69	116.99	121.00
1	E	413	ALA	C-N-CA	6.69	138.42	121.70
1	C	247	PHE	CB-CG-CD1	-6.68	116.12	120.80
1	A	420	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	C	102	CYS	N-CA-CB	6.65	122.56	110.60
1	B	210	PHE	CB-CG-CD1	-6.64	116.15	120.80
1	B	303	ASP	N-CA-CB	-6.63	98.66	110.60
1	D	451	ASP	N-CA-CB	6.63	122.53	110.60
1	A	176	LYS	N-CA-C	-6.62	93.12	111.00
1	E	367	HIS	CB-CA-C	-6.62	97.16	110.40
1	E	58	GLY	N-CA-C	-6.61	96.57	113.10
1	B	330	PHE	CB-CG-CD1	-6.61	116.17	120.80
1	C	35	TYR	CA-CB-CG	-6.61	100.84	113.40
1	D	102	CYS	N-CA-CB	6.61	122.49	110.60
1	C	125	LYS	N-CA-C	-6.59	93.19	111.00
1	D	372	ASP	N-CA-CB	6.59	122.46	110.60
1	F	373	LEU	CB-CA-C	6.58	122.70	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	205	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	D	459	ASP	C-N-CA	6.57	138.11	121.70
1	B	405	PHE	CB-CG-CD1	-6.56	116.21	120.80
1	F	83	PHE	CB-CG-CD1	-6.56	116.21	120.80
1	E	127	ASP	C-N-CA	6.55	138.08	121.70
1	D	25	ASP	N-CA-CB	-6.54	98.83	110.60
1	B	49	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	A	371	PHE	N-CA-C	6.52	128.60	111.00
1	D	229	CYS	CA-CB-SG	-6.52	102.26	114.00
1	A	363	GLU	CB-CA-C	6.51	123.43	110.40
1	B	252	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	D	364	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	C	447	PHE	CA-CB-CG	-6.51	98.27	113.90
1	C	395	MET	CB-CA-C	6.51	123.42	110.40
1	E	311	TYR	CA-CB-CG	-6.51	101.03	113.40
1	A	74	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	E	207	ALA	C-N-CA	6.50	137.94	121.70
1	F	71	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	C	59	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	D	258	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	D	443	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	F	35	TYR	CA-CB-CG	-6.48	101.08	113.40
1	F	447	PHE	CA-CB-CG	-6.48	98.35	113.90
1	D	251	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	D	330	PHE	CB-CG-CD1	-6.44	116.30	120.80
1	B	18	VAL	O-C-N	-6.43	112.41	122.70
1	E	246	MET	CG-SD-CE	-6.43	89.91	100.20
1	F	440	ASP	N-CA-C	-6.42	93.65	111.00
1	E	459	ASP	N-CA-CB	6.42	122.16	110.60
1	A	394	ASN	CA-CB-CG	-6.41	99.29	113.40
1	A	260	PHE	CB-CG-CD1	6.41	125.29	120.80
1	F	335	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	97	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	C	395	MET	CG-SD-CE	-6.39	89.97	100.20
1	B	375	PHE	CB-CG-CD1	-6.39	116.33	120.80
1	C	24	THR	C-N-CA	6.39	137.67	121.70
1	D	189	GLU	N-CA-CB	-6.38	99.12	110.60
1	C	424	SER	N-CA-CB	6.37	120.06	110.50
1	F	229	CYS	CA-CB-SG	-6.37	102.53	114.00
1	A	49	TYR	CA-CB-CG	-6.36	101.31	113.40
1	C	380	CYS	CA-CB-SG	-6.36	102.56	114.00
1	C	393	HIS	N-CA-CB	-6.35	99.18	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	GLU	N-CA-CB	-6.35	99.18	110.60
1	E	68	TYR	CA-CB-CG	-6.34	101.34	113.40
1	B	273	GLU	C-N-CA	6.34	137.54	121.70
1	C	250	LEU	CB-CA-C	-6.34	98.16	110.20
1	A	311	TYR	N-CA-C	-6.33	93.90	111.00
1	C	192	ASN	CA-CB-CG	-6.33	99.46	113.40
1	D	169	TRP	CB-CG-CD2	-6.33	118.37	126.60
1	C	62	VAL	N-CA-C	-6.31	93.97	111.00
1	B	251	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	E	68	TYR	CB-CG-CD1	-6.29	117.22	121.00
1	D	469	PHE	CB-CG-CD2	-6.28	116.40	120.80
1	C	81	ASN	CA-CB-CG	-6.28	99.59	113.40
1	E	469	PHE	N-CA-CB	-6.26	99.33	110.60
1	B	326	HIS	CA-CB-CG	-6.26	102.96	113.60
1	B	447	PHE	CB-CG-CD1	-6.25	116.42	120.80
1	B	248	PHE	CB-CG-CD1	-6.25	116.42	120.80
1	A	153	GLN	N-CA-CB	-6.24	99.37	110.60
1	F	267	MET	CG-SD-CE	-6.24	90.22	100.20
1	E	71	ARG	N-CA-CB	-6.24	99.37	110.60
1	D	42	LEU	CB-CG-CD2	6.23	121.60	111.00
1	C	35	TYR	CB-CG-CD1	-6.23	117.26	121.00
1	E	395	MET	CG-SD-CE	-6.23	90.23	100.20
1	A	109	ARG	CD-NE-CZ	-6.21	114.91	123.60
1	C	421	PHE	CA-CB-CG	6.21	128.80	113.90
1	F	403	TRP	CB-CG-CD2	-6.20	118.54	126.60
1	F	455	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	35	TYR	CA-CB-CG	-6.19	101.64	113.40
1	F	209	ASP	CB-CG-OD1	6.19	123.87	118.30
1	B	169	TRP	CA-CB-CG	-6.18	101.95	113.70
1	E	459	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	B	144	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	379	LEU	CB-CG-CD1	6.17	121.49	111.00
1	C	213	LEU	CB-CG-CD1	6.15	121.46	111.00
1	B	261	TRP	CB-CG-CD2	-6.14	118.61	126.60
1	C	461	ASP	N-CA-CB	-6.13	99.56	110.60
1	F	469	PHE	N-CA-CB	-6.13	99.56	110.60
1	B	327	ASN	CA-CB-CG	-6.13	99.92	113.40
1	F	261	TRP	CB-CG-CD2	-6.13	118.63	126.60
1	F	354	ASN	CA-CB-CG	-6.12	99.94	113.40
1	E	447	PHE	CA-CB-CG	-6.12	99.22	113.90
1	D	373	LEU	CB-CG-CD2	6.11	121.38	111.00
1	E	35	TYR	CB-CG-CD1	-6.10	117.34	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	CYS	N-CA-C	-6.08	94.58	111.00
1	B	380	CYS	CA-CB-SG	-6.08	103.06	114.00
1	F	68	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	C	413	ALA	C-N-CA	6.08	136.89	121.70
1	C	414	SER	N-CA-CB	6.07	119.60	110.50
1	A	403	TRP	CB-CG-CD1	6.06	134.87	127.00
1	D	49	TYR	CA-CB-CG	-6.05	101.90	113.40
1	B	404	ASN	CA-CB-CG	-6.04	100.10	113.40
1	C	375	PHE	CA-CB-CG	-6.04	99.41	113.90
1	B	469	PHE	N-CA-CB	-6.01	99.78	110.60
1	D	279	GLY	N-CA-C	-6.01	98.07	113.10
1	B	73	PHE	CB-CG-CD2	-6.00	116.60	120.80
1	E	169	TRP	CB-CG-CD1	6.00	134.80	127.00
1	A	144	ARG	CG-CD-NE	-5.99	99.22	111.80
1	D	202	ASP	CA-CB-CG	-5.99	100.23	113.40
1	C	364	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	E	448	TRP	CB-CG-CD2	-5.98	118.83	126.60
1	F	246	MET	CG-SD-CE	-5.98	90.63	100.20
1	E	364	TYR	CB-CG-CD1	5.97	124.58	121.00
1	B	179	THR	N-CA-CB	5.97	121.65	110.30
1	A	68	TYR	CA-CB-CG	-5.97	102.06	113.40
1	C	458	ALA	C-N-CA	5.97	136.62	121.70
1	E	314	HIS	CA-CB-CG	-5.97	103.45	113.60
1	E	125	LYS	N-CA-CB	5.96	121.33	110.60
1	C	311	TYR	N-CA-C	-5.96	94.91	111.00
1	A	386	THR	CB-CA-C	-5.96	95.51	111.60
1	C	49	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	C	459	ASP	N-CA-C	5.93	127.00	111.00
1	A	251	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	88	ASN	CB-CA-C	5.91	122.22	110.40
1	D	380	CYS	CA-CB-SG	-5.91	103.36	114.00
1	B	262	ASN	N-CA-C	-5.90	95.07	111.00
1	D	262	ASN	N-CA-C	-5.90	95.07	111.00
1	A	380	CYS	CA-CB-SG	-5.89	103.40	114.00
1	C	419	TYR	CA-CB-CG	-5.87	102.25	113.40
1	B	192	ASN	CB-CA-C	-5.87	98.66	110.40
1	B	260	PHE	CB-CG-CD1	5.87	124.91	120.80
1	C	60	GLN	CA-C-N	-5.87	104.29	117.20
1	C	258	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	345	CYS	N-CA-CB	5.85	121.14	110.60
1	E	41	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	F	388	VAL	CA-CB-CG1	5.84	119.67	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	440	ASP	O-C-N	-5.84	110.00	121.10
1	E	190	LEU	CB-CG-CD1	5.83	120.91	111.00
1	D	40	SER	CA-C-N	5.83	130.02	117.20
1	D	440	ASP	CB-CG-OD2	5.83	123.55	118.30
1	C	251	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	40	SER	N-CA-C	5.81	126.69	111.00
1	D	61	ASP	N-CA-C	-5.81	95.32	111.00
1	B	92	ASP	N-CA-C	-5.79	95.37	111.00
1	B	366	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	311	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	F	335	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	E	405	PHE	CB-CG-CD1	-5.78	116.76	120.80
1	A	459	ASP	CA-CB-CG	-5.77	100.70	113.40
1	D	421	PHE	CB-CG-CD1	-5.77	116.76	120.80
1	E	258	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	D	314	HIS	CA-CB-CG	-5.75	103.82	113.60
1	F	34	PHE	CA-CB-CG	-5.75	100.10	113.90
1	F	455	ARG	C-N-CA	5.75	136.08	121.70
1	F	43	LEU	CB-CG-CD1	5.75	120.77	111.00
1	C	200	MET	CG-SD-CE	-5.74	91.01	100.20
1	D	258	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	F	234	TYR	CB-CA-C	-5.74	98.92	110.40
1	B	210	PHE	CB-CG-CD2	5.73	124.81	120.80
1	A	387	GLU	N-CA-C	-5.73	95.53	111.00
1	C	144	ARG	N-CA-CB	-5.73	100.28	110.60
1	C	215	ASP	CB-CG-OD1	5.73	123.45	118.30
1	C	157	CYS	N-CA-CB	5.72	120.89	110.60
1	D	354	ASN	CA-CB-CG	-5.72	100.82	113.40
1	B	30	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	59	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	C	249	CYS	N-CA-CB	-5.69	100.36	110.60
1	A	273	GLU	CB-CA-C	-5.68	99.03	110.40
1	C	210	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	B	26	GLU	N-CA-CB	-5.67	100.39	110.60
1	D	92	ASP	CA-CB-CG	-5.67	100.92	113.40
1	C	373	LEU	N-CA-CB	-5.67	99.06	110.40
1	B	237	MET	CB-CA-C	5.67	121.73	110.40
1	F	209	ASP	CA-C-N	-5.66	104.74	117.20
1	C	261	TRP	CA-CB-CG	-5.66	102.95	113.70
1	C	251	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	E	394	ASN	CB-CA-C	-5.65	99.10	110.40
1	A	432	ASP	CA-CB-CG	-5.63	101.02	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	375	PHE	CB-CA-C	-5.63	99.14	110.40
1	E	258	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	B	57	ASN	CA-CB-CG	-5.62	101.03	113.40
1	E	30	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	E	312	TRP	N-CA-C	-5.62	95.81	111.00
1	B	151	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	A	307	PHE	CA-CB-CG	-5.62	100.42	113.90
1	C	223	ASP	N-CA-CB	-5.61	100.49	110.60
1	A	345	CYS	N-CA-C	-5.61	95.86	111.00
1	E	341	ASN	N-CA-C	-5.60	95.87	111.00
1	E	463	PHE	CA-CB-CG	-5.60	100.45	113.90
1	E	283	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	169	TRP	CB-CG-CD1	5.59	134.27	127.00
1	D	366	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	F	463	PHE	CB-CG-CD1	-5.59	116.89	120.80
1	B	425	ALA	N-CA-CB	5.59	117.93	110.10
1	B	375	PHE	CA-CB-CG	-5.59	100.49	113.90
1	D	244	ASP	C-N-CA	5.58	135.66	121.70
1	F	447	PHE	CB-CA-C	-5.58	99.24	110.40
1	B	364	TYR	CB-CG-CD1	5.58	124.35	121.00
1	C	345	CYS	N-CA-CB	5.57	120.62	110.60
1	B	200	MET	CG-SD-CE	-5.56	91.31	100.20
1	F	144	ARG	CB-CA-C	5.55	121.51	110.40
1	E	412	THR	CA-CB-CG2	-5.55	104.64	112.40
1	E	143	THR	C-N-CA	5.54	135.56	121.70
1	C	210	PHE	CA-CB-CG	-5.54	100.61	113.90
1	F	387	GLU	N-CA-CB	-5.54	100.63	110.60
1	A	100	TRP	CB-CG-CD2	-5.53	119.41	126.60
1	C	422	VAL	C-N-CA	5.53	135.53	121.70
1	A	30	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	283	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	18	VAL	CA-C-N	5.53	129.35	117.20
1	C	395	MET	CB-CG-SD	-5.52	95.83	112.40
1	F	123	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	D	139	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	120	HIS	CA-CB-CG	-5.52	104.22	113.60
1	C	169	TRP	CA-CB-CG	-5.52	103.22	113.70
1	E	446	LYS	CB-CA-C	-5.52	99.36	110.40
1	E	169	TRP	CA-CB-CG	-5.51	103.22	113.70
1	A	326	HIS	CA-CB-CG	-5.51	104.23	113.60
1	B	204	GLY	N-CA-C	-5.51	99.32	113.10
1	C	236	GLN	N-CA-CB	5.51	120.52	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	354	ASN	CA-CB-CG	-5.50	101.29	113.40
1	A	94	ASN	CA-CB-CG	-5.50	101.30	113.40
1	A	461	ASP	N-CA-CB	-5.50	100.70	110.60
1	D	261	TRP	CA-CB-CG	-5.50	103.25	113.70
1	F	73	PHE	CA-CB-CG	-5.50	100.71	113.90
1	A	463	PHE	CA-CB-CG	-5.49	100.72	113.90
1	C	110	GLY	N-CA-C	5.49	126.83	113.10
1	C	375	PHE	CB-CA-C	-5.48	99.43	110.40
1	A	157	CYS	N-CA-CB	5.48	120.46	110.60
1	E	49	TYR	CA-CB-CG	-5.48	102.99	113.40
1	F	189	GLU	O-C-N	-5.47	113.94	122.70
1	B	391	TYR	N-CA-CB	-5.47	100.75	110.60
1	D	237	MET	CG-SD-CE	-5.47	91.45	100.20
1	E	73	PHE	CA-CB-CG	-5.47	100.77	113.90
1	D	469	PHE	N-CA-CB	-5.46	100.77	110.60
1	F	424	SER	N-CA-C	-5.46	96.25	111.00
1	B	68	TYR	CA-CB-CG	-5.46	103.03	113.40
1	D	403	TRP	CB-CG-CD2	-5.45	119.51	126.60
1	B	463	PHE	N-CA-C	-5.45	96.28	111.00
1	A	164	ALA	C-N-CA	5.45	135.33	121.70
1	B	451	ASP	N-CA-CB	5.45	120.41	110.60
1	D	157	CYS	N-CA-CB	5.45	120.41	110.60
1	E	294	SER	CB-CA-C	-5.45	99.75	110.10
1	A	445	LEU	CB-CG-CD1	5.43	120.24	111.00
1	E	338	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	E	463	PHE	N-CA-C	-5.43	96.35	111.00
1	C	58	GLY	O-C-N	-5.42	114.03	122.70
1	E	261	TRP	CB-CG-CD2	-5.42	119.55	126.60
1	B	237	MET	CA-CB-CG	-5.41	104.11	113.30
1	C	73	PHE	CA-CB-CG	-5.41	100.92	113.90
1	E	269	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	69	GLN	CB-CG-CD	5.40	125.65	111.60
1	D	109	ARG	CD-NE-CZ	-5.40	116.04	123.60
1	C	292	SER	N-CA-CB	-5.40	102.40	110.50
1	F	311	TYR	CA-C-N	-5.38	105.35	117.20
1	E	396	ASN	N-CA-C	-5.38	96.47	111.00
1	E	412	THR	N-CA-CB	5.38	120.52	110.30
1	A	252	ARG	N-CA-CB	-5.38	100.92	110.60
1	C	70	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	E	94	ASN	CA-CB-CG	-5.38	101.57	113.40
1	B	427	VAL	N-CA-C	-5.37	96.50	111.00
1	E	109	ARG	NE-CZ-NH2	-5.37	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	419	TYR	O-C-N	-5.36	114.12	122.70
1	E	420	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	D	356	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	B	151	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	D	231	TYR	CB-CG-CD2	-5.36	117.79	121.00
1	B	111	GLN	N-CA-C	5.35	125.45	111.00
1	A	247	PHE	CB-CG-CD2	-5.35	117.06	120.80
1	E	71	ARG	CD-NE-CZ	-5.35	116.11	123.60
1	F	404	ASN	N-CA-C	-5.34	96.57	111.00
1	F	303	ASP	CA-CB-CG	-5.34	101.65	113.40
1	A	41	ARG	N-CA-CB	5.34	120.21	110.60
1	D	62	VAL	N-CA-C	-5.34	96.59	111.00
1	F	420	ARG	CG-CD-NE	-5.33	100.60	111.80
1	A	339	SER	N-CA-C	5.33	125.39	111.00
1	B	30	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	235	LEU	CB-CA-C	-5.33	100.08	110.20
1	E	413	ALA	CB-CA-C	5.32	118.08	110.10
1	F	367	HIS	N-CA-CB	5.32	120.18	110.60
1	E	325	TRP	CA-CB-CG	-5.32	103.60	113.70
1	E	377	PHE	CB-CG-CD1	-5.31	117.08	120.80
1	F	189	GLU	CB-CA-C	5.30	121.00	110.40
1	F	433	THR	N-CA-C	5.30	125.31	111.00
1	D	403	TRP	CA-CB-CG	-5.29	103.64	113.70
1	C	375	PHE	N-CA-CB	5.29	120.12	110.60
1	D	461	ASP	N-CA-CB	-5.29	101.08	110.60
1	D	25	ASP	CB-CA-C	5.29	120.98	110.40
1	B	371	PHE	N-CA-C	5.28	125.26	111.00
1	B	367	HIS	N-CA-CB	-5.28	101.09	110.60
1	C	118	SER	N-CA-CB	5.28	118.42	110.50
1	C	330	PHE	CA-CB-CG	-5.28	101.24	113.90
1	D	420	ARG	NE-CZ-NH2	5.27	122.93	120.30
1	E	424	SER	C-N-CA	5.26	134.86	121.70
1	B	263	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	E	443	ASP	CA-CB-CG	-5.26	101.82	113.40
1	A	285	ASN	CA-CB-CG	-5.26	101.83	113.40
1	C	338	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	377	PHE	CB-CA-C	-5.25	99.91	110.40
1	C	207	ALA	N-CA-CB	-5.25	102.76	110.10
1	D	463	PHE	CA-CB-CG	-5.24	101.32	113.90
1	E	440	ASP	C-N-CD	-5.24	109.07	120.60
1	B	188	LEU	N-CA-CB	-5.24	99.92	110.40
1	F	144	ARG	CG-CD-NE	-5.24	100.80	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	PHE	CA-CB-CG	-5.23	101.34	113.90
1	E	128	ASP	N-CA-CB	-5.23	101.18	110.60
1	E	176	LYS	N-CA-C	-5.23	96.88	111.00
1	D	60	GLN	CA-C-N	-5.23	105.70	117.20
1	A	248	PHE	CA-CB-CG	-5.23	101.36	113.90
1	B	372	ASP	N-CA-C	5.22	125.10	111.00
1	D	419	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	B	94	ASN	CA-CB-CG	-5.21	101.93	113.40
1	D	73	PHE	CA-CB-CG	-5.21	101.39	113.90
1	A	62	VAL	N-CA-C	-5.21	96.93	111.00
1	E	469	PHE	CB-CG-CD1	-5.21	117.15	120.80
1	F	311	TYR	CG-CD1-CE1	-5.21	117.13	121.30
1	B	39	SER	N-CA-CB	5.20	118.30	110.50
1	B	262	ASN	CB-CA-C	5.20	120.79	110.40
1	E	141	LYS	N-CA-CB	-5.20	101.25	110.60
1	D	245	SER	N-CA-CB	-5.19	102.72	110.50
1	A	73	PHE	CA-CB-CG	-5.19	101.45	113.90
1	E	24	THR	N-CA-C	5.18	125.00	111.00
1	D	42	LEU	N-CA-CB	-5.18	100.03	110.40
1	F	341	ASN	CA-CB-CG	-5.18	102.00	113.40
1	F	421	PHE	CB-CG-CD2	5.18	124.43	120.80
1	B	261	TRP	CA-CB-CG	-5.18	103.86	113.70
1	A	439	GLN	N-CA-CB	5.18	119.92	110.60
1	C	448	TRP	CA-CB-CG	-5.17	103.87	113.70
1	F	455	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	303	ASP	CA-CB-CG	-5.17	102.03	113.40
1	B	92	ASP	CB-CA-C	5.17	120.73	110.40
1	E	283	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	455	ARG	CG-CD-NE	-5.15	100.98	111.80
1	D	208	MET	CG-SD-CE	-5.15	91.96	100.20
1	C	24	THR	CA-C-N	-5.15	105.88	117.20
1	C	372	ASP	N-CA-CB	5.15	119.86	110.60
1	B	67	ALA	N-CA-C	5.14	124.89	111.00
1	B	91	TYR	N-CA-C	-5.14	97.11	111.00
1	F	447	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	B	303	ASP	CA-C-N	-5.14	105.89	117.20
1	B	107	ILE	CB-CA-C	-5.14	101.33	111.60
1	C	403	TRP	CA-CB-CG	-5.14	103.94	113.70
1	F	325	TRP	CB-CA-C	-5.13	100.13	110.40
1	C	58	GLY	C-N-CA	5.13	134.52	121.70
1	D	371	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	E	79	ASP	N-CA-CB	5.12	119.81	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	407	VAL	C-N-CA	5.11	134.48	121.70
1	F	469	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	B	190	LEU	CB-CA-C	-5.11	100.50	110.20
1	D	250	LEU	CB-CA-C	-5.11	100.50	110.20
1	C	260	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	E	117	LEU	CB-CA-C	-5.10	100.51	110.20
1	A	311	TYR	CA-CB-CG	-5.10	103.71	113.40
1	A	463	PHE	CB-CG-CD1	-5.10	117.23	120.80
1	A	410	PRO	C-N-CD	-5.10	109.38	120.60
1	B	369	GLU	C-N-CA	5.09	134.43	121.70
1	A	127	ASP	C-N-CA	5.08	134.41	121.70
1	A	467	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	298	SER	N-CA-CB	5.08	118.13	110.50
1	D	373	LEU	CB-CA-C	5.08	119.86	110.20
1	A	314	HIS	CA-CB-CG	-5.08	104.96	113.60
1	E	371	PHE	CA-CB-CG	-5.08	101.70	113.90
1	F	262	ASN	N-CA-C	-5.08	97.28	111.00
1	A	24	THR	CA-C-O	5.08	130.76	120.10
1	A	33	ILE	CB-CA-C	-5.08	101.44	111.60
1	B	457	SER	N-CA-C	-5.08	97.30	111.00
1	C	106	GLU	N-CA-CB	5.08	119.74	110.60
1	D	387	GLU	N-CA-CB	-5.07	101.47	110.60
1	E	351	SER	N-CA-C	-5.07	97.32	111.00
1	A	372	ASP	CB-CA-C	-5.06	100.28	110.40
1	B	173	THR	CA-CB-CG2	-5.06	105.31	112.40
1	C	233	ASP	CB-CA-C	-5.06	100.28	110.40
1	A	372	ASP	N-CA-CB	5.05	119.70	110.60
1	B	426	ALA	C-N-CA	5.05	134.34	121.70
1	A	175	CYS	CA-C-N	-5.05	106.08	117.20
1	A	333	VAL	C-N-CA	5.05	134.33	121.70
1	C	260	PHE	CB-CG-CD1	5.05	124.33	120.80
1	C	463	PHE	CA-CB-CG	-5.05	101.78	113.90
1	C	135	ALA	C-N-CA	5.05	134.32	121.70
1	E	39	SER	CB-CA-C	-5.04	100.52	110.10
1	F	106	GLU	N-CA-CB	5.03	119.65	110.60
1	B	60	GLN	CA-C-N	-5.03	106.14	117.20
1	B	49	TYR	CA-CB-CG	-5.02	103.86	113.40
1	D	244	ASP	CA-C-N	-5.02	106.16	117.20
1	A	469	PHE	CA-CB-CG	-5.02	101.86	113.90
1	D	234	TYR	CB-CG-CD2	-5.01	117.99	121.00
1	F	41	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	C	372	ASP	CB-CA-C	-5.01	100.38	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	291	TYR	CA-CB-CG	-5.01	103.88	113.40
1	D	311	TYR	CG-CD1-CE1	-5.01	117.29	121.30
1	F	384	LEU	N-CA-CB	-5.01	100.38	110.40
1	E	339	SER	N-CA-C	5.01	124.52	111.00
1	D	396	ASN	CA-CB-CG	-5.00	102.39	113.40
1	B	192	ASN	CA-CB-CG	-5.00	102.39	113.40
1	F	377	PHE	CB-CG-CD1	-5.00	117.30	120.80
1	F	408	THR	N-CA-CB	5.00	119.81	110.30

There are no chirality outliers.

All (253) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	A	144	ARG	Sidechain
1	A	234	TYR	Sidechain
1	A	242	TYR	Sidechain
1	A	248	PHE	Sidechain
1	A	258	ARG	Sidechain
1	A	263	ARG	Sidechain
1	A	283	ARG	Sidechain
1	A	289	TYR	Sidechain
1	A	307	PHE	Sidechain
1	A	314	HIS	Sidechain
1	A	319	LEU	Mainchain,Peptide
1	A	35	TYR	Sidechain
1	A	361	PHE	Sidechain
1	A	366	ARG	Sidechain
1	A	375	PHE	Sidechain
1	A	391	TYR	Sidechain
1	A	405	PHE	Sidechain
1	A	41	ARG	Sidechain
1	A	420	ARG	Sidechain
1	A	442	TYR	Sidechain
1	A	447	PHE	Sidechain
1	A	456	PHE	Sidechain
1	A	463	PHE	Sidechain
1	A	469	PHE	Sidechain
1	A	49	TYR	Sidechain
1	A	68	TYR	Sidechain
1	A	70	TYR	Sidechain
1	A	71	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	73	PHE	Sidechain
1	A	74	ARG	Sidechain
1	A	86	PRO	Mainchain
1	A	91	TYR	Sidechain
1	A	97	ARG	Sidechain
1	B	120	HIS	Sidechain
1	B	123	TYR	Sidechain
1	B	151	TYR	Sidechain
1	B	168	HIS	Sidechain
1	B	203	THR	Mainchain
1	B	205	TYR	Sidechain
1	B	234	TYR	Sidechain
1	B	244	ASP	Mainchain
1	B	274	SER	Mainchain
1	B	283	ARG	Sidechain
1	B	289	TYR	Sidechain
1	B	291	TYR	Sidechain
1	B	303	ASP	Mainchain,Peptide
1	B	311	TYR	Sidechain
1	B	35	TYR	Sidechain,Mainchain
1	B	364	TYR	Sidechain
1	B	375	PHE	Sidechain
1	B	377	PHE	Mainchain
1	B	385	THR	Mainchain,Peptide
1	B	393	HIS	Sidechain
1	B	403	TRP	Mainchain
1	B	419	TYR	Sidechain
1	B	420	ARG	Sidechain
1	B	421	PHE	Sidechain
1	B	425	ALA	Mainchain
1	B	442	TYR	Sidechain,Mainchain
1	B	447	PHE	Sidechain
1	B	455	ARG	Sidechain
1	B	459	ASP	Mainchain,Peptide
1	B	460	LEU	Mainchain
1	B	467	ARG	Sidechain
1	B	469	PHE	Sidechain
1	B	49	TYR	Sidechain
1	B	59	ARG	Sidechain
1	B	68	TYR	Sidechain
1	B	71	ARG	Sidechain
1	B	73	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	B	78	PRO	Mainchain
1	B	91	TYR	Mainchain
1	B	95	SER	Mainchain
1	C	109	ARG	Sidechain
1	C	144	ARG	Sidechain
1	C	151	TYR	Sidechain
1	C	168	HIS	Sidechain
1	C	174	ALA	Peptide
1	C	205	TYR	Sidechain
1	C	210	PHE	Sidechain
1	C	234	TYR	Sidechain
1	C	242	TYR	Sidechain
1	C	248	PHE	Sidechain
1	C	256	PHE	Sidechain
1	C	263	ARG	Sidechain
1	C	27	TYR	Sidechain
1	C	276	TYR	Sidechain
1	C	291	TYR	Sidechain
1	C	307	PHE	Sidechain
1	C	311	TYR	Sidechain
1	C	323	ILE	Mainchain
1	C	330	PHE	Sidechain
1	C	338	ARG	Sidechain
1	C	34	PHE	Sidechain
1	C	35	TYR	Sidechain
1	C	356	TYR	Sidechain
1	C	366	ARG	Sidechain
1	C	375	PHE	Sidechain
1	C	385	THR	Mainchain,Peptide
1	C	403	TRP	Mainchain
1	C	41	ARG	Sidechain
1	C	419	TYR	Sidechain
1	C	42	LEU	Mainchain
1	C	421	PHE	Sidechain
1	C	442	TYR	Sidechain
1	C	447	PHE	Sidechain
1	C	455	ARG	Sidechain
1	C	463	PHE	Sidechain
1	C	467	ARG	Sidechain
1	C	469	PHE	Sidechain
1	C	49	TYR	Sidechain
1	C	68	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	71	ARG	Sidechain
1	C	73	PHE	Sidechain
1	C	74	ARG	Sidechain
1	C	87	ASP	Mainchain
1	C	88	ASN	Mainchain
1	C	91	TYR	Mainchain
1	D	100	TRP	Mainchain,Peptide
1	D	109	ARG	Sidechain
1	D	144	ARG	Sidechain,Mainchain
1	D	151	TYR	Sidechain
1	D	157	CYS	Mainchain
1	D	168	HIS	Sidechain
1	D	205	TYR	Sidechain
1	D	210	PHE	Sidechain
1	D	231	TYR	Sidechain
1	D	242	TYR	Sidechain
1	D	252	ARG	Sidechain
1	D	263	ARG	Sidechain
1	D	283	ARG	Sidechain
1	D	289	TYR	Sidechain
1	D	311	TYR	Sidechain
1	D	314	HIS	Sidechain
1	D	323	ILE	Mainchain,Peptide
1	D	35	TYR	Sidechain
1	D	354	ASN	Mainchain
1	D	36	HIS	Sidechain
1	D	364	TYR	Sidechain
1	D	366	ARG	Sidechain
1	D	371	PHE	Sidechain
1	D	377	PHE	Sidechain
1	D	391	TYR	Sidechain
1	D	419	TYR	Sidechain
1	D	442	TYR	Sidechain
1	D	443	ASP	Mainchain
1	D	447	PHE	Sidechain
1	D	455	ARG	Sidechain
1	D	456	PHE	Sidechain
1	D	458	ALA	Mainchain
1	D	467	ARG	Sidechain
1	D	469	PHE	Sidechain
1	D	49	TYR	Sidechain
1	D	68	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	70	TYR	Sidechain
1	D	71	ARG	Sidechain
1	D	73	PHE	Sidechain
1	D	97	ARG	Sidechain
1	E	100	TRP	Mainchain
1	E	109	ARG	Sidechain
1	E	144	ARG	Sidechain
1	E	151	TYR	Sidechain
1	E	187	PRO	Mainchain
1	E	234	TYR	Sidechain
1	E	243	GLY	Mainchain
1	E	263	ARG	Sidechain
1	E	276	TYR	Sidechain
1	E	289	TYR	Sidechain
1	E	311	TYR	Sidechain,Mainchain,Peptide
1	E	35	TYR	Sidechain
1	E	356	TYR	Sidechain
1	E	375	PHE	Sidechain
1	E	377	PHE	Sidechain
1	E	381	LYS	Mainchain
1	E	391	TYR	Sidechain
1	E	393	HIS	Sidechain
1	E	398	THR	Mainchain
1	E	407	VAL	Mainchain
1	E	430	GLN	Mainchain
1	E	440	ASP	Mainchain
1	E	442	TYR	Sidechain
1	E	447	PHE	Sidechain
1	E	463	PHE	Sidechain
1	E	467	ARG	Sidechain
1	E	469	PHE	Sidechain
1	E	49	TYR	Sidechain
1	E	59	ARG	Sidechain,Mainchain
1	E	68	TYR	Sidechain
1	E	70	TYR	Sidechain
1	E	71	ARG	Sidechain
1	E	73	PHE	Sidechain
1	E	88	ASN	Mainchain
1	F	100	TRP	Mainchain
1	F	109	ARG	Sidechain
1	F	12	TYR	Sidechain
1	F	144	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	151	TYR	Sidechain
1	F	168	HIS	Sidechain
1	F	203	THR	Mainchain
1	F	209	ASP	Mainchain,Peptide
1	F	242	TYR	Sidechain
1	F	244	ASP	Mainchain
1	F	245	SER	Mainchain,Peptide
1	F	248	PHE	Sidechain
1	F	251	ARG	Sidechain
1	F	256	PHE	Sidechain
1	F	260	PHE	Sidechain
1	F	27	TYR	Sidechain
1	F	276	TYR	Sidechain
1	F	283	ARG	Sidechain
1	F	291	TYR	Sidechain
1	F	30	ARG	Sidechain
1	F	307	PHE	Sidechain
1	F	311	TYR	Sidechain
1	F	314	HIS	Sidechain
1	F	32	SER	Mainchain
1	F	34	PHE	Sidechain
1	F	356	TYR	Sidechain
1	F	364	TYR	Sidechain
1	F	391	TYR	Sidechain
1	F	397	THR	Mainchain,Peptide
1	F	41	ARG	Sidechain
1	F	417	ASP	Mainchain
1	F	420	ARG	Sidechain
1	F	429	CYS	Mainchain
1	F	442	TYR	Sidechain
1	F	447	PHE	Sidechain
1	F	455	ARG	Sidechain
1	F	469	PHE	Sidechain
1	F	49	TYR	Sidechain
1	F	59	ARG	Sidechain
1	F	60	GLN	Mainchain
1	F	68	TYR	Sidechain
1	F	73	PHE	Sidechain
1	F	91	TYR	Sidechain
1	F	92	ASP	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3598	0	3503	270	0
1	B	3661	0	3571	243	0
1	C	3604	0	3506	219	0
1	D	3586	0	3488	236	0
1	E	3586	0	3489	244	0
1	F	3661	0	3571	230	0
All	All	21696	0	21128	1384	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 32.

All (1384) 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:A:386:THR:O	1:A:386:THR:HG22	1.56	1.06
1:D:169:TRP:CD1	1:D:190:LEU:HD13	2.06	0.90
1:B:169:TRP:CE2	1:B:190:LEU:HD13	2.05	0.90
1:A:70:TYR:CD1	1:A:201:VAL:HG12	2.07	0.90
1:F:169:TRP:CD1	1:F:190:LEU:HD13	2.11	0.85
1:A:386:THR:O	1:A:386:THR:CG2	2.25	0.84
1:D:120:HIS:CD2	1:D:122:LEU:H	1.97	0.83
1:F:70:TYR:CD1	1:F:201:VAL:HG12	2.13	0.83
1:E:70:TYR:CD1	1:E:201:VAL:HG12	2.13	0.83
1:E:47:HIS:CD2	1:E:48:PRO:HD2	2.13	0.82
1:E:40:SER:H	1:E:455:ARG:HH12	1.23	0.81
1:F:168:HIS:CE1	1:F:191:ILE:HB	2.20	0.77
1:D:168:HIS:CE1	1:D:191:ILE:HG23	2.20	0.76
1:A:22:VAL:HG12	1:A:27:TYR:CE1	2.21	0.76
1:A:47:HIS:CD2	1:A:48:PRO:HD2	2.21	0.75
1:A:97:ARG:HB3	1:A:403:TRP:CE2	2.21	0.75
1:F:94:ASN:O	1:F:384:LEU:HD12	1.87	0.75
1:D:313:LEU:HD12	1:D:314:HIS:H	1.53	0.74
1:C:171:LYS:H	1:C:212:LEU:HD21	1.52	0.74
1:E:171:LYS:H	1:E:212:LEU:HD23	1.54	0.73
1:D:47:HIS:CE1	1:D:49:TYR:H	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:TYR:CD2	1:F:98:LEU:HD21	2.24	0.72
1:F:467:ARG:HA	1:F:470:LEU:HD12	1.70	0.71
1:A:120:HIS:CD2	1:A:122:LEU:H	2.07	0.71
1:B:341:ASN:HD21	1:B:367:HIS:CD2	2.08	0.71
1:A:460:LEU:HB2	1:A:470:LEU:HD11	1.73	0.71
1:E:47:HIS:CG	1:E:48:PRO:HD2	2.25	0.71
1:F:422:VAL:HG23	1:F:426:ALA:H	1.55	0.71
1:A:38:GLY:H	1:A:455:ARG:HB3	1.56	0.71
1:C:169:TRP:CZ2	1:C:190:LEU:HD13	2.26	0.70
1:B:167:GLU:HG3	1:B:190:LEU:HD11	1.74	0.70
1:F:107:ILE:H	1:F:107:ILE:HD12	1.56	0.70
1:D:91:TYR:CD2	1:D:98:LEU:HD21	2.26	0.70
1:A:388:VAL:O	1:A:391:TYR:CD2	2.44	0.70
1:C:393:HIS:O	1:C:397:THR:HG23	1.92	0.69
1:D:35:TYR:CE2	1:D:458:ALA:HB2	2.27	0.69
1:C:467:ARG:HA	1:C:470:LEU:HD12	1.75	0.69
1:F:47:HIS:CE1	1:F:49:TYR:HB2	2.28	0.68
1:E:47:HIS:CE1	1:E:49:TYR:H	2.11	0.68
1:A:167:GLU:HG2	1:A:190:LEU:HD11	1.75	0.68
1:B:120:HIS:CE1	1:B:222:LEU:HD21	2.29	0.68
1:E:45:VAL:HG13	1:E:367:HIS:O	1.94	0.68
1:B:120:HIS:CG	1:B:123:TYR:CD1	2.81	0.68
1:B:387:GLU:H	1:B:387:GLU:CD	1.97	0.68
1:A:416:VAL:HG23	1:A:417:ASP:H	1.57	0.67
1:F:74:ARG:HB2	1:F:447:PHE:CG	2.29	0.67
1:C:47:HIS:CE1	1:C:49:TYR:H	2.12	0.67
1:F:167:GLU:HA	1:F:192:ASN:HA	1.77	0.67
1:A:120:HIS:CD2	1:A:222:LEU:HD21	2.30	0.66
1:A:169:TRP:NE1	1:A:190:LEU:HD13	2.11	0.66
1:B:101:ALA:HB3	1:B:378:GLN:O	1.95	0.66
1:F:387:GLU:CD	1:F:387:GLU:H	1.98	0.66
1:D:235:LEU:H	1:D:235:LEU:HD12	1.60	0.66
1:F:36:HIS:CD2	1:F:463:PHE:CD1	2.83	0.66
1:A:171:LYS:H	1:A:212:LEU:HD21	1.62	0.65
1:A:388:VAL:O	1:A:392:ILE:HG13	1.95	0.65
1:D:262:ASN:HA	1:D:290:LEU:O	1.97	0.65
1:F:120:HIS:CD2	1:F:222:LEU:HD21	2.31	0.65
1:A:190:LEU:HD12	1:A:191:ILE:H	1.60	0.65
1:C:387:GLU:H	1:C:387:GLU:CD	2.00	0.65
1:A:259:HIS:CG	1:B:131:ASN:HD21	2.14	0.65
1:A:170:THR:HB	1:A:191:ILE:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LEU:H	1:B:371:PHE:H	1.45	0.65
1:C:169:TRP:CH2	1:C:190:LEU:HD13	2.32	0.65
1:A:169:TRP:CD1	1:A:190:LEU:HD13	2.32	0.64
1:A:165:ILE:HA	1:A:194:PRO:HA	1.78	0.64
1:A:91:TYR:CD2	1:A:98:LEU:HD21	2.33	0.64
1:D:36:HIS:CG	1:D:463:PHE:CE2	2.86	0.64
1:A:83:PHE:CE2	1:F:83:PHE:HA	2.33	0.64
1:E:123:TYR:CD2	1:E:147:VAL:HG21	2.32	0.64
1:B:365:ALA:C	1:B:366:ARG:HE	2.00	0.64
1:C:273:GLU:HG2	1:C:276:TYR:CE1	2.32	0.64
1:F:24:THR:O	1:F:28:VAL:HG23	1.98	0.64
1:F:70:TYR:CZ	1:F:201:VAL:HA	2.33	0.64
1:C:30:ARG:HB3	1:C:30:ARG:HH11	1.63	0.64
1:D:107:ILE:H	1:D:107:ILE:HD12	1.61	0.64
1:D:67:ALA:HB3	1:D:68:TYR:CE2	2.33	0.63
1:E:197:ASP:HB2	1:E:447:PHE:HA	1.80	0.63
1:A:398:THR:HA	1:A:401:GLU:CD	2.18	0.63
1:B:66:SER:HA	1:B:367:HIS:CD2	2.32	0.63
1:D:219:GLU:HA	1:D:263:ARG:HH22	1.62	0.63
1:C:97:ARG:HG2	1:C:384:LEU:HD11	1.81	0.63
1:D:70:TYR:CD1	1:D:201:VAL:HG12	2.33	0.63
1:A:356:TYR:CE1	1:A:361:PHE:CE2	2.87	0.63
1:A:211:LYS:HB3	1:A:211:LYS:HZ3	1.64	0.63
1:C:442:TYR:HA	1:C:445:LEU:HD12	1.80	0.63
1:E:190:LEU:HD12	1:E:191:ILE:H	1.64	0.63
1:F:70:TYR:CE1	1:F:201:VAL:HG12	2.33	0.63
1:A:42:LEU:O	1:A:370:GLU:HA	1.99	0.63
1:C:24:THR:HA	1:C:27:TYR:CZ	2.33	0.63
1:A:30:ARG:HA	1:A:380:CYS:SG	2.39	0.62
1:A:47:HIS:CE1	1:A:49:TYR:HB2	2.34	0.62
1:B:97:ARG:HB3	1:B:403:TRP:CE2	2.34	0.62
1:B:120:HIS:CD2	1:B:123:TYR:CD1	2.88	0.62
1:E:234:TYR:CZ	1:E:249:CYS:HB2	2.34	0.62
1:F:121:PRO:HD2	1:F:222:LEU:HD11	1.81	0.62
1:A:168:HIS:HB3	1:A:230:LYS:HA	1.81	0.62
1:B:47:HIS:CE1	1:B:50:PHE:H	2.18	0.62
1:C:168:HIS:CD2	1:C:191:ILE:O	2.53	0.62
1:D:448:TRP:HA	1:D:448:TRP:CE3	2.34	0.62
1:F:169:TRP:NE1	1:F:190:LEU:HD13	2.15	0.62
1:F:81:ASN:HA	1:F:98:LEU:HD12	1.81	0.62
1:A:70:TYR:CE2	1:A:201:VAL:HA	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:TYR:CE2	1:A:98:LEU:HD21	2.35	0.61
1:B:196:GLU:CD	1:B:446:LYS:H	2.03	0.61
1:F:367:HIS:CG	1:F:368:VAL:H	2.18	0.61
1:E:74:ARG:HB2	1:E:447:PHE:CG	2.35	0.61
1:D:66:SER:HA	1:D:367:HIS:CD2	2.36	0.61
1:F:99:VAL:O	1:F:379:LEU:HD12	2.00	0.61
1:B:341:ASN:HD21	1:B:367:HIS:CG	2.18	0.61
1:D:271:LEU:HD12	1:D:275:LEU:HD22	1.83	0.61
1:B:35:TYR:HB2	1:B:377:PHE:H	1.66	0.61
1:D:167:GLU:HA	1:D:192:ASN:HA	1.81	0.61
1:A:329:LEU:HD23	1:A:330:PHE:N	2.15	0.61
1:D:100:TRP:CZ3	1:D:377:PHE:HB3	2.35	0.61
1:D:460:LEU:HB2	1:D:470:LEU:HD11	1.80	0.61
1:B:220:VAL:HG22	1:B:225:CYS:HA	1.83	0.61
1:B:421:PHE:CE1	1:B:422:VAL:HG12	2.36	0.60
1:E:24:THR:HA	1:E:27:TYR:CZ	2.37	0.60
1:E:377:PHE:CD2	1:E:377:PHE:N	2.68	0.60
1:A:169:TRP:CE2	1:A:190:LEU:HD13	2.37	0.60
1:E:121:PRO:HA	1:E:146:ASN:HA	1.82	0.60
1:B:120:HIS:C	1:B:120:HIS:CD2	2.74	0.60
1:B:13:LEU:H	1:B:393:HIS:CE1	2.20	0.60
1:B:41:ARG:HB3	1:B:43:LEU:HD11	1.84	0.60
1:C:70:TYR:CE2	1:C:201:VAL:HA	2.36	0.60
1:C:120:HIS:HB2	1:C:221:PRO:HA	1.84	0.60
1:C:208:MET:HB2	1:C:213:LEU:HD21	1.83	0.60
1:F:30:ARG:HA	1:F:380:CYS:SG	2.42	0.60
1:A:399:ILE:HD12	1:A:399:ILE:H	1.67	0.60
1:B:169:TRP:CH2	1:B:190:LEU:HB2	2.37	0.60
1:B:305:GLN:CD	1:B:307:PHE:H	2.05	0.60
1:C:24:THR:HA	1:C:27:TYR:CE2	2.36	0.60
1:F:214:GLN:HB3	1:F:216:ASN:HD21	1.66	0.60
1:F:442:TYR:HA	1:F:445:LEU:HD12	1.82	0.60
1:A:171:LYS:HE3	1:A:213:LEU:HA	1.84	0.59
1:C:101:ALA:HA	1:C:324:CYS:HG	1.67	0.59
1:D:79:ASP:CA	1:D:327:ASN:HD21	2.15	0.59
1:E:424:SER:HA	1:E:425:ALA:HB3	1.85	0.59
1:E:40:SER:H	1:E:455:ARG:NH1	1.98	0.59
1:B:169:TRP:NE1	1:B:190:LEU:HD13	2.16	0.59
1:B:123:TYR:CE1	1:B:219:GLU:HA	2.37	0.59
1:B:24:THR:HA	1:B:27:TYR:CE2	2.37	0.59
1:D:169:TRP:NE1	1:D:190:LEU:HD13	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:GLN:C	1:D:467:ARG:HH21	2.06	0.59
1:E:172:GLY:H	1:E:188:LEU:HA	1.67	0.59
1:E:168:HIS:HB3	1:E:230:LYS:HA	1.85	0.59
1:E:57:ASN:HD21	1:E:61:ASP:HB3	1.68	0.59
1:F:45:VAL:HG12	1:F:368:VAL:HA	1.84	0.59
1:E:190:LEU:HD12	1:E:191:ILE:N	2.18	0.59
1:F:97:ARG:O	1:F:382:ILE:HD12	2.03	0.59
1:C:42:LEU:O	1:C:370:GLU:HA	2.03	0.58
1:F:107:ILE:HG23	1:F:373:LEU:HD22	1.83	0.58
1:A:181:VAL:HB	1:A:184:ASP:HB2	1.85	0.58
1:A:442:TYR:N	1:A:442:TYR:CD1	2.71	0.58
1:A:444:LYS:C	1:A:445:LEU:HD12	2.24	0.58
1:F:173:THR:HB	1:F:175:CYS:SG	2.43	0.58
1:D:300:VAL:HG12	1:D:301:THR:H	1.67	0.58
1:E:30:ARG:HA	1:E:380:CYS:SG	2.44	0.58
1:B:356:TYR:CD2	1:C:142:ASP:HB3	2.39	0.58
1:B:121:PRO:HA	1:B:146:ASN:HA	1.84	0.58
1:D:36:HIS:CG	1:D:463:PHE:CD2	2.90	0.58
1:D:73:PHE:CE2	1:D:448:TRP:HB3	2.38	0.58
1:E:392:ILE:HA	1:E:395:MET:SD	2.44	0.58
1:F:35:TYR:CE1	1:F:456:PHE:CD2	2.92	0.58
1:B:152:LYS:HA	1:B:297:GLY:HA2	1.85	0.58
1:D:73:PHE:HB3	1:D:450:VAL:HG21	1.85	0.58
1:C:168:HIS:HA	1:C:207:ALA:HB1	1.86	0.58
1:F:24:THR:HA	1:F:27:TYR:CE1	2.38	0.58
1:A:47:HIS:CE1	1:A:49:TYR:H	2.21	0.58
1:B:120:HIS:CD2	1:B:122:LEU:H	2.22	0.58
1:C:47:HIS:CE1	1:C:49:TYR:HB2	2.39	0.58
1:C:169:TRP:CE3	1:C:169:TRP:HA	2.38	0.58
1:C:169:TRP:CZ3	1:C:190:LEU:HA	2.39	0.58
1:B:396:ASN:HD21	1:B:398:THR:HB	1.69	0.57
1:D:97:ARG:HG3	1:D:403:TRP:CD2	2.39	0.57
1:B:344:VAL:HB	1:B:364:TYR:HB2	1.86	0.57
1:B:393:HIS:CE1	1:B:394:ASN:OD1	2.57	0.57
1:F:256:PHE:CE1	1:F:296:SER:HB3	2.39	0.57
1:F:152:LYS:HA	1:F:297:GLY:HA2	1.87	0.57
1:A:367:HIS:CG	1:A:368:VAL:H	2.22	0.57
1:B:120:HIS:CD2	1:B:123:TYR:HD1	2.22	0.57
1:F:97:ARG:HG2	1:F:384:LEU:HD11	1.86	0.57
1:B:156:LEU:HD23	1:B:157:CYS:N	2.20	0.57
1:B:164:ALA:HB1	1:B:237:MET:SD	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:PHE:CZ	1:B:250:LEU:HB2	2.39	0.57
1:F:356:TYR:CE1	1:F:361:PHE:CE2	2.91	0.57
1:B:99:VAL:O	1:B:379:LEU:HD22	2.04	0.57
1:C:91:TYR:CE2	1:C:93:PRO:HA	2.39	0.57
1:B:30:ARG:HA	1:B:380:CYS:SG	2.45	0.57
1:E:74:ARG:CZ	1:E:442:TYR:HB2	2.34	0.57
1:F:325:TRP:HB2	1:F:326:HIS:CD2	2.40	0.57
1:A:342:LEU:O	1:A:365:ALA:HA	2.04	0.56
1:A:387:GLU:HG2	1:A:388:VAL:HG23	1.87	0.56
1:A:391:TYR:C	1:A:391:TYR:CD1	2.78	0.56
1:B:220:VAL:CG2	1:B:225:CYS:HA	2.34	0.56
1:B:420:ARG:HH22	1:B:427:VAL:H	1.52	0.56
1:D:84:GLY:C	1:D:85:LEU:HD23	2.24	0.56
1:F:404:ASN:HB2	1:F:405:PHE:CE1	2.40	0.56
1:A:243:GLY:HA3	1:A:319:LEU:HD22	1.87	0.56
1:C:196:GLU:H	1:C:199:ASP:CG	2.09	0.56
1:D:91:TYR:CZ	1:D:93:PRO:HA	2.40	0.56
1:F:31:THR:H	1:F:378:GLN:NE2	2.03	0.56
1:E:259:HIS:HB2	1:E:261:TRP:CZ2	2.40	0.56
1:A:344:VAL:O	1:A:363:GLU:HA	2.05	0.56
1:A:48:PRO:HG2	1:A:49:TYR:CE2	2.39	0.56
1:B:105:VAL:HG13	1:B:375:PHE:CE1	2.41	0.56
1:C:48:PRO:HB2	1:C:49:TYR:CE2	2.40	0.56
1:B:234:TYR:CZ	1:B:249:CYS:HB2	2.40	0.56
1:C:326:HIS:HB2	1:C:328:GLN:HE21	1.70	0.56
1:D:24:THR:HA	1:D:27:TYR:CE2	2.39	0.56
1:B:47:HIS:CE1	1:B:49:TYR:CD2	2.93	0.56
1:B:89:THR:C	1:B:91:TYR:H	2.09	0.56
1:A:276:TYR:CD2	1:E:122:LEU:HD12	2.41	0.56
1:B:133:HIS:CD2	1:B:134:VAL:HA	2.41	0.56
1:E:97:ARG:HB2	1:E:382:ILE:HD12	1.87	0.56
1:E:59:ARG:NE	1:E:60:GLN:HE22	2.04	0.56
1:F:120:HIS:CD2	1:F:122:LEU:H	2.23	0.56
1:F:422:VAL:HG23	1:F:426:ALA:N	2.21	0.56
1:A:91:TYR:CZ	1:A:98:LEU:HD11	2.41	0.56
1:C:105:VAL:HG13	1:C:375:PHE:CE1	2.40	0.56
1:C:391:TYR:HA	1:C:394:ASN:HD21	1.70	0.56
1:C:440:ASP:O	1:C:443:ASP:HB2	2.06	0.56
1:E:172:GLY:HA2	1:E:189:GLU:CD	2.26	0.56
1:F:126:LEU:H	1:F:263:ARG:HA	1.71	0.56
1:A:259:HIS:HB2	1:A:261:TRP:CZ3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ALA:H	1:B:367:HIS:CE1	2.24	0.56
1:E:120:HIS:HB3	1:E:123:TYR:HB2	1.87	0.56
1:E:400:LEU:HD11	1:E:405:PHE:CE1	2.41	0.56
1:B:167:GLU:CG	1:B:190:LEU:HD11	2.35	0.55
1:E:91:TYR:CE2	1:E:98:LEU:HG	2.41	0.55
1:D:377:PHE:CD2	1:D:377:PHE:N	2.73	0.55
1:E:428:THR:HG23	1:E:430:GLN:HE21	1.71	0.55
1:E:47:HIS:CE1	1:E:50:PHE:CE1	2.95	0.55
1:A:36:HIS:CG	1:A:37:ALA:N	2.74	0.55
1:A:168:HIS:O	1:A:190:LEU:HD12	2.06	0.55
1:A:47:HIS:CG	1:A:48:PRO:HD2	2.41	0.55
1:E:469:PHE:HA	1:E:472:GLN:OE1	2.06	0.55
1:E:441:PRO:HD2	1:E:442:TYR:CE1	2.42	0.55
1:F:49:TYR:HA	1:F:223:ASP:OD2	2.07	0.55
1:F:422:VAL:HA	1:F:426:ALA:HB3	1.89	0.55
1:C:115:VAL:HG22	1:C:116:GLY:H	1.72	0.55
1:C:41:ARG:HA	1:C:371:PHE:O	2.06	0.55
1:F:121:PRO:HA	1:F:146:ASN:HA	1.89	0.55
1:F:427:VAL:HG13	1:F:429:CYS:SG	2.47	0.55
1:A:391:TYR:CZ	1:A:392:ILE:HA	2.41	0.55
1:A:69:GLN:CA	1:A:201:VAL:HG13	2.37	0.55
1:D:26:GLU:CD	1:D:26:GLU:H	2.09	0.55
1:E:109:ARG:HA	1:E:371:PHE:CE1	2.42	0.55
1:E:323:ILE:HB	1:E:325:TRP:CE2	2.42	0.55
1:F:312:TRP:HB2	1:F:314:HIS:CE1	2.42	0.55
1:A:467:ARG:HA	1:A:470:LEU:HD12	1.88	0.55
1:A:48:PRO:HB2	1:A:49:TYR:CZ	2.42	0.55
1:C:124:ASN:HA	1:C:144:ARG:CB	2.37	0.55
1:C:325:TRP:O	1:C:326:HIS:CD2	2.59	0.55
1:E:273:GLU:HA	1:E:276:TYR:CE1	2.42	0.55
1:E:102:CYS:HA	1:E:377:PHE:CD1	2.42	0.55
1:A:33:ILE:O	1:A:378:GLN:HA	2.07	0.55
1:B:85:LEU:HD23	1:B:86:PRO:N	2.21	0.55
1:E:214:GLN:CD	1:E:219:GLU:HB2	2.27	0.55
1:B:78:PRO:HD3	1:B:456:PHE:CE1	2.42	0.55
1:C:301:THR:HA	1:D:254:GLN:HA	1.89	0.55
1:C:420:ARG:HB2	1:C:423:GLN:HE22	1.72	0.55
1:A:70:TYR:CZ	1:A:201:VAL:HA	2.42	0.54
1:F:168:HIS:C	1:F:168:HIS:CD2	2.81	0.54
1:B:80:PRO:HA	1:B:83:PHE:HB2	1.89	0.54
1:C:190:LEU:HD12	1:C:191:ILE:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:ASP:HA	1:D:261:TRP:HA	1.90	0.54
1:A:169:TRP:CZ2	1:A:190:LEU:HB2	2.42	0.54
1:A:169:TRP:HB2	1:A:208:MET:HB3	1.88	0.54
1:E:100:TRP:HB2	1:E:324:CYS:SG	2.47	0.54
1:E:402:ASP:HB2	1:E:403:TRP:CD2	2.42	0.54
1:B:76:LYS:HB2	1:B:451:ASP:HA	1.89	0.54
1:E:152:LYS:HA	1:E:297:GLY:HA2	1.89	0.54
1:E:165:ILE:HD11	1:E:192:ASN:HB3	1.89	0.54
1:A:462:GLN:C	1:A:467:ARG:HH21	2.11	0.54
1:C:469:PHE:CD2	1:C:469:PHE:C	2.81	0.54
1:E:236:GLN:HE21	1:E:237:MET:HG3	1.72	0.54
1:A:273:GLU:C	1:A:275:LEU:H	2.11	0.54
1:B:123:TYR:CD2	1:B:263:ARG:NH2	2.76	0.54
1:E:357:THR:HG22	1:E:358:PRO:HD2	1.90	0.54
1:F:100:TRP:CZ3	1:F:377:PHE:HB3	2.42	0.54
1:F:340:THR:O	1:F:367:HIS:CE1	2.61	0.54
1:B:262:ASN:HA	1:B:290:LEU:O	2.07	0.54
1:E:273:GLU:H	1:E:273:GLU:CD	2.10	0.54
1:F:168:HIS:O	1:F:190:LEU:HD12	2.08	0.54
1:A:168:HIS:CE1	1:A:191:ILE:HB	2.42	0.54
1:F:107:ILE:CG2	1:F:373:LEU:HD22	2.38	0.54
1:A:81:ASN:HA	1:A:98:LEU:HD12	1.90	0.53
1:B:186:PRO:HG2	1:B:188:LEU:HD21	1.89	0.53
1:E:393:HIS:CD2	1:E:397:THR:HG22	2.44	0.53
1:E:49:TYR:HB2	1:E:50:PHE:CD2	2.43	0.53
1:A:185:CYS:HB2	1:E:364:TYR:CD2	2.44	0.53
1:A:77:LEU:H	1:A:327:ASN:HB3	1.72	0.53
1:B:107:ILE:HD12	1:B:107:ILE:H	1.71	0.53
1:B:190:LEU:HD12	1:B:191:ILE:N	2.24	0.53
1:C:150:ASP:HA	1:C:151:TYR:CZ	2.44	0.53
1:C:392:ILE:HG21	1:C:400:LEU:HD21	1.89	0.53
1:D:334:VAL:HG12	1:D:335:ASP:H	1.72	0.53
1:D:391:TYR:O	1:D:395:MET:SD	2.66	0.53
1:D:448:TRP:CD2	1:D:449:PRO:HD2	2.43	0.53
1:F:371:PHE:N	1:F:371:PHE:CD2	2.76	0.53
1:A:22:VAL:HG21	1:A:391:TYR:CZ	2.43	0.53
1:F:235:LEU:HD12	1:F:235:LEU:H	1.72	0.53
1:C:43:LEU:HA	1:C:369:GLU:O	2.08	0.53
1:D:45:VAL:HA	1:D:367:HIS:O	2.08	0.53
1:E:88:ASN:HA	1:E:90:VAL:HB	1.90	0.53
1:A:190:LEU:HD12	1:A:191:ILE:N	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:TYR:HB2	1:B:145:ASP:O	2.08	0.53
1:B:454:GLU:CD	1:B:454:GLU:H	2.11	0.53
1:B:51:LYS:HG2	1:B:63:PRO:HA	1.91	0.53
1:D:130:GLU:HA	1:D:260:PHE:CD2	2.43	0.53
1:D:273:GLU:HA	1:D:276:TYR:CE1	2.44	0.53
1:D:77:LEU:H	1:D:327:ASN:HB3	1.73	0.53
1:A:367:HIS:CG	1:A:368:VAL:N	2.76	0.53
1:A:73:PHE:CD2	1:A:448:TRP:HB3	2.43	0.53
1:B:169:TRP:HB2	1:B:208:MET:HB3	1.90	0.53
1:B:241:ALA:HB3	1:B:242:TYR:CE2	2.43	0.53
1:C:233:ASP:CG	1:C:236:GLN:H	2.12	0.53
1:D:357:THR:CB	1:D:359:THR:HG1	2.22	0.53
1:A:397:THR:HA	1:A:400:LEU:HD12	1.91	0.53
1:C:321:ASN:H	1:C:323:ILE:CD1	2.22	0.53
1:D:121:PRO:HA	1:D:146:ASN:HA	1.91	0.53
1:E:47:HIS:CE1	1:E:49:TYR:N	2.77	0.53
1:F:36:HIS:CE1	1:F:463:PHE:CE1	2.97	0.53
1:A:343:SER:HA	1:A:364:TYR:O	2.09	0.53
1:A:442:TYR:HA	1:A:445:LEU:HD13	1.91	0.53
1:D:218:SER:H	1:D:219:GLU:HG2	1.72	0.53
1:D:341:ASN:HD21	1:D:367:HIS:HB2	1.73	0.53
1:D:36:HIS:CD2	1:D:463:PHE:CG	2.96	0.53
1:D:41:ARG:HH22	1:E:233:ASP:CG	2.12	0.53
1:A:47:HIS:CE1	1:A:50:PHE:CD1	2.97	0.53
1:A:69:GLN:HB3	1:A:200:MET:SD	2.49	0.53
1:D:150:ASP:HA	1:D:151:TYR:CZ	2.44	0.53
1:B:248:PHE:C	1:B:248:PHE:CD1	2.83	0.52
1:D:100:TRP:HA	1:D:379:LEU:HD12	1.92	0.52
1:D:164:ALA:HA	1:D:165:ILE:HD12	1.90	0.52
1:D:79:ASP:HA	1:D:327:ASN:HD21	1.74	0.52
1:D:97:ARG:HG2	1:D:384:LEU:HD11	1.91	0.52
1:D:73:PHE:CD2	1:D:448:TRP:HB3	2.44	0.52
1:A:121:PRO:HA	1:A:146:ASN:HA	1.90	0.52
1:B:421:PHE:CG	1:B:422:VAL:N	2.75	0.52
1:C:78:PRO:HD3	1:C:456:PHE:CE1	2.44	0.52
1:D:196:GLU:CD	1:D:446:LYS:H	2.12	0.52
1:E:74:ARG:H	1:E:447:PHE:HB3	1.73	0.52
1:E:37:ALA:HA	1:E:455:ARG:O	2.09	0.52
1:B:169:TRP:CZ2	1:B:190:LEU:HD13	2.45	0.52
1:B:26:GLU:HB2	1:B:27:TYR:CE1	2.44	0.52
1:A:166:GLY:HA2	1:A:232:PRO:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ILE:O	1:B:378:GLN:HA	2.10	0.52
1:E:344:VAL:O	1:E:363:GLU:HA	2.10	0.52
1:E:70:TYR:CZ	1:E:201:VAL:HA	2.44	0.52
1:F:360:SER:HB2	1:F:361:PHE:CE2	2.43	0.52
1:A:99:VAL:HG12	1:A:382:ILE:HD11	1.90	0.52
1:B:423:GLN:HA	1:B:423:GLN:HE21	1.75	0.52
1:C:43:LEU:HD11	1:C:368:VAL:CG1	2.40	0.52
1:F:100:TRP:CE3	1:F:100:TRP:HA	2.45	0.52
1:A:149:VAL:HG22	1:A:150:ASP:H	1.75	0.52
1:A:47:HIS:HE1	1:A:49:TYR:HB2	1.72	0.52
1:B:35:TYR:O	1:B:376:ILE:HA	2.10	0.52
1:B:398:THR:HA	1:B:401:GLU:CD	2.30	0.52
1:E:169:TRP:CZ2	1:E:190:LEU:HB2	2.45	0.52
1:E:393:HIS:CG	1:E:408:THR:HG21	2.45	0.52
1:E:420:ARG:O	1:E:421:PHE:CD1	2.63	0.52
1:E:424:SER:HA	1:E:425:ALA:CB	2.40	0.52
1:A:157:CYS:SG	1:A:158:ILE:N	2.83	0.52
1:B:150:ASP:HA	1:B:151:TYR:CZ	2.45	0.52
1:E:33:ILE:O	1:E:378:GLN:HG3	2.10	0.52
1:A:448:TRP:CE2	1:F:419:TYR:CZ	2.98	0.52
1:A:109:ARG:HA	1:A:371:PHE:CE1	2.45	0.52
1:B:231:TYR:CD1	1:B:232:PRO:HD2	2.45	0.52
1:B:80:PRO:HB2	1:B:379:LEU:HD21	1.91	0.52
1:C:66:SER:HA	1:C:367:HIS:CG	2.45	0.52
1:D:78:PRO:HA	1:D:453:LYS:HG2	1.92	0.52
1:E:467:ARG:HA	1:E:470:LEU:HD12	1.91	0.52
1:A:196:GLU:CD	1:A:446:LYS:H	2.12	0.51
1:B:386:THR:HA	1:B:389:MET:SD	2.50	0.51
1:C:309:LYS:O	1:C:311:TYR:CZ	2.63	0.51
1:C:469:PHE:HA	1:C:472:GLN:OE1	2.09	0.51
1:D:35:TYR:CD1	1:D:456:PHE:CD2	2.99	0.51
1:D:363:GLU:N	1:E:268:GLY:H	2.09	0.51
1:F:103:VAL:HG22	1:F:376:ILE:O	2.10	0.51
1:E:160:GLY:HA3	1:E:245:SER:O	2.10	0.51
1:E:27:TYR:CD1	1:E:27:TYR:N	2.74	0.51
1:E:347:SER:HA	1:E:361:PHE:HA	1.93	0.51
1:C:120:HIS:CE1	1:C:122:LEU:C	2.83	0.51
1:C:30:ARG:HA	1:C:380:CYS:SG	2.51	0.51
1:E:25:ASP:HA	1:E:28:VAL:HB	1.93	0.51
1:F:169:TRP:CZ2	1:F:190:LEU:HB2	2.45	0.51
1:F:190:LEU:HD12	1:F:191:ILE:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:314:HIS:N	1:F:314:HIS:CD2	2.74	0.51
1:A:275:LEU:HA	1:E:226:GLN:HE21	1.75	0.51
1:B:176:LYS:HG2	1:B:178:THR:HG23	1.91	0.51
1:B:392:ILE:HG21	1:B:400:LEU:HD21	1.91	0.51
1:F:243:GLY:HA3	1:F:318:GLY:HA3	1.92	0.51
1:F:36:HIS:CG	1:F:463:PHE:CG	2.98	0.51
1:D:278:LYS:HB2	1:D:284:ALA:HA	1.91	0.51
1:F:123:TYR:C	1:F:144:ARG:HA	2.31	0.51
1:A:232:PRO:O	1:A:234:TYR:CE2	2.64	0.51
1:C:71:ARG:HH21	1:C:197:ASP:CG	2.14	0.51
1:C:34:PHE:CE1	1:C:378:GLN:HB2	2.45	0.51
1:D:120:HIS:CD2	1:D:222:LEU:HD21	2.46	0.51
1:E:454:GLU:CD	1:E:454:GLU:N	2.64	0.51
1:F:409:PRO:HB2	1:F:411:PRO:HD3	1.93	0.51
1:A:100:TRP:HA	1:A:379:LEU:HD12	1.92	0.51
1:C:27:TYR:N	1:C:27:TYR:CD1	2.79	0.51
1:C:309:LYS:O	1:C:311:TYR:CE1	2.63	0.51
1:C:48:PRO:HB2	1:C:49:TYR:CZ	2.46	0.51
1:D:210:PHE:CD2	1:D:227:SER:O	2.64	0.51
1:E:80:PRO:HD3	1:E:327:ASN:HD21	1.76	0.51
1:A:375:PHE:HB3	1:A:377:PHE:CE2	2.46	0.51
1:C:454:GLU:CD	1:C:454:GLU:H	2.13	0.51
1:D:169:TRP:CZ2	1:D:190:LEU:HB2	2.46	0.51
1:F:35:TYR:CE2	1:F:458:ALA:HA	2.46	0.51
1:F:252:ARG:HH21	1:F:253:GLU:C	2.14	0.51
1:A:38:GLY:HA2	1:A:373:LEU:O	2.10	0.50
1:B:120:HIS:CD2	1:B:122:LEU:N	2.79	0.50
1:C:310:PRO:HB2	1:C:312:TRP:CE2	2.46	0.50
1:E:209:ASP:HB3	1:E:212:LEU:HD22	1.93	0.50
1:E:91:TYR:CD2	1:E:96:GLN:HB2	2.46	0.50
1:C:97:ARG:HB2	1:C:403:TRP:CZ3	2.47	0.50
1:D:195:ILE:HD13	1:D:230:LYS:HD3	1.94	0.50
1:D:384:LEU:HD13	1:D:405:PHE:CD2	2.46	0.50
1:F:244:ASP:HB3	1:F:320:ASN:HB3	1.92	0.50
1:A:97:ARG:HB3	1:A:403:TRP:CZ2	2.46	0.50
1:D:235:LEU:H	1:D:235:LEU:CD1	2.20	0.50
1:E:200:MET:SD	1:E:229:CYS:HB2	2.52	0.50
1:F:123:TYR:O	1:F:144:ARG:HA	2.12	0.50
1:F:307:PHE:HA	1:F:307:PHE:CE1	2.40	0.50
1:A:273:GLU:HB3	1:A:278:LYS:HZ1	1.76	0.50
1:B:70:TYR:CE2	1:B:201:VAL:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:HIS:HA	1:E:207:ALA:HB1	1.94	0.50
1:F:35:TYR:CE1	1:F:456:PHE:CE2	2.99	0.50
1:A:169:TRP:CH2	1:A:190:LEU:HB2	2.46	0.50
1:A:70:TYR:CE1	1:A:201:VAL:HG12	2.45	0.50
1:B:190:LEU:HD12	1:B:191:ILE:H	1.76	0.50
1:B:165:ILE:HA	1:B:194:PRO:HA	1.94	0.50
1:B:30:ARG:HH11	1:B:378:GLN:CD	2.14	0.50
1:B:442:TYR:HA	1:B:445:LEU:HD12	1.92	0.50
1:D:467:ARG:O	1:D:471:LEU:HG	2.11	0.50
1:A:141:LYS:HD3	1:A:141:LYS:H	1.77	0.50
1:D:391:TYR:CE2	1:D:392:ILE:HD13	2.46	0.50
1:E:259:HIS:H	1:E:294:SER:HB3	1.76	0.50
1:F:232:PRO:HB2	1:F:234:TYR:CE1	2.47	0.50
1:F:262:ASN:HA	1:F:290:LEU:O	2.12	0.50
1:A:448:TRP:CD2	1:F:419:TYR:CZ	3.00	0.50
1:A:105:VAL:HG13	1:A:375:PHE:CE1	2.47	0.50
1:A:73:PHE:HB3	1:A:450:VAL:HG21	1.94	0.50
1:A:74:ARG:HB2	1:A:447:PHE:CG	2.47	0.50
1:B:35:TYR:HB2	1:B:377:PHE:HB2	1.94	0.50
1:C:209:ASP:O	1:C:213:LEU:HD13	2.12	0.50
1:D:392:ILE:HG21	1:D:400:LEU:HD21	1.94	0.50
1:D:78:PRO:CA	1:D:453:LYS:HG2	2.42	0.50
1:D:91:TYR:CZ	1:D:98:LEU:HG	2.46	0.50
1:E:169:TRP:H	1:E:207:ALA:C	2.15	0.50
1:A:448:TRP:CE2	1:F:419:TYR:CE2	3.00	0.50
1:F:439:GLN:HA	1:F:443:ASP:OD2	2.10	0.50
1:A:377:PHE:N	1:A:377:PHE:CD2	2.79	0.50
1:A:430:GLN:NE2	1:A:432:ASP:H	2.10	0.50
1:B:33:ILE:O	1:B:34:PHE:CD1	2.65	0.50
1:B:36:HIS:CG	1:B:463:PHE:CD2	3.00	0.50
1:C:105:VAL:O	1:C:311:TYR:CD2	2.65	0.50
1:D:461:ASP:HA	1:D:467:ARG:HG2	1.94	0.50
1:A:172:GLY:HA3	1:A:189:GLU:CD	2.32	0.50
1:A:26:GLU:CD	1:A:26:GLU:N	2.66	0.50
1:A:96:GLN:HA	1:A:383:THR:HA	1.93	0.50
1:C:231:TYR:CD1	1:C:232:PRO:HD2	2.47	0.50
1:C:152:LYS:HA	1:C:297:GLY:HA2	1.93	0.50
1:D:409:PRO:HB2	1:D:410:PRO:HA	1.94	0.50
1:E:42:LEU:O	1:E:370:GLU:HA	2.12	0.50
1:F:102:CYS:HA	1:F:377:PHE:CD1	2.46	0.50
1:F:107:ILE:H	1:F:107:ILE:CD1	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:ALA:HB3	1:F:242:TYR:CD2	2.47	0.50
1:A:71:ARG:O	1:A:332:THR:HA	2.12	0.49
1:A:38:GLY:H	1:A:455:ARG:CB	2.23	0.49
1:D:36:HIS:CD2	1:D:463:PHE:CD1	3.00	0.49
1:E:73:PHE:CE2	1:E:448:TRP:HB2	2.47	0.49
1:F:11:VAL:HG13	1:F:12:TYR:CE2	2.47	0.49
1:B:19:ALA:H	1:F:407:VAL:N	2.10	0.49
1:A:42:LEU:H	1:A:371:PHE:H	1.59	0.49
1:B:38:GLY:H	1:B:455:ARG:HB3	1.76	0.49
1:C:73:PHE:CD2	1:C:448:TRP:HB3	2.47	0.49
1:E:342:LEU:O	1:E:365:ALA:HA	2.12	0.49
1:A:243:GLY:HA3	1:A:319:LEU:H	1.77	0.49
1:B:464:PRO:HA	1:B:467:ARG:HD2	1.94	0.49
1:A:256:PHE:CZ	1:A:296:SER:HB3	2.47	0.49
1:B:97:ARG:CB	1:B:403:TRP:CE2	2.96	0.49
1:E:166:GLY:HA2	1:E:232:PRO:HA	1.94	0.49
1:F:385:THR:O	1:F:389:MET:HG3	2.11	0.49
1:A:448:TRP:CZ3	1:F:419:TYR:CE1	3.00	0.49
1:A:180:VAL:HG22	1:A:181:VAL:H	1.77	0.49
1:A:22:VAL:HG11	1:A:391:TYR:CE2	2.48	0.49
1:A:78:PRO:CD	1:A:456:PHE:CZ	2.95	0.49
1:A:393:HIS:CD2	1:A:394:ASN:ND2	2.81	0.49
1:B:400:LEU:HB3	1:B:405:PHE:CG	2.48	0.49
1:C:262:ASN:HA	1:C:290:LEU:O	2.11	0.49
1:E:69:GLN:N	1:E:201:VAL:HG13	2.26	0.49
1:B:168:HIS:O	1:B:190:LEU:HD12	2.12	0.49
1:B:99:VAL:C	1:B:379:LEU:HD22	2.33	0.49
1:C:388:VAL:O	1:C:392:ILE:HG12	2.13	0.49
1:D:248:PHE:CG	1:D:249:CYS:N	2.81	0.49
1:A:84:GLY:HA3	1:F:83:PHE:CE2	2.48	0.49
1:A:440:ASP:OD1	1:A:442:TYR:CD2	2.66	0.49
1:A:78:PRO:HD3	1:A:456:PHE:CE1	2.46	0.49
1:B:168:HIS:CE1	1:B:191:ILE:HB	2.48	0.49
1:C:158:ILE:HG23	1:C:248:PHE:O	2.13	0.49
1:D:346:ALA:HB1	1:E:183:GLY:C	2.33	0.49
1:E:36:HIS:CG	1:E:37:ALA:N	2.80	0.49
1:E:33:ILE:O	1:E:378:GLN:HA	2.13	0.49
1:E:413:ALA:HB3	1:E:414:SER:C	2.33	0.49
1:F:35:TYR:CE1	1:F:457:SER:C	2.86	0.49
1:B:169:TRP:CZ2	1:B:190:LEU:HB2	2.48	0.49
1:B:385:THR:O	1:B:388:VAL:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ASN:O	1:C:384:LEU:HD12	2.13	0.49
1:D:234:TYR:HA	1:D:237:MET:SD	2.53	0.49
1:E:165:ILE:HA	1:E:194:PRO:HA	1.95	0.49
1:B:121:PRO:HD2	1:B:222:LEU:HD11	1.95	0.49
1:C:345:CYS:HA	1:C:363:GLU:HG3	1.93	0.49
1:D:165:ILE:N	1:D:165:ILE:HD12	2.28	0.49
1:B:173:THR:H	1:F:427:VAL:HG23	1.78	0.49
1:B:252:ARG:HB3	1:B:306:LEU:HD11	1.94	0.48
1:C:33:ILE:O	1:C:378:GLN:HG2	2.13	0.48
1:D:169:TRP:HE1	1:D:190:LEU:HD22	1.77	0.48
1:D:426:ALA:HB3	1:D:427:VAL:C	2.34	0.48
1:E:210:PHE:CD2	1:E:227:SER:O	2.66	0.48
1:E:259:HIS:HB2	1:E:261:TRP:CH2	2.48	0.48
1:F:25:ASP:HA	1:F:28:VAL:HB	1.95	0.48
1:F:33:ILE:O	1:F:378:GLN:HA	2.13	0.48
1:E:242:TYR:HA	1:E:319:LEU:HD12	1.95	0.48
1:F:210:PHE:CD2	1:F:227:SER:O	2.67	0.48
1:F:79:ASP:HA	1:F:327:ASN:HD21	1.78	0.48
1:A:80:PRO:HG3	1:A:379:LEU:HD11	1.94	0.48
1:B:312:TRP:HB2	1:B:314:HIS:CE1	2.49	0.48
1:B:97:ARG:HB2	1:B:403:TRP:CH2	2.49	0.48
1:C:75:VAL:O	1:C:328:GLN:HA	2.14	0.48
1:D:47:HIS:CE1	1:D:49:TYR:N	2.79	0.48
1:E:73:PHE:O	1:E:330:PHE:HA	2.13	0.48
1:B:85:LEU:HD21	1:B:87:ASP:OD2	2.13	0.48
1:C:208:MET:HG3	1:C:210:PHE:CZ	2.48	0.48
1:D:120:HIS:CE1	1:D:218:SER:HA	2.48	0.48
1:E:193:THR:HB	1:E:230:LYS:HD3	1.94	0.48
1:E:440:ASP:HB3	1:E:442:TYR:CZ	2.48	0.48
1:E:464:PRO:HA	1:E:467:ARG:CZ	2.42	0.48
1:A:232:PRO:HB2	1:A:234:TYR:CE1	2.49	0.48
1:A:279:GLY:H	1:A:284:ALA:HA	1.78	0.48
1:A:416:VAL:CG2	1:A:417:ASP:H	2.27	0.48
1:B:76:LYS:HD2	1:B:76:LYS:H	1.77	0.48
1:C:259:HIS:HB2	1:C:261:TRP:CH2	2.49	0.48
1:C:469:PHE:CD1	1:C:472:GLN:OE1	2.67	0.48
1:F:455:ARG:HH11	1:F:455:ARG:HB3	1.78	0.48
1:A:375:PHE:CB	1:A:377:PHE:CE2	2.97	0.48
1:A:420:ARG:HH11	1:F:370:GLU:HG2	1.78	0.48
1:B:438:LYS:HG2	1:B:439:GLN:H	1.78	0.48
1:C:126:LEU:HB3	1:C:262:ASN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:HIS:O	1:D:190:LEU:HD12	2.13	0.48
1:D:48:PRO:HB2	1:D:49:TYR:CE1	2.48	0.48
1:E:370:GLU:O	1:E:371:PHE:CD2	2.67	0.48
1:E:97:ARG:HA	1:E:97:ARG:HD3	1.75	0.48
1:A:322:GLY:C	1:A:323:ILE:HD12	2.34	0.48
1:A:361:PHE:CD2	1:A:361:PHE:N	2.81	0.48
1:A:102:CYS:HA	1:A:377:PHE:CD1	2.48	0.48
1:B:250:LEU:HD11	1:B:306:LEU:HD13	1.96	0.48
1:B:96:GLN:HA	1:B:384:LEU:HG	1.96	0.48
1:D:172:GLY:HA2	1:D:189:GLU:HB2	1.95	0.48
1:F:166:GLY:HA2	1:F:232:PRO:HA	1.95	0.48
1:A:24:THR:HG23	1:A:320:ASN:HA	1.96	0.48
1:A:43:LEU:HA	1:A:369:GLU:O	2.14	0.48
1:B:350:SER:HA	1:C:182:GLN:CD	2.34	0.48
1:C:248:PHE:CZ	1:C:250:LEU:HB2	2.49	0.48
1:C:325:TRP:C	1:C:326:HIS:CG	2.87	0.48
1:C:469:PHE:CZ	1:C:473:LEU:HD21	2.48	0.48
1:D:256:PHE:CE1	1:D:296:SER:HB3	2.49	0.48
1:D:364:TYR:HB3	1:D:366:ARG:CZ	2.44	0.48
1:D:469:PHE:CD2	1:D:469:PHE:C	2.85	0.48
1:E:210:PHE:C	1:E:212:LEU:H	2.17	0.48
1:E:391:TYR:HA	1:E:394:ASN:ND2	2.29	0.48
1:E:442:TYR:HA	1:E:445:LEU:HD12	1.96	0.48
1:E:464:PRO:O	1:E:468:LYS:HG3	2.14	0.48
1:A:309:LYS:O	1:A:311:TYR:CE2	2.66	0.48
1:B:341:ASN:ND2	1:B:367:HIS:CD2	2.79	0.48
1:B:73:PHE:CD2	1:B:448:TRP:HB3	2.49	0.48
1:C:33:ILE:O	1:C:378:GLN:CG	2.61	0.48
1:C:391:TYR:CZ	1:C:395:MET:SD	3.07	0.48
1:D:379:LEU:HG	1:D:380:CYS:N	2.29	0.48
1:E:47:HIS:CE1	1:E:50:PHE:CD1	3.02	0.48
1:A:22:VAL:HG21	1:A:391:TYR:CE1	2.49	0.47
1:B:100:TRP:CZ2	1:B:456:PHE:CE2	3.01	0.47
1:B:174:ALA:HB2	1:B:187:PRO:HG3	1.96	0.47
1:C:350:SER:HA	1:D:182:GLN:HG2	1.94	0.47
1:E:440:ASP:CG	1:E:442:TYR:CE2	2.88	0.47
1:F:171:LYS:HA	1:F:188:LEU:HD23	1.95	0.47
1:F:373:LEU:C	1:F:375:PHE:CZ	2.87	0.47
1:F:38:GLY:HA2	1:F:375:PHE:CE2	2.48	0.47
1:C:169:TRP:CH2	1:C:190:LEU:HB2	2.49	0.47
1:C:168:HIS:CE1	1:C:193:THR:OG1	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:GLU:HG2	1:D:27:TYR:CD1	2.49	0.47
1:D:346:ALA:HB1	1:E:183:GLY:O	2.15	0.47
1:A:262:ASN:HA	1:A:290:LEU:O	2.14	0.47
1:A:326:HIS:CE1	1:A:399:ILE:HG13	2.48	0.47
1:B:13:LEU:HD12	1:B:390:SER:HA	1.96	0.47
1:C:73:PHE:CE2	1:C:448:TRP:HB3	2.49	0.47
1:F:387:GLU:CD	1:F:387:GLU:N	2.66	0.47
1:F:393:HIS:CD2	1:F:393:HIS:C	2.86	0.47
1:F:397:THR:HA	1:F:400:LEU:HD12	1.96	0.47
1:F:36:HIS:CD2	1:F:463:PHE:CG	3.03	0.47
1:F:464:PRO:HD3	1:F:467:ARG:HH21	1.78	0.47
1:A:96:GLN:HA	1:A:382:ILE:O	2.15	0.47
1:B:13:LEU:O	1:B:393:HIS:CE1	2.68	0.47
1:F:43:LEU:HD13	1:F:43:LEU:C	2.35	0.47
1:D:379:LEU:HG	1:D:380:CYS:H	1.80	0.47
1:D:469:PHE:CE1	1:D:472:GLN:NE2	2.82	0.47
1:D:470:LEU:HD23	1:D:473:LEU:HD11	1.96	0.47
1:D:47:HIS:CD2	1:D:48:PRO:HD2	2.49	0.47
1:D:91:TYR:CE2	1:D:96:GLN:HB2	2.50	0.47
1:D:148:SER:HB3	1:E:291:TYR:CD1	2.49	0.47
1:E:356:TYR:C	1:E:356:TYR:CD2	2.88	0.47
1:B:179:THR:OG1	1:B:181:VAL:HG23	2.15	0.47
1:B:240:ASP:CG	1:B:243:GLY:H	2.18	0.47
1:C:460:LEU:HD22	1:C:470:LEU:HG	1.96	0.47
1:C:356:TYR:CD1	1:E:277:ILE:HD12	2.50	0.47
1:F:165:ILE:HA	1:F:194:PRO:HA	1.96	0.47
1:F:391:TYR:CD1	1:F:391:TYR:C	2.87	0.47
1:A:444:LYS:HB2	1:A:445:LEU:HD12	1.97	0.47
1:B:24:THR:HA	1:B:27:TYR:CZ	2.50	0.47
1:B:312:TRP:CZ3	1:B:469:PHE:HB2	2.50	0.47
1:C:169:TRP:CZ3	1:C:190:LEU:CA	2.98	0.47
1:E:91:TYR:CE1	1:E:93:PRO:HB3	2.49	0.47
1:F:26:GLU:CD	1:F:26:GLU:N	2.68	0.47
1:A:36:HIS:HD1	1:A:457:SER:HB3	1.80	0.47
1:A:80:PRO:CB	1:A:379:LEU:HD11	2.45	0.47
1:B:405:PHE:CD2	1:B:406:GLY:N	2.83	0.47
1:C:97:ARG:CG	1:C:384:LEU:HD11	2.44	0.47
1:D:70:TYR:CZ	1:D:201:VAL:HA	2.50	0.47
1:D:81:ASN:HA	1:D:98:LEU:HD12	1.96	0.47
1:E:323:ILE:HB	1:E:325:TRP:CZ2	2.49	0.47
1:A:83:PHE:CD2	1:F:84:GLY:HA2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASN:HA	1:A:144:ARG:HB3	1.95	0.47
1:A:121:PRO:HD2	1:A:222:LEU:HD11	1.96	0.47
1:A:313:LEU:HD12	1:A:314:HIS:H	1.79	0.47
1:C:91:TYR:HB3	1:C:381:LYS:HE2	1.96	0.47
1:D:162:VAL:HG21	1:D:244:ASP:HB2	1.96	0.47
1:D:334:VAL:HG12	1:D:335:ASP:N	2.30	0.47
1:D:34:PHE:HA	1:D:377:PHE:O	2.15	0.47
1:E:373:LEU:HB3	1:E:375:PHE:CZ	2.50	0.47
1:E:385:THR:O	1:E:388:VAL:HB	2.15	0.47
1:E:466:GLY:O	1:E:470:LEU:HG	2.15	0.47
1:F:190:LEU:HD12	1:F:191:ILE:H	1.79	0.47
1:A:170:THR:CB	1:A:191:ILE:HD11	2.45	0.47
1:A:317:GLN:HG3	1:A:318:GLY:H	1.80	0.47
1:A:459:ASP:O	1:A:463:PHE:CD2	2.68	0.47
1:A:47:HIS:CD2	1:A:48:PRO:CD	2.95	0.47
1:B:256:PHE:CZ	1:B:296:SER:HB3	2.50	0.47
1:B:328:GLN:O	1:B:329:LEU:HD12	2.15	0.47
1:C:319:LEU:HD22	1:C:319:LEU:N	2.30	0.47
1:D:392:ILE:HG22	1:D:392:ILE:O	2.14	0.47
1:E:373:LEU:HB3	1:E:375:PHE:CE2	2.50	0.47
1:F:43:LEU:HD21	1:F:45:VAL:HG13	1.95	0.47
1:A:121:PRO:CD	1:A:222:LEU:HD11	2.45	0.46
1:C:391:TYR:CD2	1:C:392:ILE:HD13	2.50	0.46
1:C:346:ALA:HB1	1:D:183:GLY:HA2	1.97	0.46
1:D:209:ASP:HB3	1:D:212:LEU:HB3	1.97	0.46
1:E:168:HIS:CD2	1:E:191:ILE:HD12	2.50	0.46
1:F:170:THR:HG22	1:F:171:LYS:N	2.30	0.46
1:F:256:PHE:CZ	1:F:296:SER:HB3	2.51	0.46
1:A:169:TRP:CZ2	1:A:190:LEU:HD22	2.50	0.46
1:A:395:MET:C	1:A:395:MET:SD	2.94	0.46
1:A:391:TYR:CE1	1:A:395:MET:HB2	2.51	0.46
1:B:277:ILE:HG23	1:B:278:LYS:O	2.16	0.46
1:C:173:THR:H	1:C:189:GLU:CD	2.19	0.46
1:C:374:GLN:O	1:C:375:PHE:CE1	2.67	0.46
1:C:78:PRO:CD	1:C:456:PHE:CE1	2.99	0.46
1:E:175:CYS:SG	1:E:176:LYS:HD2	2.55	0.46
1:E:169:TRP:HE1	1:E:190:LEU:HD22	1.80	0.46
1:F:259:HIS:HB2	1:F:261:TRP:CH2	2.51	0.46
1:F:310:PRO:HG2	1:F:312:TRP:CZ2	2.50	0.46
1:F:99:VAL:HB	1:F:382:ILE:HD11	1.96	0.46
1:B:208:MET:SD	1:B:210:PHE:CD2	3.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:LEU:HB3	1:C:375:PHE:CE2	2.51	0.46
1:C:47:HIS:HE1	1:C:50:PHE:CE2	2.32	0.46
1:F:36:HIS:CG	1:F:37:ALA:N	2.83	0.46
1:F:374:GLN:OE1	1:F:463:PHE:HB3	2.16	0.46
1:A:36:HIS:CD2	1:A:463:PHE:CG	3.02	0.46
1:A:74:ARG:HH22	1:A:440:ASP:CG	2.18	0.46
1:B:421:PHE:CE2	1:B:422:VAL:HB	2.51	0.46
1:B:462:GLN:N	1:B:462:GLN:CD	2.69	0.46
1:D:120:HIS:C	1:D:120:HIS:CD2	2.87	0.46
1:D:70:TYR:CE2	1:D:201:VAL:HA	2.50	0.46
1:D:104:GLY:HA2	1:D:311:TYR:O	2.15	0.46
1:E:30:ARG:HD3	1:E:378:GLN:OE1	2.16	0.46
1:E:78:PRO:N	1:E:453:LYS:HG2	2.30	0.46
1:F:367:HIS:CG	1:F:368:VAL:N	2.83	0.46
1:A:196:GLU:H	1:A:199:ASP:CG	2.19	0.46
1:A:100:TRP:CE2	1:A:379:LEU:HD13	2.51	0.46
1:C:208:MET:HG3	1:C:210:PHE:CE1	2.50	0.46
1:C:424:SER:H	1:C:428:THR:HG21	1.79	0.46
1:E:34:PHE:HA	1:E:377:PHE:O	2.15	0.46
1:B:47:HIS:CG	1:B:48:PRO:HD2	2.50	0.46
1:C:123:TYR:CE2	1:C:263:ARG:NH1	2.84	0.46
1:C:73:PHE:HB3	1:C:450:VAL:HG21	1.96	0.46
1:D:169:TRP:H	1:D:208:MET:HA	1.80	0.46
1:D:389:MET:HA	1:D:392:ILE:HG12	1.98	0.46
1:D:97:ARG:HB3	1:D:403:TRP:CZ2	2.49	0.46
1:F:153:GLN:OE1	1:F:253:GLU:HA	2.15	0.46
1:A:61:ASP:O	1:F:423:GLN:HB3	2.15	0.46
1:B:70:TYR:CD1	1:B:201:VAL:HG12	2.51	0.46
1:B:74:ARG:HB2	1:B:447:PHE:CG	2.51	0.46
1:C:312:TRP:CH2	1:C:469:PHE:HA	2.50	0.46
1:E:248:PHE:CG	1:E:249:CYS:N	2.84	0.46
1:E:55:GLY:O	1:E:57:ASN:HA	2.14	0.46
1:F:419:TYR:CE1	1:F:420:ARG:CZ	2.99	0.46
1:F:422:VAL:HG11	1:F:428:THR:HA	1.96	0.46
1:C:41:ARG:HH21	1:C:370:GLU:HG3	1.81	0.46
1:D:48:PRO:HA	1:D:65:VAL:O	2.16	0.46
1:E:323:ILE:HG21	1:E:325:TRP:CZ3	2.51	0.46
1:F:385:THR:O	1:F:388:VAL:HG12	2.15	0.46
1:B:19:ALA:H	1:F:407:VAL:H	1.64	0.46
1:A:309:LYS:HB2	1:A:311:TYR:CE1	2.50	0.46
1:A:346:ALA:HB1	1:B:183:GLY:HA2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:O	1:A:34:PHE:CD1	2.69	0.46
1:B:91:TYR:CE2	1:B:97:ARG:HA	2.50	0.46
1:C:421:PHE:C	1:C:423:GLN:H	2.19	0.46
1:C:77:LEU:HD12	1:C:327:ASN:HA	1.97	0.46
1:D:172:GLY:H	1:D:188:LEU:HA	1.81	0.46
1:D:27:TYR:N	1:D:27:TYR:CD1	2.83	0.46
1:E:343:SER:HA	1:E:364:TYR:O	2.15	0.46
1:F:120:HIS:CE1	1:F:122:LEU:HB2	2.51	0.46
1:F:404:ASN:HB3	1:F:405:PHE:CD2	2.51	0.46
1:F:42:LEU:O	1:F:370:GLU:HA	2.16	0.46
1:A:107:ILE:HB	1:A:307:PHE:CE1	2.51	0.46
1:A:172:GLY:HA3	1:A:189:GLU:HB2	1.98	0.46
1:B:12:TYR:CE2	1:B:13:LEU:HD21	2.51	0.46
1:B:391:TYR:CE1	1:F:408:THR:HG23	2.50	0.46
1:B:47:HIS:CD2	1:B:48:PRO:HD2	2.51	0.46
1:C:153:GLN:HB3	1:C:254:GLN:HG2	1.98	0.46
1:C:33:ILE:O	1:C:378:GLN:HA	2.15	0.46
1:C:196:GLU:OE2	1:C:445:LEU:HA	2.15	0.46
1:D:375:PHE:HB2	1:D:377:PHE:CE2	2.51	0.46
1:D:460:LEU:HA	1:D:466:GLY:HA3	1.98	0.46
1:E:388:VAL:O	1:E:391:TYR:HB3	2.15	0.46
1:E:91:TYR:CD2	1:E:98:LEU:HD21	2.51	0.46
1:A:393:HIS:HA	1:A:400:LEU:HD12	1.98	0.45
1:B:157:CYS:SG	1:B:158:ILE:N	2.89	0.45
1:D:126:LEU:HB3	1:D:262:ASN:O	2.16	0.45
1:D:24:THR:HA	1:D:27:TYR:CZ	2.52	0.45
1:F:75:VAL:HG13	1:F:450:VAL:HB	1.98	0.45
1:A:252:ARG:HH22	1:A:254:GLN:HB3	1.82	0.45
1:B:448:TRP:CE2	1:B:449:PRO:HD2	2.50	0.45
1:C:36:HIS:CG	1:C:37:ALA:N	2.82	0.45
1:C:68:TYR:H	1:C:69:GLN:HG2	1.81	0.45
1:D:120:HIS:CE1	1:D:122:LEU:C	2.90	0.45
1:D:153:GLN:HB3	1:D:254:GLN:HB3	1.98	0.45
1:D:393:HIS:CG	1:D:394:ASN:N	2.84	0.45
1:E:139:ASP:CG	1:E:141:LYS:HZ1	2.19	0.45
1:E:32:SER:C	1:E:34:PHE:CE2	2.90	0.45
1:F:102:CYS:HA	1:F:377:PHE:CG	2.51	0.45
1:A:172:GLY:H	1:A:188:LEU:HA	1.81	0.45
1:A:47:HIS:HE1	1:A:50:PHE:CG	2.35	0.45
1:A:73:PHE:N	1:A:73:PHE:CD1	2.82	0.45
1:A:77:LEU:HG	1:A:327:ASN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ALA:HA	1:B:427:VAL:HG13	1.97	0.45
1:C:210:PHE:CD2	1:C:227:SER:O	2.69	0.45
1:E:109:ARG:HD3	1:E:110:GLY:N	2.32	0.45
1:E:167:GLU:HG2	1:E:231:TYR:O	2.16	0.45
1:E:98:LEU:HB3	1:E:379:LEU:HD21	1.98	0.45
1:F:68:TYR:C	1:F:201:VAL:HG13	2.37	0.45
1:B:78:PRO:HB2	1:B:100:TRP:HE1	1.81	0.45
1:C:43:LEU:HD11	1:C:368:VAL:HG12	1.99	0.45
1:C:80:PRO:HD3	1:C:100:TRP:HE1	1.81	0.45
1:D:170:THR:HG22	1:D:191:ILE:CG2	2.46	0.45
1:D:24:THR:HG21	1:D:320:ASN:HA	1.99	0.45
1:D:305:GLN:CD	1:D:307:PHE:H	2.20	0.45
1:A:330:PHE:CD2	1:A:330:PHE:N	2.81	0.45
1:A:398:THR:HA	1:A:401:GLU:OE1	2.17	0.45
1:B:117:LEU:HD21	1:C:260:PHE:CE1	2.52	0.45
1:B:43:LEU:HA	1:B:369:GLU:O	2.17	0.45
1:B:356:TYR:CE2	1:C:142:ASP:HB3	2.52	0.45
1:D:107:ILE:HB	1:D:308:ASN:H	1.82	0.45
1:A:43:LEU:O	1:F:419:TYR:HB2	2.15	0.45
1:B:273:GLU:HA	1:B:276:TYR:CE1	2.51	0.45
1:C:214:GLN:CD	1:C:219:GLU:H	2.20	0.45
1:C:391:TYR:O	1:C:395:MET:HB3	2.16	0.45
1:D:208:MET:HG2	1:D:210:PHE:CE1	2.51	0.45
1:C:362:LYS:HD2	1:D:268:GLY:HA2	1.98	0.45
1:E:35:TYR:O	1:E:376:ILE:HA	2.17	0.45
1:E:438:LYS:HG2	1:E:439:GLN:H	1.81	0.45
1:E:70:TYR:N	1:E:199:ASP:O	2.50	0.45
1:E:80:PRO:HG2	1:E:98:LEU:HB2	1.98	0.45
1:F:35:TYR:CD1	1:F:456:PHE:CD1	3.05	0.45
1:A:347:SER:HA	1:A:361:PHE:CD1	2.51	0.45
1:A:68:TYR:O	1:A:201:VAL:HG22	2.17	0.45
1:B:77:LEU:CD1	1:B:100:TRP:CD1	3.00	0.45
1:C:392:ILE:CG2	1:C:400:LEU:HD21	2.46	0.45
1:D:397:THR:HA	1:D:400:LEU:HD12	1.97	0.45
1:E:33:ILE:O	1:E:34:PHE:CD1	2.69	0.45
1:E:96:GLN:HA	1:E:382:ILE:O	2.16	0.45
1:E:402:ASP:HB2	1:E:403:TRP:CE3	2.52	0.45
1:E:36:HIS:CG	1:E:463:PHE:CG	3.05	0.45
1:F:436:PRO:HA	1:F:439:GLN:OE1	2.16	0.45
1:A:256:PHE:CE1	1:A:296:SER:HB3	2.51	0.45
1:A:27:TYR:N	1:A:27:TYR:CD1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:TRP:HB2	1:A:326:HIS:CE1	2.52	0.45
1:A:78:PRO:HD3	1:A:456:PHE:CZ	2.52	0.45
1:A:35:TYR:CE1	1:A:457:SER:N	2.84	0.45
1:A:460:LEU:HD12	1:A:470:LEU:HD21	1.99	0.45
1:C:242:TYR:OH	1:C:395:MET:HA	2.17	0.45
1:D:326:HIS:CE1	1:D:399:ILE:CG1	2.99	0.45
1:D:373:LEU:C	1:D:375:PHE:CZ	2.90	0.45
1:E:168:HIS:CB	1:E:207:ALA:HA	2.47	0.45
1:E:114:GLY:H	1:E:338:ARG:HA	1.82	0.45
1:F:47:HIS:HE1	1:F:49:TYR:HB2	1.79	0.45
1:A:367:HIS:CE1	1:A:368:VAL:O	2.69	0.45
1:A:464:PRO:O	1:A:468:LYS:HG3	2.15	0.45
1:B:172:GLY:HA2	1:B:189:GLU:HB2	1.99	0.45
1:B:24:THR:O	1:B:28:VAL:HG23	2.17	0.45
1:D:33:ILE:O	1:D:378:GLN:HA	2.17	0.45
1:D:100:TRP:CZ2	1:D:379:LEU:HD13	2.51	0.45
1:E:171:LYS:N	1:E:212:LEU:HD23	2.29	0.45
1:E:391:TYR:O	1:E:395:MET:SD	2.75	0.45
1:F:70:TYR:CG	1:F:201:VAL:HG12	2.51	0.45
1:F:209:ASP:CG	1:F:212:LEU:HG	2.37	0.45
1:F:43:LEU:HA	1:F:369:GLU:O	2.17	0.45
1:C:43:LEU:HG	1:C:369:GLU:O	2.17	0.45
1:C:73:PHE:CD1	1:C:73:PHE:N	2.85	0.45
1:D:356:TYR:CE1	1:D:361:PHE:CE2	3.05	0.45
1:D:442:TYR:HB3	1:D:445:LEU:HD12	1.99	0.45
1:E:447:PHE:N	1:E:447:PHE:CD2	2.84	0.45
1:A:121:PRO:HA	1:A:146:ASN:CA	2.46	0.44
1:B:387:GLU:N	1:B:387:GLU:CD	2.68	0.44
1:B:420:ARG:NH2	1:B:427:VAL:H	2.16	0.44
1:C:278:LYS:HZ2	1:C:278:LYS:H	1.66	0.44
1:D:272:PRO:HB2	1:D:275:LEU:HD13	1.99	0.44
1:D:329:LEU:HA	1:D:329:LEU:HD12	1.88	0.44
1:E:97:ARG:HG3	1:E:403:TRP:CD2	2.52	0.44
1:E:47:HIS:CE1	1:E:50:PHE:CZ	3.05	0.44
1:F:200:MET:HB3	1:F:229:CYS:SG	2.58	0.44
1:F:422:VAL:CG1	1:F:428:THR:HA	2.47	0.44
1:B:175:CYS:HB2	1:F:428:THR:HG21	1.98	0.44
1:A:23:SER:O	1:A:27:TYR:CE1	2.70	0.44
1:A:416:VAL:HB	1:F:41:ARG:HD2	2.00	0.44
1:B:172:GLY:CA	1:B:189:GLU:HB2	2.47	0.44
1:B:222:LEU:HD23	1:B:225:CYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LEU:C	1:B:43:LEU:HG	2.37	0.44
1:B:47:HIS:CE1	1:B:49:TYR:N	2.84	0.44
1:C:121:PRO:HA	1:C:146:ASN:HA	1.99	0.44
1:C:167:GLU:HG3	1:C:231:TYR:O	2.17	0.44
1:C:419:TYR:HA	1:C:421:PHE:HB3	1.99	0.44
1:C:47:HIS:CD2	1:C:48:PRO:N	2.86	0.44
1:D:35:TYR:CE1	1:D:457:SER:C	2.91	0.44
1:E:172:GLY:N	1:E:187:PRO:O	2.50	0.44
1:E:234:TYR:H	1:E:251:ARG:NH2	2.15	0.44
1:E:388:VAL:HG12	1:E:392:ILE:HD12	1.99	0.44
1:F:51:LYS:CE	1:F:61:ASP:HB2	2.48	0.44
1:A:69:GLN:HA	1:A:199:ASP:O	2.17	0.44
1:A:100:TRP:CD2	1:A:379:LEU:HD12	2.53	0.44
1:B:460:LEU:HA	1:B:463:PHE:HD2	1.83	0.44
1:C:176:LYS:HB2	1:C:177:PRO:HD2	1.98	0.44
1:C:125:LYS:HE2	1:C:261:TRP:CD1	2.52	0.44
1:C:99:VAL:HB	1:C:382:ILE:HD11	1.99	0.44
1:C:392:ILE:HG22	1:C:392:ILE:O	2.17	0.44
1:C:73:PHE:CE2	1:C:448:TRP:CB	3.00	0.44
1:C:91:TYR:CE2	1:C:98:LEU:HG	2.53	0.44
1:E:409:PRO:HB2	1:E:410:PRO:HD3	1.99	0.44
1:E:51:LYS:HG3	1:E:62:VAL:O	2.16	0.44
1:F:372:ASP:C	1:F:373:LEU:HD23	2.37	0.44
1:A:99:VAL:HG22	1:A:100:TRP:N	2.33	0.44
1:B:464:PRO:O	1:B:468:LYS:HG3	2.18	0.44
1:C:70:TYR:CD1	1:C:201:VAL:HG12	2.53	0.44
1:D:167:GLU:H	1:D:231:TYR:H	1.65	0.44
1:D:209:ASP:OD1	1:D:211:LYS:HD2	2.18	0.44
1:D:97:ARG:HG3	1:D:403:TRP:CE3	2.53	0.44
1:E:79:ASP:O	1:E:83:PHE:CD1	2.70	0.44
1:F:28:VAL:HG13	1:F:380:CYS:SG	2.57	0.44
1:F:396:ASN:OD1	1:F:398:THR:HG23	2.17	0.44
1:A:154:THR:H	1:A:336:THR:CG2	2.31	0.44
1:A:41:ARG:O	1:F:417:ASP:HB2	2.16	0.44
1:B:65:VAL:O	1:B:367:HIS:CD2	2.70	0.44
1:B:379:LEU:HD13	1:B:380:CYS:N	2.32	0.44
1:B:398:THR:O	1:B:402:ASP:CG	2.56	0.44
1:B:81:ASN:HD21	1:B:403:TRP:HE1	1.66	0.44
1:B:76:LYS:HD2	1:B:76:LYS:N	2.33	0.44
1:C:45:VAL:HA	1:C:367:HIS:O	2.18	0.44
1:D:120:HIS:CD2	1:D:121:PRO:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:PHE:CD1	1:D:260:PHE:N	2.85	0.44
1:A:385:THR:O	1:A:389:MET:N	2.50	0.44
1:B:48:PRO:HA	1:B:65:VAL:O	2.18	0.44
1:C:454:GLU:CD	1:C:454:GLU:N	2.71	0.44
1:C:460:LEU:HB2	1:C:470:LEU:HD11	2.00	0.44
1:D:169:TRP:CH2	1:D:189:GLU:C	2.91	0.44
1:D:25:ASP:HA	1:D:28:VAL:HB	1.98	0.44
1:D:300:VAL:HG12	1:D:301:THR:N	2.33	0.44
1:E:169:TRP:HB2	1:E:207:ALA:O	2.16	0.44
1:E:259:HIS:H	1:E:294:SER:CB	2.30	0.44
1:E:379:LEU:HG	1:E:380:CYS:N	2.32	0.44
1:F:156:LEU:HD12	1:F:157:CYS:CA	2.47	0.44
1:F:167:GLU:N	1:F:231:TYR:O	2.50	0.44
1:F:29:THR:HB	1:F:381:LYS:HB2	1.99	0.44
1:F:391:TYR:O	1:F:395:MET:N	2.50	0.44
1:A:43:LEU:HB3	1:F:418:THR:HA	1.98	0.44
1:A:133:HIS:CE1	1:A:134:VAL:HG12	2.52	0.44
1:B:120:HIS:CG	1:B:123:TYR:CE1	3.06	0.44
1:B:20:LYS:HG2	1:B:21:VAL:H	1.82	0.44
1:B:248:PHE:CZ	1:B:250:LEU:CB	3.01	0.44
1:B:360:SER:HB2	1:B:361:PHE:CE2	2.53	0.44
1:B:384:LEU:H	1:B:384:LEU:HG	1.55	0.44
1:B:430:GLN:NE2	1:B:430:GLN:HA	2.33	0.44
1:B:70:TYR:CZ	1:B:201:VAL:HA	2.53	0.44
1:B:69:GLN:O	1:B:71:ARG:HD2	2.18	0.44
1:C:26:GLU:HB2	1:C:27:TYR:CD1	2.52	0.44
1:C:37:ALA:HA	1:C:455:ARG:O	2.17	0.44
1:C:97:ARG:HD2	1:C:403:TRP:CD1	2.52	0.44
1:C:419:TYR:HA	1:C:421:PHE:CB	2.48	0.44
1:D:259:HIS:O	1:D:294:SER:N	2.51	0.44
1:D:356:TYR:CE2	1:D:358:PRO:HA	2.52	0.44
1:D:346:ALA:HB3	1:D:364:TYR:HE1	1.81	0.44
1:D:30:ARG:HA	1:D:380:CYS:SG	2.58	0.44
1:D:326:HIS:CE1	1:D:399:ILE:HG13	2.52	0.44
1:D:39:SER:O	1:D:372:ASP:CG	2.55	0.44
1:D:451:ASP:OD2	1:D:453:LYS:HG3	2.18	0.44
1:E:120:HIS:CD2	1:E:122:LEU:H	2.35	0.44
1:F:323:ILE:HB	1:F:325:TRP:CZ2	2.52	0.44
1:C:101:ALA:HA	1:C:324:CYS:SG	2.58	0.44
1:D:121:PRO:HD2	1:D:222:LEU:HD11	2.00	0.44
1:D:263:ARG:H	1:D:290:LEU:HG	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:ASN:CG	1:D:323:ILE:HD12	2.39	0.44
1:D:441:PRO:HD2	1:D:442:TYR:CE2	2.53	0.44
1:D:91:TYR:CE2	1:D:98:LEU:HD21	2.53	0.44
1:D:461:ASP:CG	1:E:20:LYS:HZ2	2.21	0.44
1:F:120:HIS:HA	1:F:222:LEU:HG	1.98	0.44
1:A:469:PHE:C	1:A:469:PHE:CD2	2.91	0.44
1:B:70:TYR:CE1	1:B:201:VAL:HG12	2.53	0.44
1:B:454:GLU:CD	1:B:454:GLU:N	2.72	0.44
1:B:97:ARG:NH1	1:B:97:ARG:HG2	2.33	0.44
1:D:77:LEU:HG	1:D:327:ASN:O	2.17	0.44
1:D:472:GLN:C	1:D:472:GLN:CD	2.77	0.44
1:D:83:PHE:CE1	1:D:85:LEU:HB2	2.52	0.44
1:E:78:PRO:HB3	1:E:83:PHE:CZ	2.53	0.44
1:F:312:TRP:HD1	1:F:314:HIS:HE2	1.66	0.44
1:C:278:LYS:NZ	1:C:278:LYS:H	2.15	0.43
1:C:422:VAL:HG22	1:C:431:LYS:HE2	2.00	0.43
1:D:254:GLN:HE21	1:D:254:GLN:C	2.22	0.43
1:E:124:ASN:HA	1:E:144:ARG:HB3	1.99	0.43
1:F:128:ASP:HA	1:F:261:TRP:HA	1.99	0.43
1:F:79:ASP:CG	1:F:81:ASN:H	2.21	0.43
1:A:231:TYR:CD1	1:A:232:PRO:HD2	2.53	0.43
1:A:46:GLY:N	1:A:65:VAL:HB	2.32	0.43
1:A:47:HIS:CE1	1:A:50:PHE:CG	3.07	0.43
1:B:41:ARG:HH22	1:C:233:ASP:CG	2.21	0.43
1:C:91:TYR:CD2	1:C:93:PRO:HA	2.53	0.43
1:C:97:ARG:HG2	1:C:97:ARG:HH11	1.82	0.43
1:D:312:TRP:CE2	1:D:472:GLN:HG3	2.53	0.43
1:E:273:GLU:N	1:E:273:GLU:CD	2.71	0.43
1:E:325:TRP:C	1:E:326:HIS:CD2	2.91	0.43
1:F:161:CYS:HA	1:F:329:LEU:HA	2.00	0.43
1:F:102:CYS:HB2	1:F:377:PHE:CZ	2.53	0.43
1:A:425:ALA:HB3	1:F:60:GLN:H	1.82	0.43
1:F:68:TYR:CD2	1:F:68:TYR:N	2.86	0.43
1:F:71:ARG:HE	1:F:71:ARG:HA	1.83	0.43
1:A:70:TYR:HB2	1:A:199:ASP:HB2	2.00	0.43
1:A:469:PHE:O	1:A:472:GLN:HB3	2.18	0.43
1:A:80:PRO:CG	1:A:379:LEU:HD11	2.48	0.43
1:B:46:GLY:HA3	1:B:63:PRO:HG2	2.01	0.43
1:C:119:GLY:O	1:C:222:LEU:HG	2.18	0.43
1:C:259:HIS:HB2	1:C:261:TRP:CZ2	2.53	0.43
1:D:160:GLY:HA2	1:D:247:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:TRP:CE2	1:D:449:PRO:HD2	2.53	0.43
1:E:119:GLY:O	1:E:120:HIS:HB2	2.18	0.43
1:F:305:GLN:OE1	1:F:307:PHE:CD2	2.72	0.43
1:A:382:ILE:N	1:A:382:ILE:HD12	2.34	0.43
1:B:27:TYR:N	1:B:27:TYR:CD1	2.84	0.43
1:D:345:CYS:SG	1:D:361:PHE:HB3	2.58	0.43
1:D:357:THR:HB	1:D:359:THR:HG1	1.83	0.43
1:D:447:PHE:N	1:D:447:PHE:CD2	2.85	0.43
1:E:312:TRP:CZ3	1:E:469:PHE:HB2	2.53	0.43
1:A:234:TYR:CD2	1:A:234:TYR:N	2.82	0.43
1:C:155:GLN:HA	1:C:335:ASP:HA	1.99	0.43
1:D:267:MET:SD	1:D:288:SER:HA	2.59	0.43
1:E:155:GLN:HE22	1:E:305:GLN:NE2	2.16	0.43
1:F:341:ASN:HD21	1:F:367:HIS:CD2	2.36	0.43
1:A:448:TRP:CH2	1:F:419:TYR:CE1	3.07	0.43
1:A:124:ASN:HA	1:A:144:ARG:CB	2.48	0.43
1:A:356:TYR:CZ	1:A:361:PHE:CD2	3.07	0.43
1:C:272:PRO:HG2	1:C:275:LEU:HD23	2.01	0.43
1:C:113:LEU:HD22	1:C:337:THR:HB	2.01	0.43
1:D:162:VAL:HG21	1:D:244:ASP:CB	2.49	0.43
1:D:373:LEU:HB2	1:D:375:PHE:CZ	2.53	0.43
1:D:460:LEU:CB	1:D:470:LEU:HD11	2.48	0.43
1:F:201:VAL:C	1:F:229:CYS:HG	2.21	0.43
1:F:27:TYR:CD2	1:F:27:TYR:C	2.92	0.43
1:F:36:HIS:NE2	1:F:463:PHE:CD1	2.86	0.43
1:F:392:ILE:HG22	1:F:400:LEU:HD11	2.00	0.43
1:B:130:GLU:CD	1:B:260:PHE:H	2.21	0.43
1:A:112:PRO:HB3	1:B:231:TYR:CE1	2.53	0.43
1:B:341:ASN:HD21	1:B:367:HIS:CE1	2.36	0.43
1:B:389:MET:O	1:B:393:HIS:HB3	2.19	0.43
1:B:441:PRO:HD2	1:B:442:TYR:CD1	2.54	0.43
1:B:73:PHE:CE2	1:B:448:TRP:CB	3.01	0.43
1:C:452:LEU:O	1:C:456:PHE:CD1	2.71	0.43
1:C:466:GLY:O	1:C:469:PHE:HB3	2.18	0.43
1:C:47:HIS:CE1	1:C:49:TYR:N	2.83	0.43
1:F:210:PHE:HB2	1:F:211:LYS:HZ3	1.84	0.43
1:F:347:SER:HA	1:F:361:PHE:CD1	2.53	0.43
1:A:262:ASN:HA	1:A:291:TYR:HA	2.01	0.43
1:A:47:HIS:CE1	1:A:49:TYR:CB	3.01	0.43
1:C:248:PHE:C	1:C:248:PHE:CD2	2.92	0.43
1:C:256:PHE:CZ	1:C:296:SER:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ARG:HB2	1:C:447:PHE:CG	2.53	0.43
1:D:111:GLN:HB3	1:D:112:PRO:HD2	2.01	0.43
1:D:167:GLU:OE2	1:D:190:LEU:HG	2.18	0.43
1:D:375:PHE:HB2	1:D:377:PHE:CZ	2.54	0.43
1:E:162:VAL:HB	1:E:245:SER:HB3	2.00	0.43
1:E:45:VAL:HG22	1:E:368:VAL:HA	2.01	0.43
1:E:36:HIS:HB3	1:E:457:SER:HB2	2.00	0.43
1:F:186:PRO:HG2	1:F:188:LEU:HD21	2.00	0.43
1:F:438:LYS:O	1:F:442:TYR:CD2	2.72	0.43
1:F:469:PHE:CZ	1:F:473:LEU:HD21	2.54	0.43
1:A:164:ALA:O	1:A:195:ILE:N	2.51	0.43
1:C:47:HIS:O	1:C:64:LYS:HG3	2.19	0.43
1:D:312:TRP:HB2	1:D:314:HIS:CE1	2.54	0.43
1:D:395:MET:SD	1:D:395:MET:N	2.92	0.43
1:D:47:HIS:NE2	1:D:49:TYR:CD2	2.84	0.43
1:E:210:PHE:N	1:E:210:PHE:CD2	2.86	0.43
1:E:324:CYS:SG	1:E:324:CYS:O	2.77	0.43
1:A:144:ARG:CZ	1:E:356:TYR:HB2	2.48	0.43
1:E:469:PHE:C	1:E:469:PHE:CD2	2.92	0.43
1:A:180:VAL:HG22	1:A:181:VAL:N	2.33	0.43
1:A:208:MET:SD	1:A:208:MET:C	2.97	0.43
1:A:220:VAL:HB	1:A:224:ILE:HD11	2.01	0.43
1:A:96:GLN:HG2	1:A:96:GLN:H	1.54	0.43
1:C:199:ASP:OD1	1:C:446:LYS:NZ	2.50	0.43
1:D:157:CYS:SG	1:D:158:ILE:N	2.91	0.43
1:D:444:LYS:HG3	1:D:445:LEU:HG	2.00	0.43
1:D:78:PRO:N	1:D:453:LYS:HG2	2.34	0.43
1:E:167:GLU:CD	1:E:233:ASP:HB2	2.39	0.43
1:E:324:CYS:SG	1:E:327:ASN:HA	2.59	0.43
1:E:48:PRO:HD3	1:E:341:ASN:OD1	2.19	0.43
1:F:69:GLN:HA	1:F:199:ASP:O	2.18	0.43
1:F:472:GLN:CD	1:F:472:GLN:C	2.78	0.43
1:A:32:SER:C	1:A:34:PHE:CE2	2.92	0.42
1:A:76:LYS:HB3	1:A:451:ASP:HA	2.01	0.42
1:B:154:THR:H	1:B:336:THR:CG2	2.32	0.42
1:B:73:PHE:CD1	1:B:73:PHE:N	2.84	0.42
1:C:169:TRP:CZ3	1:C:190:LEU:HB2	2.54	0.42
1:C:464:PRO:O	1:C:468:LYS:HG3	2.19	0.42
1:F:34:PHE:HA	1:F:377:PHE:O	2.19	0.42
1:F:73:PHE:CD1	1:F:73:PHE:N	2.84	0.42
1:A:234:TYR:O	1:A:238:SER:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:THR:C	1:B:341:ASN:HD22	2.21	0.42
1:B:369:GLU:OE2	1:B:371:PHE:CE2	2.73	0.42
1:B:47:HIS:CE1	1:B:50:PHE:CD1	3.07	0.42
1:B:300:VAL:HB	1:C:255:VAL:HG13	2.02	0.42
1:B:299:VAL:HG23	1:C:256:PHE:HB3	1.99	0.42
1:B:142:ASP:CG	1:C:283:ARG:HE	2.22	0.42
1:C:392:ILE:O	1:C:396:ASN:N	2.51	0.42
1:C:441:PRO:HG2	1:C:442:TYR:CE2	2.55	0.42
1:C:36:HIS:CE1	1:C:463:PHE:CE1	3.06	0.42
1:C:47:HIS:HB3	1:C:50:PHE:O	2.20	0.42
1:D:157:CYS:SG	1:D:331:LEU:HD11	2.59	0.42
1:D:271:LEU:HD11	1:D:276:TYR:CD1	2.54	0.42
1:B:356:TYR:CD1	1:D:277:ILE:HD12	2.54	0.42
1:E:150:ASP:HA	1:E:151:TYR:CZ	2.54	0.42
1:F:111:GLN:HB3	1:F:112:PRO:HD2	2.02	0.42
1:A:34:PHE:HA	1:A:377:PHE:O	2.19	0.42
1:A:47:HIS:CE1	1:A:50:PHE:CE1	3.07	0.42
1:B:32:SER:O	1:B:34:PHE:CD2	2.72	0.42
1:B:467:ARG:O	1:B:471:LEU:HG	2.19	0.42
1:B:68:TYR:CD2	1:B:68:TYR:N	2.87	0.42
1:C:460:LEU:CB	1:C:470:LEU:HD11	2.50	0.42
1:C:76:LYS:HA	1:C:327:ASN:O	2.20	0.42
1:D:448:TRP:HA	1:D:449:PRO:HD2	1.85	0.42
1:D:91:TYR:CE1	1:D:93:PRO:HB3	2.54	0.42
1:E:440:ASP:CB	1:E:442:TYR:H	2.32	0.42
1:F:79:ASP:HA	1:F:327:ASN:ND2	2.34	0.42
1:F:399:ILE:H	1:F:399:ILE:CD1	2.28	0.42
1:A:149:VAL:HG22	1:A:150:ASP:N	2.34	0.42
1:A:183:GLY:HA2	1:E:346:ALA:HB1	2.01	0.42
1:A:26:GLU:C	1:A:27:TYR:CD1	2.93	0.42
1:A:319:LEU:HD22	1:A:319:LEU:N	2.35	0.42
1:A:328:GLN:HB3	1:A:330:PHE:CE2	2.53	0.42
1:A:460:LEU:H	1:A:460:LEU:HG	1.47	0.42
1:B:167:GLU:HA	1:B:192:ASN:HA	2.01	0.42
1:B:97:ARG:HG3	1:B:403:TRP:CD2	2.55	0.42
1:B:312:TRP:CH2	1:B:469:PHE:HA	2.54	0.42
1:C:91:TYR:CE1	1:C:93:PRO:HB3	2.54	0.42
1:E:26:GLU:CD	1:E:26:GLU:N	2.72	0.42
1:E:105:VAL:HG22	1:E:375:PHE:CD1	2.54	0.42
1:E:385:THR:N	1:E:389:MET:SD	2.92	0.42
1:E:46:GLY:O	1:E:367:HIS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:CYS:SG	1:F:376:ILE:O	2.77	0.42
1:A:209:ASP:C	1:A:213:LEU:HD12	2.40	0.42
1:B:158:ILE:HG12	1:B:249:CYS:HA	2.00	0.42
1:C:36:HIS:HA	1:C:375:PHE:O	2.20	0.42
1:D:197:ASP:HB2	1:D:447:PHE:HA	2.02	0.42
1:D:43:LEU:HD11	1:D:368:VAL:CG2	2.50	0.42
1:E:398:THR:HA	1:E:401:GLU:HB3	2.01	0.42
1:F:107:ILE:N	1:F:107:ILE:HD12	2.31	0.42
1:F:68:TYR:HB3	1:F:201:VAL:HG22	2.02	0.42
1:F:54:LYS:HG3	1:F:61:ASP:HA	2.02	0.42
1:A:108:GLY:N	1:A:372:ASP:O	2.52	0.42
1:A:33:ILE:HD13	1:A:33:ILE:N	2.35	0.42
1:A:370:GLU:O	1:A:371:PHE:CD2	2.73	0.42
1:A:400:LEU:O	1:A:404:ASN:N	2.53	0.42
1:A:76:LYS:HA	1:A:327:ASN:O	2.19	0.42
1:B:97:ARG:CB	1:B:403:TRP:CD2	3.02	0.42
1:B:421:PHE:CZ	1:B:422:VAL:HG12	2.55	0.42
1:B:467:ARG:HA	1:B:470:LEU:HD12	2.00	0.42
1:B:97:ARG:HB2	1:B:403:TRP:CZ3	2.54	0.42
1:C:74:ARG:HD2	1:C:447:PHE:CD2	2.54	0.42
1:E:169:TRP:NE1	1:E:190:LEU:HD13	2.34	0.42
1:E:231:TYR:CE1	1:E:232:PRO:HD2	2.54	0.42
1:E:464:PRO:HA	1:E:467:ARG:NE	2.35	0.42
1:E:68:TYR:N	1:E:68:TYR:CD2	2.88	0.42
1:E:70:TYR:C	1:E:71:ARG:HE	2.23	0.42
1:F:460:LEU:HB2	1:F:470:LEU:HD11	2.02	0.42
1:A:312:TRP:CH2	1:A:469:PHE:HA	2.53	0.42
1:A:75:VAL:HA	1:A:450:VAL:HB	2.02	0.42
1:B:36:HIS:CG	1:B:37:ALA:N	2.85	0.42
1:B:76:LYS:HG3	1:B:328:GLN:NE2	2.34	0.42
1:C:23:SER:O	1:C:27:TYR:CE1	2.73	0.42
1:C:48:PRO:HB3	1:C:341:ASN:HD21	1.84	0.42
1:E:25:ASP:N	1:E:26:GLU:OE1	2.52	0.42
1:E:70:TYR:CE2	1:E:201:VAL:HA	2.54	0.42
1:F:462:GLN:HB2	1:F:463:PHE:CE2	2.55	0.42
1:A:56:GLY:O	1:A:60:GLN:HB2	2.19	0.42
1:C:100:TRP:CE3	1:C:456:PHE:CE2	3.07	0.42
1:C:47:HIS:CD2	1:C:48:PRO:CD	3.02	0.42
1:D:155:GLN:HB2	1:D:252:ARG:HB3	2.01	0.42
1:D:373:LEU:HB2	1:D:375:PHE:CE1	2.55	0.42
1:E:68:TYR:CA	1:E:201:VAL:HG22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:PHE:CZ	1:E:249:CYS:O	2.73	0.42
1:E:43:LEU:HD12	1:E:369:GLU:O	2.20	0.42
1:E:453:LYS:HG3	1:E:453:LYS:H	1.69	0.42
1:E:461:ASP:HA	1:E:467:ARG:HG3	2.01	0.42
1:F:404:ASN:HB3	1:F:405:PHE:CG	2.55	0.42
1:F:96:GLN:HA	1:F:382:ILE:O	2.20	0.42
1:C:168:HIS:HD1	1:C:230:LYS:HA	1.84	0.42
1:B:364:TYR:CE2	1:C:185:CYS:HB2	2.55	0.42
1:C:248:PHE:CE2	1:C:250:LEU:HB2	2.54	0.42
1:C:271:LEU:HA	1:C:272:PRO:HD2	1.94	0.42
1:C:43:LEU:HD11	1:C:368:VAL:HG13	2.02	0.42
1:D:186:PRO:HA	1:D:187:PRO:HD3	1.87	0.42
1:E:438:LYS:CG	1:E:439:GLN:H	2.33	0.42
1:E:441:PRO:O	1:E:444:LYS:HG2	2.18	0.42
1:F:325:TRP:C	1:F:326:HIS:CG	2.92	0.42
1:A:158:ILE:HB	1:A:332:THR:HB	2.02	0.42
1:A:360:SER:HG	1:A:361:PHE:HE2	1.67	0.42
1:B:205:TYR:CE2	1:B:295:PRO:HG3	2.55	0.42
1:C:196:GLU:CD	1:C:446:LYS:H	2.22	0.42
1:E:157:CYS:SG	1:E:248:PHE:CE2	3.13	0.42
1:E:168:HIS:CE1	1:E:193:THR:HB	2.55	0.42
1:E:210:PHE:HB2	1:E:211:LYS:HD3	2.01	0.42
1:D:301:THR:HA	1:E:254:GLN:HA	2.01	0.42
1:E:374:GLN:OE1	1:E:463:PHE:HB3	2.19	0.42
1:E:197:ASP:CB	1:E:447:PHE:HA	2.47	0.42
1:F:216:ASN:HB2	1:F:218:SER:HB2	2.02	0.42
1:F:259:HIS:C	1:F:260:PHE:CD1	2.94	0.42
1:F:100:TRP:CE3	1:F:377:PHE:HB3	2.55	0.42
1:A:320:ASN:HD21	1:A:323:ILE:H	1.68	0.41
1:A:404:ASN:C	1:A:405:PHE:CG	2.94	0.41
1:C:128:ASP:HA	1:C:261:TRP:CD1	2.55	0.41
1:C:391:TYR:CE1	1:C:395:MET:SD	3.13	0.41
1:D:24:THR:O	1:D:27:TYR:CG	2.73	0.41
1:D:459:ASP:O	1:D:463:PHE:CD2	2.74	0.41
1:E:248:PHE:CE2	1:E:250:LEU:HB2	2.55	0.41
1:E:71:ARG:O	1:E:332:THR:HA	2.20	0.41
1:A:420:ARG:HB3	1:F:43:LEU:HD12	2.01	0.41
1:A:22:VAL:H	1:A:22:VAL:HG23	1.46	0.41
1:A:347:SER:HB3	1:A:361:PHE:HE1	1.84	0.41
1:C:38:GLY:HA3	1:C:374:GLN:HA	2.02	0.41
1:C:392:ILE:HA	1:C:395:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:ASP:CG	1:D:241:ALA:N	2.73	0.41
1:E:196:GLU:OE1	1:E:446:LYS:N	2.53	0.41
1:E:96:GLN:HG2	1:E:383:THR:HA	2.01	0.41
1:E:79:ASP:OD2	1:E:81:ASN:HB2	2.21	0.41
1:F:35:TYR:CZ	1:F:458:ALA:HA	2.54	0.41
1:A:160:GLY:HA3	1:A:245:SER:O	2.20	0.41
1:A:160:GLY:HA3	1:A:246:MET:HA	2.02	0.41
1:B:125:LYS:HA	1:B:263:ARG:CZ	2.51	0.41
1:B:49:TYR:HA	1:B:223:ASP:OD2	2.20	0.41
1:B:276:TYR:N	1:B:276:TYR:CD1	2.89	0.41
1:B:84:GLY:O	1:B:86:PRO:HD3	2.21	0.41
1:C:105:VAL:HG13	1:C:375:PHE:CD1	2.55	0.41
1:C:124:ASN:HA	1:C:144:ARG:HA	2.03	0.41
1:C:259:HIS:CB	1:C:261:TRP:CZ2	3.03	0.41
1:D:48:PRO:HB2	1:D:49:TYR:CZ	2.54	0.41
1:F:121:PRO:HA	1:F:146:ASN:CA	2.51	0.41
1:F:261:TRP:CD2	1:F:261:TRP:N	2.88	0.41
1:F:386:THR:HA	1:F:389:MET:CE	2.49	0.41
1:F:388:VAL:O	1:F:392:ILE:HG12	2.20	0.41
1:F:47:HIS:CD2	1:F:365:ALA:O	2.73	0.41
1:A:329:LEU:HD23	1:A:330:PHE:H	1.86	0.41
1:A:335:ASP:CG	1:A:337:THR:H	2.24	0.41
1:A:461:ASP:OD1	1:A:462:GLN:HG2	2.20	0.41
1:B:309:LYS:O	1:B:311:TYR:CE2	2.73	0.41
1:B:389:MET:HA	1:B:392:ILE:HD12	2.01	0.41
1:C:105:VAL:HG13	1:C:375:PHE:HE1	1.83	0.41
1:C:313:LEU:C	1:C:314:HIS:CG	2.93	0.41
1:C:40:SER:H	1:C:455:ARG:HH12	1.67	0.41
1:D:209:ASP:OD1	1:D:209:ASP:C	2.59	0.41
1:D:28:VAL:HA	1:D:382:ILE:HG12	2.01	0.41
1:D:422:VAL:HG23	1:D:423:GLN:OE1	2.21	0.41
1:D:57:ASN:C	1:D:59:ARG:HA	2.41	0.41
1:E:156:LEU:O	1:E:333:VAL:HG23	2.20	0.41
1:E:360:SER:HB2	1:E:361:PHE:CE2	2.56	0.41
1:E:408:THR:N	1:E:409:PRO:HD2	2.35	0.41
1:F:392:ILE:HA	1:F:395:MET:CB	2.51	0.41
1:F:441:PRO:HG2	1:F:442:TYR:CD1	2.55	0.41
1:A:447:PHE:N	1:A:447:PHE:CD2	2.86	0.41
1:A:47:HIS:CE1	1:A:49:TYR:C	2.93	0.41
1:D:32:SER:C	1:D:34:PHE:CE2	2.94	0.41
1:D:388:VAL:O	1:D:392:ILE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:GLY:O	1:E:205:TYR:CD1	2.73	0.41
1:E:109:ARG:HG3	1:E:307:PHE:CD2	2.56	0.41
1:E:440:ASP:HB3	1:E:442:TYR:H	1.86	0.41
1:E:81:ASN:HA	1:E:98:LEU:HD12	2.02	0.41
1:F:169:TRP:CE3	1:F:170:THR:N	2.89	0.41
1:F:77:LEU:HG	1:F:327:ASN:O	2.20	0.41
1:A:130:GLU:CD	1:A:260:PHE:H	2.24	0.41
1:A:97:ARG:O	1:A:382:ILE:HD12	2.20	0.41
1:A:451:ASP:CG	1:A:452:LEU:N	2.74	0.41
1:B:210:PHE:CD2	1:B:227:SER:O	2.73	0.41
1:B:102:CYS:HA	1:B:377:PHE:CD1	2.55	0.41
1:B:37:ALA:O	1:B:375:PHE:N	2.54	0.41
1:C:256:PHE:N	1:C:256:PHE:CD1	2.89	0.41
1:C:347:SER:HB3	1:C:361:PHE:CE1	2.56	0.41
1:C:462:GLN:C	1:C:467:ARG:HH21	2.23	0.41
1:D:100:TRP:CZ3	1:D:377:PHE:CB	3.03	0.41
1:D:391:TYR:CZ	1:D:395:MET:HE1	2.55	0.41
1:E:170:THR:CG2	1:E:189:GLU:HB2	2.50	0.41
1:A:266:THR:O	1:E:363:GLU:HG2	2.21	0.41
1:E:462:GLN:HB2	1:E:463:PHE:CZ	2.56	0.41
1:E:91:TYR:CE2	1:E:93:PRO:HA	2.54	0.41
1:F:211:LYS:H	1:F:211:LYS:HD3	1.85	0.41
1:F:419:TYR:HB3	1:F:420:ARG:H	1.73	0.41
1:A:141:LYS:HB2	1:E:357:THR:HA	2.03	0.41
1:B:202:ASP:CG	1:B:204:GLY:H	2.24	0.41
1:B:261:TRP:N	1:B:261:TRP:CD2	2.88	0.41
1:B:396:ASN:HD21	1:B:398:THR:CB	2.32	0.41
1:B:451:ASP:CG	1:B:453:LYS:H	2.24	0.41
1:B:51:LYS:HE2	1:B:53:PRO:HA	2.02	0.41
1:B:91:TYR:CG	1:B:92:ASP:N	2.87	0.41
1:C:232:PRO:HB2	1:C:234:TYR:CE1	2.56	0.41
1:C:325:TRP:HB2	1:C:326:HIS:NE2	2.35	0.41
1:D:118:SER:O	1:D:148:SER:HA	2.20	0.41
1:D:312:TRP:CH2	1:D:469:PHE:HA	2.55	0.41
1:E:243:GLY:HA3	1:E:318:GLY:HA3	2.02	0.41
1:F:36:HIS:CG	1:F:463:PHE:CD1	3.09	0.41
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.93	0.41
1:B:448:TRP:C	1:B:448:TRP:CD1	2.94	0.41
1:D:222:LEU:HD23	1:D:222:LEU:HA	1.91	0.41
1:D:275:LEU:N	1:D:275:LEU:CD1	2.83	0.41
1:D:459:ASP:O	1:D:463:PHE:CE2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:LEU:HD13	1:E:144:ARG:CZ	2.51	0.41
1:E:392:ILE:HA	1:E:395:MET:CE	2.51	0.41
1:E:419:TYR:HA	1:E:421:PHE:CE1	2.55	0.41
1:E:68:TYR:HA	1:E:201:VAL:HG22	2.03	0.41
1:F:120:HIS:O	1:F:123:TYR:HB2	2.20	0.41
1:F:18:VAL:HG13	1:F:19:ALA:H	1.86	0.41
1:F:160:GLY:HA3	1:F:246:MET:HA	2.03	0.41
1:F:361:PHE:N	1:F:361:PHE:CD2	2.88	0.41
1:A:40:SER:H	1:A:455:ARG:NH1	2.18	0.41
1:B:390:SER:HA	1:B:393:HIS:HB3	2.02	0.41
1:B:91:TYR:CD2	1:B:96:GLN:O	2.73	0.41
1:C:70:TYR:CG	1:C:201:VAL:HG12	2.56	0.41
1:D:150:ASP:CG	1:D:151:TYR:H	2.24	0.41
1:E:461:ASP:C	1:E:463:PHE:H	2.23	0.41
1:F:122:LEU:O	1:F:144:ARG:HB2	2.20	0.41
1:F:77:LEU:CA	1:F:453:LYS:HG2	2.50	0.41
1:A:152:LYS:HA	1:A:297:GLY:HA2	2.02	0.41
1:B:107:ILE:HB	1:B:307:PHE:CD2	2.55	0.41
1:B:35:TYR:CB	1:B:377:PHE:H	2.32	0.41
1:C:30:ARG:HH12	1:C:378:GLN:CD	2.24	0.41
1:C:396:ASN:OD1	1:C:398:THR:HG23	2.19	0.41
1:C:441:PRO:C	1:C:443:ASP:H	2.24	0.41
1:C:77:LEU:HD13	1:C:100:TRP:CD1	2.56	0.41
1:D:123:TYR:O	1:D:144:ARG:HA	2.20	0.41
1:D:392:ILE:HA	1:D:395:MET:SD	2.61	0.41
1:E:234:TYR:CE1	1:E:249:CYS:SG	3.13	0.41
1:E:267:MET:HG2	1:E:267:MET:H	1.65	0.41
1:E:319:LEU:H	1:E:319:LEU:HG	1.58	0.41
1:E:396:ASN:O	1:E:399:ILE:HD12	2.21	0.41
1:E:46:GLY:N	1:E:65:VAL:HB	2.36	0.41
1:F:233:ASP:O	1:F:237:MET:SD	2.78	0.41
1:F:252:ARG:C	1:F:252:ARG:HE	2.24	0.41
1:F:393:HIS:HA	1:F:400:LEU:HD12	2.02	0.41
1:A:109:ARG:C	1:A:109:ARG:CD	2.90	0.41
1:A:148:SER:HB3	1:B:291:TYR:CD1	2.56	0.41
1:A:233:ASP:OD1	1:A:235:LEU:HG	2.21	0.41
1:A:273:GLU:O	1:A:276:TYR:CD1	2.74	0.41
1:B:312:TRP:HB2	1:B:314:HIS:NE2	2.36	0.41
1:C:325:TRP:HB2	1:C:326:HIS:CE1	2.55	0.41
1:C:361:PHE:HB3	1:C:363:GLU:OE1	2.21	0.41
1:D:398:THR:O	1:D:402:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:TYR:CE1	1:E:112:PRO:HB3	2.56	0.41
1:E:23:SER:O	1:E:26:GLU:HB2	2.20	0.41
1:E:36:HIS:HA	1:E:375:PHE:O	2.20	0.41
1:E:97:ARG:CB	1:E:382:ILE:HD12	2.49	0.41
1:E:451:ASP:OD1	1:E:453:LYS:HG3	2.20	0.41
1:A:240:ASP:CG	1:A:244:ASP:H	2.25	0.40
1:A:45:VAL:HA	1:A:367:HIS:O	2.21	0.40
1:A:469:PHE:HA	1:A:472:GLN:HB3	2.03	0.40
1:A:71:ARG:C	1:A:73:PHE:CE1	2.94	0.40
1:B:155:GLN:OE1	1:B:306:LEU:HG	2.21	0.40
1:B:13:LEU:HB2	1:B:393:HIS:ND1	2.36	0.40
1:B:65:VAL:HG12	1:B:367:HIS:CG	2.56	0.40
1:B:93:PRO:O	1:B:97:ARG:NH1	2.52	0.40
1:C:202:ASP:HA	1:C:206:GLY:HA3	2.03	0.40
1:C:208:MET:CB	1:C:213:LEU:HD21	2.51	0.40
1:D:138:VAL:HG13	1:D:141:LYS:HG2	2.04	0.40
1:D:231:TYR:CG	1:D:232:PRO:CD	3.05	0.40
1:D:289:TYR:HA	1:D:291:TYR:CZ	2.56	0.40
1:D:43:LEU:HD11	1:D:368:VAL:HG22	2.03	0.40
1:E:169:TRP:CB	1:E:208:MET:HA	2.50	0.40
1:E:48:PRO:HG2	1:E:49:TYR:CD2	2.56	0.40
1:F:126:LEU:HD22	1:F:264:SER:OG	2.21	0.40
1:F:152:LYS:HA	1:F:297:GLY:CA	2.50	0.40
1:F:365:ALA:O	1:F:366:ARG:NE	2.54	0.40
1:F:398:THR:HA	1:F:401:GLU:HB3	2.03	0.40
1:A:84:GLY:HA3	1:F:83:PHE:CZ	2.57	0.40
1:B:181:VAL:HG12	1:B:182:GLN:N	2.35	0.40
1:B:209:ASP:OD1	1:B:210:PHE:N	2.54	0.40
1:B:30:ARG:HD3	1:B:378:GLN:HE22	1.86	0.40
1:C:162:VAL:HG12	1:C:163:PRO:N	2.36	0.40
1:C:311:TYR:HB2	1:C:313:LEU:HD21	2.03	0.40
1:C:347:SER:HA	1:C:361:PHE:CD1	2.56	0.40
1:C:97:ARG:HB3	1:C:403:TRP:CE2	2.56	0.40
1:D:69:GLN:CA	1:D:201:VAL:HG13	2.51	0.40
1:D:391:TYR:O	1:D:394:ASN:ND2	2.54	0.40
1:D:35:TYR:CE1	1:D:456:PHE:CD2	3.09	0.40
1:D:460:LEU:O	1:D:463:PHE:O	2.39	0.40
1:D:47:HIS:CD2	1:D:48:PRO:CD	3.05	0.40
1:E:128:ASP:CG	1:E:129:THR:H	2.25	0.40
1:A:183:GLY:CA	1:E:347:SER:O	2.69	0.40
1:E:47:HIS:CG	1:E:48:PRO:CD	3.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:VAL:CG2	1:F:225:CYS:HA	2.50	0.40
1:F:389:MET:O	1:F:393:HIS:N	2.53	0.40
1:A:69:GLN:N	1:A:201:VAL:HG13	2.36	0.40
1:B:333:VAL:HG22	1:B:334:VAL:N	2.37	0.40
1:B:429:CYS:O	1:B:430:GLN:HB2	2.21	0.40
1:B:77:LEU:HD12	1:B:100:TRP:CD1	2.56	0.40
1:C:289:TYR:HA	1:C:291:TYR:CE2	2.56	0.40
1:C:197:ASP:HB2	1:C:447:PHE:HA	2.03	0.40
1:C:91:TYR:CE2	1:C:97:ARG:HA	2.56	0.40
1:D:120:HIS:ND1	1:D:123:TYR:HA	2.36	0.40
1:D:399:ILE:HG13	1:D:399:ILE:H	1.60	0.40
1:D:71:ARG:C	1:D:73:PHE:CE1	2.95	0.40
1:D:81:ASN:ND2	1:D:403:TRP:HE1	2.19	0.40
1:F:204:GLY:O	1:F:205:TYR:CG	2.74	0.40
1:F:231:TYR:HA	1:F:232:PRO:HD3	1.85	0.40
1:F:36:HIS:CE1	1:F:37:ALA:C	2.95	0.40
1:A:307:PHE:CD1	1:A:308:ASN:N	2.89	0.40
1:A:434:ALA:HA	1:A:435:PRO:HD3	1.89	0.40
1:B:111:GLN:HB3	1:B:112:PRO:HD2	2.04	0.40
1:B:444:LYS:N	1:B:444:LYS:HD3	2.36	0.40
1:C:374:GLN:N	1:C:375:PHE:CZ	2.90	0.40
1:C:77:LEU:O	1:C:327:ASN:HB3	2.21	0.40
1:D:102:CYS:SG	1:D:376:ILE:O	2.80	0.40
1:D:109:ARG:HA	1:D:371:PHE:CD1	2.57	0.40
1:D:169:TRP:N	1:D:207:ALA:O	2.53	0.40
1:D:21:VAL:HG22	1:D:22:VAL:N	2.36	0.40
1:D:271:LEU:HD11	1:D:276:TYR:CE1	2.57	0.40
1:D:421:PHE:CE1	1:D:426:ALA:HB1	2.57	0.40
1:D:85:LEU:HD23	1:D:85:LEU:N	2.37	0.40
1:E:167:GLU:CG	1:E:231:TYR:O	2.69	0.40
1:E:220:VAL:HB	1:E:221:PRO:CD	2.52	0.40
1:E:390:SER:H	1:E:390:SER:HG	1.62	0.40
1:F:341:ASN:HD21	1:F:367:HIS:CG	2.39	0.40
1:F:91:TYR:CD1	1:F:93:PRO:HD3	2.57	0.40
1:A:102:CYS:SG	1:A:375:PHE:HB3	2.61	0.40
1:A:235:LEU:HA	1:A:238:SER:OG	2.22	0.40
1:A:47:HIS:CE1	1:A:49:TYR:N	2.88	0.40
1:A:87:ASP:CG	1:A:89:THR:HG23	2.41	0.40
1:B:124:ASN:HD21	1:B:265:GLY:N	2.19	0.40
1:B:196:GLU:H	1:B:199:ASP:CG	2.25	0.40
1:B:460:LEU:HD12	1:B:470:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:TRP:CH2	1:B:469:PHE:CA	3.05	0.40
1:B:144:ARG:H	1:C:283:ARG:NH2	2.20	0.40
1:D:170:THR:HG22	1:D:191:ILE:HG21	2.04	0.40
1:D:325:TRP:CD2	1:D:325:TRP:N	2.85	0.40
1:D:460:LEU:HD13	1:D:470:LEU:HD21	2.04	0.40
1:E:323:ILE:HG21	1:E:325:TRP:CH2	2.56	0.40
1:E:51:LYS:NZ	1:E:63:PRO:HA	2.36	0.40
1:F:23:SER:HB3	1:F:26:GLU:OE1	2.22	0.40
1:F:28:VAL:HG12	1:F:28:VAL:O	2.21	0.40
1:F:196:GLU:CD	1:F:446:LYS:H	2.25	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	454/500 (91%)	359 (79%)	59 (13%)	36 (8%)	1	19
1	B	462/500 (92%)	356 (77%)	65 (14%)	41 (9%)	1	17
1	C	455/500 (91%)	363 (80%)	57 (12%)	35 (8%)	1	20
1	D	452/500 (90%)	370 (82%)	53 (12%)	29 (6%)	2	25
1	E	452/500 (90%)	351 (78%)	70 (16%)	31 (7%)	1	22
1	F	462/500 (92%)	367 (79%)	62 (13%)	33 (7%)	1	22
All	All	2737/3000 (91%)	2166 (79%)	366 (13%)	205 (8%)	3	20

All (205) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	50	PHE

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Mol	Chain	Res	Type
1	A	67	ALA
1	A	86	PRO
1	A	404	ASN
1	A	405	PHE
1	A	410	PRO
1	A	411	PRO
1	A	417	ASP
1	A	423	GLN
1	A	436	PRO
1	A	437	VAL
1	B	86	PRO
1	B	91	TYR
1	B	298	SER
1	B	339	SER
1	B	411	PRO
1	B	418	THR
1	B	419	TYR
1	B	436	PRO
1	B	441	PRO
1	C	67	ALA
1	C	207	ALA
1	C	225	CYS
1	C	227	SER
1	C	278	LYS
1	C	307	PHE
1	C	411	PRO
1	C	418	THR
1	C	421	PHE
1	C	424	SER
1	C	436	PRO
1	D	140	THR
1	D	192	ASN
1	D	227	SER
1	D	298	SER
1	D	339	SER
1	D	386	THR
1	D	411	PRO
1	D	453	LYS
1	E	115	VAL
1	E	142	ASP
1	E	144	ARG
1	E	293	PRO

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Mol	Chain	Res	Type
1	E	298	SER
1	E	339	SER
1	E	386	THR
1	E	399	ILE
1	E	421	PHE
1	E	422	VAL
1	E	425	ALA
1	E	440	ASP
1	E	441	PRO
1	F	18	VAL
1	F	57	ASN
1	F	88	ASN
1	F	210	PHE
1	F	244	ASP
1	F	299	VAL
1	F	414	SER
1	F	417	ASP
1	F	425	ALA
1	A	27	TYR
1	A	66	SER
1	A	129	THR
1	A	181	VAL
1	A	240	ASP
1	A	274	SER
1	A	308	ASN
1	A	421	PHE
1	A	439	GLN
1	A	454	GLU
1	B	11	VAL
1	B	19	ALA
1	B	67	ALA
1	B	90	VAL
1	B	111	GLN
1	B	205	TYR
1	B	286	PRO
1	B	415	LEU
1	B	421	PHE
1	B	424	SER
1	B	427	VAL
1	B	433	THR
1	B	440	ASP
1	C	19	ALA

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Mol	Chain	Res	Type
1	C	22	VAL
1	C	115	VAL
1	C	136	SER
1	C	138	VAL
1	C	339	SER
1	C	416	VAL
1	C	422	VAL
1	C	426	ALA
1	C	437	VAL
1	C	459	ASP
1	D	137	ALA
1	D	175	CYS
1	D	194	PRO
1	D	225	CYS
1	D	409	PRO
1	D	415	LEU
1	D	420	ARG
1	E	111	GLN
1	E	129	THR
1	E	186	PRO
1	E	213	LEU
1	E	404	ASN
1	F	11	VAL
1	F	125	LYS
1	F	152	LYS
1	F	205	TYR
1	F	227	SER
1	F	228	ILE
1	F	240	ASP
1	F	317	GLN
1	F	339	SER
1	F	420	ARG
1	F	435	PRO
1	F	453	LYS
1	A	131	ASN
1	A	407	VAL
1	B	48	PRO
1	B	140	THR
1	B	152	LYS
1	B	175	CYS
1	B	184	ASP
1	B	264	SER

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Mol	Chain	Res	Type
1	B	275	LEU
1	B	288	SER
1	B	308	ASN
1	B	337	THR
1	B	416	VAL
1	B	430	GLN
1	C	91	TYR
1	C	245	SER
1	C	413	ALA
1	C	438	LYS
1	D	32	SER
1	D	89	THR
1	D	111	GLN
1	D	246	MET
1	D	359	THR
1	D	413	ALA
1	D	414	SER
1	D	435	PRO
1	E	87	ASP
1	E	353	PRO
1	E	396	ASN
1	F	132	SER
1	F	142	ASP
1	F	410	PRO
1	F	413	ALA
1	F	421	PHE
1	A	24	THR
1	A	163	PRO
1	A	298	SER
1	A	384	LEU
1	A	416	VAL
1	A	431	LYS
1	B	404	ASN
1	B	423	GLN
1	C	90	VAL
1	C	131	ASN
1	C	134	VAL
1	C	274	SER
1	C	286	PRO
1	D	125	LYS
1	D	130	GLU
1	D	139	ASP

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Mol	Chain	Res	Type
1	D	440	ASP
1	E	152	LYS
1	E	206	GLY
1	E	432	ASP
1	F	14	PRO
1	A	422	VAL
1	B	281	ASP
1	B	409	PRO
1	B	417	ASP
1	C	208	MET
1	E	48	PRO
1	E	174	ALA
1	E	428	THR
1	F	134	VAL
1	F	352	ILE
1	F	429	CYS
1	A	85	LEU
1	A	111	GLN
1	A	125	LYS
1	A	453	LYS
1	B	176	LYS
1	C	221	PRO
1	E	143	THR
1	E	134	VAL
1	E	90	VAL
1	E	204	GLY
1	F	111	GLN
1	A	206	GLY
1	B	14	PRO
1	C	80	PRO
1	D	85	LEU
1	D	437	VAL
1	F	48	PRO
1	F	409	PRO
1	C	410	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	406/444 (91%)	341 (84%)	65 (16%)	3	21
1	B	414/444 (93%)	353 (85%)	61 (15%)	4	24
1	C	407/444 (92%)	343 (84%)	64 (16%)	3	22
1	D	405/444 (91%)	328 (81%)	77 (19%)	2	13
1	E	405/444 (91%)	332 (82%)	73 (18%)	2	15
1	F	414/444 (93%)	334 (81%)	80 (19%)	2	13
All	All	2451/2664 (92%)	2031 (83%)	420 (17%)	6	18

All (420) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	24	THR
1	A	25	ASP
1	A	26	GLU
1	A	33	ILE
1	A	35	TYR
1	A	47	HIS
1	A	52	VAL
1	A	61	ASP
1	A	66	SER
1	A	71	ARG
1	A	77	LEU
1	A	88	ASN
1	A	91	TYR
1	A	96	GLN
1	A	109	ARG
1	A	123	TYR
1	A	124	ASN
1	A	141	LYS
1	A	145	ASP
1	A	149	VAL
1	A	162	VAL
1	A	189	GLU
1	A	193	THR
1	A	208	MET
1	A	211	LYS
1	A	221	PRO
1	A	223	ASP

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Mol	Chain	Res	Type
1	A	226	GLN
1	A	234	TYR
1	A	242	TYR
1	A	247	PHE
1	A	251	ARG
1	A	252	ARG
1	A	260	PHE
1	A	283	ARG
1	A	307	PHE
1	A	317	GLN
1	A	319	LEU
1	A	325	TRP
1	A	345	CYS
1	A	359	THR
1	A	360	SER
1	A	369	GLU
1	A	384	LEU
1	A	386	THR
1	A	387	GLU
1	A	391	TYR
1	A	393	HIS
1	A	395	MET
1	A	403	TRP
1	A	404	ASN
1	A	405	PHE
1	A	410	PRO
1	A	418	THR
1	A	423	GLN
1	A	430	GLN
1	A	433	THR
1	A	436	PRO
1	A	440	ASP
1	A	442	TYR
1	A	454	GLU
1	A	457	SER
1	A	461	ASP
1	A	462	GLN
1	B	24	THR
1	B	27	TYR
1	B	41	ARG
1	B	44	THR
1	B	60	GLN

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Mol	Chain	Res	Type
1	B	66	SER
1	B	69	GLN
1	B	76	LYS
1	B	88	ASN
1	B	91	TYR
1	B	92	ASP
1	B	99	VAL
1	B	107	ILE
1	B	109	ARG
1	B	122	LEU
1	B	123	TYR
1	B	127	ASP
1	B	128	ASP
1	B	139	ASP
1	B	140	THR
1	B	144	ARG
1	B	150	ASP
1	B	151	TYR
1	B	162	VAL
1	B	165	ILE
1	B	168	HIS
1	B	176	LYS
1	B	205	TYR
1	B	208	MET
1	B	213	LEU
1	B	220	VAL
1	B	242	TYR
1	B	244	ASP
1	B	248	PHE
1	B	260	PHE
1	B	277	ILE
1	B	281	ASP
1	B	289	TYR
1	B	302	SER
1	B	304	SER
1	B	305	GLN
1	B	315	LYS
1	B	340	THR
1	B	366	ARG
1	B	378	GLN
1	B	379	LEU
1	B	387	GLU

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Mol	Chain	Res	Type
1	B	388	VAL
1	B	393	HIS
1	B	397	THR
1	B	423	GLN
1	B	427	VAL
1	B	430	GLN
1	B	436	PRO
1	B	439	GLN
1	B	442	TYR
1	B	444	LYS
1	B	450	VAL
1	B	454	GLU
1	B	457	SER
1	B	472	GLN
1	C	25	ASP
1	C	27	TYR
1	C	30	ARG
1	C	50	PHE
1	C	51	LYS
1	C	59	ARG
1	C	60	GLN
1	C	66	SER
1	C	69	GLN
1	C	77	LEU
1	C	91	TYR
1	C	96	GLN
1	C	109	ARG
1	C	126	LEU
1	C	140	THR
1	C	141	LYS
1	C	145	ASP
1	C	151	TYR
1	C	154	THR
1	C	163	PRO
1	C	168	HIS
1	C	177	PRO
1	C	187	PRO
1	C	196	GLU
1	C	205	TYR
1	C	211	LYS
1	C	213	LEU
1	C	223	ASP

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Mol	Chain	Res	Type
1	C	226	GLN
1	C	234	TYR
1	C	244	ASP
1	C	246	MET
1	C	251	ARG
1	C	252	ARG
1	C	260	PHE
1	C	267	MET
1	C	278	LYS
1	C	289	TYR
1	C	290	LEU
1	C	300	VAL
1	C	326	HIS
1	C	329	LEU
1	C	334	VAL
1	C	339	SER
1	C	340	THR
1	C	362	LYS
1	C	366	ARG
1	C	371	PHE
1	C	379	LEU
1	C	391	TYR
1	C	394	ASN
1	C	397	THR
1	C	401	GLU
1	C	409	PRO
1	C	422	VAL
1	C	423	GLN
1	C	427	VAL
1	C	428	THR
1	C	429	CYS
1	C	430	GLN
1	C	438	LYS
1	C	454	GLU
1	C	464	PRO
1	C	472	GLN
1	D	20	LYS
1	D	27	TYR
1	D	35	TYR
1	D	36	HIS
1	D	41	ARG
1	D	42	LEU

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Mol	Chain	Res	Type
1	D	45	VAL
1	D	59	ARG
1	D	69	GLN
1	D	85	LEU
1	D	87	ASP
1	D	89	THR
1	D	105	VAL
1	D	109	ARG
1	D	117	LEU
1	D	121	PRO
1	D	125	LYS
1	D	129	THR
1	D	132	SER
1	D	138	VAL
1	D	139	ASP
1	D	142	ASP
1	D	145	ASP
1	D	151	TYR
1	D	185	CYS
1	D	191	ILE
1	D	193	THR
1	D	211	LYS
1	D	216	ASN
1	D	223	ASP
1	D	224	ILE
1	D	226	GLN
1	D	234	TYR
1	D	235	LEU
1	D	242	TYR
1	D	244	ASP
1	D	246	MET
1	D	247	PHE
1	D	249	CYS
1	D	254	GLN
1	D	260	PHE
1	D	261	TRP
1	D	289	TYR
1	D	292	SER
1	D	294	SER
1	D	305	GLN
1	D	307	PHE
1	D	324	CYS

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Mol	Chain	Res	Type
1	D	325	TRP
1	D	332	THR
1	D	336	THR
1	D	339	SER
1	D	340	THR
1	D	341	ASN
1	D	343	SER
1	D	345	CYS
1	D	357	THR
1	D	359	THR
1	D	360	SER
1	D	363	GLU
1	D	364	TYR
1	D	366	ARG
1	D	369	GLU
1	D	373	LEU
1	D	387	GLU
1	D	391	TYR
1	D	401	GLU
1	D	404	ASN
1	D	409	PRO
1	D	415	LEU
1	D	421	PHE
1	D	429	CYS
1	D	431	LYS
1	D	456	PHE
1	D	461	ASP
1	D	464	PRO
1	D	472	GLN
1	E	27	TYR
1	E	33	ILE
1	E	41	ARG
1	E	57	ASN
1	E	59	ARG
1	E	82	LYS
1	E	88	ASN
1	E	91	TYR
1	E	109	ARG
1	E	111	GLN
1	E	115	VAL
1	E	124	ASN
1	E	127	ASP

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Mol	Chain	Res	Type
1	E	129	THR
1	E	140	THR
1	E	150	ASP
1	E	151	TYR
1	E	155	GLN
1	E	157	CYS
1	E	159	ILE
1	E	176	LYS
1	E	185	CYS
1	E	189	GLU
1	E	190	LEU
1	E	208	MET
1	E	212	LEU
1	E	216	ASN
1	E	219	GLU
1	E	223	ASP
1	E	242	TYR
1	E	247	PHE
1	E	252	ARG
1	E	266	THR
1	E	267	MET
1	E	273	GLU
1	E	282	ILE
1	E	285	ASN
1	E	289	TYR
1	E	292	SER
1	E	300	VAL
1	E	307	PHE
1	E	315	LYS
1	E	317	GLN
1	E	329	LEU
1	E	332	THR
1	E	334	VAL
1	E	340	THR
1	E	345	CYS
1	E	362	LYS
1	E	363	GLU
1	E	387	GLU
1	E	391	TYR
1	E	393	HIS
1	E	395	MET
1	E	396	ASN

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Mol	Chain	Res	Type
1	E	401	GLU
1	E	403	TRP
1	E	404	ASN
1	E	407	VAL
1	E	408	THR
1	E	410	PRO
1	E	412	THR
1	E	415	LEU
1	E	419	TYR
1	E	421	PHE
1	E	428	THR
1	E	430	GLN
1	E	432	ASP
1	E	444	LYS
1	E	450	VAL
1	E	459	ASP
1	E	464	PRO
1	E	472	GLN
1	F	15	PRO
1	F	26	GLU
1	F	30	ARG
1	F	33	ILE
1	F	35	TYR
1	F	36	HIS
1	F	43	LEU
1	F	45	VAL
1	F	51	LYS
1	F	64	LYS
1	F	69	GLN
1	F	85	LEU
1	F	87	ASP
1	F	90	VAL
1	F	126	LEU
1	F	128	ASP
1	F	132	SER
1	F	142	ASP
1	F	150	ASP
1	F	151	TYR
1	F	156	LEU
1	F	159	ILE
1	F	161	CYS
1	F	165	ILE

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Mol	Chain	Res	Type
1	F	169	TRP
1	F	184	ASP
1	F	192	ASN
1	F	195	ILE
1	F	208	MET
1	F	211	LYS
1	F	221	PRO
1	F	237	MET
1	F	244	ASP
1	F	246	MET
1	F	247	PHE
1	F	251	ARG
1	F	252	ARG
1	F	278	LYS
1	F	281	ASP
1	F	289	TYR
1	F	295	PRO
1	F	304	SER
1	F	308	ASN
1	F	312	TRP
1	F	317	GLN
1	F	324	CYS
1	F	328	GLN
1	F	333	VAL
1	F	339	SER
1	F	345	CYS
1	F	363	GLU
1	F	367	HIS
1	F	371	PHE
1	F	373	LEU
1	F	387	GLU
1	F	388	VAL
1	F	391	TYR
1	F	393	HIS
1	F	399	ILE
1	F	401	GLU
1	F	410	PRO
1	F	412	THR
1	F	416	VAL
1	F	419	TYR
1	F	422	VAL
1	F	430	GLN

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Mol	Chain	Res	Type
1	F	431	LYS
1	F	436	PRO
1	F	439	GLN
1	F	443	ASP
1	F	444	LYS
1	F	448	TRP
1	F	450	VAL
1	F	451	ASP
1	F	453	LYS
1	F	454	GLU
1	F	455	ARG
1	F	461	ASP
1	F	465	LEU
1	F	472	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	88	ASN
1	A	120	HIS
1	A	153	GLN
1	A	314	HIS
1	A	326	HIS
1	A	462	GLN
1	B	131	ASN
1	B	236	GLN
1	B	285	ASN
1	B	341	ASN
1	B	367	HIS
1	B	423	GLN
1	C	47	HIS
1	C	153	GLN
1	C	226	GLN
1	C	270	GLN
1	C	317	GLN
1	C	321	ASN
1	C	326	HIS
1	C	394	ASN
1	C	423	GLN
1	C	472	GLN
1	D	120	HIS

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Mol	Chain	Res	Type
1	D	168	HIS
1	D	216	ASN
1	D	236	GLN
1	D	254	GLN
1	D	327	ASN
1	D	462	GLN
1	D	472	GLN
1	E	120	HIS
1	E	133	HIS
1	E	168	HIS
1	E	226	GLN
1	E	326	HIS
1	E	430	GLN
1	E	472	GLN
1	F	120	HIS
1	F	168	HIS
1	F	354	ASN
1	F	393	HIS
1	F	472	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.